

High Level Requirements for the Nuclear Energy – Knowledge Base for Advanced Modeling and Simulation (NE-KAMS)

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EXECUTIVE SUMMARY

The U.S. Department of Energy, Office of Nuclear Energy (DOE-NE), has been tasked with the important mission of ensuring that nuclear energy remains a compelling and viable energy source in the U.S. The motivations behind this mission include cost-effectively meeting the expected increases in the power needs of the country, reducing carbon emissions, and reducing dependence on foreign energy sources. In the near term, to ensure that nuclear power remains a key element of U.S. energy strategy, the DOE-NE will be working with the nuclear industry to support safe and efficient operations of existing nuclear power plants. In the long term, the DOE-NE will be investing in research and development (R&D) and working in concert with the nuclear industry to build new, safer and more efficient nuclear power plants. The safe and efficient operations of existing nuclear power plants and designing and licensing new reactor designs, however, will require the extensive use of advanced modeling and simulation (M&S). Thus, it is expected that M&S will play a key role in ensuring the safe and efficient operation of existing and new nuclear reactors.

The complexity of nuclear reactor power plants, as well as the cost and difficulty associated with testing nuclear reactor systems makes the use of M&S a desirable tool for nuclear reactor design, analysis and licensing. Thus, engineering analysis and performance characterization of existing and new reactor designs will employ advanced M&S tools, such as computational fluid dynamics (CFD) and computational structural mechanics (CSM), in addition to the traditional thermal hydraulics (T/H) and systems analysis codes. The DOE-NE, in fact, has been actively developing and promoting the use of advanced M&S in reactor design and analysis through its R&D programs, *e.g.*, the Nuclear Energy Advanced Modeling and Simulation (NEAMS) and Consortium for Advanced Simulation of Light Water Reactors (CASL) programs. Also, nuclear reactor vendors are already using CFD and CSM, for design, analysis, and licensing. However, these M&S tools cannot be used with confidence for nuclear reactor applications unless supported by verification and validation (V&V) and uncertainty quantification (UQ) which provide quantitative measures of uncertainty for specific applications.

V&V and UQ are the primary means to assess the accuracy and reliability of M&S and, hence, to establish confidence in M&S. Though the nuclear industry has established standards and processes for carrying out V&V and UQ for systems analysis codes and simulations, at present, similar standards and processes for high fidelity M&S tools such as CFD have not reached the same level of maturity. However, the nuclear industry recognizes that such standards and processes are needed and that the resources required to support V&V and UQ for CFD for nuclear applications is significant. In fact, no single organization, whether a commercial company or government laboratory, has the resources required to organize, develop and maintain the needed V&V and UQ program. What is needed is a standardized program for V&V and UQ at a national or even international level, with a consortium of partners from government, academia and industry. Specifically, what is needed is a structured knowledge base for V&V and UQ that collects, evaluates and maintains V&V and UQ data and information, and provides guidance and resources for performing V&V and UQ assessments. This kind of a knowledge base can promote collaboration and provide for sharing of resources needed to support the use of M&S for engineering and licensing applications.

The Nuclear Energy Knowledge base for Advanced Modeling and Simulation (NE-KAMS) is being developed at the Idaho National Laboratory in conjunction with Bettis Laboratory, Sandia

National Laboratories, Argonne National Laboratory, Utah State University and others. The objective of this consortium is to establish a comprehensive and web-accessible knowledge base to provide V&V and UQ resources for M&S for nuclear reactor design, analysis and licensing. The knowledge base will serve as an important resource for technical exchange that will enable credible computational models and simulations for application to nuclear power. NE-KAMS will serve as a valuable resource for the nuclear industry, academia, the national laboratories, the U.S. Nuclear Regulatory Commission (NRC), and the public, and will help ensure the safe, economical and reliable operation of existing and future nuclear reactors.

Existing V&V databases, such as the European Research Community on Flow, Turbulence and Combustion (ERCOfTAC), the European QNET-CFD, and the U.S. NPARC Alliance databases, serve only as repositories for V&V cases. In addition to its V&V benchmark databases, the NE-KAMS knowledge base will provide guidance for progressive levels of V&V completeness, assessment of V&V benchmarks, and improved best practices for V&V. Specifically, the NE-KAMS knowledge base will assist analysts, model developers, experimentalists, designers, and regulators by:

- Establishing accepted standards, requirements and best practices for V&V and UQ of computational models and simulations,
- Establishing accepted standards and procedures for assessing experimental and numerical benchmark data,
- Providing readily accessible databases with long-term storage for code verification and validation benchmark data that can be used in V&V assessments and methods development,
- Providing a searchable knowledge base of information, documents and data on V&V and UQ, and
- Providing web-enabled tools and utilities for V&V and UQ activities, data assessment and processing, and information and data searches.

From its inception, NE-KAMS will directly support nuclear energy R&D programs within the U.S. Department of Energy (DOE), including CASL, NEAMS, Light Water Reactor Sustainability (LWRS), Small Modular Reactors (SMR), and Next Generation Nuclear Power Plant (NGNP). These programs all involve M&S for nuclear reactor systems and it is envisioned that NE-KAMS will facilitate collaboration and sharing of resources and expertise across these programs. The initial focus for the NE-KAMS effort will be on supporting the use of CFD for simulation of nuclear reactor systems, but will eventually expand to include, materials, fuel system performance and other areas of M&S as time and funding allow.

NE-KAMS High Level Requirements

The NE-KAMS knowledge base will be developed, implemented, and deployed for use in stages and will grow and evolve over time. In particular, the primary elements of the knowledge base along with the attendant hardware, software and facility infrastructure will be developed and implemented in stages as funding and available resources allow. Similarly, select parts of the knowledge base, *e.g.*, standards, requirements and best practices for V&V and UQ of computational models and simulations, will become available for use when ready.

The successful realization and future vitality of the NE-KAMS knowledge base require the identification and successful implementation of the key elements, features and functions of the knowledge base. This document describes the high level requirements, specifically the key elements, features, and functions of the NE-KAMS knowledge base, that will guide the development and implementation the NE-KAMS knowledge base. The high level requirements for NE-KAMS are categorized as follows:

- Programmatic requirements (elements, features and functions required by the supported DOE M&S programs and other nuclear energy sciences and engineering communities)
- Technical requirements (the key elements and software and hardware components of the knowledge base)
- Operational requirements (the actual operations of the knowledge base)
- User feedback requirements (the collection of recommendations for NE-KAMS content from potential users of the knowledge base)
- Funding requirements (required funding to perform prioritized tasks to establish the NE-KAMS knowledge base)
- Development requirements (targeted funding for R&D in support of V&V and UQ data needs and improved practices and procedures)

Next Steps for NE-KAMS Development

A list of prioritized tasks is given as the next steps for the development of the NE-KAMS knowledge base. These include:

- A survey and analysis of existing DOE data and knowledge bases for connection and integration with NE-KAMS.
- Continued development of NE-KAMS V&V and UQ standards, requirements and best practices.
- Evaluation and testing of NE-KAMS V&V benchmark data standards and requirements.
- Development of NE-KAMS implementation specifications.

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ACRONYMS

ANL	Argonne National Laboratory
CASL	Consortium for Advanced Simulation of Light Water Reactors
CFD	computational fluid dynamics
CSAU	Code Scaling, Applicability and Uncertainty
DOE	Department of Energy
DOE-NE	Department of Energy – Office of Nuclear Energy
EPRI	Electric Power Research Institute
INL	Idaho National Laboratory
LWRS	Light Water Reactor Sustainability
M&S	modeling and simulation
NE-KAMS	Nuclear Energy Knowledge base for Advanced Modeling and Simulation
NE-KM	Nuclear Energy Knowledge Management Program
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NGNP	Next Generation Nuclear Plant
NRC	Nuclear Regulatory Commission
PIRT	Phenomenon Identification Ranking Table
R&D	Research and Development
SMR	Small Modular Reactors
SNL	Sandia National Laboratories
UQ	uncertainty quantification
USU	Utah State University
V&V	verification and validation

1. Introduction

This document describes the high level requirements that will guide the development, implementation and operations of the Nuclear Energy Knowledge base for Advanced Modeling and Simulation (NE-KAMS). The requirements presented here represent an overview of the high level functions and features that are required for the knowledge base. The high level requirements for the NE-KAMS knowledge base are categorized into the following sets of requirements: programmatic, technical, operational, user feedback, funding, development and system software. More detailed requirements will be developed in the future based on these high level requirements such that the required features and functions of the NE-KAMS knowledge base can be fully implemented. It is noted that the detailed description of the software requirements for the NE-KAMS knowledge base will be provided in the future via the NE-KAMS implementation specification documents. In addition, this document describes the prioritized set of near term tasks and activities which will support the development of the NE-KAMS knowledge base.

