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NEAMS Nuclear Waste Management IPSC: Evaluation and Selection of Tools for the Quality Environment

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Abstract

The objective of the U.S. Department of Energy Office of Nuclear Energy Advanced Modeling and Simulation Nuclear Waste Management Integrated Performance and Safety Codes (NEAMS Nuclear Waste Management IPSC) is to provide an integrated suite of computational modeling and simulation (M&S) capabilities to quantitatively assess the long-term performance of waste forms in the engineered and geologic environments of a radioactive-waste storage facility or disposal repository. These M&S capabilities are to be managed, verified, and validated within the NEAMS Nuclear Waste Management IPSC *quality environment*. M&S capabilities and the supporting analysis workflow and simulation data management tools will be distributed to end-users from this same quality environment. The same analysis workflow and simulation data management tools that are to be distributed to end-users will be used for verification and validation (V&V) activities within the quality environment. This strategic decision reduces the number of tools to be supported, and increases the quality of tools distributed to end users due to rigorous use by V&V activities. This report documents an evaluation of the needs, options, and tools selected for the NEAMS Nuclear Waste Management IPSC quality environment.

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Nomenclature

ADM	analysis data management
CM	configuration management
DOE	Department of Energy
IPSC	Integrated Performance and Safety Codes
M&S	modeling and simulation
NEAMS	Nuclear Energy Advanced Modeling and Simulation
PCMM	Predictive Capability Maturity Model
Sandia	Sandia National Laboratories
SQE	software quality engineering
THCM	thermal-hydrological-chemical-mechanical
THCMBR	thermal-hydrological-chemical-mechanical-biological-radiological
UQ	uncertainty quantification
V&V	verification and validation
V&V and UQ	verification and validation and uncertainty quantification

1 Introduction

The objective of the U.S. Department of Energy (DOE) Office of Nuclear Energy Advanced Modeling and Simulation Nuclear Waste Management Integrated Performance and Safety Codes (NEAMS Nuclear Waste Management IPSC) program element is to provide an integrated suite of computational modeling and simulation (M&S) capabilities to assess quantitatively the long-term performance of waste forms in the engineered and geologic environments of a radioactive-waste storage facility or disposal repository. This objective will be fulfilled by acquiring and developing M&S capabilities, and establishing a defensible level of confidence in these M&S capabilities. The foundation for assessing the level of confidence is based upon the rigor and results from verification, validation, and uncertainty quantification (V&V and UQ) activities.

M&S capabilities are to be managed, verified, and validated within the NEAMS Nuclear Waste Management IPSC quality environment. M&S capabilities and the supporting analysis workflow and simulation data management tools will be distributed to end-users from this same quality environment. The same analysis workflow and simulation data management tools that are to be distributed to end-users will be used for verification and validation (V&V) activities within the quality environment. This strategic decision reduces the number of tools to be supported, and increases the quality of tools distributed to end users due to rigorous use by V&V activities.

NEAMS Nuclear Waste Management IPSC V&V and UQ practices and evidence management goals are documented in the V&V Plan [1]. This V&V plan includes a description of the quality environment into which M&S capabilities are imported and V&V and UQ activities are managed. The first phase of implementing the V&V plan is to deploy an initial quality environment through the acquisition and integration of a set of software tools. An evaluation of the needs, options, and tools selected for the quality environment is given in this report.

1.1 Deploying the Quality Environment

As illustrated in Figure 1-1, codes for the NEAMS Nuclear Waste Management IPSC may be developed and integrated in many development environments. Codes will be developed, tested, integrated, and updated within development environments at Sandia or elsewhere. However, there is a single NEAMS Nuclear Waste Management IPSC *quality environment* that will be managed by the NEAMS Nuclear Waste Management IPSC team. This quality environment will serve as a clearinghouse from which end-users will be acquiring codes, models, and tools.

The quality environment will serve as a repository for M&S capabilities. Assuring accessibility and tracking provenance are some of the responsibilities of a repository. An excellent in-depth discussion of the responsibilities of a repository has been compiled in the “Reference Model for an Open Archival Information System (OAIS)” (CCSDS 650.0-B-1).

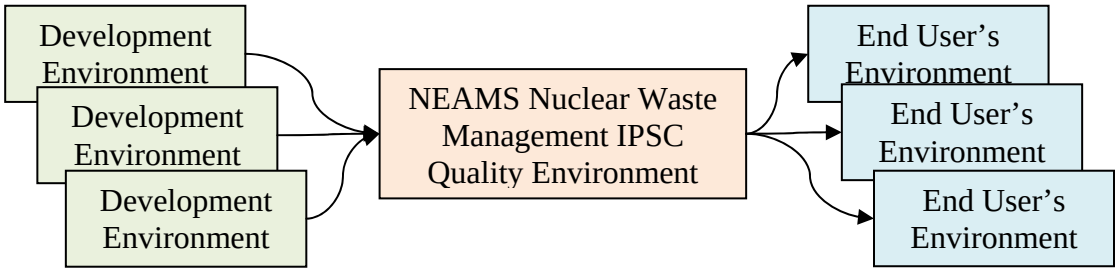

Figure 1-1. Flow of M&S capabilities from development projects through quality environment to end-user environments.

