SANDIA REPORT
SAND2012-10208
Unlimited Release
Printed November 2012

Development of an Advanced Performance Assessment Modeling Capability for Geologic Disposal of Nuclear Waste: Methodology and Requirements

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Abstract

This report describes the planning and initial development of an advanced disposal system PA modeling capability to facilitate the science-based evaluation of disposal system performance for a range of fuel cycle alternatives in a variety of geologic media and generic disposal system concepts. The advanced modeling capability will provide a PA model framework that facilitates PA model development, execution, and evaluation within a formal PA methodology.

The PA model framework will provide a formalized structure that enables (a) representation and implementation of a range of generic geologic disposal system options, (b) representation of subsystem processes and couplings at varying levels of complexity in an integrated disposal system model, (c) flexible, modular representation of multi-physics processes, including the use of legacy codes, (d) evaluation of system- and subsystem-level performance, (e) uncertainty and sensitivity analyses to isolate key subsystem processes and components, (f) data and configuration management functions, and (g) implementation in HPC environments.

The PA model framework includes two main components: a multi-physics modeling capability and a computational framework capability. These capabilities are implemented through integrated suites of computer codes. The multi-physics codes provide the conceptual and mathematical representations of the relevant FEPs. The computational framework codes provide the supporting functions to facilitate the numerical integration (coupling) and implementation of the multi-physics, computationally efficient code execution, and analysis and configuration management of results. The development of an advanced disposal system PA modeling capability for UFD attempts to balance efforts towards these two components; it must provide an adequate range of multi-physics process models and it must facilitate adequate multi-physics couplings across the entire disposal system. And, to the extent possible, the code development

and integration will be performed in an open-source environment and will leverage existing legacy and utility codes.

The report outlines specific requirements for a multi-physics modeling capability and for a computational framework capability and identifies and summarizes existing codes with the potential to address those requirements. No single existing code addresses all of the requirements. However, the list of requirements is quite comprehensive; a PA modeling capability that satisfies all of the requirements would represent a significant advancement in the state-of-the-art. T herefore, the approach to develop an advanced PA model framework capability will involve (1) an integration of multiple codes and/or code capabilities, rather than a single code, (2) a phased implementation, where requirements are prioritized and iteratively re-evaluated as UFD program needs evolve, and (3) leveraging relevant ongoing open-source code development efforts.

Three existing code development efforts are identified as having the best combination of readily available open-source development, appropriate multi-physics capabilities, and HPC capabilities. Two of these codes, ASCEM and Albany, are computational framework codes that include multi-physics capabilities. The third code, PFLOTRAN, is a THC multi-physics modeling code that includes some limited computational framework capabilities.

The multi-physics modeling and computational framework capabilities of these three codes will be further evaluated in FY2013. T he evaluation will focus on the existing capabilities and necessary enhancements required to apply each code to solve a U FD-relevant demonstration problem. The development and application of these three codes to the demonstration problem will provide a gap analysis relative to the PA model framework requirements. The results of the gap analysis will help to identify which of the three codes (or combination of capabilities from the codes) provides the most favorable path forward for further development of advanced disposal system PA modeling capabilities.

This work supports the Office of Used Nuclear Fuel Disposition (UFD) within the U.S. Department of Energy (DOE) Office of Nuclear Energy (NE) Fuel Cycle Technologies (FCT) Program.

ACKNOWLEDGEMENTS

This work was supported by the U.S. Department of Energy, Office of Nuclear Energy, Fuel Cycle Technologies Program, Office of Used Nuclear Fuel Disposition.

Helpful review comments were provided by Paul Mariner and S. David Sevougian.

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FIGURES

TABLES

ACRONYMS

1D	one-dimensional
2D	two-dimensional
3D	three-dimensional
ADSM	advanced disposal system modeling
ASC	Advanced Simulation and Computing
ASCEM	Advanced Simulation Capability for Environmental Management
DOE	U.S. Department of Energy
DRZ	disturbed rock zone
EBS	engineered barrier system
EDZ	excavation disturbed zone
FEP	feature, event, and process
FY	fiscal year
GDSM	generic disposal system modeling
GPAM	Generic Performance Assessment Model
GUI	graphical user interface
HLW	high-level radioactive waste
HPC	high-performance computing
IAEA	International Atomic Energy Agency
INL	Idaho National Laboratory
IPSC	Integrated Safety and Performance Codes
LHS	Latin hypercube sampling
LLW	low-level radioactive waste
NE	Office of Nuclear Energy
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NRC	U.S. Nuclear Regulatory Commission
PA	performance assessment
PDE	partial differential equation
PNNL	Pacific Northwest National Laboratory
QA	quality assurance
R&D	research and development
SC	Office of Science
SciDAC	Scientific Discovery through Advanced Computing
SNL	Sandia National Laboratories
THCMBR	thermal-hydrological-chemical-mechanical-biological-radiological
UFD	Office of Used Nuclear Fuel Disposition
UNF	used nuclear fuel
UQ	uncertainty quantification
V&V	verification and validation
WIPP	Waste Isolation Pilot Plant
YMP	Yucca Mountain Project

1. INTRODUCTION

This report describes the planning and initial development of an advanced performance assessment (PA) modeling capability for the evaluation of disposal system performance in a variety of geologic disposal system options to support the Office of Used Nuclear Fuel Disposition (UFD). The UFD operates under the U.S. Department of Energy (DOE) Office of Nuclear Energy (NE) Fuel Cycle Technologies (FCT) Program. The mission of the UFD is to identify alternatives and conduct scientific research and technology development to enable storage, transportation and disposal of used nuclear fuel and wastes generated by existing and future nuclear fuel cycles (DOE 2010a, Section 3.7.1). To support the UFD mission, DOE has established a number of short-term (i.e., 5-year) and long-term objectives. UFD objectives specific to disposal system modeling include (DOE 2010a, Section 3.7.1):

- Short-Term Objective 4: Develop a comprehensive understanding of the current technical bases for disposing of used nuclear fuel (UNF), low-level radioactive waste (LLW), and high-level radioactive waste (HLW) in a range of potential disposal environments to identify opportunities for long-term research and development.

- Short-Term Objective 5: Continue model development for the evaluation of disposal system performance in a variety of geologic media and generic disposal system concepts.

- Long-Term Objective 3: Develop a fundamental understanding of disposal system performance in a range of geologic media for potential wastes that could arise from future nuclear fuel cycle alternatives through theory, simulation, testing, and experimentation.

- Long-Term Objective 4: Develop a computational modeling capability for the performance of storage and disposal options for a range of fuel cycle alternatives, evolving from generic models to more robust models of performance assessment.

To address these UFD objectives, DOE has further identified research and development (R&D) topics for safe and secure disposition and disposal. The focus of R&D supporting disposal system modeling is on the development of computational models for evaluating the long-term performance of generic geologic disposal systems comprised of waste forms, engineered barriers, and the natural barriers. The scope of recommended R&D in this area includes (DOE 2010a, Section 3.7.2):

- New high-performance computing (HPC) applications to achieve better transparency on disposal system performance while reducing the need for large-scale testing
- Science-based disposal system performance modeling, to help in the determination of appropriate geologic disposal concepts with an appropriate geologic barrier and an effective engineered barrier
- Advanced modeling of cladding and UNF performance in a disposal environment
- Advanced modeling and simulation capabilities for near-field and far-field analyses
- Advanced modeling capabilities for all generic disposal system environments for once-through, modified open and closed fuel cycles

- Experimental R&D in the laboratory and field, leveraging international partnerships, to further understanding and validate the models.

UFD activities that address the disposal system modeling objectives and R&D scope are managed within the Generic Disposal System Modeling (GDSM) and Advanced Disposal System Modeling (ADSM) work packages. The GDSM work package activities are focused on the development of disposal system modeling capabilities to support the evaluation of a range of generic geologic disposal options at varying levels of complexity. The ADSM work package activities augment the GDSM activities by focusing on the acquisition or development of a PA model framework for implementing the generic disposal system modeling capabilities. The combined objective of these activities is to create an advanced disposal system PA modeling capability that (a) facilitates science-based evaluation of disposal system performance for a range of fuel cycle alternatives in a variety of geologic media and generic disposal system concepts, and (b) takes advantage of HPC technologies.

The remainder of this report describes progress and future plans towards the development of an advanced disposal system PA modeling capability. The advanced modeling capability will provide a PA model framework that facilitates PA model development, execution, and evaluation within a formal PA methodology. Section 2 provides an overview of the components of a PA model framework that can facilitate advanced PA modeling. Section 3 identifies high-level requirements for a PA model framework. Section 4 identifies existing computational codes that may address some of the PA model framework requirements. Section 5 outlines future plans to examine the candidate PA model frameworks against the relevant requirements, including the identification of a demonstration problem. Section 6 provides a summary.

This report corresponds to DOE Document Number FCRD-UFD-2012-000227 and satisfies DOE Milestone Number M3FT-12SN0808062.

2. PA MODEL METHODOLOGY AND FRAMEWORK OVERVIEW

UFD analyses of generic disposal system performance will follow a formal PA methodology. An overview of the PA methodology is presented in Section 2.1. The advanced modeling capability will provide a PA model framework that facilitates PA model development, execution, and evaluation within the PA methodology. The PA model framework should (in no specific order):

- provide the flexibility to examine multiple generic and site-specific geologic disposal options at levels of complexity that are expected to increase as the UFD program matures,
- enable the evaluation of system- and subsystem-level performance,
- enable uncertainty and sensitivity analyses to isolate key subsystem processes and components,
- facilitate the modular integration of representations of subsystem processes and couplings, where the level of complexity of the representation may vary with intended use or relative importance to the total system,
- provide the capability to accommodate new or alternative subsystem process representations, including the use of legacy codes,
- provide data and configuration management functions,
- be developed and distributed in an open source environment,
- leverage existing utilities (e.g., meshing, visualization, matrix solvers, etc.), and
- facilitate implementation across a range of computing environments from laptops to HPC networks, including distributed code execution.

The PA model framework includes two main components:

- a generic multi-physics model framework that facilitates development of (a) a conceptual model of the important features, events, and processes (FEPs) and scenarios that describe the multi-physics phenomena of a specific UFD disposal system and its subsystem components, and (b) a mathematical model (e.g., governing equations) that implements the representations of the important FEPs and their couplings; and

- a computational framework that facilitates the integration of the system analysis workflow (e.g., input pre-processing, integration and numerical solution of the mathematical representations of the conceptual model components, output post-processing), and the supporting capabilities (e.g., mesh generation, input parameter specification and traceability, matrix solvers, visualization, uncertainty quantification and sensitivity analysis, file configuration management including verification and validation (V&V) and quality assurance (QA) functions, and compatibility with HPC environments).