1.1 Background

The US Department of Energy, Office of Nuclear Energy (DOE-NE), has been tasked with the important mission of ensuring that nuclear energy remains a compelling and viable energy source in the U.S. The motivations behind this mission include cost-effectively meeting the expected increases in the power needs of the country, reducing carbon emissions, and reducing dependence on foreign energy sources. In the near term, to ensure that nuclear power remains a key element of U.S. energy strategy, the DOE-NE will be working with the nuclear industry to support safe and efficient operations of existing nuclear power plants. In the long term, the DOE-NE will be investing in research and development (R&D) and working in concert with the nuclear industry to build new, safer and more efficient nuclear power plants. The safe and efficient operations of existing nuclear power plants and designing and licensing new reactor designs, however, will require the extensive use of advanced modeling and simulation (M&S). Thus, it is expected that M&S will play a key role in ensuring the safe and efficient operation of existing and new nuclear reactors.

The complexity of nuclear reactor power plants, as well as the cost and difficulty associated with testing nuclear reactor systems makes the use of M&S a desirable tool for nuclear reactor design, analysis and licensing. Thus, engineering analysis and performance characterization of existing and new reactor designs will employ advanced M&S tools, such as computational fluid dynamics (CFD) and computational structural mechanics (CSM), in addition to the traditional thermal hydraulics (T/H) and systems analysis codes. The DOE-NE, in fact, has been actively developing and promoting the use of advanced M&S in reactor design and analysis through its R&D programs, *e.g.*, the Nuclear Energy Advanced Modeling and Simulation (NEAMS) and Consortium for Advanced Simulation of Light Water Reactors (CASL) programs. Also, nuclear reactor vendors are already using CFD and CSM, for design, analysis, and licensing. However, these M&S tools cannot be used with confidence for nuclear reactor applications unless supported by verification and validation (V&V) and uncertainty quantification (UQ) which provide quantitative measures of uncertainty for specific applications.

V&V and UQ are the primary means to assess the accuracy and reliability of M&S and, hence, to establish confidence in M&S. Though the nuclear industry has established standards and processes for carrying out V&V and UQ for systems analysis codes and simulations, at present, similar standards and processes for high fidelity M&S tools such as CFD have not reached the same level of maturity. However, the nuclear industry recognizes that such standards and processes are needed and that the resources required to support V&V and UQ for CFD for nuclear applications is significant. In fact, no single organization, whether a commercial company or government laboratory, has the resources required to organize, develop and maintain the needed V&V and UQ program. What is needed is a standardized program for V&V and UQ at a national or even international level, with a consortium of partners from government, academia and industry. Specifically, what is needed is a structured knowledge base for V&V and UQ that collects, evaluates and maintains V&V and UQ data and information, and provides guidance and resources for performing V&V and UQ assessments. This kind of a knowledge base can promote collaboration and provide for sharing of resources needed to support the use of M&S for engineering and licensing applications.

The NE-KAMS knowledge base is being developed at the Idaho National Laboratory (INL) in conjunction with Bettis Laboratory, Sandia National Laboratories (SNL), Argonne National Laboratory (ANL), Utah State University and others. The objective of this consortium is to establish a comprehensive and web-accessible knowledge base to provide V&V and UQ resources for M&S for nuclear reactor design, analysis and licensing. The knowledge base will serve as an important resource for technical exchange that will enable credible computational models and simulations for application to nuclear power. NE-KAMS will serve as a valuable resource for the nuclear industry, academia, the national laboratories, the U.S. Nuclear Regulatory Commission (NRC), and the public, and will help ensure the safe, economical and reliable operation of existing and future nuclear reactors.

The initial focus for the NE-KAMS effort will be on supporting the use of CFD for simulation of nuclear reactor systems. To better define the scope of the effort required to develop the NE-KAMS knowledge base and its V&V benchmark databases, a survey and evaluation of existing CFD V&V and assessment databases or related efforts, including commercial databases, were performed. Understanding the functionality of these databases is needed to leverage existing efforts and to be able to articulate the added value of NE-KAMS by contrasting the intended functionality for the new knowledge base with existing ones.

The results of the survey showed that V&V and assessment databases presently exist for CFD, mostly outside of the nuclear domain, such as the European Research Community On Flow, Turbulence And Combustion (ERCOFTAC), the European QNET-CFD, and the U.S. NPARC Alliance databases. The evaluation of these V&V databases surveyed showed that they are essentially repositories for V&V cases, and related documents. In general, all that these databases do is maintain mostly validation cases, which have been collected or submitted to the database over time. The quality and amount of the V&V case data as well as the attendant documentation vary significantly, ranging from good quality data that is well documented to poor quality data with little or no documentation. There are few standards and requirements with these CFD databases, and little guidance for best practices for V&V and UQ. There is no process of quality assurance, such as procedures for assessing and classifying V&V benchmark data. It is noted that over time, most of these CFD V&V and assessment databases have either

become defunct or fallen out of date due to lack of use and interest. The details of the survey and evaluation of existing CFD V&V and assessment databases are provided in Appendix A.

From its inception, NE-KAMS will directly support nuclear energy research, development and demonstration programs within the U.S. Department of Energy (DOE), including the CASL, NEAMS, Light Water Reactor Sustainability (LWRS), Small Modular Reactors (SMR), and Next Generation Nuclear Power Plant (NGNP) programs. These programs all involve M&S of nuclear reactor systems, components and processes, and it is envisioned that NE-KAMS will help to coordinate and facilitate collaboration and sharing of resources and expertise for V&V and UQ across these programs. Standards, requirements and best practices for CFD V&V will be established in support of the application of CFD to nuclear reactor design and safety analysis. The NE-KAMS effort will later expand to include materials, fuel system performance and other areas of M&S as time and funding allow.

1.2 Purpose

The successful realization and future vitality of the NE-KAMS knowledge base require the identification and successful implementation of the key elements, features and functions of the knowledge base. This document describes the high level requirements, specifically the key elements, features, and functions of the NE-KAMS knowledge base, which will guide the development and implementation the NE-KAMS knowledge base. The high level requirements for NE-KAMS are categorized as follows:

- Programmatic requirements (elements, features and functions required by the supported DOE M&S programs and other nuclear energy sciences and engineering communities)
- Technical requirements (the key elements and software and hardware components of the knowledge base)
- Operational requirements (the actual operations of the knowledge base)
- User feedback requirements (the collection of recommendations for NE-KAMS content from potential users of the knowledge base)
- Funding requirements (required funding to perform prioritized tasks to establish the NE-KAMS knowledge base)
- Development requirements (targeted funding for R&D in support of V&V and UQ data needs and improved practices and procedures)

This document is intended to communicate the high level requirements for the aforementioned key aspects of the NE-KAMS knowledge base to the NEAMS Program Manager and the technical experts/vendors responsible/contracted to develop the NE-KAMS knowledge base. The proposed audience is, therefore, stakeholders, potential users, program managers, technical experts, software vendors, hardware vendors, computer scientists and software quality engineers.

As other organizations become involved in either the development of NE-KAMS or defining its usage and requirements, this document will be updated. Other organizations that could become involved include:

- DOE Office of Science
- Other government agencies, *e.g.*, Department of Defense (DOD)
- Technical agencies and organizations such as the Organization for Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA)
- Industry, *e.g.*, Electric Power Research Institute (EPRI), Westinghouse, AREVA
- Technical societies
- Academia
- Commercial modeling and simulation software vendors

1.3 Scope

This document provides the high level requirements for the key elements, features and functions of the NE-KAMS knowledge base. Specific or detailed requirements for these aspects of the knowledge base, especially those for the system software required in the operations of the knowledge base, will be developed later and provided via the NE-KAMS implementation specification documents. These high level requirements will be used to guide the initial set of development tasks identified for the NE-KAMS effort that will support the development and implementation of NE-KAMS V&V benchmark databases.

2. NE-KAMS Knowledge Base Overview Description

The NE-KAMS knowledge base will provide guidance for progressive levels of V&V completeness, assessment of submitted V&V benchmarks, improved best practices, and computational methods development. Specifically, the NE-KAMS knowledge base will assist computational analysts, physics model developers, experimentalists, nuclear reactor designers, and federal regulators by:

- Establishing accepted standards, requirements and best practices for V&V of computational models and simulations,
- Establishing accepted standards and procedures for assessing V&V (numerical and experimental) benchmark data,
- Providing readily accessible databases with long-term storage for V&V (code verification and validation) benchmark data that can be used in V&V assessments and computational methods development,
- Providing a searchable knowledge base of information, documents and data on V&V and UQ, and
- Providing web-enabled applications, tools and utilities for V&V and UQ activities, data assessment and processing, and information and data searches.

NE-KAMS will deploy state-of-the-art technology in information and data management systems and web services, leveraging the latest advances in high performance computing (HPC) and web/internet technologies to maximize the benefit to its users in industry, academia and

government. This section describes the main elements of the NE-KAMS knowledge base and how they will be implemented.

2.1 NE-KAMS Standards, Databases and Infrastructure

The NE-KAMS knowledge base will be developed, implemented, and deployed for use in stages and will grow and evolve over time. In particular, the primary elements of the knowledge base along with the attendant hardware, software and facility infrastructure will be developed and implemented in stages as funding and available resources allow. Similarly, select parts of the knowledge base, *e.g.*, standards, requirements and best practices for V&V and UQ of computational models and simulations, will become available for use when ready.