1.2 Implementing the V&V Plan

Implementing the V&V plan requires deployment of software tools in the quality environment to support enabling practices such as version control, acquisition, build and test, and integration testing. The V&V plan also requires deployment of a V&V evidence information management system within the quality environment. The goals for this system are defined in Section 5 of the V&V plan and summarized here.

EVIM Goal I.	Develop an electronic repository of V&V M&S evidence and traceability.
EVIM Goal II.	Allow for the timely capture and update of information described in Goal I.
EVIM Goal III.	Enable derived V&V metrics for M&S capabilities coupled by composition hierarchies and interscale relationships.
EVIM Goal IV.	Establish and maintain data quality.
EVIM Goal V.	Allow for searching of the M&S V&V evidence and traceability.
EVIM Goal VI.	Provide an estimated level of confidence assessment, including uncertainty, for a prediction or prediction capability.
EVIM Goal VII.	Establish an operational production infrastructure.

1.3 Supporting End-User Needs for Tools

End-users will exercise NEAMS Nuclear Waste Management IPSC to analyze disposal alternatives, designing waste forms and engineered environments, and generate evidence to support licensing of a waste disposal system design. Each of these uses will require a degree of confidence that is commensurate with the associated risks or is required by the end users' stakeholders – such as the U.S. Nuclear Regulatory Commission (NRC). Confidence is established through (a) verification, validation, and uncertainty quantification of both M&S capabilities and end users' analyses; (b) establishing justifiable arguments for confidence in the validity of computer models; and (c) effective communication of the confidence arguments and supporting body of evidence to the stakeholders.

The NEAMS Nuclear Waste Management IPSC will provide end-users with M&S capabilities as well as analysis workflow, simulation data management, and evidence management tools. The end-user needs for these tools are similar, if not identical, to the tools needed to support V&V and UQ activities. As such the NEAMS Nuclear Waste Management IPSC will deploy software tools in the quality environment which support V&V and UQ workflows and evidence management analysis, *and* can be distributed to support the end users' analysis workflows and evidence management needs. The strategy to use the same tools for V&V and UQ workflows and evidence management as will be provided to end users (sometimes referred to in the software community as "eating your own dog food") causes these tools to be extensively exercised by the NEAMS Nuclear Waste Management IPSC team before they are deployed to the end users – leading to greater confidence in the quality of the tools.

1.4 Evaluating and Selecting Tools

The needs and options for software tools have been evaluated with respect to the goals of providing a repository for M&S capabilities, implementing the V&V plan, and supporting end-user analysis workflow and evidence management needs. Existing commercial, public domain, and DOE laboratory supported tools were considered. However, a significant non-technical consideration in this evaluation and selection was to <u>not require an end-user to purchase a commercial product with significant acquisition, maintenance, or licensing costs</u>.

2 V&V and UQ Evidence Management

2.1 Motivation

Delivered M&S capabilities must have a defensible level of confidence that is commensurate with the risks associated with the intended uses these capabilities. The foundation for assessing the level of confidence is based upon the rigor and results from V&V and UQ activities. Because it is economically impractical to apply the maximum V&V and UQ rigor to each and every M&S capability, these capabilities will be ranked according to (1) their anticipated impact on the performance of waste forms and systems and (2) the risks associated with how the M&S capabilities are used. Those M&S capabilities with greater impact (e.g., radionuclide transport) or higher risk (e.g., assessing a proposed disposal site near a populated area) will require a greater level of confidence and a correspondingly greater investment in V&V and UQ. The difference between required and assessed levels of confidence in M&S capabilities will influence how program resources for V&V, UQ, and M&S are prioritized and allocated.

2.1.1 Risk-Based / Evidence-Based Approach

Large-scale, multi-physics NEAMS M&S capabilities will always have some degree of uncertainty due to inherent M&S complexity, variability, and difficulty. Use of these M&S capabilities in decision-support applications requires risk analysis, where the uncertainties and potential consequences of reliance on simulation results must be considered. An evidence-based approach is required to establish justifiable confidence in M&S capabilities.

The traditional approach to software engineering takes customer requirements as a focus and provides a number of approaches for negotiating clear requirements and then verifying and validating when those requirements are met. In the case of computer modeling of natural phenomena the basis for validity is a scientific understanding of the phenomena. Scientific theories are constantly subject to revision as new theoretical arguments and empirical data emerge [3]. Furthermore, modeling efforts themselves can drive revision of theories. As such complex computer models cannot assume a simple, conventional software engineering closed context for V&V.

V&V and UQ for computer modeling of natural phenomena are tied to the ongoing, epistemically open process of scientific theory formation. V&V and UQ are an exploratory process that is driven by complex arguments from emerging empirical evidence and theoretical problems. Thus an evidence-base approach is required where V&V and UQ evidence is generated and managed in an open context; i.e., the body of evidence will change over time.

