Nuclear Energy CFD Application Management System

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Abstract

In modeling and simulation (M&S), it is virtually impossible to separately evaluate the effectiveness of the model from the data used because the results produced rely heavily on the interaction between the two. Both the data and the simulation are responsible for achieving the ultimate goal of providing defensible research and development (R&D) products and decisions. It is therefore vital that data verification and validation (V&V) activities, along with stringent configuration management, be considered part of the overall M&S accreditation process. In support of these goals is the Nuclear Energy CFD Application Management System (NE-CAMS) for nuclear system design and safety analysis. Working with Bettis Laboratory and Utah State University, a plan of action is being developed by the Idaho National Laboratory (INL) that will address the highest and most immediate needs to track and manage computational fluid dynamics (CFD) models and experimental data in an electronic database. The database will intrinsically incorporate the Nuclear Regulatory Commission (NRC) approved policies and procedures for quality. The quality requirements will be such that the model and data must conform to the quality specifications outlined by the NRC before they can be entered into the database. The primary focus of this database is CFD V&V for nuclear industry needs and will, in practice, serve as the best practice guideline that will accommodate NRC regulations. Such a database, along with a prescriptive methodology for how to utilize it, will provide the NRC with accepted CFD results that could potentially be used for licensing.

Input from major organizations in government and industry have shown the need to develop a coordinated strategy at a national level to effectively accelerate the use of CFD for nuclear systems design and safety analysis. The growth of CFD for nuclear applications is evident from publications, both in journals and conferences, where CFD is shown to be an essential tool in nuclear reactor design and safety analyses. The nuclear industry arguably has the most stringent and technically sophisticated regulatory body which carefully watches and scrutinizes not only the analysis results but even more so the tools used for such analysis. It is critical that the applied CFD technology is brought to the level, through developments and demonstrations, such that the NRC will rule on requirements for using CFD in nuclear systems design and safety related applications and enforce them. To this end is the critical need for NE-CAMS, a CFD database that will incorporate the required V&V activities capable of producing results accepted by the NRC.

NE-CAMS will incorporate data V&V as key precursors to the distribution of nuclear systems design and safety data, ensuring that these data are appropriate for use in a particular M&S application. Verification will be conducted to provide a level of confidence that the data selected are the most appropriate for the simulation and are properly prepared, i.e., they are complete, correct and conform to predefined procedures and requirements. Validation will ensure that the data accurately represent the real world activity that is being simulated, ensuring the analytical quality of the data. The level of detail and stringency applied against the data V&V activities will

be based on a graded approach principle; the higher the risk, the more rigorous the V&V activities. For the V&V activities to be complete, it will be necessary to scrutinize the physical and statistical properties of the extracted data during the overall process. Regardless of the specific technique or methodology, data V&V will be an important component of NE-CAMS.

Introduction

Over the past decade, there has been a worldwide increase in the use of modeling and simulation (M&S) for the analysis of nuclear reactors. M&S provides a more affordable approach to scientific insights into a nuclear reactor than traditional testing and demonstration. With the advent of high resolution computing resources, modern information technologies and advanced modeling, government agencies, industry and academia are using M&S as means to virtually explore the physical structure and assess the performance of a nuclear reactor. The Department of Energy Office of Nuclear Energy (DOE-NE), for example, is not only investing in these capabilities but has formally established a national M&S research, development and demonstration program referred to as the Consortium of Advanced Simulation for Light Water Reactors (CASL). Similarly, in nuclear systems design and safety analysis, computational fluid dynamics (CFD) is one of several M&S tools that are increasingly being used to understand the operation and structural integrity of a nuclear reactor. For CFD to be useful, however, the models in CFD codes, i.e., models for simulating turbulence, heat transfer, multiphase flows, chemical reactions, etc., and experimental data utilized to develop those models must be verified and validated to ensure the level of quality needed and expected for their intended use. To that end and in support of the general M&S accreditation process for the use of M&S in nuclear systems design and safety analysis, the effort to develop and implement the Nuclear Energy CFD Application Management System (NE-CAMS) was initiated. It is envisioned that NE-CAMS, when implemented, will serve as a readily accessible knowledge base and repository for critical CFD applications in nuclear systems design and safety analysis, including experimental data sets, CFD models and simulation input decks, to the nuclear energy community.