The challenge in developing an advanced disposal system PA modeling capability is one of allocating efforts toward these two components. An over-emphasis on computational framework development can result in a very robust framework code with extensive functionality, but may fail to provide adequate capabilities to address the range of multi-physics needed to represent the

system being modeled. The result is an elegant computational framework tool that cannot be used to address issues regarding disposal system performance because of a lack of multi-physics modeling capabilities. This over-focus on computational framework development is a common cause leading to the cessation or failure of system modeling framework development projects, because the ultimate objective should be to solve a multi-physics problem. Conversely, an over-emphasis on the development of specific process modeling capabilities can result in very accurate conceptual and numerical representations of independent subsystem processes, but may fail to provide a mechanism to integrate those subsystem processes into a robust total system model or to integrate the multi-physics within or across subsystems. The result is a good representation of subsystem processes, but a limited ability to address issues related to integrated disposal system performance. The initial development of an advanced disposal system PA modeling capability for UFD needs to balance these two efforts; it must provide an adequate range of process models and it must facilitate adequate multi-physics couplings across the entire disposal system.

An overview of the components of a generic multi-physics model framework is presented in Section 2.2. This includes a discussion of disposal system options and FEPs relevant to UFD. An overview of the components of a computational framework needed to support the multi-physics model framework is presented in Section 2.3.

To ensure consistent terminology throughout this report, the following definitions are used to distinguish models and codes:

- Conceptual model: A representation of the behavior of a real-world process, phenomenon, or object as an aggregation of scientific concepts, so as to enable predictions about its behavior. Such a model consists of concepts related to geometrical elements of the object (size and shape); dimensionality (1-, 2-, or 3-D); time dependence (steady-state or transient); applicable conservation principles (mass, momentum, energy); applicable constitutive relations; significant processes; boundary conditions; and initial conditions. (NRC 1999, Appendix C)

- Mathematical Model: A representation of a conceptual model of a system, subsystem, or component through the use of mathematics. Mathematical models can be mechanistic, in which the causal relations are based on physical conservation principles and constitutive equations. In empirical models, causal relations are based entirely on observations. (NRC 1999, Appendix C)

- Numerical model: An approximate representation of a mathematical model that is constructed using a numerical description method such as finite volumes, finite differences, or finite elements. A numerical model is typically represented by a series of program statements that are executed on a computer. (NRC 2003, Glossary)

- Computer code: An implementation of a mathematical model on a digital computer generally in a higher-order computer language such as FORTRAN or C. (NRC 1999, Appendix C)

2.1. PA Methodology

Over a period of nearly 40 years, Sandia National Laboratories (SNL) has developed and applied a PA methodology – a methodology for probabilistic risk analysis of radioactive waste disposal methods, facilities, and systems. The SNL PA methodology has been used to inform key decisions concerning radioactive waste management both in the United States (e.g., the Waste Isolation Pilot Plant (WIPP) and the Yucca Mountain Project (YMP)) and internationally (Meacham et al. 2011, Section 1.1).

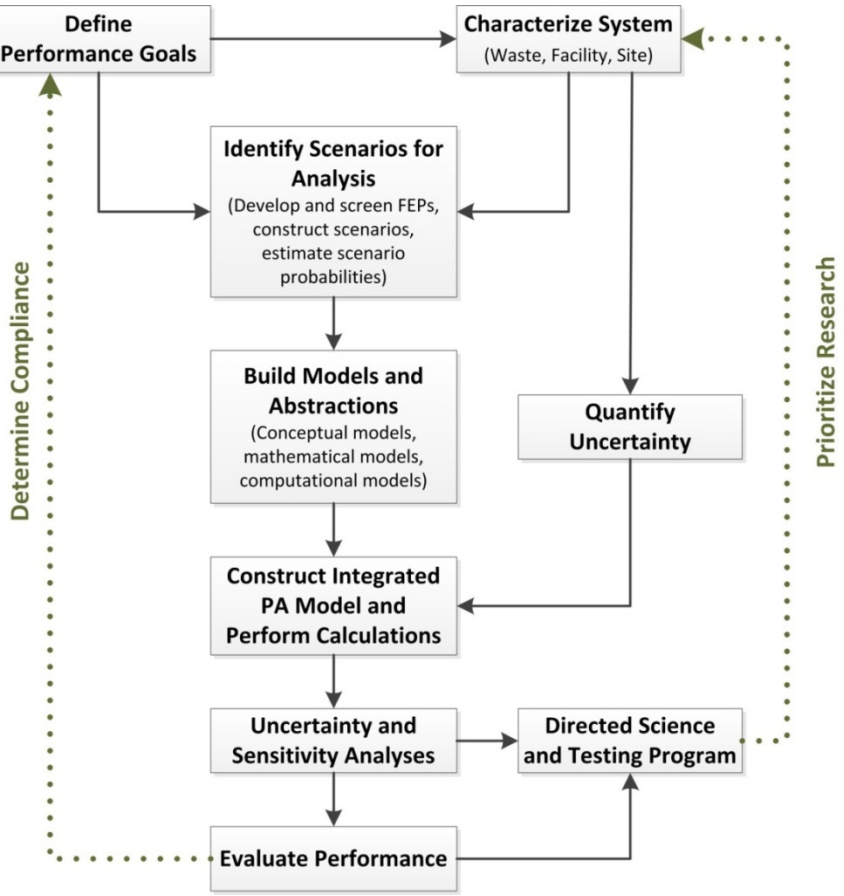
The following excerpts from Meacham et al. (2011, Section 1.2.1) summarize the SNL PA methodology:

> *The PA methodology provides the framework for assembling, organizing, and assessing the large quantity of data and information needed to evaluate the performance of complex systems, such as radioactive waste disposal systems. The PA methodology incorporates data and information from multiple sources and organizes them in a logical manner to support decision making, explicitly taking into consideration the different sources of uncertainty that will influence the analysis. It also provides a framework that enhances the traceability, transparency, reproducibility, and retrievability of the technical work. Finally, it allows for the analysis of how the different components (i.e., subsystems) of the disposal system behave in isolation and in conjunction with each other.*
>
> *SNL has demonstrated in numerous projects that applying the PA methodology in an iterative manner ensures that research and development activities are closely linked to the behavior and performance of subsystems and of the total system. The results of the analyses typically improve with successive iterative applications of the methodology as more data and information become available and understanding of the system improves.*
>
> *In the very early phase of a radioactive waste disposal project, applications of the PA methodology tend to be exploratory in nature and rely on relatively simple models focused on the identification of opportunities for improving understanding of the system under consideration. As the project evolves, more detailed models are incorporated into the methodology. In the intermediate phases of the project, applications of the methodology provide opportunities to review alternative models, conduct uncertainty and sensitivity analyses, identify shortcomings in the analysis or model implementation, and communicate with stakeholders. Eventually, once the understanding of the disposal system is sufficiently mature to proceed to the licensing phase, the application of the PA methodology provides the foundation for the safety analysis that informs the licensing decision.*

The PA methodology generally consists of the following steps (Meacham et al. 2011, Section 1.2.2):

1. Define performance goals;
2. Characterize system (waste, facility and site);
3. Identify scenarios for analysis;
    a. Identify and screen relevant FEPs
    b. Construct and screen scenarios
    c. Estimate scenario probabilities
4. Build models and abstractions;
    a. Conceptual models
    b. Mathematical models
    c. Computational models
5. Quantify uncertainty;
6. Construct integrated PA model and perform calculations
7. Perform uncertainty and sensitivity analyses;
8. Evaluate performance; and
9. As needed, direct science and testing program.

Figure 2-1 shows the sequential and iterative nature of these nine steps. Details of the general application of each of the steps are provided in Meacham et al. (2011, Section 1.2.2).



from Meacham et al. (2011, Figure 2)

Figure 2-1. PA Methodology

Within the formalized structure of the PA methodology, PA modeling and simulation must capture the fundamental behaviors of the phenomena (i.e., FEPs) that affect long-term disposal system performance, must appropriately capture uncertainty, and must be based on data and information gathered from laboratory experiments and field investigations. To be of practical value, this information must be integrated into the disposal system PA model in a way that is transparent and traceable. The disposal system PA model framework facilitates PA model development, execution, and evaluation. More specifically, the two components of the PA model framework (generic multi-physics model framework and computational framework) are designed to facilitate the implementation of steps 3 through 8 of the PA methodology. Section 2.2 describes how the generic multi-physics model framework facilitates FEP analysis and scenario development (step 3), and conceptual and mathematical model development (steps 4a and 4b). Section 2.3 describes how the computational framework facilitates computational model development (step 4c), construction and execution of an integrated PA model (step 6) uncertainty quantification and sensitivity analysis (steps 5 and 7), and performance evaluation (step 8).

2.2. Generic Multi-Physics Model Framework Components

Objectives of the PA model framework (described in Section 2) that are relevant to the generic multi-physics model framework include:

- facilitate the science-based evaluation of disposal system performance for a range of geologic disposal system options (i.e., multiple fuel cycle alternatives in a variety of geologic media and generic disposal system concepts)
- provide the flexibility to examine generic and site-specific geologic disposal systems (and their subsystems) at varying levels of complexity

To support these objectives, the function of a generic multi-physics model framework is to facilitate:

- FEP analysis and scenario development - the identification of important disposal system FEPs and scenarios that describe the multi-physics phenomena of a specific disposal system option (PA methodology step 3)
- conceptual and mathematical model development – the identification of governing equations that implement the mathematical representations of the important FEPs and their couplings (PA methodology steps 4a and 4b)
- modular integration of representations of subsystem processes and couplings into a "science-based" disposal system model, where the level of complexity of the representation may vary with intended use or relative importance to the total system (PA methodology steps 4 and 6)

The term "science-based" implies a model that captures the fundamental physics and chemistry of the phenomena that affect long-term performance, appropriately captures uncertainty, and is based on data and information gathered from laboratory experiments and field investigations.

Four generic disposal system options are currently under consideration by the UFD: mined geologic repositories in salt, clay, and crystalline rock (granite); and deep borehole disposal in crystalline rock (Vaughn et al. 2012, Section 1.5). The preliminary development of a conceptual framework, the Generic Performance Assessment Model (GPAM), to represent these four generic disposal options is described in Clayton et al. (2011, Sections 4 and 4.1). The GPAM conceptual framework is broad and flexible and provides the basis for the advanced generic conceptual model components described here. The GPAM conceptual framework is organized around four common disposal system regions (Figure 2-2): Source; Near Field; Far Field; and Receptor. Each of the four GPAM Regions, in turn, consists of one or more common features. Collectively, these regions and features are the generic disposal system conceptual model components.