The following elements of the NE-KAMS knowledge base will be developed and implemented:

- Standards, requirements and best practices for performing V&V assessments of computational models and simulations for nuclear reactor design and safety analysis will be developed and implemented. Initially the NE-KAMS effort will focus on establishing V&V standards, requirements and best practices. This effort will build from and leverage previous efforts in V&V standards and guides of the American Institute of Aeronautics and Astronautics (AIAA) and the American Society of Mechanical Engineers (ASME). In addition, NE-KAMS will coordinate all future work in V&V standards, guides and practices with these organizations and with technical organizations in the nuclear energy sciences and engineering, such as the American Nuclear Society (ANS) and the Organization for Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA). It is envisioned that these standards, requirements and best practices for V&V developed by the NE-KAMS effort should become the accepted standards, requirements and best practices for V&V of computational models and simulations for the various nuclear energy sciences and engineering communities.
- Standards and procedures for the evaluation and classification of experimental and numerical benchmark data for use in V&V assessments of computational models and simulations will be developed and implemented. These standards and procedures will additionally provide clear guidelines on what is required to generate high-quality V&V benchmark data by highlighting the importance of several key quality classification categories. These standards and procedures can also be used to assess the pedigree of legacy experimental data. This NE-KAMS effort is unique in that currently no accepted standards or procedures exist for assessing the quality of numerical and experimental benchmark data used in V&V assessments. It is envisioned that these standards and procedures developed by the NE-KAMS effort can become the accepted standards and procedures for assessing and classifying code verification and validation benchmark data for use in V&V of computational models and simulations for the various nuclear energy sciences and engineering communities.
- Quality-assessed, web-accessible databases for nuclear energy related V&V (numerical and experimental) benchmark data and metadata that can be used in V&V assessments will be developed and deployed. It is expected that over time, an extensive database of V&V benchmark cases will be developed that are applicable to a wide variety of applications in nuclear energy sciences and engineering. The NE-KAMS V&V benchmark databases will be supported by and used in conjunction with the NE-KAMS

V&V standards, requirements, and best practices, providing a unique resource and capability for V&V and quality assurance of computational models and simulations. It is expected that the NE-KAMS V&V benchmark databases will become a valuable resource for the nuclear industry, academia, national laboratories and the U.S. NRC.

- A knowledge base of searchable information, documents and data related to V&V and UQ of computational models and simulations will be developed and implemented. The NE-KAMS knowledge base will include such items as examples of credible V&V and UQ assessments, validation pyramids and Phenomenon Identification Ranking Table (PIRT) charts for applicable nuclear reactor designs and systems, and reference documents and technical reports on V&V and UQ. It is envisioned that over time a large amount of information and data on V&V and UQ will be collected, processed and formatted and made available to NE-KAMS knowledge base users as a searchable knowledge base. All the information, documents and data will not reside in the NE-KAMS knowledge base. Appropriate links and connections will be provided to other sources of information, documents and data, including other data and knowledge bases, as needed. It is thus envisioned that the NE-KAMS knowledge base will become a valuable resource of cohesive reference information and data for the nuclear industry, academia, national laboratories and the U.S. NRC.

The NE-KAMS knowledge base will maximize the benefits to its users by providing the means to easily access the required information and data and efficiently and effectively utilize them in support of V&V and UQ assessments and methods development. To that end, NE-KAMS will deploy state-of-the-art technology in information management systems and web services to leverage the latest advances in high performance computing and web technologies. The NE-KAMS infrastructure will include knowledge base systems software, web-based user interface systems, HPC and storage systems, and high performance networks. Web-enabled applications, tools and utilities for V&V and UQ activities, data access and processing, and information and data searches will be developed and deployed.

As mentioned above, it is expected that the NE-KAMS knowledge base will have links to other data and knowledge bases, especially those of the DOE, such as the Office of Scientific and Technical Information (OSTI) and the Nuclear Energy Knowledge Management Program (NE-KM), and, as such, will serve as an access portal for a much larger and more extensive body of knowledge to its users. The NE-KAMS knowledge base will be implemented and operated with the required security infrastructure and protocols to accommodate both proprietary and public information.

The realization of the described vision for NE-KAMS knowledge base will require a focused effort with sustained funding and dedicated staff and resources for several years. To that end, it should be recognized that the initial implementation of the NE-KAMS knowledge base will be technically and organizationally complex, as well as costly, and the long-term success of the NE-KAMS knowledge base requires a sound starting point, with broad consensus from all the interested parties about goals, use, access and funding over the long term.

3. NE-KAMS High Level Requirements

This section describes the high level requirements for the NE-KAMS knowledge base which will guide the development, implementation and operations of NE-KAMS. The requirements

presented here represent an overview of the high level functions and features that are required to be in the knowledge base. More detailed requirements will be developed in the future based on these requirements such that these required functions and features of the knowledge base can be fully implemented. The high level knowledge base system software requirements are presented in section 4 since these requirements encompass most of, if not all, the high level requirements presented in this section. It is noted that the detailed description of the software requirements for the NE-KAMS knowledge base will be provided in the future via specification documents.

3.1 Programmatic Requirements

The programmatic requirements for NE-KAMS identify those programs or communities for which NE-KAMS will provide V&V and UQ support and resources that are needed in developing and employing computational modeling and analyses for nuclear reactor design, analysis and licensing. The NE-KAMS knowledge base will support all the DOE-NE M&S programs as well as the nuclear industry and academia. To that end, it will support both the science based and existing engineering/licensing based approaches to V&V and UQ.

NE-KAMS will provide V&V and UQ support and resources for the following DOE-NE M&S programs: CASL, NEAMS, LWRS, SMR, and NGNP. Future M&S programs that are initiated in DOE-NE will also be supported by NE-KAMS. Specific details on how NE-KAMS will support the current DOE-NE M&S programs are as follows:

- NEAMS – NE-KAMS is an integral part of the NEAMS Program and, as such, it will attempt to support all the V&V activities and processes of NEAMS. Initially, NE-KAMS will focus on supporting the CFD component of NEAMS.
- CASL – In the near term, NE-KAMS will focus on supporting the V&V activities and processes for the use of CFD in the CASL Program: single- and two-phase flows and fluid structure interaction. In the longer term, NE-KAMS will provide support for chemical-kinetics, materials and fuel system performance.
- LWRS – NE-KAMS will focus on supporting the V&V activities and processes for the use of next generation reactor systems code R7 and related T/H analysis codes in the LWRS Program.
- SMR – NE-KAMS will focus on supporting the V&V activities and processes for the use of CFD in the SMR Program. It is expected that CFD will be used extensively in the SMR Program to assess the behavior and performance of integral SMR designs where the reactor systems are tightly coupled to the containment.
- NGNP – NE-KAMS will focus on connecting to and making available data captured under the NGNP Program and leveraging V&V and UQ resources.

NE-KAMS will also provide similar V&V and UQ support and resources for the nuclear industry and academia. In addition, it is expected that NE-KAMS, through its focused development activities and V&V application case studies, will support the use of computational M&S in the nuclear industry by developing guidelines and recommended practices aimed at reducing uncertainty and improving applicability of existing analysis methods. In the longer term, steps that will be taken to expand the capabilities and scope of NE-KAMS to support a broader user community, not only in the nuclear energy sciences and engineering fields, but also users in other disciplines and industries.

3.2 Technical Requirements

The technical requirements for NE-KAMS identify the key elements of the knowledge base that will be developed, implemented and maintained as part of the NE-KAMS effort. Unlike most V&V databases which just serve as repositories for V&V cases and documents, NE-KAMS will provide value-added V&V, UQ and methods development technical support services to its users. To that end, the following elements of the NE-KAMS knowledge base will have to be implemented:

- Standards, requirements and best practices for performing V&V and UQ assessments in establishing credibility in computational analyses of nuclear reactor systems, components and processes;
- Standards and procedures for the evaluation and classification of numerical and experimental benchmark data for use in V&V assessments, which will characterize the quality of the data used in V&V assessments via quality classification categories;
- Quality-assessed, web-accessible knowledge bases and databases for nuclear energy related V&V benchmark data and attendant metadata that can be used in V&V assessments of computational models and methods development;
- A knowledge base of searchable information, documents and data related to V&V and UQ of computational models and simulations, including examples of credible V&V assessment and uncertainty analysis;
- Focused and targeted V&V case studies of nuclear reactor systems, components and processes to enable reduction in uncertainty and improvement in applicability of computational models and simulations used in the nuclear industry;
- Validation pyramids and PIRT charts for applicable nuclear reactor designs and systems;
- Development and implementation of knowledge base system software, hardware and facility infrastructure for information and data collection, processing, qualification, storage and utilization with the goal of retaining and maximizing access to both the data and the metadata;
- Web-enabled applications, tools and utilities for V&V and UQ activities, data assessment and processing, and information and data searches.

The initial focus for the NE-KAMS effort will be on supporting the use of CFD for M&S of nuclear reactor systems, components and processes. CFD validation datasets, both existing and legacy experimental data, will be sought first for inclusion in the NE-KAMS validation database. The initial standards, requirements and procedures for validation data evaluation and classification will be specific to CFD, but are expected to be generalizable. It is expected that the NE-KAMS CFD validation datasets will be composed of two types of experimental data:

- Single-phase flow experimental data from CFD validation experiments;
- Single-phase and heated flow experimental data from separate-effects T/H and reactor systems validation experiments.