NE-CAMS

NE-CAMS is being developed by the Idaho National Laboratory (INL) with the primary objective of building a CFD database that collects, stores and maintains CFD models and experiment data for nuclear systems design and safety analysis. There are two key premises associated with this database, 1) a focus on CFD and experiments specific to the nuclear energy field and 2) work closely with the Nuclear Regulatory Commission (NRC) to define a best practice guideline that incorporates NRC regulations and policies. In the NE-CAMS project, verification and validation (V&V), uncertainty analysis and configuration control will be used to provide a methodical, industry-inclusive approach to developing and applying CFD technology, to the point that CFD models can be used as a qualifiable predictive tool for nuclear reactor design. To achieve this, rigorous standards and support methods are required for CFD models (model development, qualification and application) experimental data (testing, data analysis, data/information storage). Availability of these models and their data, along with the associations between them, as implemented in NE-CAMS, will provide the basic technology needed to support the DOE-NE Advanced Modeling and Simulation Vision, i.e., "*To rapidly create and deploy verified and validated nuclear energy modeling and simulation capability for the design, implementation, and operation of future nuclear energy systems to improve the U.S. energy security future.*[1]

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[1] Larzelere, Alex R. Advanced Modeling and Simulation Facilities Requirements, Presentation, Office of Nuclear Energy, Fuel Cycle Management (NE-5)

NE-CAMS will be developed to satisfy several high-level primary goals, specifically to

- Develop, implement, maintain and promote a database that incorporates CFD models and experiments involving relevant physical processes that span a parameter range of interest to the NRC.
- Provide a selected set of data (experiments) that a CFD code must be benchmarked against before its results can be included in the database.
- Standardize experimental and computational procedures from the perspective of data collection, processing, storage and qualification with the ultimately goal of maximizing and retaining the value of both the physical and numerical data.
- Apply V&V activities against the models and data that result in well-defined, well-characterized and defensible CFD analysis.
- Develop knowledge-based tools and procedures, e.g., best practices, for industrial application of CFD.
- Provide high performance computing and visualization support, including tools and utilities for V&V activities, data access and processing, and physics exploration.
- Make the models, data and utilities available to the nuclear energy community via the web.
- Include controls for security, integrity, and configuration management.

The proposed NE-CAMS database will provide the foundation for identifying, collecting, and validating new experimental and high-fidelity CFD data that can be used for qualifying integrated performance and safety codes and ultimately used for NRC licensing. It will intrinsically incorporate NRC approved policies and procedures for quality. The requirements will be such that the data must conform to the quality specification outlined by the NRC before they can be entered into the database. Such a database, along with a prescriptive methodology for how to utilize it, will provide the NRC with accepted CFD results that can be used for licensing.

Data V&V

Today, most nuclear energy programs rely on expert knowledge to ensure that decisions are supported by the data of the type and quality needed and expected for their intended use. This expertise is usually localized to the site or lab in which the data and/or models were generated, and is rarely codified and exported for more global application. Because of the critical nature of nuclear engineering programs and the need to provide quality nuclear engineering data to a distributed community, the current expert-based V&V process must be expanded to include metadata, documenting the broader architecture that transforms physical observations to generalizations and meaningful insights. Without metadata, it is difficult to extract the meaningful information needed to create the knowledge to produce actionable insights and correct decisions.

In the NE-CAMS project, to accomplish the goal of providing quality nuclear engineering data and the corresponding meta-data documenting the proper usage of data to a distributed community of users, a set of V&V activities will be defined and conducted during the planning, implementation, and assessment phases of data collection. Specifically, the data quality V&V assessment workflow will include the following components:

- Data origin and integrity checks
- Data integration tags and metadata definitions

- Statistical data scrutiny, exploratory data analysis, and data mining approaches
- Standard reference data, dimensional analysis, and scaling
- Qualification of data generated from models
- Adherence to appropriate data quality standards

Thus, using a holistic approach with a strong emphasis on data V&V, the implemented methods (derived from different perspectives, e.g., physical, statistical, and engineering) could also be used to facilitate further use of the data for analyses. In addition, the V&V processes and methods used to achieve these ends must be defined and automated with a robust data integration environment that includes controls for security, integrity, and configuration management.

One of the primary deliverables associated with the NE-CAMS project is the data management plan. This plan will specifically describe the data analysis and management that will be done to support the modeling and simulation nuclear energy programs including descriptions of the data and collection and storage methods. It will also describe the methods under consideration for data qualification and validation activities and data security.

Data used in nuclear engineering projects have a configuration management (CM) burden that must be accommodated. Part of that burden is due to the critical nature of the engineering tasks, but a large part is also due to the legacy data and the models and program codes derived from and applied to that data. Thus, in this environment the nuclear engineering data CM activity must be an extremely disciplined operation that requires maintaining accurate records of *all* transactions involving the data. An appropriate Configuration Management Plan (CMP) must therefore define the requirements and procedures necessary for all configuration management activities, including methodologies for generating configuration identifiers, controlling engineering changes, maintaining status accounting with time stamped logs for check-ins and check-outs, automatically triggering reviews and inspections upon detecting violations or discrepancies, and support for maintenance and longevity.