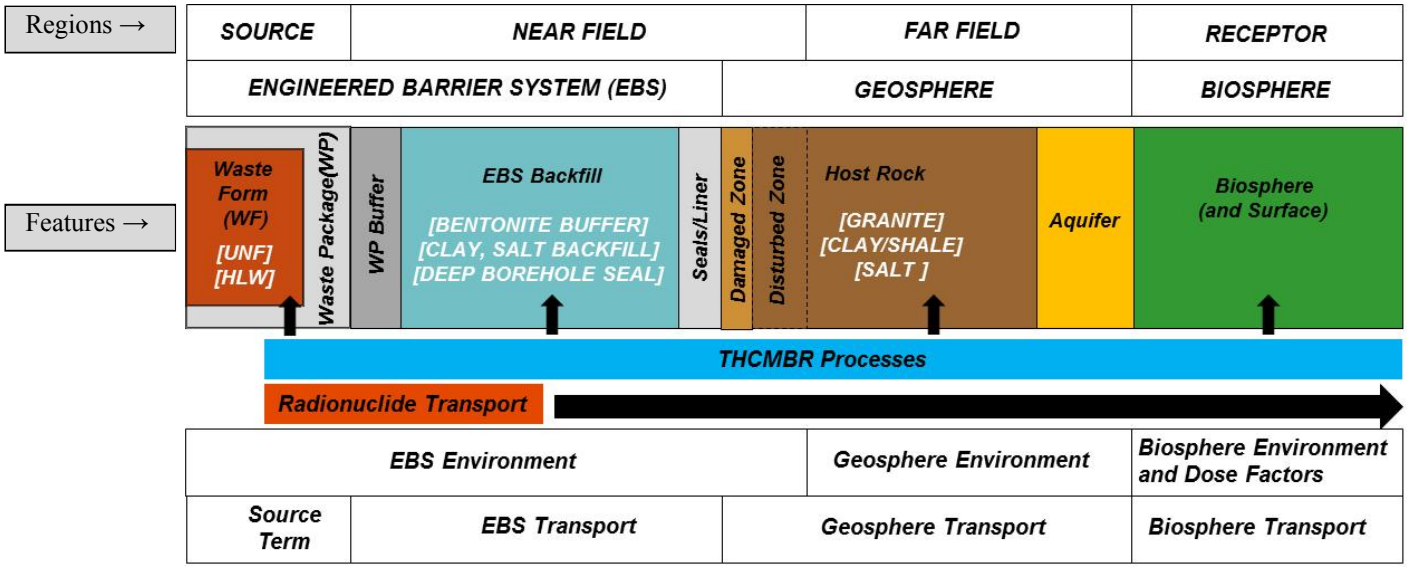


Figure 2-2. Schematic Illustration of Generic Disposal System Components and Phenomena

Figure 2-2 also illustrates the relationship between the GPAM Regions and alternate terms that are commonly used to describe a disposal system: engineered barrier system (EBS), geosphere, and biosphere. The near field encompasses the EBS and as well as the interface with, and adjacent portion of, the host rock that experiences durable (but not necessarily permanent) changes due to the presence of the repository. In some cases, it is useful to further subdivide this adjacent portion of the host rock into a "damaged" zone, where the repository-induced changes to the host rock are permanent (e.g., mechanical alteration due to excavation), and a "disturbed" zone, where the repository-induced changes to the host rock are time-dependent but not permanent (e.g., thermal effects due to radioactive decay of waste). The adjacent portions of the host rock are of sometimes referred to (individually or collectively) as the "excavation damaged zone", the "excavation disturbed zone" (EDZ), or the "disturbed rock zone" (DRZ). The far field encompasses the remainder of the geosphere. The receptor is located within, and has behaviors and characteristics consistent with, the biosphere. Further discussion of the generic EBS components is provided in Vaughn et al. (2012, Section 3.5.3.3.2); further discussion of the

generic natural system (geosphere) components is provided in Vaughn et al. (2012, Section 3.5.3.2.1.1).

The bottom half of Figure 2-2 illustrates how radionuclide movement from the waste form to the biosphere is influenced by multi-physics phenomena that can act upon and within each of the GPAM Regions and Features. These multi-physics phenomena include, at a high level, the thermal-hydrologic-chemical-mechanical-biological-radiological (THCMBR) processes and external events (e.g., seismicity) that describe (1) waste degradation and radionuclide release from the Source Region, (2) radionuclide transport through the Near Field and Far Field Regions, and (3) radionuclide transport, uptake, and health effects in the Receptor Region. In addition to their direct effects on radionuclide transport, the THCMBR processes also influence the physical and chemical environments (e.g., temperature, fluid chemistry, biology, mechanical alteration) in the EBS, geosphere, and biosphere, which in turn affect water movement, degradation of EBS components, and radionuclide transport. Further discussion of the generic EBS processes is provided in Vaughn et al. (2012, Section 3.5.3.3.1) and Hardin (2012, Sections 2 and 3); further discussion of the generic natural system (geosphere) processes is provided in Vaughn et al. (2012, Section 3.5.3.2.1.2) and Arnold et al. (2012, Sections 2 and 3).

A geologic disposal system generally relies on the performance attributes of both the engineered and natural barriers that serve to isolate waste from the environment and limit the migration of materials that could be released from the disposal facility. These barriers have different performance attributes depending on the waste being disposed of, the type of barrier, and the natural and perturbed characteristics of the disposal environment. The barrier capabilities of the EBS and geosphere also vary with time. In general the EBS provides a shorter-term barrier capability than the geosphere. They work in unison to provide the overall disposal system with effective isolation and containment performance.

The generic regions and features, and the associated THCMBR processes and events, are consistent with the generic features defined in the UFD FEP list (Freeze et al. 2010a; Freeze et al. 2011a). A FEP generally encompasses a single phenomenon; typically it is a process or event acting upon a feature (or region). As described in Freeze et al. (2010a, Section 2), the UFD FEP list derived from an international FEP list that included phenomena from 10 different national radioactive waste disposal programs covering a wide range of waste forms, disposal concepts, and geologic settings. As a result, the UFD FEP list represents a comprehensive set of phenomena potentially relevant to a wide range of disposal system options. Correspondingly, the generic GPAM Regions and Features are a comprehensive set of disposal system components applicable to a wide range of potential disposal options, including the four UFD disposal options mentioned previously and three additional open emplacement concepts identified by Hardin (2012, Section 2). The UFD FEP list contains 208 FEPs that are classified using a hierarchical numbering scheme that associates each FEP with a specific feature. In Figure 2-3 the FEP classification and numbering hierarchy is overlain on the schematic illustration of the generic disposal system components. Figure 2-3 also illustrates how each of the generic features can be acted upon by THCMBR processes and events (i.e., external factors).

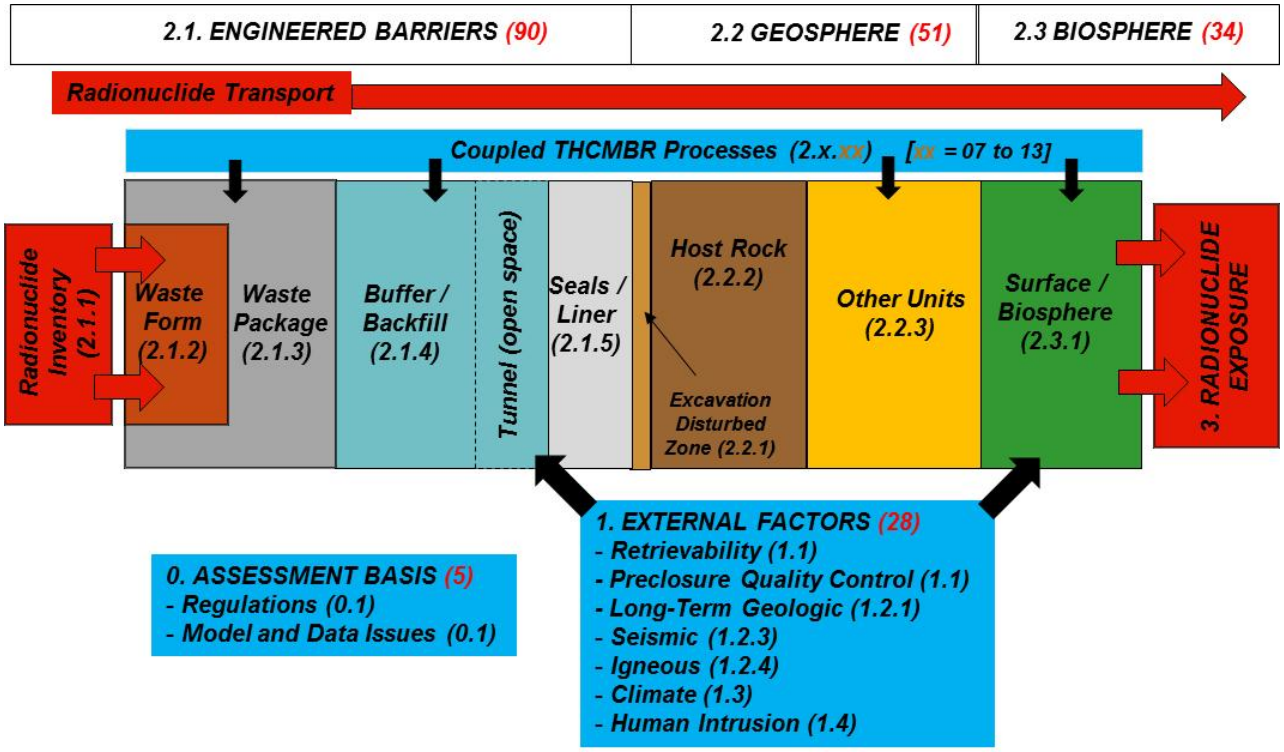


Figure 2-3. Mapping of UFD FEP Classification and Numbering Hierarchy to Generic Disposal System Components

The combination of generic disposal system components and THCMBR phenomena forms the basis of the multi-physics model framework. The generic multi-physics model framework is modular such that, for a specific disposal system option, relevant system components and FEPs can be identified and formed into scenarios – combinations of important FEPs that represent possible future states of the system. The goal of scenario development is to construct a set of scenarios that (1) represent all of the important (i.e., included) FEPs, and (2) cover the spectrum of possible future states of the disposal system. Scenario development typically results in the creation of a nominal scenario (sometimes referred to as undisturbed or expected or reference) and one or more disturbed scenarios (sometimes referred to as alternative or disruptive). The nominal scenario is typically, but not necessarily, considered to represent the most likely or expected evolution of the disposal system. Disturbed scenarios described the evolution of the system if altered by phenomena such as human intrusion, seismicity, volcanism, or unexpected component failures. Scenario development is described further in Vaughn et al. (2012, Section 3.5.4.3).