V&V and UQ of M&S capabilities will depend upon multiple scientific disciplines, many of which are still developing. Thus evidence for complex multiphysics models will rely on a variety of corroborations from different disciplines, using differing methods, different rhetorical conventions, and potentially different standards for acceptance. An

evidence-based approach cannot be the simple accumulation of supporting data. An evidence-based approach must (a) combine a body of evidence into a coherent assessment of the degree to which confidence in the model's results is justified and (b) insure the proper use of those results in a decision process.

There is unlikely to be a single measure of adequacy that can be applied to these diverse concerns, methods, and measures to render a conclusive argument for confidence in model results. Rather, coherent, robust explanatory arguments must be constructed from this complex web of evidence [4]. Such arguments will combine the diverse quantitative and qualitative evidence into an explanatory structure that supports ongoing evaluation, refinement, and decision-making.

2.1.2 Decision Support

The difficulties of a risk-based, evidentiary approach are complicated by the nature of the decision-processes involved in policy analysis, regulation, legal decisions, and other applications. Using M&S in these applications confronts the problems of introducing scientific arguments into debates where values, economics, politics, culture and other areas of human interest exert an influence equal to or greater than science [5-7]. This is particularly evident in risk calculations, where the evaluation of the consequences of various risks depends fundamentally on the subjective values people give to potential environmental, economic, political, and lifestyle effects.

V&V and UQ of M&S capabilities must establish justifiable arguments for confidence in the validity of computer models, and must make those arguments accessible to a decision process that is often driven by subjective values, political interests, and legal constraints. These integrated needs lead to unique objectives for management of V&V and UQ evidence.

2.1.3 Patterns of Use

V&V and UQ evidence management must effectively support patterns of information and analysis underlying risk assessment, and evidentiary reasoning with an evolving foundation of science. For risk analysis, these patterns include the measurement of uncertainties in the model and its theoretical basis, and the assessment of the nature and consequences of potential failures inherent in these uncertainties. Evidence management must also support teams of phenomena domain experts, model developers, and quality assurance specialists in generating and linking complex chains of evidentiary reasoning to establish justifiable confidence in models. Finally, evidence management must be robust enough to support application of information in scientific, regulatory, legal, and political decision-making.

2.2 Evidence Traceability

The management and traceability of V&V and UQ evidence is critical to support risk-informed decisions. This evidence will not be developed or obtained at one time, it will be accumulated and change over the multidecade lifetime of the NEAMS Nuclear Waste

Management IPSC. For accumulated evidence to be useful, it must be managed in a way that it can be efficiently queried and reported. Hardcopy output does not provide an expeditious means of either querying or reporting, and electronic file keeping is only marginally better than hardcopy output, unless indexing and traceability information is introduced to speed up retrieval. V&V and UQ evidence management traceability requirements from the V&V plan are summarized here.

2.2.1 Traceability for M&S Components and V&V Evidence

Modeling and simulating a physical system requires conceptual modeling, mathematical modeling, numerical modeling, and software development (Figure 2-1). Each component of M&S should have an associated artifact. For example, the conceptual model for a real physical system to be simulated should document what phenomena are required to be modeled (or not) and justifications for those requirements. Similarly mathematical and numerical models for phenomena are typically documented in publications or reports. Artifacts associated with these M&S components must be traceable to one another as illustrated in Figure 2-1.