While it is premature at this point to define the nuclear engineering data V&V CMP, a tentative outline of its contents includes:

1. Definitions and acronyms
2. Data domains, tags, identifiers
3. Configuration Control Board (CCB) definition
4. Baseline data pre-check-in procedures
5. Data check-out procedures
6. Modified data check-in procedures
7. Procedures for modifying the CMP
8. Forms and templates

All the nuclear engineering data – with associated meta-data, models, and program codes – will be deposited into NE-CAMS using the proposed CMP and its associated CM tools, i.e., data will be supported and maintained under configuration and versioning control.

Data V&V Methods and Tools

The complexity of modern engineering systems, as well as the cost and difficulty associated with experimentally verifying system and subsystem design makes the use of M&S a future alternative for design and development. The predictive ability of simulations such as CFD and computational structural mechanics (CSM) has matured significantly. However, for numerical simulation to be used with confidence in design and development, quantitative measures of uncertainty must be available. As such, methods for assessing computational uncertainty are one of the focused areas of research for the computational science and engineering community. In general, the approaches for dealing with computational uncertainty can be divided into method V&V, i.e., code verification and model validation, and prediction uncertainty quantification (UQ), i.e., solution verification, uncertainty analysis, uncertainty propagation and sensitivity analysis. The generally accepted definitions for these terms are given below:

Model V&V

- Code verification – The process of gathering evidence that the mathematical model as implemented and its solution are correct.
- Model validation – The quantitative determination that the model is an accurate representation of the real world for its intended use.

Prediction UQ

- Solution verification – The estimation of residual discretization error.
- Uncertainty analysis – The identification and characterization of uncertainty sources.
- Uncertainty propagation – The propagation of the uncertainty into the system response quantities.
- Sensitivity analysis – The determination of the most important uncertainty contributors.

The NE-CAMS as envisioned will include a suite of V&V and UQ methods and tools in support of the general M&S accreditation process for the use of M&S in nuclear systems design and safety analysis. As noted, the effort will initially concentrate on developing and implementing technically sound and V&V process-vetted, best practice guidelines for applying CFD analysis to obtain reliable and consistent results for nuclear systems design and safety analysis applications. Toward this end, a focused and system program for CFD V&V will be implemented as a part of the NE-CAMS. In particular, a bottom-up approach for CFD V&V will be implemented where the assessments of fundamental, unit and separate-effects physics, flow configurations are performed to develop the large body of knowledge required to implement knowledge-based tools and procedures, *e.g*., best practices and design guidelines, for managing uncertainty and improving reliability of CFD analysis and simulations. In this approach, the flow field data obtained from validation experiments require a higher level of fidelity, resolution and documentation, including a complete and thorough description of the boundary and initial conditions driving the flows, the as-built geometry of the validation experiment and an appropriate uncertainty analysis of the experimental data. Datasets which meet these standards are termed validation-level datasets. It is expected that over time, the amount of validation-level data in the NE-CAMS CFD V&V database and the knowledge gained from CFD V&V assessments will be sufficient to assure the accuracy of the associated CFD predictions over a wide range of applications with a minimal amount of additional, confirmatory physical testing. In time, automated and standardized CFD V&V methodology with associated best practices, design guidelines, and uncertainty quantification methods will provide a predictive capability in which sufficient confidence can be placed in CFD predictions that CFD analysis can replace large, semi-scale physical testing and allow for designs to be developed using CFD up front in the design process.

It is suggested that the current bottom-up approach for CFD V&V should create, over time, an extensive validation database that would be applicable to a wide variety of applications in nuclear systems design and safety analysis. This validation database made up predominantly of physics-based, unit and separate-effects physics validation assessments can then serve as a vehicle for developing and extending a generally applicable knowledge base from which validation to higher levels of confidence for a given application can be performed, as needed. In fact, as the validation database gets well populated with these more detailed, physics-based validation assessments, it is expected that extending an existing set of validation assessments to a specific application will become more straightforward and comparatively fewer validation assessments would be needed. In time, validation assessments for new applications will begin to systematically use and leverage existing validation assessments in the validation database so that synergy will be maximized and duplication and redundancy will be minimized. Thus, over time, the validation domain will begin to approach the application domain for large classes of thermal hydraulic analysis problems needed for nuclear systems design and safety analysis.