In addition, CFD V&V assessments of a select set of existing and legacy experimental data will be performed. This industry-focused effort will evaluate legacy experimental data that is in common use for T/H analysis, including experimental data for

- Wall friction
- Heat transfer
- Pressure loss coefficients
- Thermal and species mixing
- Natural convection and buoyant flows
- Multi-phase flows

This NE-KAMS effort will also consider and evaluate Code Scaling, Applicability, and Uncertainty (CSAU) methodology for CFD analysis, especially in the context of assessing the applicability of PIRT charts and validation pyramids.

Once NE-KAMS has reached a sufficient level of functionality for CFD, the same graded approach will be applied to develop and implement other databases that are pertinent to nuclear reactor design and safety analysis, such as the materials and fuel system performance databases.

3.3 Operational Requirements

The operational requirements for NE-KAMS identify the functionality that the knowledge base needs to have to support the day-to-day operations of the knowledge base. These operational requirements are categorized into knowledge base, interface and communications, hardware, facility and staffing requirements. The operational requirements for NE-KAMS are:

- Knowledge Base Requirements
 - Capability to capture, preserve and utilize M&S, V&V and UQ knowledge and data
 - Capture and preservation of DOE-NE M&S, V&V and UQ data and information, both new and legacy data and information
 - Support for both proprietary and public data and information
 - Web-accessible and secure, rapid and coherent access to data and information
 - Web-enabled, infrastructure for knowledge management and utilization
 - Access to V&V and UQ standards and requirements
 - Access to recommended V&V and UQ best practices and procedures
 - Access to quality-assessed V&V benchmark databases
 - Provide web-enabled knowledge base tools and utilities
 - Tools and utilities for V&V and UQ activities
 - Tools and utilities for data assessment and processing
 - Tools and utilities for data classification and qualification
 - Tools and utilities for data and information searches and exploration
 - Access portal to other knowledge and data bases, *e.g.*, DOE OSTI
- Interface and Communications Requirements
 - Secure, web-enabled user interfaces
 - Secure connections and communications with other knowledge and data bases
- Hardware Requirements

- Web-based interface and communication systems
- HPC compute and high-capacity, hierarchical storage systems
- HPC networks
- Facility Requirements
 - Dedicated physical facility at the INL that houses the primary NE-KAMS knowledge base
- Staffing Requirements
 - Availability of NE-KAMS technical staff and consultants to provide specific support and educational services to knowledge base users
 - Full time staff that maintains the NE-KAMS software and hardware and provide daily operations support

3.4 User Feedback Requirements

The requirements for users relate to specific content that potential users of NE-KAMS may want to see included in the knowledge base that will benefit them in their performance of V&V and/or UQ of models and simulations for their particular applications. Efforts will be made to survey potential NE-KAMS customers to obtain their recommendations for knowledge base content including:

- DOE-NE programs,
- Nuclear reactor vendors,
- Nuclear utilities,
- University partners, and
- U.S. NRC.

3.5 Development Requirements

The requirements for development relate to the unique position in which the NE-KAMS knowledge base will be able to operate. That is, the NE-KAMS technical staff will be able to recognize where dedicated research will be able to help develop processes that pertain to V&V and UQ activities, and where more research is needed. Additionally, the NE-KAMS staff will be able to consult with DOE-NE program managers to see where there are gaps in the V&V benchmark data that are needed for particular nuclear energy sciences and engineering applications. Thus, it seems appropriate that NE-KAMS is provided with some funds to be able to fund researchers to help fill in gaps in knowledge and needed data. The requirements for applications are given as:

- Funding to improve V&V and UQ assessment capability, such as new ways to perform numerical error estimation on very large grids that are not suitable for grid refinement and better ways to obtain isotropically refined grids.
- Funding to sponsor experiments, primarily at universities, to fill in gaps identified in the V&V benchmark database needed for V&V assessments of computational modeling and simulation of nuclear reactor systems, components and processes.
- Funding to address other areas that should be developed to improve credibility of engineering analyses for CFD, T/H or other disciplines.

3.6 Funding Requirements

The requirements for funding identify funds needed to develop, operate and maintain the NE-KAMS knowledge base. The greater the initial funding, the more development can be performed for the knowledge base. The NE-KAMS funding support can be categorized as:

- Near-term funding to develop NE-KAMS
- Long-term funding to implement, deploy, operate and maintain NE-KAMS

The prioritized set of initial tasks identified for the development of NE-KAMS is detailed in Section 5 below.

4. High Level System Software Requirements

The functionality of NE-KAMS will depend on the reliable operation of system software and hardware for the knowledge base. The knowledge base will need to be able to perform a number of functions and will actually have a series of different characteristics for each function. Detailed software requirements will be developed in another document to fully describe the associated requirements necessary to provide the desired functionalities. These functionalities and their specific functions are listed at a high level in the following sub-sections.

4.1 Website

Access to the NE-KAMS knowledge base will be via an internet website and web portal. The website software should have the following functionality:

- allow login and logout ability
- allow website browsing
- provide sitemap
- maintain linkages within the knowledge base
- maintain linkages to other sites
 - software interfaces
 - hardware interfaces
- provide for webmaster editing and control

4.2 Search Engine

It will be important for NE-KAMS users to be able to quickly find what they are looking for on the NE-KAMS knowledge base.

- Federated search engine to rapidly and coherently search the NE-KAMS knowledge base and linked knowledge and data bases.

4.3 Communications

It will be important to be able to communicate with NE-KAMS staff and perhaps with other users. Communication will require the following functions:

- provide communication to NE-KAMS staff and others

- e-mail
- instant messaging
- web-based telephone

4.4 Experimental Data Repository

A primary function of NE-KAMS is to provide experimental data for validation purposes. Therefore, NE-KAMS will include an experimental data repository with the following functions:

- create and use experimental data storage formats
- upload data
- display information about each dataset
- download data
- reformat data into desired formats
- store petabytes of experimental data
- partition data into several physics bases
- display documents
- plot data

4.5 Numerical Data Repository

NE-KAMS will provide numerical data for code verification purposes. The numerical data repository will need to have the following functions:

- create and use numerical data storage formats
- upload numerical data
- display information about codes, files, data, etc.
- upload source codes and input files
- reformat data into desired formats
- store codes, files and output data
- read stored simulation files
- access simulation files with website software (not the creator software)
- plot numerical data
- create data videos
- reformat numerical data into neutral formats
- download numerical data

4.6 Document Repository

Documents will be stored along with experimental and numerical data to provide for metadata as well as recommended practices and procedures for performing V&V and UQ. The documents repository will have the following functions:

- upload documents
- archive documents

- display documents
- play videos
- download documents

4.7 Computing Support on the Knowledge Base

An added value of NE-KAMS will be the addition of web-enabled computer tools and utilities that can be used to perform V&V and UQ activities that can be performed on the NE-KAMS HPC systems available through the NE-KAMS web-enabled interface. The functions needed for the computing include the following:

- Maintain suite of web-enabled computing tools/utilities
- perform computations using computing tools/utilities
- plot and display results
- create and play videos
- download data/plots/videos

4.8 Training

In order to provide maximum value to users, users may need training on how to use the knowledge base:

- provide for online, web-enabled training tutorials and related material
- provide access to NE-KAMS knowledge base during tutorial operations or related training session

4.9 Security

A very important system software requirement is to provide security for the knowledge base. The functions required are summarized as:

- maintain backup of knowledge base data and information
- provide security of stored data and documents
- provide multiple, secured levels of access to stored data
- provide security protection from unauthorized users and cyber attack

Security details for DOE-NE knowledge management have been previously developed and are provided in Appendix B.

4.10 Site Usage Monitoring

It is important that usage of the knowledge base be recorded:

- Usage statistics will be captured and managed for the NE-KAMS system.

5. NE-KAMS Implementation: Next Steps

This section describes the near term tasks which will be performed during the initial development phase of NE-KAMS. These developmental tasks will be prioritized and performed in stages as funding and available resources will allow.

5.1 Survey and Analysis of Existing Data and Knowledge Bases

To better define the scope and breadth of the NE-KAMS effort, a state of the art survey will be performed to assess all the major ongoing M&S, V&V and UQ database efforts, including the DOE and commercial databases. Understanding the architecture and functionality of these databases, *i.e.*, how the data are collected/acquired, reviewed, processed, formatted, stored and accessed, will be needed in order to not only leverage existing database efforts in the NE-KAMS development and implementation, but also to articulate the true value of NE-KAMS by highlighting the unique set of value-added functionality and services that the NE-KAMS knowledge base will provide to its users.

The NE-KAMS knowledge base will have links and connections to other data and knowledge bases, especially those of the DOE, such as OSTI, and, as such, the survey will be needed to identify and understand the requirements for integrating NE-KAMS with other data and knowledge bases. In particular, early in FY12, the DOE Gen IV Materials Handbook Database at Oak Ridge National Laboratory and DOE Environmental Management Groundwater and Soil Database at Pacific Northwest National Laboratory will be assessed to identify and understand the requirements for integrating these databases to the NE-KAMS knowledge base. It is expected that over time, the NE-KAMS knowledge base will serve as an access portal for a much larger and extensive body of knowledge to its users in industry, government and academia.