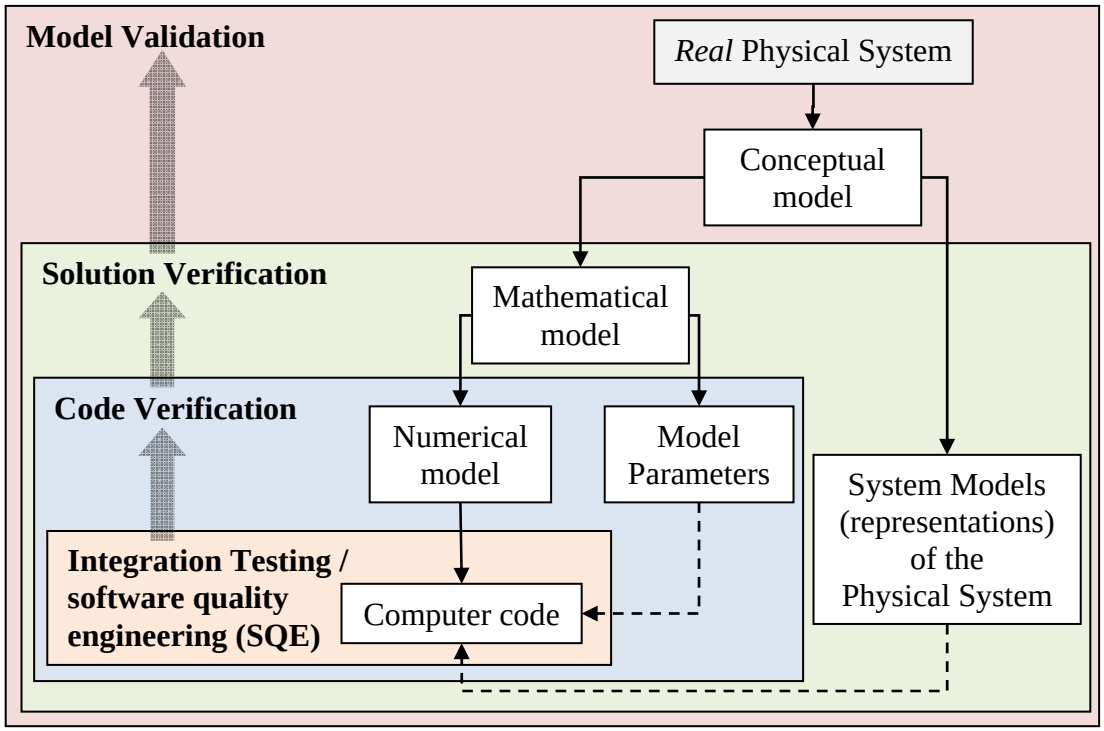

Figure 2-1. Components of M&S capabilities and associated V&V practices.

For each M&S component illustrated in Figure 2-1 there should also exist associated V&V and UQ evidence. Figure 3-1 should be interpreted starting at the upper right-hand side. The development of M&S capabilities begins with the real physical system, in the form of a conceptual model, and progresses downward as increasingly more complex models must be produced until the models are implemented in computer code. At that point the V&V practices (or activities) on the left-hand side of the figure come into play,

with the order of these practices typically occurring from bottom to top. These V&V practices generate evidence for confidence in the associated code or model. For example, integration testing is performed to establish confidence that the computer code is free of fundamental coding errors, but the next phase of code verification is required to establish confidence that the numerical model is correctly implemented.

2.2.2 Traceability for M&S Integration Hierarchies

Complex M&S capabilities will be formed by integrating other simpler M&S capabilities. V&V evidence for integrated M&S capabilities will depend upon V&V evidence for the component capabilities as well V&V of the integrated assembly. The integration of M&S capabilities defines a hierarchical structure with its own traceability needs. This type of hierarchical mapping frequently is referred to as a bill of material. Figure 2-2 shows an example of a conceptual hierarchical structure.

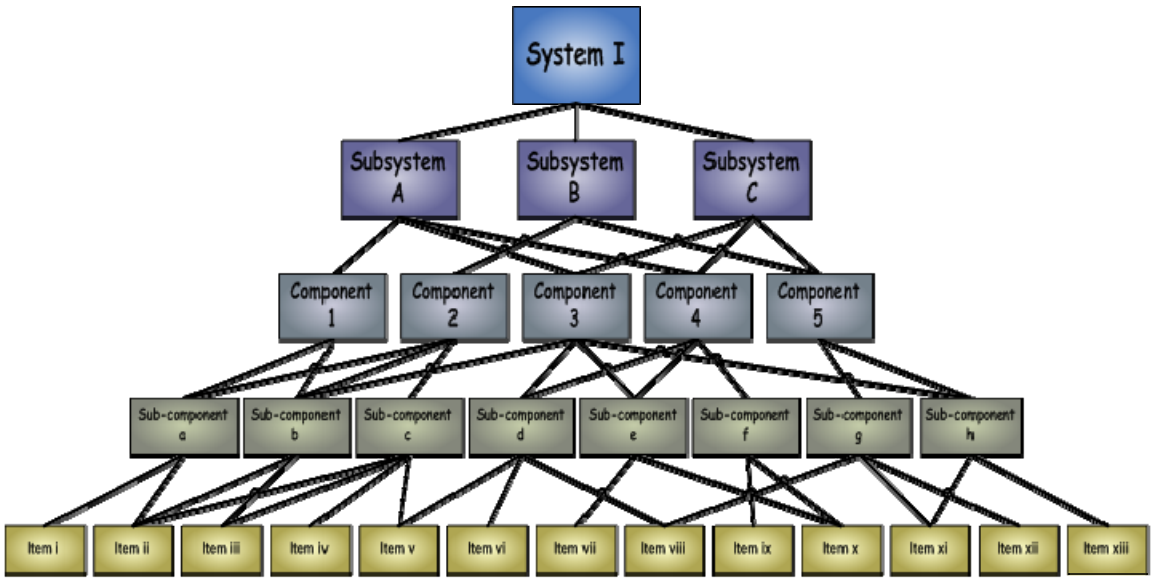

Figure 2-2. Hierarchical integration of components.

In a hierarchical integration structure, tracing can go in two directions, forward and backward. A forward trace begins at the top level or at a middle level and goes down. A backward trace begins at a middle level or a bottom level and goes up. Generally, a forward trace is used for an impact analysis to answer the question: What is the impact if I make a change at this level? For example, using Figure 2-2, the impact analysis of changing component 4 would include evaluating the effect on subcomponents d, e, and f and on items v, vi, vii, viii, ix, and x. A backward trace, on the other hand, is a traceability analysis. It generally answers questions like the following: Why do I have this item? How did this item originate? Do I need this item? A backward trace also can be used to provide roll-up information. For example, verification of higher-level requirements may depend on verification of lower-level requirements, so when verification is completed at a lower level, it is rolled up to the level directly above.