This CFD V&V approach has some other significant and practical advantages. First, because the underpinning validation assessments are performed predominantly at the base of the validation pyramid, one is dealing with simpler geometry and physics, which, in turn, makes the difficult tasks of a validation assessment more tractable. For instance, assessing and quantifying the uncertainty of computational results (grid convergence study and numerical uncertainty estimation) and experimental data (uncertainty analysis and propagation of uncertainty) are far easier tasks when one is dealing with the simpler geometries and flow physics at the lower tiers of the validation pyramid versus those at the top tiers. Second, because in this approach one is performing validation assessments with high-quality, high-resolution flow field data obtained from validation-level experiments, one is more likely to develop a better understanding of various physical phenomena embodied in the validation experiments. This better understanding of physical phenomena, in turn, can be used to develop knowledge-based procedures for applying CFD analysis or aid in developing physical models. As such, in this CFD V&V approach, the high-fidelity, high-resolution experimental data obtained from validation experiments can be used for other design related activities, such as physical modeling and methods development, in addition to validation assessments. Finally, the most important advantage of this CFD V&V approach is that it can foster and promote collaboration among interested parties and organizations in expanding the validation range of CFD analysis to cover a larger application space. In particular, because most of the flow geometries and unit or separate-effects physics at the base of the validation pyramid are not likely to be directly related to a proprietary application or design, interested parties are more likely to collaborate and share CFD V&V resources and knowledge. It is in everyone's interest to have access to a well populated CFD validation database made up of fundamental, unit and separate-effects physics validation assessments to draw upon to support their CFD V&V efforts.

Data Standards Clearing Committee

A data standards clearing committee will be established to ensure that the data validation process has been completed per NE-CAMS policies and procedures. The committee is expected to meet at least annually with the specific and ongoing responsibility to:

- Review the data quality objectives and ensure data that are entered into NE-CAMS meet the objectives.
- Conduct a preliminary data review.
- Ensure that strategies to address potential threats to the program's success have been identified, costed and approved, and that the threats are regularly re-assessed.

- Be genuinely interested in the initiative to preserve experimental data and models, and the outcomes being pursued.
- Review and steer NE-CAMS to ensure program feasibility and success.
- Provide guidance to the development of NE-CAMS to ensure that the effort and expenditure are appropriate to stakeholder expectations.
- Provide recommendations to address any issues which have major implications for NE-CAMS.
- Attend an annual oversight meeting and report findings that include an assessment of progress, recommendations to improve capabilities, and the risks associated with scope, schedule, and budget.

Challenges

There are several challenges associated with NE-CAMS that will need to be addressed. First, because of the wide variety of thermo-fluid conditions in nuclear reactor thermal hydraulics, a large number of small scale, unit physics or separate-effects experiments will be required to develop the knowledge base and technical underpinning for V&V processes at the base of the validation pyramid.. Second, for large nuclear energy programs, the cost of designing, building and conducting the required set of separate-effects and integrated-effects experiments could be prohibitive to any one program. Third, the resources needed to collect and process large, petabyte size, data sets and the infrastructure required to store and manage them are not readily available. Finally, proprietary information and data can be difficult to obtain and share, and in general cannot be shared with non-US citizens.

Benefits of NE-CAMS

Several benefits can be realized with the implementation of NE-CAMS.

Globalization – with modeling and simulation programs being widely dispersed across industry, DOE national laboratories and universities, NE-CAMS will reduce the valuable time and resources that are wasted by recreating models that already exist and make available valuable data sets that have gone through a rigorous V&V process.

Sharing of best practices – Millions of dollars per year could be saved by leveraging what geographically already exists, expanding modeling and simulation applications that have already been implemented and applying those models in similar situations elsewhere.

Culture of quality – The widespread use of NE-CAMS creates an incentive to produce "benchmark-quality" products and encourages uncertainty quantification and best practices.

Expertise – Applied expertise can enhance the value of M&S programs, making both the models and experimental data available will reduce the gap between hands on experience and modeling and simulation.

These and other benefits foster improved problem solving and more rapid adaptation to program changes.

3. Conclusion

Because the nuclear energy community is geographically dispersed and fragmented, effectively communicating and collaborating with one another is difficult but this situation can be improved and further enhanced by making important and useful nuclear systems design and safety analysis models and data readily available to the nuclear energy community through a trusted central exchange or repository. Thus, we recognize the strategic importance of implementing NE-CAMS and ensuring that it aligns with the business needs of the nuclear energy community. And more precisely, the business case for establishing NE-CAMS is simple: Without a concerted effort to preserve, evaluate, document and disseminate existing nuclear systems design and safety analysis models and data, over time, they will be irretrievably lost; the money and resources invested to create them will be wasted and future generations will have to duplicate the R&D work to regenerate these models and data if nuclear energy is to be a factor in our energy future.

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