The development of a conceptual model for a specific disposal option (i.e., step 4a of the PA methodology) thus involves selecting relevant system components, performing FEP identification and screening, and constructing plausible scenarios (i.e., step 3 of the PA methodology). To perform a quantitative evaluation of the specific disposal option, mathematical representations of the conceptual model FEPs and scenarios need to be developed (i.e., step 4b of the PA methodology). The modularity of the generic multi-physics model framework described here permits the mathematical model representations to range from simple

abstractions to complex coupled multi-physics processes. While the generic disposal system components and FEPs described above provide a useful basis for developing a disposal system conceptual model, the development of mathematical models (and subsequent computational models) for a specific disposal system option requires a number of additional modeling details to be addressed. These modeling details, which generally are dependent on the level of complexity of the conceptual model and/or the desired mathematical models, include:

- Spatial representation of the disposal system – the number of features, regions, and/or components and the corresponding spatial discretization

- Mathematical representations of the FEPs and scenarios – governing equations describing the geometry (e.g., one-dimensional (1D) or three-dimensional (3D)), representation of the key THCMBR processes (ranging from simplified to very detailed), and degree of multi-physics process coupling

- Numerical implementation of the mathematical models – numerical methods and solution techniques (which may include the application of HPC capabilities) to solve the governing equations deriving from the multi-physics processes and couplings

These modeling details, which are inter-related, provide an interface between the multi-physics model framework (via the governing equations describing the coupled multi-physics) and the computational framework (via the numerical model implementation). HPC capabilities can enhance the efficiency of the numerical solution and thus allow for more complex and/or fundamental multi-physics representations, as needed. HPC capabilities include: object oriented design, advanced numerical methods (e.g., spatial and temporal integration methods, linear and nonlinear solvers), parallel execution, agile code development, software reuse (e.g., Trilinos and SIERRA Toolkit libraries), ability to use new computer hardware architectures, embedded uncertainty quantification, and 3D animated graphics.

The following subsections present an overview of considerations in conceptual model development (Section 2.2.1) and numerical implementation (Section 2.2.2) to address these modeling details, based on more detailed documentation provided by Hardin (2012) and Arnold et al. (2012).

2.2.1. Considerations in Conceptual Model Development

Arnold et al. (2012) provides an overview of considerations in developing a generic natural system conceptual model that can support an advanced disposal system PA modeling capability. The report develops a generic conceptual model that can represent the important natural system FEPs in each of the four UFD disposal system options, lays out the mathematical governing equations for those FEPs, identifies alternative strategies for numerical implementation of the mathematical models of groundwater flow and radionuclide transport, describes requirements for interfaces with other components of the system model (e.g., the EBS and Biosphere). Hardin (2012) provides a similar overview of considerations in developing a generic EBS conceptual model. The two reports also collectively outline an overarching conceptual framework for

integrating the EBS and the natural system models that derives from, and expands upon, the generic multi-physics model framework introduced in Section 2.2.

The basic generic disposal system conceptual model requirements include (modified from Arnold et al. (2012, Section 1.2):

- Flexibility: The generic disposal system model should be flexible enough to accommodate the four disposal system options currently under consideration as well as other potential future alternatives. This requirement includes flexibility with regard to variations in waste forms and inventory, engineered components, geologic environment, and boundary conditions associated with different options. In addition, the generic disposal system model must have the flexibility to handle differences in EBS degradation processes, specific geologic media (e.g., porous versus fractured media) and in the processes related to groundwater flow and radionuclide transport (e.g., advection-dominated transport versus diffusion-dominated transport). Ideally, the generic disposal system model should have the flexibility of a set of switches built into the numerical framework that allow certain individual FEPs to be turned on or off, as needed.

- Inclusiveness: The generic conceptual model should include all FEPs relevant to postclosure repository performance, assembled into a coherent disposal system model. Relevant FEPs consist of all FEPs that are identified as included, or potentially included, in the FEPs screening process. If a particular FEP is screened in for any of the disposal system options, then functionality for that FEP must be included in the generic disposal system model. It may also be desirable to include numerical functionality for some FEPs that have been screened out as excluded, for the purpose of demonstrating low consequences of that FEP or for consideration of alternative conceptual models.

- Comprehensiveness: The generic disposal system model should fully incorporate the execution of component, subsystem models. It is desirable to minimize the abstraction and external execution of component models and limit the use of conservative assumptions. Where possible, subsystem process models should be more fundamental models based on first principles rather than highly abstracted models. Full integration of subsystem models into the system model will enhance the transparency and traceability of postclosure risk analyses, and provide augmented quality assurance control over simulation results. An important example of comprehensiveness is radionuclide transport simulation for all radionuclides in decay chains. Comprehensive incorporation of all radionuclides being transported in the natural system enhances clarity and realism of disposal system simulations.

- Integration: The generic natural system model components should be integrated with regard to the exchange of state variables, thermal and chemical environment, groundwater flow, radionuclide transport, geometric boundaries, model assumptions, numerical implementation, and values for common parameters. The interface between the EBS and natural system models is particularly critical and challenging; the nature of the coupling required between the two regions may vary from decoupled to fully coupled depending on the disposal system option, the multi-physics processes under

consideration, and the relative importance of each region to system performance. For example, in a salt repository the negligible groundwater flow in the bedded salt of the EBS may be assumed to be decoupled from groundwater flow in overlying strata in the natural system. In a clay repository a uni-directional coupling for radionuclide transport may be assumed for diffusive migration of radionuclides from the EBS and clay into overlying and underlying more transmissive strata in the generic natural system model. In contrast, simulations of heat transport may require implicit bi-directional coupling (see Appendix A) between the EBS and the near-field portion of the natural system for some period of time. Bi-directional coupling of processes or model regions implies that each depends in some way on the other and there is a two-way exchange of information.

- Numerical Efficiency: Numerical simulations for multi-realization (e.g., Monte Carlo) analyses must be performed within the computational budget of the generic disposal system model. Numerous aspects of the system model impact the numerical performance, including number of radionuclides tracked, number and complexity of processes simulated, degree of coupling between component models, heterogeneity of the system, grid resolution, time step size, and numerical methods used. Although exact constraints on the computational budget are difficult to determine a priori, the general requirement for numerical efficiency should be considered in development of the generic disposal system model. Greater numerical efficiency promotes the ability to include more fundamental processes, which in turn can result in increased model transparency.

Based on preliminary generic FEP analyses for the EBS (Hardin (2012, Section 3)) and for the natural system (Arnold et al. (2012, Section 2 and Appendix A)), the generic disposal system conceptual model should have the capability to represent, at a minimum, the following spatially-variable and time-dependent multi-physics processes:

- Source Region (Waste Form and Waste Package):
  - Radionuclide inventory (heat generation, decay and ingrowth)
  - Waste form degradation (dissolution processes)
  - Waste package degradation (corrosion processes, mechanical damage, early failures)
  - Gas generation
  - Radionuclide release and transport (mobilization, early release (e.g., from gap and grain boundaries), precipitation/dissolution)

- Near Field (Buffer, Backfill, Seals/Liner, and Disturbed Zone):
  - Evolution/degradation of EBS components and DRZ
  - Effects from rockfall, drift collapse (e.g., salt creep)
  - Fluid flow and radionuclide transport (advection, dispersion, diffusion, sorption, decay and ingrowth)
  - Chemical interactions (aqueous speciation, mineral precipitation/dissolution, reaction with degraded materials, surface complexation, radiolysis)
  - Thermal effects on flow and chemistry
  - Effects from disruptive events (seismicity, human intrusion)

- Far Field (Host Rock, Aquifer)
  - Fluid flow and radionuclide transport (advection, dispersion, diffusion, sorption, decay and ingrowth)
  - Effects of fracture flow (e.g., dual porosity/permeability, discrete fracture)
  - Groundwater chemistry

- Biosphere
  - Dilution due to mixing of contaminated and uncontaminated waters
  - Receptor characteristics (basis for converting radionuclide concentrations in groundwater to dose)

The degree to which these processes are captured in a disposal system model is dependent on their importance to the performance and safety of the disposal system. Simpler process representation may be sufficient in early PA iterations, with more complex representations introduced, as needed, during later iterations. For example, flow and transport may initially consider only single-phase, fully saturated conditions. However, for some disposal options (e.g., salt) gas generation processes may be important, and the capability to evaluate unsaturated and multi-phase flow and transport will eventually be needed. The basic generic multi-physics processes are shown schematically in Figure 2-4.