2.2.3 Traceability between Three Scales of M&S

The NEAMS Nuclear Waste Management IPSC will use three scales of M&S, as illustrated in Figure 2-3, to address requirements for validation, UQ, and sensitivity analysis. Subgrid-scale analyses will be used in conjunction with experimental data to characterize material properties and mechanistic processes. Results of coordinated subgrid-scale simulations and experimental investigations will be used to develop and verify continuum-scale models. Continuum-scale models will be integrated as necessary to analyze coupled phenomena, i.e., thermal-hydrological-chemical-mechanical-biological-radiological (THCMBR). Capabilities for M&S are abstracted from the continuum-scale simulations to be "robust and fast" for the performance assessment of waste forms, engineered barriers, and geologic settings over large spatial and temporal scales.

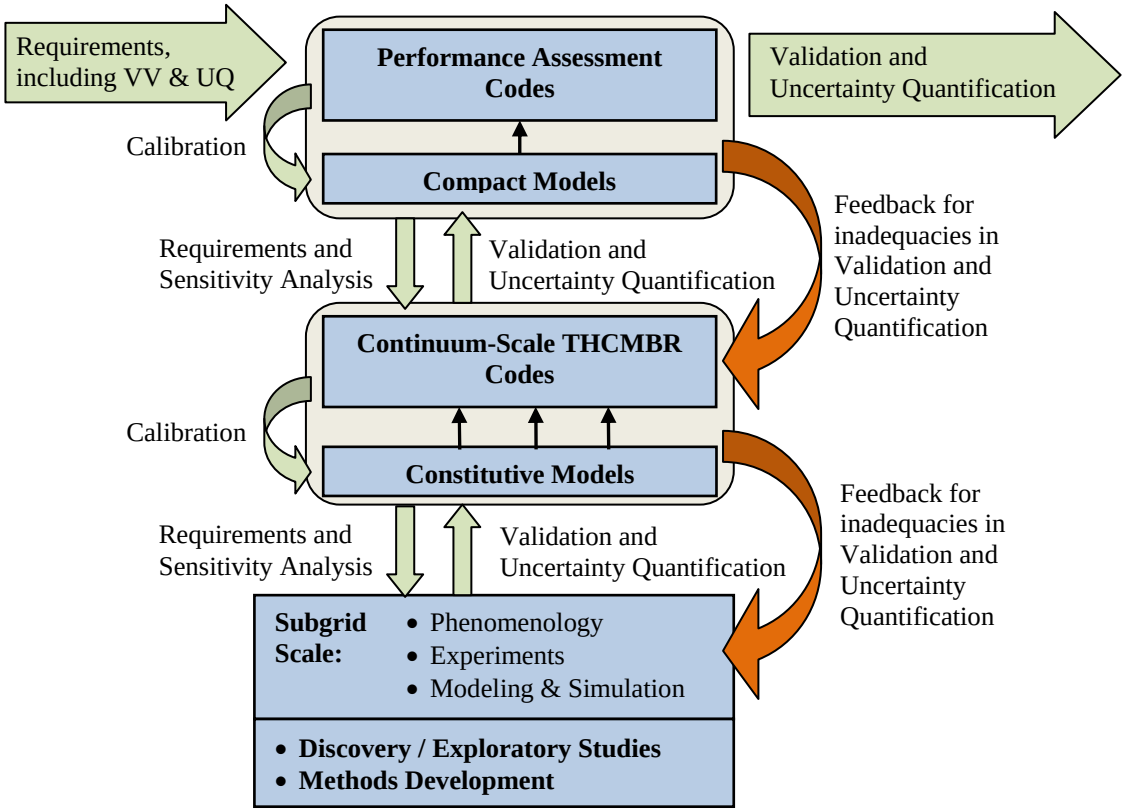

Figure 2-3. Three scales of M&S with requirements, sensitivity analysis, UQ, and validation traceability relationships.

The strategy for three scales of M&S introduces additional M&S and V&V evidence traceability requirements. Mathematical models for the same phenomena at different scales are required to be traceable to the common conceptual model or associated requirements. In addition, M&S capabilities that derived from or validated against M&S capabilities from a finer scale must also be traceable to those M&S capabilities and their associated V&V evidence.

2.2.4 Traceability for Changing M&S Capabilities

It is expected for M&S capabilities to be changed and improved over time. As such analyses and evidence associated with old versions of M&S capabilities will not be applicable to the new versions and new V&V evidence must be generate for the new version. Thus evidence and traceability of evidence to M&S capabilities must include version identification for both the M&S capability and re-generated evidence.

Typically, version identification will be a version number, a date, or a combination of the two. A basic version identifier for an evolving model (model X) might be version 1.5. Mapping to versions is a particularly important dimension of traceability because items being traced, such as requirements, software codes, and tests, commonly evolve over time, which means new versions are created and the new versions create new versions of results. Version 1.6 of model X, for example, might contain only slight adjustments that are improvements to version 1.5. Nevertheless, version 1.5 of model X would need to be retained because it is evidence that supported something that occurred at a previous time. Results and other supporting evidence related to a particular version identifier need to be adequately connected, i.e., cross-referenced, to their source; otherwise, the trace is incomplete or inaccurate. For example, it would be necessary to link the results of a validation exercise performed of the specific version of model X that was used to produce those results. Furthermore, the versions of the codes and tests must be accessible evidence to reproduce and confirm the test results.