5.2 Development of NE-KAMS V&V Standards, Requirements and Best Practices

The focused effort to develop and improve standards, requirements and best practices for CFD V&V will be ongoing. The overarching goal of this activity is to increase confidence in CFD analysis results and predictions for nuclear reactor design, safety analyses, and licensing applications. To that end, the newly developed NE-KAMS V&V standards and requirements for CFD will be further developed, refined and updated, as needed. In parallel, this effort will be augmented by the following related activities:

- Assessment of methods and approaches for processing, formatting, documenting, storing and retrieving V&V benchmark data.
- Assessment of methods and approaches for linking V&V benchmark data with attendant metadata.
- Assessment of methods and approaches for incorporating, linking and presenting V&V benchmark datasets in the higher level context of applicable PIRT charts and validation pyramids (validation hierarchy).

The effort to develop the NE-KAMS best practices guidelines for V&V assessments will be initiated. The V&V benchmark data standards and requirements identify the quality levels for V&V benchmark data, including the ideal case. The role of the NE-KAMS V&V best practices

guidelines is to bridge the gap between the ideal V&V assessments and V&V assessments that can be done in a practical engineering setting to support the use of CFD for nuclear reactor design, safety analysis and licensing applications. The NE-KAMS best practices guidelines for V&V will also be an ongoing effort with frequent revisions and updates, as needed.

5.3 NE-KAMS Evaluation and Testing

As part of the NE-KAMS development process, tasks will be performed to evaluate and/or test the NE-KAMS V&V benchmark data standards and requirements and software and hardware components of the NE-KAMS knowledge base in support of the NE-KAMS development and implementation. Some of these tasks will be performed to better understand the requirements for implementing the NE-KAMS knowledge base and other tasks will be performed to test out various NE-KAMS software and hardware components at a small-scale and reduced scope to develop various implementation specifications for the NE-KAMS knowledge base. The expected set of evaluations and testing will include the following:

- V&V benchmark data assessments – Initially, seven V&V benchmark datasets (four code verification and three validation benchmark datasets) will be assessed relative to the newly developed NE-KAMS V&V standards and requirements for CFD. This assessment will aid in the development of the processes, standards and requirements for evaluating the quality of V&V benchmark data for inclusion in the CFD V&V databases. The details of these seven code verification and validation benchmark datasets are provided in Appendix C.
- Database software evaluation and testing – Various database software packages, including commercial software, will be evaluated and tested for potential use in the NE-KAMS knowledge base.
- Knowledge base interface systems evaluation – Various candidate interface systems for the NE-KAMS knowledge base will be evaluated, including the web-enabled user interface system. This evaluation will also consider interface systems for linking and connecting the NE-KAMS knowledge base to other data and knowledge base systems.
- Web-enabled database tools and utilities evaluation – Various web-enabled database tools and utilities will be evaluated for potential use and incorporation into the NE-KAMS knowledge base.
- Software and utilities evaluation – Various techniques for front-end virtualization that will be needed to support computing in NE-KAMS will be evaluated. The front end virtualization when developed and implemented will allow the NE-KAMS users to run their V&V and UQ applications in the NE-KAMS HPC clusters and servers using lightweight devices or terminals on their desktops.

5.4 NE-KAMS Implementation Specifications

As part of the initial NE-KAMS development process, tasks will be performed to develop implementation specifications for various software and hardware components of the NE-KAMS knowledge base in conjunction with the other development tasks identified in this section. The knowledge gained and lessons learned from the state of the art survey of existing M&S, V&V and UQ databases and evaluations and testing of various NE-KAMS software and hardware components will be incorporated into the NE-KAMS implementation specifications, *e.g.*, NE-

KAMS software requirements specification document. The expected set of NE-KAMS implementation specifications includes:

- NE-KAMS Software Requirements Specification
- NE-KAMS System Software Design Specification
- NE-KAMS Interface Systems Design Specification
- NE-KAMS Hardware Specifications
- NE-KAMS Facility and Infrastructure Specifications
- NE-KAMS Cyber Security Master Plan

6. Concluding Remarks

Because the nuclear energy community is geographically dispersed and fragmented, effectively communicating and collaborating with one another is difficult and unreliable. However, this situation can be greatly improved by making important V&V data and related metadata readily available to the nuclear energy sciences and engineering communities through a trusted knowledge base for technical exchange and collaboration. Thus, we recognize the strategic importance of implementing NE-KAMS and ensuring that it aligns with the business needs of the nuclear energy sciences and engineering communities. More precisely, the business case for establishing NE-KAMS is simple: Without a concerted effort to evaluate and preserve nuclear reactor 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.

7. Reference Materials

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APPENDIX A

A SURVEY OF EXISTING CFD V&V AND ASSESSMENT DATABASES

Verification and validation (V&V) are the primary means to assess the accuracy and reliability of computational simulations. V&V methods and procedures have fundamentally improved the credibility of simulations in several high-consequence fields, such as nuclear reactor safety, underground nuclear waste storage, and nuclear weapon safety. However, significant improvements in the methodology and practice of V&V are necessary to achieve improved credibility in computational sciences and engineering. One element of needed improvements is the design, construction, and use of highly demanding V&V benchmarks to improve the accuracy and reliability of physics models and codes. In particular, these V&V benchmarks should be of high quality such that they can be viewed as engineering reference standards. To that end, the concept of *strong sense benchmarks* (SSBs) was formulated by Oberkampf et al. [1]. As such, one of the key components of the Nuclear Energy – Knowledge base for Advanced Modeling and Simulation (NE-KAMS) is its V&V benchmark databases with SSBs for code verification and validation. Code verification benchmarks and validation benchmarks have been constructed for a number of years in every field of computational simulation. However, the comprehensive approach embodied in NE-KAMS with its quality-assessed V&V benchmark databases, V&V standards, requirements, and best practice guidelines, and related support services for the construction and use of SSBs in V&V has not been proposed.

The goal of the V&V benchmark database within NE-KAMS is to improve the reliability of the computer software, the estimation of numerical accuracy, the quality of the physics models used, the quantification of uncertainty, and the training and expertise of users of the codes. To better define the scope and breadth of the effort required to develop, implement and deploy NE-KAMS V&V benchmark databases, a survey and evaluation of existing V&V and assessment databases or related development efforts, including commercial V&V and assessment databases, were performed. Understanding the architecture, features and functionality of these databases, *i.e.*, how the V&V benchmark or assessment data is acquired/collected, reviewed, processed, formatted, stored, accessed and used, is needed in order to not only leverage existing database efforts in the development of NE-KAMS, but also to articulate the true value of NE-KAMS by highlighting the unique set of value-added functionality and services that the NE-KAMS knowledge base will provide to its users.

The results of the survey showed that V&V and assessment databases presently exist, mostly outside of the nuclear domain, such as the European Research Community On Flow, Turbulence And Combustion (ERCOFTAC) [2], QNET-CFD [3], and NPARC Alliance [4] databases. These databases are mostly computational fluid dynamics (CFD) V&V and assessment databases. This is not surprising since it is accurate to say that computationalists (code users and code developers) and experimentalists in the field of fluid dynamics have been the pioneers in the development of terminology, methodology, and procedures for V&V. A good summary of the development of many of the methodologies and procedures for V&V of CFD can be found in the seminal book on V&V by Roache [5]. In addition, Oberkampf and Blottner [6] and Oberkampf and Trucano [7] provide a comprehensive review of the history and development of V&V from the perspective of the CFD community. Recently, Oberkampf and Trucano [8] and

Oberkampf and Roy [9] have extended and generalized the terminology, methodology, and procedures for V&V to a broader domain of computational sciences and engineering.

The evaluation of the V&V and assessment databases surveyed showed that these databases are essentially repositories for V&V cases, V&V assessment results, and related documents. In general, all that these databases do is maintain V&V cases, mostly validation cases, which have been collected or submitted to the database over time. The quality and amount of the V&V case data as well as the attendant documentation vary significantly, ranging from good quality data that is well documented to poor quality data with a little or no documentation. The users interface with the database via a website and search manually through a listing of links, directories or folders to find the V&V benchmark data and related documentation to download for use offline. There are no standards, requirements or best practices guidance for V&V and uncertainty quantification (UQ) associated with these databases. There is also no process of quality assurance, such as procedures for assessing and classifying the quality of V&V benchmark data or a review and approval procedure for entries into the database, associated with these databases. In fact, it can be stated that there is a little or no organizational control or protocol on the operations of these databases. Once one gains access to these databases, how one uses these databases is, by and large, up to the user. Other than some brief web page documentation or an overview tutorial on V&V, there is no technical support services associated with these databases. It is noted that over time, most of these CFD V&V and assessment databases have either become defunct or fallen out of date due to lack of use and interest. For most of these databases, the content of the database have not changed and there have been a little or no updating of the V&V cases in the database. It is also noted that the terms “V&V cases” were used to describe the V&V data in the existing databases instead of “V&V benchmarks.” This was deliberate because most of the V&V data in these databases were not of required quality and resolution and did not have the required level of detailed documentation such that they can be viewed as engineering reference standard, *i.e.*, strong sense benchmarks.