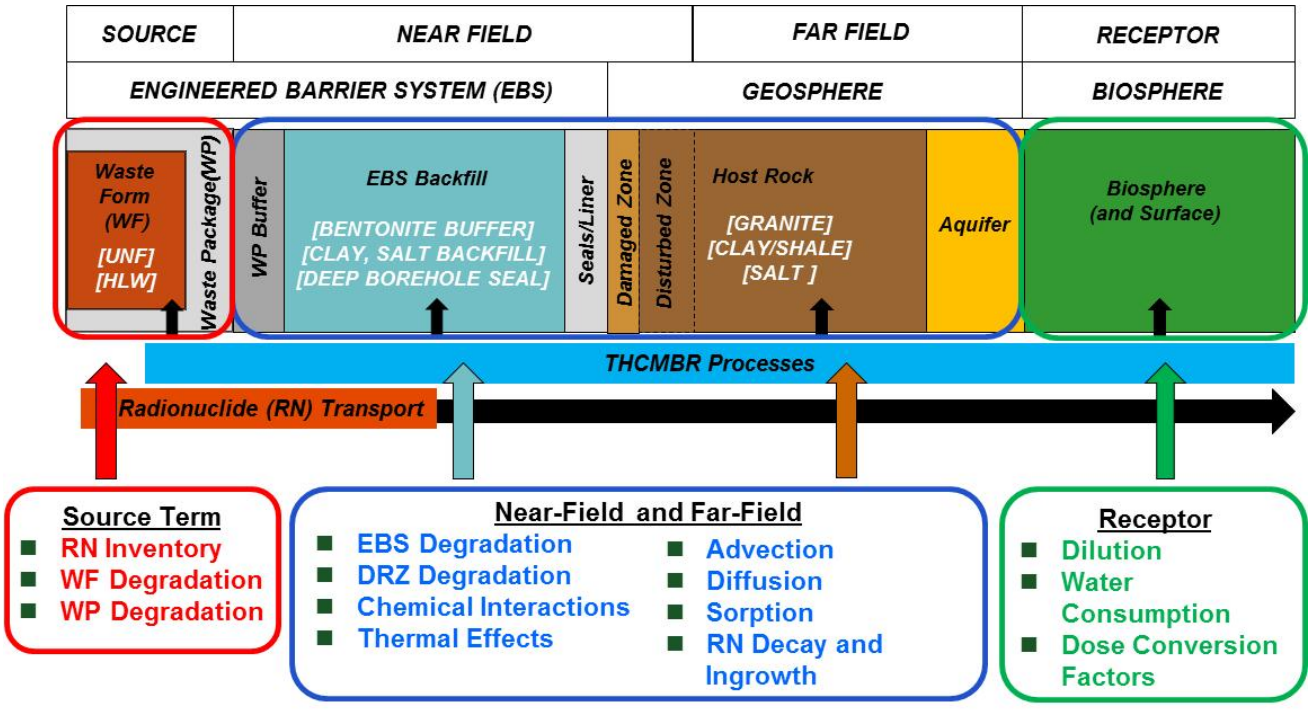


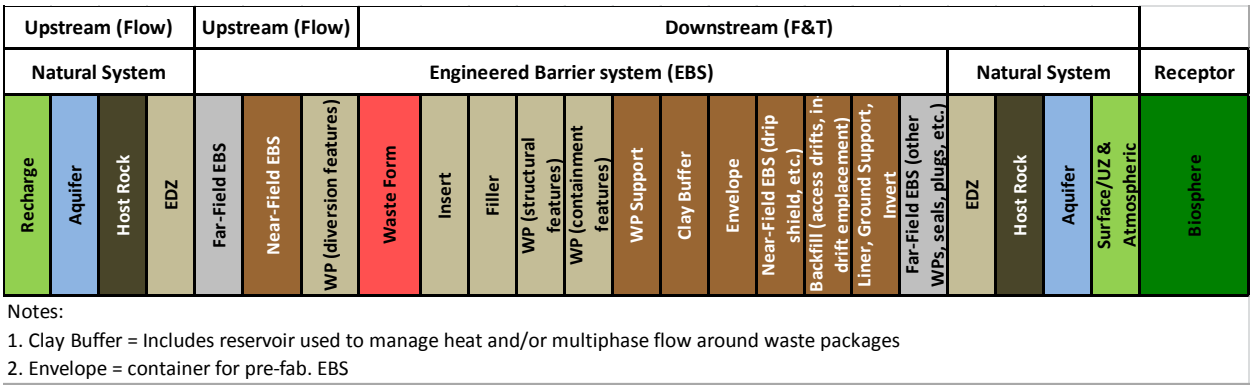
Figure 2-4. Schematic Illustration of Key Processes in a Generic Disposal System

The proposed conceptual approach for representing of these generic disposal system features and processes is to have the EBS embedded within the natural system or geosphere (Arnold et al.

2012, Section 4.3; Hardin 2012, Section 3). As described in Arnold et al. (2012, Section 4.1), the proposed geosphere conceptual model consists of a three-dimensional domain that has sufficient spatial extent to contain all significant THCMBR perturbations caused by the presence of the repository. Reasonable assumptions about the groundwater, thermal, mechanical, and chemical initial and boundary conditions can be made on the basis of "typical" natural system characteristics and assuming that a site with generally favorable characteristics would be chosen for a repository disposal system.

Ideally, the model domain would extend to natural groundwater flow boundary conditions, such as no-flow groundwater divides and surface discharge locations, zero-flux confining units at the lower boundary, and natural recharge conditions at the topographic surface. Thermal and mechanical boundary conditions would be set far enough from the repository or disposal boreholes that they have little impact on the temperature and stress calculations related to waste heat. These boundary conditions correspond to a location with low to moderate heat flow in a tectonically stable environment without a large differential in ambient horizontal stress. Steady-state, equilibrium conditions for groundwater flow and chemistry, heat flow, and mechanical stress are generally justifiable as the initial conditions for the generic disposal system model.

Consistent with the representation of an EBS embedded within a geosphere model domain defined by exterior natural boundary conditions, it is useful to consider additional detail in the representation of EBS and geosphere/natural system components. Figure 2-5 distinguishes between fluid flow in the natural system (deriving from the boundary conditions) and EBS upstream of the waste form and fluid and flow and radionuclide transport in the EBS and natural system downstream of the waste form. Figure 2-5 also provides additional detail in the EBS components beyond that shown in Figure 2-2.



(From Hardin 2012, Figure A-1)

Figure 2-5. Detailed Representation of a Generic Disposal System Components

For a specific representation of disposal system option, the EBS components and natural system features may be combined or further subdivided depending on the modeling needs. For example (Arnold et al. (2012, Section 4.1), the host rock, aquifer, and near-surface unsaturated zone may all be a single fractured granite bedrock hydrogeologic unit in the case of a mined repository in

crystalline rock. For a clay or salt repository, the aquifer system may consist of several distinct hydrogeologic units that correspond to multiple aquifers and aquitards in the stratified sedimentary system overlying the repository.

The generic disposal system conceptual model must contain interfaces between the geosphere and the EBS (both upstream and downstream) and between the geosphere and biosphere. These interfaces must be defined conceptually, geometrically, and with regard to the exchange of information describing the multi-physics processes controlling radionuclide transport.

Two general modeling approaches, one simple and one more complex, are proposed for representing the EBS embedded within the geosphere and the interface between the EBS and the surrounding geosphere (Hardin 2012, Section 3):

- **Simple "Lumped EBS"** – The EBS and near field around each waste package are embedded within the geosphere model, and are assigned to a subset of elements within the geosphere simulation grid. Multiple waste packages can be embedded in a single "lumped EBS" representation, with mass and energy conserved. This approach uses batch model concepts to represent the waste form, other waste package internals, the waste package itself, and the EBS features surrounding the package. The geosphere model would run as the "host" simulation and could have any defensible complexity and dimensionality (even 1D). The embedded "lumped EBS" would be treated as a uniform source term (although it could vary over time in a stepwise fashion) for radionuclides released from a repository with homogeneous, average thermal, hydrologic, chemical, and mechanical properties representative of the entire EBS for a given time step. Although simple, the lumped EBS would still rely on fundamental models wherever possible to directly calculate the state of the EBS during simulations, thereby avoiding the use of lookup tables or response surfaces that may have to be regenerated to conduct analyses that may be outside of the applicability range.

  The lumped EBS approach is intended to use reduced dimensionality and limited multi-physics couplings to simplify and speed up the system model, and will have only limited (or perhaps no) feedback-coupling from the geosphere. The lumped EBS approach resembles previous PA models but all components would be run simultaneously. It is a starting point for developing more complex and coupled generic PA models. Also, as an intermediate step, the boundary enclosing the region where the lumped multi-physics are applied may shift as process modeling capabilities improve (e.g., shift inward from enclosing the buffer to enclosing the waste package, with higher-fidelity representation of buffer behavior for clay-based buffers).

- **Complex "High-fidelity EBS"** – The EBS and near-field features (e.g., individual waste disposal drifts, or even individual waste packages) are explicitly represented within the geosphere simulation grid. EBS and near-field processes are represented by constitutive relationships that describe the physical and chemical evolution of the EBS. Explicit multi-physics couplings between EBS elements and geosphere elements are supported.

The complexity of the interface between the EBS and the geosphere would be commensurate with the complexity, spatial resolution, and importance to disposal system performance of each subsystem. Explicit representation of individual repository drifts would require high-resolution gridding in both the EBS and geosphere, and would probably require HPC for the numerical implementation of such a conceptual model (Arnold et al., 2012, Section 4.3).

With either approach the interface between the EBS and the geosphere must also be defined at a level sufficient for intended use, e.g., in terms of groundwater flow, radionuclide transport, possible heat and/or chemical flux, and, in the extreme, possible mechanical stress or displacement. Considerations in defining the interface are summarized below, based on Arnold et al. (2012, Section 4.3):

- Groundwater flow between the EBS and geosphere should be fairly limited in the three mined disposal options (salt, clay, crystalline), as long as the buffer materials, grouting, and repository seals remain effective. For the deep borehole disposal system there would be more interaction between fluids in the host rock and the EBS disposal zone. In either case, the interface between the EBS and the geosphere should allow for groundwater flow between the two model subsystems.

- Radionuclide transport between the EBS and the geosphere would be controlled by either advection or diffusion depending on t he hydrogeologic conditions. Uni-directional transport from the EBS to the geosphere is a justifiable simplification and could be implemented with a specified radionuclide flux coupling between the two subsystems.

- Coupling of heat flux and fluid flow in the EBS and near-field geosphere should be bi-directional to obtain accurate estimates of the near-field temperature history in the EBS. In the case of the deep borehole disposal system this coupling at the interface between the EBS and geosphere is particularly important because of the role in thermal-hydrologic effects in driving groundwater flow.

- Mechanical and thermo-mechanical effects are probably less important in the geosphere and could be implemented in a simplified fashion.

A lumped EBS representation will likely initially be used (many issues can be addressed adequately by simpler calculations), but the generic multi-physics framework should not be constructed in a way that precludes the capability to implement a more complex high-fidelity EBS, as needed, during future repository planning, siting, characterization, design, and licensing activities (Hardin 2012, Section 4).

The representation of the interface between the geosphere and the biosphere will initially be simplified. As described in Arnold et al. (2012, Section 4.3), numerous potential scenarios are plausible for the release of radionuclides to the biosphere. R eleases could occur at natural groundwater discharge locations, such as springs, rivers, lakes, or the ocean. M ore directly, radionuclide releases could occur in a hypothetical future pumping well that supplies groundwater for drinking, household use, and/or agriculture. In most performance assessment

models, the biosphere and receptor characteristics and the corresponding interface with the geosphere are defined by regulations. With the current uncertain status of UNF and HLW regulations in the U.S., the generic disposal system model biosphere will need to make some assumptions about how radionuclides move from the geosphere to the receptor. An example is the International Atomic Energy Agency BIOMASS Example Reference Biosphere (ERB) 1A and 1B dose models (IAEA 2003, Sections A.3.2 and C.2.6.1). These dose models assume that the receptor is an individual adult who obtains his drinking water from a pumping well drilled into an aquifer in the geosphere. A simplified mathematical representation converts dissolved radionuclide concentration in the geosphere to annual radionuclide dose to the receptor based on aquifer characteristics, well pumping rate, water consumption rate, and dose coefficients. The multi-physics model framework allows for greater complexity in the biosphere model to be added in the future, if needed.