2.2.5 Traceability for Complex Workflows

An analysis workflow is defined by the execution of a sequence of simulations and tools with a defined data flow between these simulations and tools. Complex workflows are best managed within an analysis workflow framework. Requirements for such a framework are defined in Section 6 of the NEAMS Waste Forms and Systems IPSC System Design Specification distributed in September 2009.

Complex analysis workflows will be used in V&V activities as well as by end-users' analyses. Resulting evidence must be traceable to the entire sequence of simulations and tools used in the workflow. Furthermore, a significant requirement is for sufficient traceability information to be maintained so that the workflow and resulting evidence can be reproduced.

3 Analysis Workflow Framework

An analysis workflow framework exists within a computational environment consisting of foundational services that the framework uses and analysis tools that the framework orchestrates, as illustrated in Figure 3-1. In this layered environment the analysis tools utilize services of the analysis framework and foundational services, and the analysis framework and foundational services are independent of any particular analysis tool. This layered architecture allows multiple analysis tools to be introduced into the computational environment without impacting the existing underlying analysis workflow framework or foundational services.

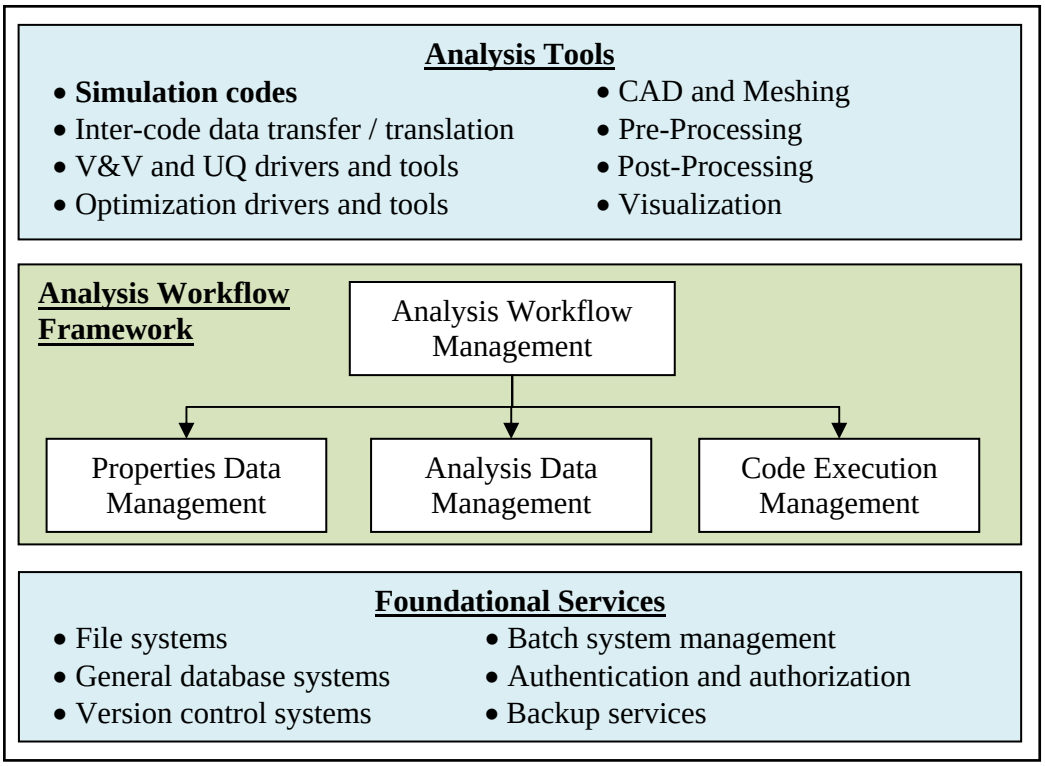

Figure 3-1 Layers and components of an analysis framework within a computational environment

Existing analysis workflow frameworks are available as commercial products, public domain packages, and from DOE projects. While several commercial products meet the technical needs of the NEAMS Nuclear Waste Management IPSC the licensing costs are an obstacle to subsequent distribution of the framework. Furthermore, the analysis data management (ADM) capability embedded within these commercial frameworks is most often based upon proprietary technology. Use of a proprietary ADM incurs significant risks for limited portability of accumulated information to new ADM tools, limited support for configuring the ADM to program and project specific needs, and limited support for integrating analysis tools with the framework.

3.1 Priority: Analysis Data Management (ADM)

Analysis data management is *the* critical tool within an analysis workflow framework. The ADM tool must manage, trace, and query analysis data throughout its lifecycle. Management encompasses access control, configuration management, and sustainability of potentially very large analysis data sets that can reside on storage systems outside of the ADM tools' repository. Traceability encompasses the provenance of acquired data, codes and inputs utilized to produce analysis data, reviews and other quality assurance activities applied to analysis data.