Unlike most V&V and assessment databases which just serve as repositories for V&V cases and related documents, the NE-KAMS knowledge base will provide value-added V&V, UQ and computational methods development technical support services to its users. This will be accomplished by (a) establishing standards, requirements and best practices for V&V and UQ assessments, (b) establishing standards and procedures for qualifying and classifying experimental and numerical benchmark data, (c) providing readily accessible databases for experimental and numerical benchmark data for V&V assessments, (d) providing a searchable knowledge base of information, documents and data, and (e) providing web-enabled tools and utilities for V&V and UQ activities. The NE-KAMS knowledge base encompasses the following elements:

- Standards, requirements and best practices for performing V&V and UQ assessments in establishing credibility in computational analyses of nuclear reactor systems, components and processes;
- Standards and procedures for the evaluation and classification of experimental and numerical benchmark data for use in V&V assessments, which will characterize the quality of the data used in V&V assessments via quality classification categories, and provide clear guidelines on what is required to generate high-quality V&V benchmark data by highlighting the importance of several key quality classification categories;

- Quality-assessed, web-accessible databases for nuclear energy related experimental and numerical benchmark data and attendant metadata that can be used in V&V assessments of computational models and simulations and computational methods development; metadata includes information about the experiment such as data uncertainty analyses, instrumentation used, the as-tested geometry and the experimental procedures followed to obtain the data;
- A knowledge base of searchable information, documents and data related to V&V and UQ of computational models and simulations, including examples of credible V&V assessment and uncertainty analysis;
- Focused and targeted V&V case studies of nuclear reactor systems, components and processes to enable reduction in uncertainty and improvement in applicability of computational models and simulations used in the nuclear industry;
- Validation pyramids and Phenomena Identification and Ranking Tables (PIRT charts) for applicable nuclear reactor designs and systems;
- Development and implementation of the knowledge base system software, hardware and facility infrastructure for data collection, processing, qualification, storage and utilization with the goal of retaining and maximizing access to both the data and the metadata;
- Web-enabled applications, tools and utilities for V&V and UQ activities, data assessment and processing, and information and data searches.

The next two sections provide the results of the survey and evaluation of existing V&V and assessment databases for computational modeling and simulations. In particular, the results of the survey are reported as a) verification benchmark and assessment databases and b) validation benchmark and assessment databases.

Verification Benchmark and Assessment Databases

During the last two decades, the National Agency for Finite Element Methods and Standards (NAFEMS) has developed some of the most widely known V&V benchmarks [10]. Roughly 30 verification benchmarks have been constructed by NAFEMS. The majority of these benchmarks have targeted solid mechanics simulations, though some of the more recent benchmarks have been in fluid dynamics. Most of the NAFEMS verification benchmarks consist of an analytical solution or an accurate numerical solution to a simplified physical process described by a partial differential equation (PDE). The NAFEMS benchmark set is carefully defined, numerically demanding, and well documented. However, these benchmarks are currently very restricted in their coverage of various mathematical and/or numerical difficulties and in their coverage of physical phenomena. Further, the performance of a given code on the benchmark is subject to interpretation by the user of the code. It is also likely that the performance of a code on the benchmark is dependent on the experience and skill of the user.

Several large commercial computer-aided engineering (CAE) code companies specializing in solid mechanics have developed an extensive set of well-documented verification benchmarks that can be exercised by licensed users of their codes. Such benchmarks are intended to be applied only to a particular code, and they describe how that code performed on the benchmark problems. The performance results of a code tested on the benchmark problems by a commercial company can be clearly compared with the results obtained by a user who tests the code with the

same benchmark problems. These company- and user-testing activities give the user a better understanding of the minimal performance that can be expected from a code. It should be noted here that information about a code's performance on a set of benchmark problems prior to purchase of the code is often difficult to obtain, as this information is proprietary.

Two examples of commercial codes with well-documented verification benchmarks are computational structural mechanics (CSM) codes ANSYS [11] and ABAQUS [12]. ANSYS and ABAQUS have roughly 270 formal verification test cases. The careful description and documentation of the ANSYS and ABAQUS benchmark sets is impressive. However, the primary goal in essentially all of these documented benchmarks is to demonstrate the “engineering accuracy” of the codes, not to precisely and carefully quantify the numerical error in the solutions as one would need to do in code verification assessments. Noticeably absent from the discussion of commercial codes above are CFD software packages. We have surveyed all the major commercial CFD codes available, including FLUENT [13], CFX [14] and STAR-CD [15] and we have not found extensive, formally documented verification benchmark sets for the codes examined.

The nuclear reactor engineering fields as a group have not focused on code verification benchmarks, but the nuclear reactor safety community placed great emphasis on developing validation benchmarks. Many of these validation benchmarks are closely related to the operations of actual reactors at near-safety-critical conditions, as opposed to being more fundamental-physics benchmarks. These validation benchmarks are described in more detail in the next section.

Probably the most important challenge in the design and computation of verification benchmarks for use in V&V process is to assess the mathematical accuracy of the benchmark solution. The AIAA Guide [16] suggests the following hierarchical organization with respect to the accuracy of benchmark solutions (from highest to lowest): analytical solutions, highly accurate numerical solutions to the ordinary differential equations (ODEs), and highly accurate numerical solutions to the partial differential equations (PDEs). In the AIAA Guide, as well as in Oberkampf et al. [1], analytical solutions included manufactured solutions that were constructed by the “Method of Manufactured Solutions” (MMS) [5,17]. Recently, however, Oberkampf and Trucano [8] have concluded that the manufactured solutions should be considered as a separate type of highly accurate solutions. This conclusion was based on two reasons: (a) manufactured solutions do not correspond to physically meaningful phenomena, and (b) they do not suffer from numerical accuracy issues that commonly occur with analytical solutions. Thus, the hierarchical organization of code verification benchmarks in NE-KAMS V&V benchmark databases is expanded to include the following four types of highly accurate solutions (from highest to lowest): (type 1) analytical solutions with no numerical approximations (such as MMS), (type 2) analytical solutions with numerical approximations (such as an infinite series solution), (type 3) numerical solutions of ODEs, and (type 4) numerical solutions of PDEs.

Validation Benchmark and Assessment Databases

A number of efforts have been undertaken in the development of validation databases that could mature into well-founded benchmarks. In the United States, the NPARC Alliance has developed a validation database that has roughly 20 different flows [4]. In Europe, starting in the early 1990s, there has been a much more organized effort to develop validation databases. These

databases have primarily focused on aerospace applications. The ERCOFTAC database has collected a number of experimental datasets for validation applications [2]. QNET-CFD is a thematic network on quality and trust for the industrial applications of CFD [3]. This network has more than 40 participants from several countries that represent research establishments and many sectors of the industry, including commercial CFD software companies. For a history and review of the various efforts, see Rizzi and Vos [18] and Vos et al. [19].

In the field of nuclear reactor engineering, the Nuclear Energy Agency (NEA), Committee on the Safety of Nuclear Installations (CSNI) devoted significant resources toward developing validation benchmarks, which they refer to as International Standard Problems (ISPs). This effort began in 1977 with recommendations for the design, construction, and use of ISPs for loss-of-coolant accidents (LOCAs) [20]. The CSNI recognized the importance of issues such as (a) providing a detailed description of the actual operational conditions in the experimental facility, not those conditions that were requested or desired; (b) preparing careful estimates of the uncertainty in experimental measurements and informing the analyst of the real estimate; (c) reporting the initial and boundary conditions that were realized in the experiment, not those conditions that were desired; and (d) conducting a sensitivity analysis to determine the most important factors that affect the predicted system responses of interest. The CSNI has continually refined the guidance for ISPs such that the most recent recommendations for the ISPs address any type of experimental benchmark, not just benchmarks for LOCA accidents [21]. Thus, the primary goal of the ISPs remains the same for all types of benchmarks: “to contribute to a better understanding of postulated and actual events” that could affect the safety of nuclear power plants.

In addition, the nuclear reactor safety community has over the years held benchmarking exercises or workshops to obtain experimental data for use in assessments of CFD and reactor systems codes for specific problems relating to nuclear reactor safety, such as boron dilution, pressurized thermal shock and thermal fatigue. Specific details on these validation data are provided in the following subsection.

A complete list of existing validation benchmark and assessment databases surveyed and evaluated are provided below with a brief description of each database:

Existing Validation Benchmark and Assessment Databases (Non-Nuclear)

- **Validation Tests Performed by Major CFD Code Vendors:** Basic validation procedures of a generic type have been undertaken by all the major code vendors. Information and data used were taken from established databases concerned with basic flow situations, such as flow over a backward facing step, jet impingement, *etc.*
- **ERCOFTAC:** ERCOFTAC is an association of research, educational, and industrial groups whose main objectives are to promote joint efforts through centers and industrial application of research, and to create Special Interest Groups (SIGs) in certain areas. One such special interest group is the ERCOFTAC Database Interest Group. The database was started in 1995 and is maintained by the University of Manchester, UK. It contains experimental as well as “high-quality” numerical data relevant to both academic and applied CFD applications. ERCOFTAC holds regular workshops on turbulence modeling around Europe, information from which is used to update and refine the

database. The Classic Data Base is open to public (though a simple registration procedure has to be followed before data may be downloaded). There are more than 80 documented cases, containing either experimental data or with highly accurate DNS (Direct Numerical Simulation) data available. Each case contains at least a brief description, some data to download, and references to published work. Some of the cases could be used also in nuclear reactor safety applications, such as a flow in curved channels, mixing layers, separated flows, impinging jets, and flows through tube bundles.