The final consideration in the development of a generic disposal system multi-physics model is the mathematical representation of the important FEPs in each of the various EBS and geosphere features and the interactions between the FEPs across features. Mathematical models for fluid flow, radionuclide transport, and associated disposal system processes generally assume (modified from Arnold et al. (2012, Section 3.1)):

- Porous media are comprised of distinct phases and with material properties that change abruptly; however, discrete treatment of porous media geometry is not feasible over length scales of the geosphere model. It is assumed that a representative scale exists over which material properties average out and continuous equations suitably describe the system. This enables the use of a single continuum representation of porous media or a dual continuum representation for fractured media.

- Fluid flow in porous media is tightly coupled to the transport of mass and energy in the subsurface. Fluid advection is a very efficient method of transporting dissolved solutes and thermal energy, thus it exerts primary control on chemical and temperature distribution in the subsurface. In turn, the fluid chemistry and temperature can affect fluid and material properties thus controlling the fluid flow field; however, the concentration of the dissolved radionuclides is typically not sufficient to influence the hydrology or thermal transport.

- Multi-phase fluid flow may under conditions of gas generation. This is particularly true in low-permeability host rocks such as salt, and possibly clay, where gas generation from corrosion processes has the potential to produce repository pressures well in excess of hydrostatic (DOE 1996).

- Alternative mathematical models exist for some processes (e.g., linear and nonlinear mathematical models of sorption). Generally, simpler alternative mathematical models of important processes can be chosen for the initial development of the generic disposal system model. The modular conceptual framework will allow for more complex models to be implemented as needed.

Specific to the development of generic disposal system models, governing equations for single- and multi-phase fluid flow, solute and energy transport, chemical reaction, and mechanical deformation consistent with these assumptions can be found in DOE (2010b), Freeze et al. (2011b, Section 4), Clayton et al. (2011, Section 4.1.1), Wang et al. (2011, Section 3), Arnold et al. (2012, Section 3), and Hardin (2012, Sections 3.3 and 3.4).

2.2.2. Considerations in Numerical Implementation

As noted in Section 2.2.1, a generic disposal system can be represented by 3D fluid flow and radionuclide transport through a geosphere, driven by a radionuclide source term in an EBS embedded within the geosphere. Arnold et al. (2012, Section 5) provides an overview of numerical methods that can be applied to 3D flow and transport models. The following discussion is excerpted from Arnold et al. (2012, Section 5.1):

> *Several numerical methods using spatial discretization or gridding of the problem domain are commonly used in numerical models of groundwater flow, solute transport, heat transport, and solid mechanics. These methods include finite difference, finite element, finite volume, and integrated finite difference techniques. These methods use an Eulerian frame of reference in which flow and transport are analyzed from a spatially rigid perspective. Alternatively, flow and transport can be analyzed from a Lagrangian frame of reference in which individual parcels of fluid or solute mass are tracked through space. The Lagrangian approach can be advantageous in simulating solute transport in groundwater flow systems, as a particle tracking algorithm.*
>
> *Eulerian numerical methods like the finite element method are very successful for simulating generally highly diffusive properties of the natural system such as fluid pressure in groundwater flow, temperature in heat transport, and stress in solid mechanics, particularly in homogeneous or mildly heterogeneous media. The grid resolution and the associated computational burden required to accurately model these processes is related to the magnitude of the gradients in the dependent properties and the degree of heterogeneity in the media. As examples, the grid resolution near a pumping well must be higher to accurately represent the gradient in hydraulic head and the grid resolution near the EBS must be higher to accurately simulate the gradients in temperature associated with repository heat. A moderate amount of heterogeneity in permeability within the medium can be accurately represented with a uniform grid; however, highly heterogeneous media and explicit representation of discrete fractures require extremely high grid resolution in the strictly Eulerian approach.*
>
> *For solute transport in systems that are advectively dominated, strictly Eulerian numerical methods are much less successful. Very high grid resolution, particularly at the front of an advancing solute plume is required to obtain an accurate numerical solution. This is because numerical dispersion inherent in Eulerian methods overwhelms physical dispersion, leading to "smearing" of the simulated solute plume and unrealistically low simulated solute concentrations. Solute mass balance errors can also be a problem in Eulerian methods.*

Lagrangian numerical methods have the advantage in solute transport simulations of limited numerical dispersion that is generally independent of grid resolution (e.g., see Zheng, 1990). Often implemented as a particle tracking method, the Lagrangian approach also enforces solute mass balance in solute transport modeling. In addition, Lagrangian numerical methods are numerically much more efficient than Eulerian methods for solute transport.

Hybrid methods that combine the respective strengths of the Eulerian and Lagrangian numerical approaches can be used to model the natural system for performance assessment analyses. Three-dimensional Eulerian modeling of groundwater flow, thermal processes, and mechanics would be used in combination with particle tracking to define paths for radionuclide transport through the generic natural system model. Essentially one-dimensional modeling would then be used to simulated radionuclide transport from the EBS to the biosphere. The one-dimensional modeling of transport can be directly coupled to the three-dimensional modeling of other processes to capture transient effects in flow and heat transport or time-invariant flow paths can be extracted for simplified, decoupled simulation of radionuclide transport. Examples of numerical methods using hybrid approaches that are relevant to nuclear waste disposal and natural system modeling include Arnold et al. (2003), Robinson et al. (2010), and Painter et al. (2008).

Furthermore, numerical methods applied to numerical models of groundwater flow, solute transport, heat transport, and solid mechanics are dependent on the conceptual simplifications applied to the media in the natural system. These alternative implementation methods of conceptual flow models are summarized in Altman et al. (1996) and include the following alternatives, listed from least to most complex:

- *Equivalent Porous Medium Continuum – All processes and material properties treated as a porous medium in a single continuum. Equivalent material properties are based on effective characteristics of the medium.*

- *Composite Porosity Continuum - All processes and material properties treated as a porous medium in a single continuum. Some material properties (e.g., relative permeability – capillary pressure relationships) are altered to reflect the effects of fractures.*

- *Dual Porosity – Processes and materials are represented by two collocated continua, the fracture continuum and the matrix continuum. Flow occurs only in the fracture continuum, but fluid and solute exchange occurs between the fracture continuum and the matrix continuum.*

- *Dual Permeability - Processes and materials are represented by two collocated continua, the fracture continuum and the matrix continuum. Flow occurs both in the fracture continuum and in the matrix continuum. Fluid and solute exchange also occur between the fracture continuum and the matrix continuum.*

- *Discrete Fracture Network – Individual fractures are discretely represented. Flow and transport only occur in the fractures.*

- *Discrete Fracture Network with Matrix - Individual fractures are discretely represented. Flow and transport occur in both the fractures and matrix. Fluid and solute exchange also occur between the fractures and the matrix.*

Different alternative implementation methods may be appropriate for different units within the generic natural system model and for different disposal system options. The equivalent porous medium approach is valid for aquifers consisting of granular media and probably for low-permeability host rock such as clay. The dual-porosity approach is appropriate for densely fractured units, such as fractured carbonate aquifers and for fractured crystalline rock as some sites. The discrete fracture network with matrix approach may be required for granite host rock at some sites.

The appropriate implementation method may also be a function of spatial scale. For example, radionuclide transport of a few hundred meters through fractured crystalline rock from a mined repository may require a discrete fracture network approach, whereas transport of a few thousand meters through fractured crystalline rock from deep borehole disposal might appropriately use a continuum dual-porosity approach. Computationally efficient methods have also been developed that effectively upscale solute transport behavior in discrete fracture networks for implementation with a continuum approach (e.g., Painter and Cvetkovic, 2005).

Based on the preceding discussion from Arnold et al. (2012, Section 5.1), the following recommendations can be made for the numerical implementation of 3D flow and transport as part of a generic disposal system model:

- Groundwater flow can be simulated using a three-dimensional model based on Eulerian methods. An equivalent porous medium representation may be sufficient for some units, but a dual-porosity, dual-permeability, or discrete fracture representation may be required in other units. Large-scale discrete fracture network representations with matrix participation for the entire natural system model are generally beyond the computational reach of standard finite-element formulations. However, advanced finite-element gridding methods to explicitly include discrete fracture networks at large scales are under development. (Arnold et al. 2012, Section 5.2)

- Heat transport and mechanics can be simulated using a three-dimensional model based on Eulerian methods. Heat transport and mechanics can be accommodated using a continuum representation for all units in the natural system. The option should exist to turn off the heat transport and mechanics processes in the model (completely or at specified times and/or sub-domains), which may be acceptable for many disposal system applications, and will lead to significantly greater computational efficiency. (Arnold et al. 2012, Sections 5.2 and 5.3). The dynamics of mechanical coupling to the host rock is not likely to be considered in the disposal system PA model at this time or in the foreseeable

future; however, detailed process level mechanics modeling will be needed to inform the approach to be taken.

- Radionuclide transport (including advection, dispersion, diffusion, sorption, matrix diffusion in fractured media, colloid-facilitated transport, and radionuclide decay and ingrowth) can be simulated using Lagrangian methods or Eulerian methods.

  Eulerian methods can be applied to preserve an implicit coupling between flow and transport processes, as long as numerical dispersion can be minimized. The corresponding fine grid resolution may require numerical solutions that take advantage of HPC to produce acceptable runtimes. Eulerian methods are more straight forward than Lagrangian methods and, a as result, can be more desirable, if these numerical limitations can be overcome.

  Lagrangian methods can be applied along essentially 1D flow pathways using multiple stochastically generated particle tracks representing packets of radionuclide mass. The 1D nature of the solute transport solution could be computationally efficient. (Arnold et al. 2012, Section 5.2). However, particle tracking can require a very large number of particles to obtain an accurate solution for contaminant concentrations in groundwater, particularly for very low concentrations at the margins of a plume. Simulating decay chains directly may also require a large number of particles and/or very small time steps. These limitations may be partially overcome by extending simple particle tracking to the method-of-characteristics numerical method.

  Different numerical solution techniques that are appropriate for local conditions could be applied to different segments of the transport pathway through the system to improve computational efficiency (Arnold et al. 2012, Section 5.2). For example, for those portions of the flow path in which diffusion dominates, a simplified equivalent porous medium, diffusion-only solution would be implemented. For locations along the particle path in which groundwater flow dominates transport, an advection-dispersion solution would be applied, with potentially dual-porosity mass transfer applied in fractured units. An additional option, if needed, could allow the groundwater flow solution to be "frozen" under steady-state conditions. Radionuclide transport would be simulated along one-dimensional flow paths that have been determined using particle tracking methods in the three-dimensional model (Arnold et al. 2012, Section 5.3).