V&V and UQ activities are analysis activities, as such requirements for V&V and UQ evidence information management includes requirements ADM. Because of this overlap in requirements it is desirable to have a single data management tools that will both satisfy the complex needs of V&V and UQ evidence management and have a suitably simpler interface for the simpler needs of ADM.

The properties data management tool is an important but less critical tool in that M&S codes will typically have their own data formats for properties as opposed to accessing a shared repository. Code execution management is needed to simplify and automate the steps required to run simulation codes on distributed computational resources (*i.e.*, in a computational resource "cloud"). When extremely useful, codes can be run in the absence of such a tool. Analysis workflow management is necessary for the orchestration of complex workflows and reliable repeatability of those workflows. However, workflow management is necessarily dependent upon the existence of analysis data management.

3.2 Existing ADM Tools

Existing ADM tools were evaluated and a single tool selected with the intent to address needs for ADM, and V&V and UQ evidence management.

1. DOE ASCEM Velo – The Selected Tool

The DOE Advanced Simulation Capability for Environmental Management (ASCEM) program is developing the Velo data / knowledge management tool. This tool enhances the public domain media wiki technology for version controlled large data files, defined collections of data files, links to externally managed data files, and traceability relationships between data files and collections of data files. Velo is configurable to define and evolve the artifacts, attributes, and relationships of the information managed within Velo. Velo will be available to ASCEM and NEAMS Nuclear Waste Management IPSC end-users as a DOE provided capability with similar terms and conditions as the supported M&S capabilities.

Selection of the ASCEM Velo tool establishes a collaborative relationship between the DOE ASCEM and NEAMS programs. Releases of Velo will be imported into the quality environment and existing data and evidence migrated from old to new releases. Releases of Velo and procedures for migrating data and evidence will be available to end-users.

ASCEM data management requirements defined in Section 12 of the System Requirements for ASCEM Platform and Integrated Toolsets, ASCEM-PIT-102610-Rev.3, dated June 17, 2010.

2. DOE ASC DART Workbench

The DOE Advanced Simulation & Computing (ASC) program developed the DART Workbench is a complete analysis workflow framework supporting ASC M&S codes. The DART Workbench is an SNL-hosted capability which is not currently intended to be distributable. The DART Workbench the DASSAULT SYSTEMES (http://www.3ds.com) Matrix product embedded to support ADM functionality.

3. DOE NGNP Data Management System

The DOE Next Generation Nuclear Plant (NGNP) Data Management System (NDMAS) is intended to serve the ADM needs of the NGNP program. This system is hosted at Idaho National Laboratory (INL) and integrates the Phoenix Integration (http://www.phoenix-int.com) Analysis Explorer and Model Center and Microsoft Sharepoint tools for data management.

4. Open Source SALOME

SALOME (http://www.salome-platform.org) is an open source analysis workflow framework and collection of analysis tools. SALOME was evaluated for use by the NEAMS Nuclear Waste Management IPSC. The SALOME framework provides extensive capabilities for code execution management and analysis workflow management through CORBA technology. However, the ADM capability was extremely limited and not suitable V&V and UQ evidence management.

5. Commercial products

The following commercial options were examined prior to “discovery” of the ASCEM Velo capability. All of these commercial options have the obstacle of a per-seat or per-named-user licensing model such that a cost increases with each additional user.

- Phoenix Integration AnalysisLibrary (http://www.phoenix-int.com)
- SIEMANS Teamcenter (http://www.plm.automation.siemens.com/en_us)
- Altair HyperWorks Data Manager (http://www.altairhyperworks.com)
- ANSYS Engineering Knowledge Manager (http://www.ansys.com)
- MSC Software SimManager (http://www.mscsoftware.com)
- PTC Windchill (http://www.ptc.com/)

3.3 Acquisition of DOE-EM ASCEM Velo

In March 2011, a beta distribution of DOE-EM ASCEM Velo was installed in the NEAMS Nuclear Waste Management IPSC Software Quality Environment. This is the first installation of Velo external to the Velo development environment. This installation was on a Linux server which is within Sandia's network firewalls and is managed by Sandia's Common Engineering Environment (CEE) team. Early installation and configuration of Velo in the NEAMS Software Quality Environment has been essential for early identification of key configuration issues and additional requirements for installing and using Velo within a restricted access network.

3.3.1 Dependent Software

Prerequisite software packages to support the current version of Velo include the following.

Table 1. DOE ASCEM Velo Prerequisite Software Packages

Prerequisite Software	Version	Options and Configuration
Apache web server	2.x	mod_ssl (for user authentication) php5_module
ActiveMQ	5.4.2 or greater	Required for Alfresco
MySQL	5.x	client + server
Perl	5.x	libXML libraries
Subversion	1.x	
Alfresco[1] (will replace Subversion in new version)	3.4.c	
PHP	5.2.x	Curl, MySQL enabled
Python	2.5 or greater	with ElementTree module
Java	1.6.x	
Ant	1.7 or greater	
ImageMagick	6.x	
Pdftotext		
Firefox or Mozilla web browser		

Installation and configuration of prerequisite software was performed collaboratively between NEAMS Infrastructure support personnel and Sandia National Laboratories (SNL) system support personnel under terms of the NEAMS Software Quality Environment Service Level Agreement (SLA).