- **QNET-CFD Knowledge Base:** QNET-CFD knowledge base was developed from the QNET-CFD web-based thematic network, which was a part-funded European project to promote the quality of CFD and trust in the industrial application of CFD. Several years were spent in assembling and collating knowledge and know-how across a range of hierarchically structured application areas: aerodynamics, combustion and heat transfer, chemical and process engineering, thermal hydraulics and nuclear safety, civil construction and HVAC (heating, ventilation and air conditioning), and environmental flows and turbomachinery. For each application case, its description, test data, CFD simulations, evaluation, best practice advice, and information on related flow regimes are all available. Between 2000 and 2004, a knowledge base containing 43 application cases was established, later expanded, and finally brought online by means of a Wiki-based website, which had been developed from the prototype pioneered by QNET-CFD network. The Wiki pages now come under the administration of the ERCOFTAC organizations.
- **NPARC Alliance Database:** Chiefly oriented towards the aerodynamics community, the CFD Verification and Validation section provides a tutorial as well as measurements and data for CFD cases. There is a link to data archive of NASA, which is particularly useful. Data are available in the following areas: incompressible, turbulent flow over a flat plate, RAE 2822 transonic airfoil, S-Duct, subsonic conical diffuser, hydrogen-air combustion in a channel, two-stream mixing, and laminar flow over a circular cylinder. Many of the basic flow configurations are relevant to nuclear reactor safety analyses at a fundamental level.
- **AIAA (American Institute of Aeronautics and Astronautics):** The society participates in the definition of standards for CFD in its *Verification and Validation Guide* [16] and has important links to websites containing lists of references (papers, books, author coordinates) related to CFD V&V. Also, there are various links to other websites, containing information of (principally) aeronautical interest, *e.g.*, NASA benchmarks and workshops. Some of these links may be useful for CFD validation, but would need to be assessed for relevance to nuclear reactor design, analysis and licensing applications.
- **VATTENFALL Database:** The Vattenfall database [22] is not a validation benchmark or assessment database, but it includes experimental data that could be used in V&V assessments. In particular, Vattenfall database includes some high quality turbulence measurements from various experiments that were conducted at Vattenfall, Sweden.

Existing Validation Benchmark and Assessment Databases (Nuclear)

- **Boron Dilution:** Experiments focusing on boron dilution generally try to reproduce the mixing in reactor downcomers and the lower plenum upstream of the reactor core inlets. The databases are well-established and have been used previously for benchmarking exercises.
 - University of Maryland Tests (USA): Formed the basis of International Standard Problem ISP-43
 - ROCOM Test Facility (Germany) [23]: Benchmarking exercise within European Commission (EC) 5th Framework Program (FWP) FLOWMIX-R [24]
 - OKB GIDROPRESS (Russia): Benchmarking exercise within EC 5th FWP FLOWMIX-R
 - VATTENFALL (Sweden): Benchmarking exercise within EC 5th FWP FLOWMIX-R
- **Pressurized Thermal Shock (Single-Phase) [25]:** During a Small-Break Loss of Cooling Accident (SB-LOCA) scenario in a pressurized water reactor (PWR), Emergency Core Cooling (ECC) water is injected into the cold-leg pipe and mixes with any water remaining in the pipe. The combined streams flow toward the downcomer, where further mixing takes place. In the case of incomplete mixing of the streams, the cold water from the ECC line will come in direct contact with the reactor pressure vessel wall and may lead to large temperature gradients inside the vessel material, generating high thermal stresses. Knowledge of such thermal loads is important for plant-life extension assessment, since during its service life the reactor pressure vessel will have become subject to radiation-embrittlement. Below are data for single-phase pressurized thermal shock. Generally, these data are restricted, though exceptions have been made within a particular context. For example, data from two UPTF tests were made available to participants in the EC 5th FWP ECORA [26].
 - CREARE 1:5/1:2 (USA)
 - IVO FORTUM 2:5 (Finland)
 - PURDUE 1:2 (USA)
 - HDR 1:4/1:2 (Germany)
 - UPTF 1:1 (Germany)
- **Thermal Fatigue (Mixing Tees):** Flow-induced failures of parts of structural components of nuclear power plants caused by high-cycle thermal fatigue include Genkai Unit 1 (Japan), Tihange Unit 1 (Belgium), Farley Unit 2 (USA), PFR (UK), Tsuruga Unit 2 (Japan), and Loviisa (Finland). As a result of these incidents, considerable research effort has been devoted to the phenomenon, and both experimental and numerical information has been gathered to aid understanding. Thermal fatigue (or thermal

striping) has been studied mainly for two geometric configurations: T-junctions and for two or more parallel jets in contact with a neighboring structure. Under this latter category is included the thermal striping threat to the reactor pressure vessel caused by pressurized thermal shock. For both types, the problem is complex, involving several scientific disciplines (and consequently several types of computer codes): calculation of velocity and temperature fields in the fluid, the temperature fields in the solid materials, estimation of the associated mechanical stresses, and the behavior of cracks in the solid. Any experimental database should reflect and comprehensively cover all of these disciplines. Moreover coupling between temperature fields is two-way, which means fluid-dynamic and structural-dynamic computations have to be carried out simultaneously, the data from each being appropriately interfaced. Most of these data are only available under agreement. However, the data from several SPG tests were released to partners in the EC 5th FWP THERFAT [27], and data from one of the tests made by VATTENFALL area the basis of an Organization for Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA) benchmark [28].

- SPG (Germany)
- FATHERINO (France)
- PSI (Switzerland)
- VATTENFALL (Switzerland)
- WALTON (Japan)

It is noted that validation benchmarks are much more difficult to construct and use than verification benchmarks. The primary difficulty in constructing validation benchmarks is that experimental measurements in the past have rarely been designed to provide true validation benchmark data. Oberkampf and Aeschliman [29], Aeschliman and Oberkampf [30], Oberkampf and Blottner [6], Oberkampf and Trucano [7], Roy et al., [31,32], and Lee and Bauer [33] give an in-depth discussion of the characteristics of validation experiments, as well as examples of experiments that were specifically designed to be a true validation benchmark. The validation benchmarks that have been compiled and documented by organized efforts, some of which were referenced above, are indeed instructive and useful to users of the codes and to developers of physics models. However, much more needs to be incorporated into the validation benchmarks, both experimentally and computationally, to achieve the next level of usefulness and critical assessment.

Oberkampf et al. [1] introduced the concept of strong-sense benchmarks in V&V. Oberkampf et al. argue that SSBs should be of a high-enough quality that they can be viewed as *engineering reference standards*. These authors state that SSBs are test problems that have the following four characteristics: (1) the purpose of the benchmark is clearly understood, (2) the definition and description of the benchmark is precisely stated, (3) specific requirements are stated for how comparisons are to be made with the results of the benchmark, and (4) acceptance criteria for comparison with the benchmark are defined. In addition, these authors require that information on each of these characteristics be “promulgated,” *i.e.*, the information is well documented and publicly available. Although a number of benchmarks are available, a few of which were discussed previously, these authors assert that SSBs do not presently exist in computational

physics or engineering. They suggested that professional societies, academic institutions, governmental or international organizations, and newly formed nonprofit organizations would be the most likely to construct SSBs. It is the goal of NE-KAMS knowledge base to become the center of excellence for the development and use of SSBs in V&V of computational models and simulations in support of nuclear reactor design, analysis and licensing.

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APPENDIX B

NE-KAMS CYBER SECURITY PLAN

Overview

The draft *Cyber Security Master Plan for the Office of Nuclear Energy Knowledge Management (NE-KM) Program* developed in FY11 will be used for NE-KAMS. The security plan is based on the National Institute of Standards and Technology (NIST) series of new guidance documents that restructure the certification and accreditation process (NIST-SP 800-37, *Guide for the Security Certification and Accreditation of Federal Information Systems*) by requiring demonstrations of the processes and controls used to ensure a defense-in-depth computer security architecture. NIST stipulates that the information security program must include documentation and reports that clearly describe how information is being protected. In addition to the Guide, DOE has published several policies relating to the security of information. To address the requirements laid out by both NIST and the Department of Energy (DOE), eleven separate references were used to create this Master Plan.

It is important to note that until this plan has gone through several reviews, including a review by the NE-KM Working Group, the document will not be considered final. However, because it was developed based on the NIST and DOE standards, it can serve as guidance for NE-KAMS information security activities.

Authorization and Authentication

Although authorization and authentication policies are outlined in the Cyber Security Master Plan, this section provides more detailed information as to how user accounts will be established and managed. In general, this section outlines the security requirements for establishing user accounts, enabling user access and ensuring the user is properly authenticated before accessing NE-KAMS.

- A user access request shall be required for all users requesting access; all access requests are for public information only, unless otherwise stated.
- User access requests shall require the following information:
 - First, middle and last name
 - Title
 - Affiliation
 - Department
 - Phone
 - Justification
- Two-factor identification and authorization shall be used that includes a user ID and user specified password.
- User IDs shall consist of the first letter of the first name, first letter of the middle name, followed by the first six letters of the requestor's last name.