2.3. Computational Framework Components

Objectives of the PA model framework (described in Section 2) that are relevant to the computational framework include:

- develop advanced disposal system modeling and simulation capabilities that facilitate the modular integration of the subsystem processes (e.g., waste form, near-field and far-field analyses) described by the conceptual and mathematical models
- support the evaluation of generic disposal system conceptual and mathematical models of varying levels of complexity

- develop HPC applications to achieve better computational efficiency and better transparency on disposal system performance – HPC environments enable better computational efficiency which permits disposal system PA models to include more fundamental process representations and avoid highly-abstracted submodels. The use of more fundamental processes improves transparency because physically meaningful parameters can be more readily identified.

To support these objectives, the function of a computational framework is to facilitate:

- computational model development – the numerical implementation of the mathematical representations of the conceptual model components and the supporting capabilities (e.g., mesh generation, matrix solvers, uncertainty quantification, compatibility with HPC environments) (PA methodology steps 4c and 5)
- construction and execution of an integrated disposal system PA model – the integration of the system analysis workflow (e.g., input pre-processing, numerical solution of the governing equations, output post-processing) and the supporting capabilities (e.g., input parameter specification and traceability including uncertainty, file configuration management) (PA methodology step 6)
- sensitivity analysis and performance evaluation – the application of analysis techniques (e.g., sensitivity analyses, visualization) to evaluate system- and subsystem-level performance and isolate key processes and components (PA methodology steps 7 and 8).

In addition, the computational framework should:

- be developed and distributed in an open source environment,
- leverage existing utilities (e.g., meshing, visualization, matrix solvers, etc.),
- not preclude the use of legacy codes, and
- facilitate implementation across a range of computing environments from laptops to HPC networks, including distributed code execution.

Preliminary development of a computational framework to support disposal system PA modeling within the UFD is described in Clayton et al. (2011, Section 4), Arnold et al. (2012), and Hardin (2012). Additional efforts to develop HPC-based computational frameworks capable of facilitating disposal system PA modeling have been initiated by the DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program and the DOE Advanced Simulation Capability for Environmental Management (ASCEM) project.

The objectives of the NEAMS Waste Integrated Performance and Safety Codes (Waste IPSC) are very similar to those for the UFD advanced disposal system PA modeling capability. Multi-physics model and computational framework components and requirements for the NEAMS Waste IPSC are documented in SNL (2009), Freeze et al. (2010b), Freeze et al. (2011b), Edwards et al. (2011a) Wang et al. (2011), Edwards et al. (2011b), and Arguello et al. (2011).

The ASCEM project is focused on developing a computational framework for simulation of environmental remediation systems. The far-field flow and transport processes considered by ASCEM are similar to those required by UFD. ASCEM multi-physics model and computational

framework components and requirements are documented in DOE (2010b), DOE (2010c), DOE (2010d), Brown et al. (2011), DOE (2012), and Schuchardt et al. (2012).

And finally, Fewell et al. (2000) documented the requirements for the DeskTop PA computational framework, based on experience gained from the WIPP PA.

In Section 2, the computational framework was described as facilitating "the integration of the system analysis workflow (e.g., input pre-processing, integration and numerical solution of the mathematical representations of the conceptual model components, output post-processing), and the supporting capabilities (e.g., mesh generation, input parameter specification and traceability, matrix solvers, visualization, uncertainty quantification and sensitivity analysis, file configuration management including V&V and QA functions, and compatibility with HPC environments)". This definition addresses the desired functional capabilities outlined at the beginning of this section, is consistent with the computational frameworks described in the above publications, and provides an outline for identifying necessary computational framework components. The necessary components, shown in Figure 2-6, are:

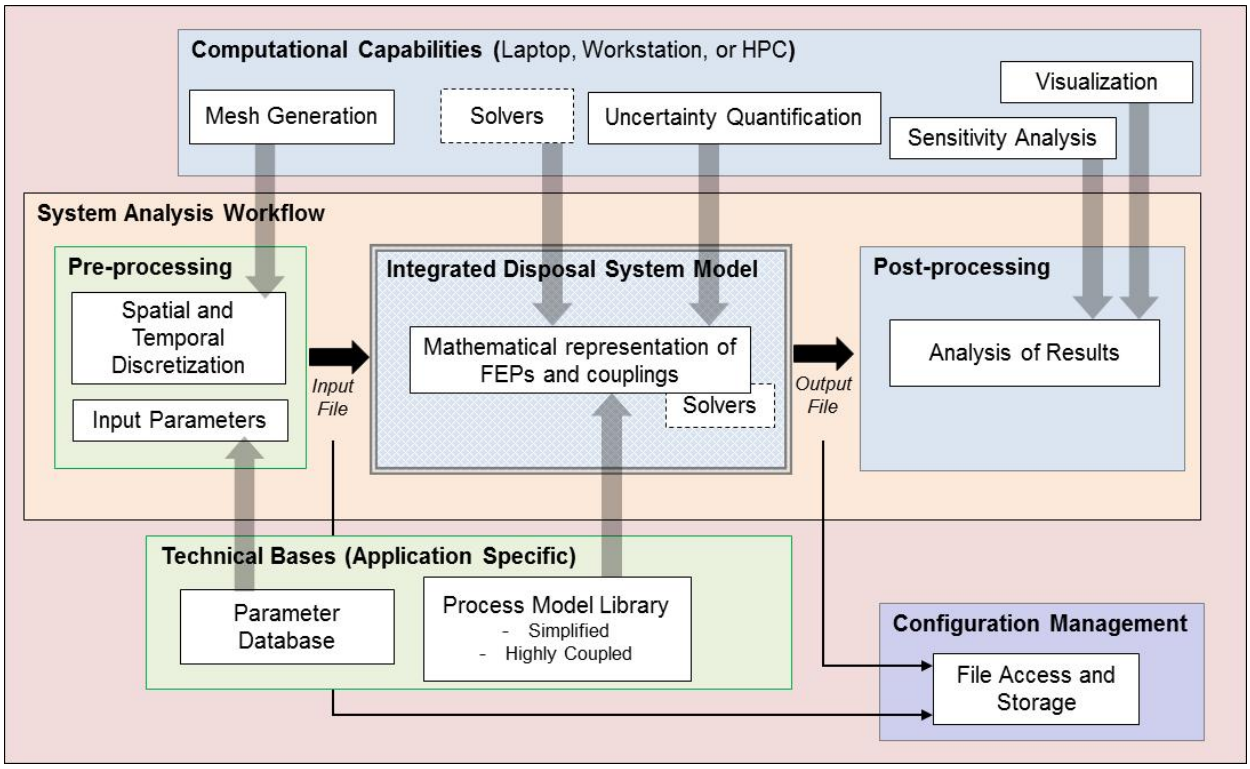


Figure 2-6. Computational Framework Components

System Analysis Workflow: controls the development and execution of the integrated system model through:

- pre-processing (spatial and temporal discretization, input parameter specification and traceability),
- integrated system model implementation and execution (mathematical representations of FEPs and couplings), and
- post-processing (analysis of results)

Computational Capabilities: enables the System Analysis Workflow by supporting:

- input development (mesh generation),
- system model development and execution (data structure and matrix solvers, uncertainty quantification), and
- output management (visualization, sensitivity analyses)

Configuration Management and Technical Bases: enables the System Analysis Workflow by supporting:

- input development (parameter database, file access and storage),
- system model development and execution (process model/governing equation library, data structure and matrix solvers, uncertainty quantification), and
- output management (file access and storage)

As shown in Figure 2-6, the integrated disposal system model is central to the System Analysis Workflow component, which in turn is the central component of the computational framework. Within the computational framework, the integrated disposal system model is the integrated set numerical representations of the subsystem components and multi-physics phenomena (i.e., the governing equations describing the included FEPs) for a specific disposal system option, developed as described in Section 2.2.1. More specifically, the integrated disposal system model is defined by the governing equations, initial and boundary conditions, and input parameters that describe the integrated disposal system FEPs and scenarios. The System Analysis Workflow component is described in more detail in Section 2.3.1.

The Computational Capabilities component enables the numerical solution of the integrated set of governing equations by providing capabilities for mesh generation (to support spatial and temporal discretization), uncertainty quantification, and numerical solution techniques. The flexibility of the PA model framework to be applied to different disposal system options and multi-physics processes is dependent on its ability to integrate different sets of governing equations from various sources (i.e., multi-physics codes and code objects, including legacy codes) contained in the process model library. The Computational Capabilities component also enables analyses of model results by providing capabilities for visualization and sensitivity analysis. The Computational Capabilities component is described in more detail in Section 2.3.2.

The Configuration Management and Technical Bases component supports the development of the integrated disposal system model by providing capabilities for specification of input parameters and distributions (from the parameter database), and of process models that comprise the integrated disposal system model (from the process model library). This component also provides a configuration management function for the parameter database, process model library,

and input and output files. The Configuration Management and Technical Bases component is described in more detail in Section 2.3.3.

An additional component of the computational framework, not explicitly identified in Figure 2-6, is the Graphical User Interface (GUI). For ease of use, the computational framework should include a GUI that facilitates the implementation of the other component functions. The GUI component is described in more detail in Section 2.3.4.

The computational framework components, which collectively support the development, execution, and analysis of disposal system PA model, are implemented as computer utility codes. One of the functions of the computational framework is to provide a structure to integrate the various utility and multi-physics codes. For example, most of the governing equations for process models exist in various legacy codes that are most commonly written in FORTRAN. Conversely, utility codes supporting functions like mesh generation and data structures supporting advanced solution techniques compatible with HPC are most commonly written in object-oriented languages like C++. The computational framework must provide a mechanism for these different codes to be integrated.

A key computational consideration relates to the development of the integrated disposal system model from the process models representing the subsystem FEPs. The generic disposal system PA model framework must accommodate the construction of a range of disposal system options from a modular library of subsystem process models that can range in complexity in their representation of (a) THCMBR multi-physics processes, and (b) the degree of coupling between the processes (e.g., how important is bi-directional process coupling, the two-way exchange of information between two coupled processes). The various representations of the multi-physics processes residing in the process model library may include stand-alone numerical codes (i.e., legacy codes) and/or independent code objects describing mathematical models/governing equations.

Computational framework codes, such as those listed in Section 4.1, can facilitate the numerical integration of multi-physics process models. Approaches to integrate the process models include:

- Weakly-Coupled or "Linked" Integration – The numerical implementation of the mathematical models of the processes exists in multiple independent codes. Each independent code typically has its own spatial and temporal discretization and a built-in numerical solution. The process coupling is numerically explicit; the codes are "linked" by mapping each of the independent spatial grids and time stepping schemes to a "master" spatial and temporal grid and passing values for state variables between the independent codes. This weakly-coupled (or linked) integration approach is numerically efficient, but has a limited capability for bi-directional process coupling. However, some bi-directional coupling may be inherent within of one of linked codes, thus providing the system model with this capability. Numerical considerations for weakly-coupled integration (i.e., "feed forward" coupling) are discussed in more detail in Appendix A.