[1] http://www.alfresco.com/

3.3.2 Installation and Configuration Issues

Security policies require that system administrator or "root" privileges for the server are restricted to Sandia's CEE team – the NEAMS Infrastructure team does not have these access privileges. As such, system administration support was required for installation or configuration of most of the prerequisite software packages and Velo itself. In addition, many of the required versions of prerequisite software were not, by default, present on the servers supported by Sandia's CEE team. Instead, the required versions had to be acquired, configured, and installed specifically for the NEAMS Software Quality Environment.

Velo was successfully installed; however, the current version cannot be used within Sandia's firewalls due to a user authentication issue. Configuration of Velo is on-hold until the next version of Velo is acquired and installed. The new version will address the requirement to allow user authentication to occur through Sandia's user authentication system as an alternative to Velo's current use of a Subversion Apache module for user authentication. User authentication requirements will be addressed in the next Velo distribution; which is expected in May 2011.

3.4 Existing Properties Data Management Tools

Properties data management, primarily for material model property data, represents a complex capability when accounting for the diversity of material models and supporting property data. Development of the mature materials information management tool GRANTA (http://www.grantadesign.com) was sponsored by a consortium which includes Los Alamos National Laboratory, Oak Ridge National Laboratory, as well as DOD and NASA laboratories. GRANTA products include the materials information management tool and numerous materials information databases.

It has been recommended that the NEAMS Enabling Computation Technologies (ECT) program element evaluate a NEAMS program-wide adoption of the GRANTA materials information management tool.

3.5 Code Execution and Analysis Workflow Management

Code execution and analysis workflow management tools will be considered at a later phase.

4 Foundational Services

Foundational services include common tools in the computational environment for which public domain or affordable commercial options are available and commonly used.

4.1 Computational Environment

The computational environment procured in 2010 for the quality environment is a multiprocessor server with 1.7 terabyte storage capacity for code and data repositories, running the Linux operating system, and residing on the SNL internal network. It is expected that this server will be replaced or upgraded as necessary throughout the life of the NEAMS program. The Linux operating system was selected for compatibility with a majority of high performance computing (HPC) M&S codes and tools. A service level agreement is in place with the SNL computing facilities organization to provide routine maintenance and backups.

4.2 Software Configuration Management

Selected software configuration management tools currently include version control and software construction tools. Issue tracking, change request, and software test harness tools will be selected at a later time.

1. The Git (http://git-scm.com) public domain tool is selected version control. This tool is the latest generation software version control tool and is use by many large software projects such as the Linux Kernel, Perl, Eclipse, Gnome, KDE, and others. The SNL Trilinos and SIERRA Mechanics projects also use git.

2. The CMake (http://www.cmake.org) public domain tool is selected for software construction. Development and maintenance of CMake was sponsored in part by the DOE ASC program and SNL. The SNL Trilinos project currently uses CMake and the SIERRA Mechanics project plans to migrate to using CMake.

4.3 Requirements Management

A requirements management repository will be required to manage the NEAMS Nuclear Waste Management IPSC phenomenological and computational requirements. The phenomenological requirements have overlapping scope with other DOE programs addressing M&S for nuclear waste such as the Used Fuel Disposition Campaign and Waste Forms Campaign. In addition phenomenological requirements exist from the DOE Yucca Mountain Project and an international database of nuclear waste disposal features, events, and processes (FEPs).

It is desirable to establish some degree of sharing and commonality among these programs' requirements and databases. As such the selection of a requirements management tool has been deferred until the potential for sharing and collaboration on requirements management has been explored.

4.4 Project Management

Project management for the NEAMS Nuclear Waste Management IPSC occurs at two contexts: a local day-to-day context and within the global context of the DOE Fuel Cycle Research and Development (FCR&D) program. In the global FCR&D context project management use the FCPICS tool (http://www.fcpics.com). In the local context project information and tasks are managed with the Trac (http://trac.edgewall.org) open source tool.

The Trac tool integrates wiki and ticket management technology for a minimalistic approach to web-based project management. The Trac tool does not provide cost estimation or Gantt-like task planning and traceability functionality as would be found in a tool such as Microsoft Project.

5 Conclusion and Path Forward

The selected tools identified in this report represent current, but not necessarily permanent, selections for the quality environment. These tools will be exercised and evaluated within the context of the NEAMS Nuclear Waste Management IPSC Challenge Problem milestones [2]. It is intended that this experience will lead to improvements in the use of selected tools, feedback to tool developers for improvements to the tools, or possibly require selection of new tools. Strategic plans, based upon the anticipated limited level funding and staffing, are for a slow evolution of the quality environment into its "final" architecture and toolset by 2015.

The first set of tools identified in this report will be applied to the 2011 Challenge Problem milestone and associated V&V and UQ activities to exercise and evaluate the tools in an operational context. This evaluation will appear in a subsequent NEAMS Nuclear Waste Management IPSC milestone report.

Evaluation and selection of the deferred tools (*e.g.*, code execution management, analysis workflow management, and requirements management) will be planned for subsequent years as funding permits.

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