- User IDs shall be unique and shall not be replicated; in cases where user-ids could result in replication, the middle initial shall be replaced with a number to ensure uniqueness.
- A user-defined password shall be required to authenticate the user and grant access to NE-KAMS.
- User defined passwords shall be eight characters in length, must begin and end with a letter, and must contain at least two special characters and/or numbers.
- The number of consecutive attempts to enter an incorrect password shall be limited to prevent password guessing attacks, after three unsuccessful attempts to enter a password, the involved user-ID shall be either 1) suspended until reset by a system administrator, 2) temporarily disabled or 3) if dial-up or other external network connections are involved – disconnected.
- To ensure individual accountability, users shall not be allowed to conduct multiple simultaneous on-line sessions without management approval.
- If there is no activity for 15 minutes, the NE-KAMS system must automatically sign the user out of the system and restrict access. Re-establishment of access may occur after the user has logged back onto the system.
- All access rights or privileges granted to users shall be documented and kept on file for review/audit purposes.
- Access controls shall be implemented to protect information resources within the NE-KAMS system, i.e., there shall be two separate NE-KAMS implementations, one classified and one public.
- Only management approved access controls shall be used for classified access.

APPENDIX C

INITIAL CFD V&V BENCHMARK DATASETS

One of the overarching goals of the NE-KAMS knowledge base is to increase confidence in CFD analysis results and predictions for nuclear reactor design, safety analyses, and licensing applications. To that end, one of tasks that will be performed during the development process for NE-KAMS is V&V benchmark data assessments. The goal of this task is to provide a systematic and structured approach for assessing and classifying the quality of V&V benchmark data for use in CFD V&V assessments. In this initial assessment, seven V&V benchmark datasets (four code verification and three validation benchmark datasets) will be evaluated relative to the newly developed NE-KAMS V&V standards and requirements for CFD. This assessment will aid in the development of the processes, standards and requirements for evaluating the quality of V&V benchmark data for inclusion in the NE-KAMS CFD V&V database. The V&V benchmark data assessment will include the following:

- Evaluation and improvement of the NE-KAMS V&V processes, standards and requirements.
- Assessment and quality classification of four code verification and three validation benchmark datasets using the code verification and validation benchmark completeness tables, respectively with accompanying documentation.
- Assessment of database methods and approaches for collecting/acquiring, processing, formatting, documenting, storing and retrieving V&V benchmark data.
- Assessment of database methods and approaches for linking V&V benchmark data with attendant metadata.
- Assessment of database methods and approaches for incorporating, linking and presenting V&V benchmark datasets in the higher level context of applicable Phenomenon Identification Ranking Table (PIRT) charts and validation pyramids (validation hierarchy).

NE-KAMS V&V benchmark database will classify code verification benchmarks as:

1. Analytical solution with no numerical approximations (such as Method of Manufactured Solutions)
2. Analytical solutions with numerical approximations (such as an infinite series solution)
3. Numerical solutions of ordinary differential solutions (ODEs)
4. Numerical solutions of partial differential equations (PDEs)

In this initial assessment, we will assess and classify the quality of four code verification benchmarks, one from each of the four categories identified above. Some examples of code verification benchmarks under consideration for each category are:

- 1a. Incompressible, unsteady, 2-D, laminar flow over an oscillating plate (Stokes oscillating plate) given in Panton, R. L. (1984). *Incompressible Flow*, New York, John Wiley, pp. 266-272.

- 1b. Incompressible, steady, axisymmetric 2-D (could also be used as 3-D Cartesian), laminar, impinging jet flow, given in Pelletier, D., E. Turgeon and D. Tremblay (2004). "Verification and Validation of Impinging Round Jet Simulations Using and Adaptive FEM," *International Journal for Numerical Methods in Engineering*, 44, 737-763.
- 1c. Incompressible, steady, 2-D, turbulent, wall-bounded flow with two turbulence models (Method of Manufactured Solution case), given in Eça, L., M. Hoekstra, A. Hay and D. Pelletier (2007). "On the Construction of Manufactured Solutions for One and Two-Equation Eddy-Viscosity Models," *International Journal for Numerical Methods in Fluids*, 54(2), 119-154.
- 2a. Incompressible, steady, axisymmetric 2-D, laminar flow in a circular tube with a discontinuous change in wall temperature (Graetz problem), given in White, F. M. (1991). *Viscous Fluid Flow*, New York, McGraw Hill, pp. 127-130.
- 2b. Incompressible, unsteady, axisymmetric 2-D, laminar flow in a circular tube impulsively started (Szymanski flow), given in White, F. M. (1991). *Viscous Fluid Flow*, New York, McGraw Hill, pp. 133-134.
- 3a. Incompressible, steady, 2-D, laminar stagnation flow on a flat plate (Hiemenz flow), given in White, F. M. (1991). *Viscous Fluid Flow*, New York, McGraw Hill, pp. 152-157.
- 4a. Incompressible, steady, 2-D, laminar flow in a driven cavity (with the singularities removed), given in Prabhakar, V. and J. N. Reddy (2006). "Spectral/hp Penalty Least-Squares Finite Element Formulation for the Steady Incompressible Navier-Stokes Equations," *Journal of Computational Physics*, 215(1), 274-297.
- 4b. Incompressible, steady, 2-D, laminar flow over a back-step, given in Gartling, D. K. (1990), "A Test Problem for Outflow Boundary Conditions-Flow Over a Backward-Facing Step." *International Journal for Numerical Methods in Fluids*, 11, 953-967.
- 4c. Recently published Direct Numerical Solution (DNS) solutions that are an improvement over past DNS "benchmarks."

These code verification benchmarks are high quality benchmarks that are relevant to nuclear power CFD and they cover a range of flow types. Some do not have all of the detailed pedigree that we would like, but will be considered in this assessment because one of the main reasons for doing this assessment is to assess the capability and applicability of the newly developed NE-KAMS V&V standards and requirements for CFD and to do that we need to assess these standards and requirements with V&V benchmarks of varying quality.

In this initial assessment, we will also assess and classify the quality of three CFD validation benchmarks (experimental datasets), two of the three experimental datasets are from Bettis

Laboratory and the third is from Utah State University. The three experimental datasets are described below:

1. **Flow in a Cylinder Array** (Utah State University): Experimental data was obtained for time-varying flow through a confined bank of cylinders. The test unit mimics the lower plenum of a high temperature reactor and is arranged with the cylinders on equilateral triangles with pitch to diameter ratio of 1.7. Time-resolved Particle Image Velocimetry (PIV) measurement coupled with pressure measurements along the facilities walls were obtained for comparisons to both the Unsteady Reynolds Averaged Navier Stokes (URANS) k-omega model and the Detached Eddy Simulation (DES) models. Spatial (*i.e.*, time-averaged bulk velocity and pressure losses and local velocity distributions) and temporal (*i.e.*, dominant frequencies and correlations) validation parameters derived from the experimental data on both the local and global scale were used in the CFD validation assessment.

Reference:

“Velocity and Pressure Measurements Along a Row of Confined Cylinders,” B. L. Smith, J. J. Stepan, D. M. McEligot (2007), Journal of Fluids Engineering, Vol. 129, pp. 1314-1327.

2. **High Reynolds Number Pipe Flow** (Bettis Laboratory): Pressure drops of single and multiple piping elbows were experimentally determined in order to reduce uncertainties in the currently used methods for predicting irrecoverable pressure losses and also to provide a validation database for CFD codes. Experimental data was obtained from a series of test configurations, including those with optical access to perform Laser Doppler Velocimetry (LDV) measurements. The experimental series culminated with obtaining irrecoverable pressure loss data at Reynolds numbers in excess of 40×10^6 .

Reference:

“Irrecoverable Pressure Loss Coefficients for a Short Radius of Curvature Piping Elbow at High Reynolds Numbers,” R. D. Coffield et al., (1998), ASME Fluids Engineering Division Summer Meeting, FEDSM 98-5146, Washington, D.C.

3. **Bluff Bodies in Cross Flow** (Bettis Laboratory): Experiments to characterize flow across bluff bodies were performed at the Pennsylvania State University / Applied Research Laboratory (PSU/ARL). The goal of these experiments was to provide data for CFD validation. Three bluff bodies were installed in a six inch water tunnel in two different orientations so the experimental series included six test configurations. The flow was at a Reynolds number of 1.5×10^6 based on the tunnel cross-section near the test article and a Reynolds number of 2.5×10^5 based on the bluff body characteristic dimension. This is higher Reynolds number than what is typically available in open literature. LDV, PIV, and static pressure measurements are available upstream and downstream of the bluff body to provide boundary conditions and to provide data for the comparison to CFD results. LDV data was used for quantitative comparisons and boundary condition generation. Flow visualizations from low pressure cavitation runs and surface painting are also available for qualitative comparisons.

These candidate validation benchmarks are judged to be of high quality and are relevant to nuclear power CFD. These experimental datasets do not have the detailed pedigree that we would like for a strong sense validation benchmark, but will be assessed in this initial evaluation because one of the main reasons for doing this evaluation is to assess the capability and applicability of the newly developed NE-KAMS V&V standards and requirements for CFD and to do that we need to assess these standards and requirements with validation benchmarks of varying quality.