Within a computational framework, weakly-coupled linked integration can be achieved by (a) defining a master spatial and temporal grid, (b) mapping the spatial and temporal grids and state variables between the stand-alone codes and to the master grids, and (c) developing computer code to implement the linkages. Modularity in the specification of system model processes can be achieved by substituting different stand-alone codes. The stand-alone codes may represent different levels of process complexity (from simple 1D algorithms to complex 3D finite element representations) as long as they are defined in terms of common state variables. The flexibility to include a range of processes is controlled by the availability of stand-alone codes, the ability to map between different discretization and solution schemes, and the numerical efficiency that can be achieved (e.g., stand-alone FORTRAN-based codes may not be able to take full advantage of HPC capabilities).

Strongly-Coupled Integration – The numerical implementation of the mathematical models of the processes exists in a single computational framework. The processes (i.e., the multiple sets of governing equations) are coupled through state variables and then solved simultaneously on a common spatial and temporal grid. The strongly-coupled integration approach is more numerically intensive, but provides a greater capability for bi-directional process coupling. Numerical considerations for strongly-coupled integration (i.e., "operator split" or "fully implicit time integration" coupling) are discussed in more detail in Appendix A.

Within a computational framework, strongly-coupled integration can be achieved by (a) defining a master spatial and temporal grid, (b) developing the coupling equations that relate the sets of governing equations, and (c) developing computer code to implement the couplings. Modularity in the specification of system model process can be achieved by substituting different sets of governing equations. The governing equations may represent different levels of process complexity as long as they can be related through common state variables. The flexibility to include a range of processes is controlled by the availability of stand-alone codes and by the ability to map between different discretization and solution schemes.

The preceding discussion of weakly- and strongly-coupled integration inferred that the coupling involved multiple multi-physics codes facilitated by a computational framework. However, there are some stand-alone codes that provide limited multi-physics coupling. For example, flow and transport codes (such as those listed in Section 4.2) that includes a simple reaction term to represent the radionuclide source term could be applicable to disposal system PA modeling. In these cases, the multi-physics capabilities (e.g., TH, TM, or THC) and the degree of coupling (typically weak feed forward) are pre-defined by the stand-alone code. Enhancement of the multi-physics capabilities would require code modification. Some stand-alone codes are optimized for HPC application (e.g., parallel processing) and may also include some peripheral computational framework capabilities such as mesh generation. The computational framework capabilities of these stand-alone codes could also be expanded through the use of shell codes, such as for uncertainty quantification and sensitivity analysis (e.g., DAKOTA or PEST, see Section 4.3). This approach might be applicable for a simulation of a simplified disposal system,

and might not even require a formal external computational framework beyond what is already provided by the stand-alone and shell codes.

In summary, strongly-coupled integration provides greater flexibility to represent multiple disposal system processes and implicit bi-directional couplings. However, it also requires a robust computational framework, and greater computational resources that may be offset by the application of HPC capabilities. Weakly-coupled integration provides greater computational efficiency for specific disposal system options and may be available in a stand-alone code. However, it may not be as flexible in representing the range of processes and couplings required, and may not be able to take full advantage of HPC capabilities. The computational framework should provide the capability for both weakly- and strongly-coupled integration.

The following subsections provide additional details regarding the computational framework components and their functions. Requirements necessary for implementing these component functions are presented in Section 3.

2.3.1. System Analysis Workflow

The System Analysis Workflow component is central to the computational framework and to the entire PA model framework. The System Analysis Workflow controls the development, execution, analysis, and reproducibility of the integrated disposal system model. The integrated disposal system model is the numerical representation of a disposal-option-specific conceptual model (developed as described in Section 2.2.1) defined by the governing equations, initial and boundary conditions, and input parameters that describe the FEPs and scenarios important to that disposal option. The System Analysis Workflow component facilitates the following functions:

- Integrated system model implementation – mathematical representations of FEPs and couplings,
- Pre-processing – spatial and temporal discretization, input parameter specification and traceability,
- Integrated system model execution, and
- Post-processing – analysis of results

These functions are described below.

Integrated System Model Implementation: System model implementation involves the identification and integration of subsystem component models. System model implementation functions include:

- specification of mathematical and numerical representations of FEPs and couplings – integration (linking or coupling) of governing equations, objects, or codes from the process model library

Ideally, the component numerical models, governing equations, codes, and/or code objects selected to describe the system model components do not require modification to the source code

or executable. This permits the V&V of the specific system component models and codes to remain intact without repeating the V&V activities.

The system model implementation function may be integrated with the pre-processing function.

Pre-Processing: Pre-processing supports system model execution by facilitating input file generation and converting data into a form expected by the system model components. Pre-processing functions include:

- spatial discretization - geometry definition and meshing
- temporal discretization
- input parameter specification – specification of input parameter values and/or distributions, with traceability to a parameter database where appropriate
- uncertainty quantification sampling
- data conversion and input file generation

The data obtained from the parameter database or from another component model in the system may require some conversion. This is accomplished in a traceable way through the use of pre-processor tools. Pre-processing is typically supported by a GUI (see Section 2.3.4).

Integrated System Model Execution: System model execution controls the System Analysis Workflow, from pre-processing to create an input file, to management of the simulation, to post-processing of output files. System model execution functions include:

- code execution and workflow management - control and integration of the execution of multi-physics codes and supporting/integrating computational codes.

Code execution and workflow management includes: management of inputs, multi-physics code integration and coupling, and outputs for a single simulation; control of multiple simulations, as needed, for optimization, uncertainty quantification and sensitivity analysis; optimization of numerical solutions; and distribution of computational workload across available computing resources (end-user local workstations, remote servers, and/or distributed computational resources). This function must be done in a way that does not compromise traceability. It includes the following:

- identification of available computational platforms/environments
- identification of all codes and code inputs
- transfer of code inputs and outputs between codes and to and from computational resources and databases
- execution of the codes

The capability to run on a variety of local and remote computing environments (e.g., Windows, Unix, or HPC) facilitates widespread use by being compatible with readily available and popular hardware. This also leverages existing software solutions, and can take advantage of large processing capacity and advanced system modeling capabilities such as with HPC.

For example, when conducting Monte Carlo simulations to address uncertainty, sufficient numerical efficiency may be achieved by simply distributing each of the Monte Carlo realizations to a different node or processor on a computational platform. Further efficiency can be realized by taking advantage of parallel solution techniques, which distribute the solution of a given Monte Carlo simulation to multiple processors.

Post-Processing: Post-processing supports the analysis and presentation of results. Post-processing functions include:

- statistical reduction
- sensitivity analysis
- plotting
- visualization and animation
- simulation reporting

While it is useful to have some of these post-processing functions as an integrated part of the computational framework, it is not absolutely necessary. As long as these post-processing tools can be accessed through the framework in a transparent fashion to the user, it is acceptable. Such access can be accomplished either by exporting results after post-processing in a format suitable for external analysis tools or by integrating the analysis tools into the framework. The disadvantage of the former is that traceability of the results and subsequent analysis may be lost.

2.3.2. Computational Capabilities

The Computational Capabilities component supports the System Analysis Workflow component (Section 2.3.1) by providing functions that enable the development, execution, and analysis of the integrated disposal system model. These functions include:

- Mesh generation,
- Uncertainty quantification,
- Numerical solution techniques – data structure and matrix solvers,
- Sensitivity analysis, and
- Visualization

These functions are described below.

Mesh Generation: Mesh generation utilities can support the development of structured and/or unstructured grids depending on the data structure and solution techniques. Mesh generation is commonly supported by a GUI (see Section2.3.4).

Mesh generation supports the pre-processing function of spatial discretization.

Uncertainty Quantification (UQ): UQ involves the specification of parameter value distributions for uncertain parameters and the incorporation of those uncertainties into a simulation. UQ is most commonly incorporated using multiple realizations (e.g., Monte Carlo analysis) of a disposal system model with varying values of uncertain parameters. However,

there are also methods to use embedded UQ (SNL 2009, Sections 6.2.2, 6.2.3.1, and 6.2.3.2). UQs methods propagate epistemic and/or aleatory uncertainty through the disposal system model. This propagation of uncertainty permits sensitivity analysis.

Uncertainty quantification supports the pre-processing functions of input parameter specification and uncertainty quantification sampling and the post-processing function of sensitivity analysis.

Numerical Solution Techniques: Numerical solution techniques are dependent of the inter-related nature of the governing equations, the degree of multi-physics coupling, the discretization scheme, and the data structure (e.g., PETSc, Trilinos, etc.). Numerical solution algorithms may require parameters that define and optimize the solution scheme for a specific numerical problem. Numerical solution techniques associated with multi-physics coupling are discussed further in Appendix A.

The numerical solution techniques support the system model execution function.

Sensitivity Analysis: Sensitivity analysis is the evaluation of disposal system performance to identify important system attributes. Sensitivity analysis most commonly involves the quantification of the effect of uncertainty in an input parameter on the value of one or more system or subsystem performance measures. Common sensitivity analysis techniques applied to disposal system PA models include: scatter plots, cobweb plots, pattern recognition, correlation and partial correlation analysis, stepwise regression analysis, rank transforms, and non-parametric regression (Sallaberry 2012).

Sensitivity analysis supports post-processing and the analysis of results.

Visualization: The capability to produce visualizations of model results (and also some spatial inputs) supports the understanding, traceability, and analysis of a disposal system PA model. Visualization includes 2D and 3D plots and animations.

Visualization supports the post-processing function.

2.3.3. Configuration Management and Technical Bases

The Configuration Management and Technical Bases component supports the System Analysis Workflow component (Section 2.3.1) by providing functions that enable the development, execution, and reproducibility of the integrated disposal system model. These functions include:

- Parameter database – specification of input parameter values and distributions,
- Process model library – specification of conceptual and mathematical representations of multi-physics processes and couplings, and
- Configuration Management – access and storage of input files, output files, parameter database, and process model/governing equation library

These functions are described below.

Parameter Database: The parameter database provides traceability of input parameter values to properties data. Properties data includes material properties and multi-physics parameters. Parameter values or distributions (including units) used in a model should be traceable to underlying experimental or literature values, including references to raw data and descriptions of any data manipulations performed.

The parameter database supports the pre-processing function of input parameter specification.

Process Model Library: The process model library contains mathematical representations (numerical models, analytic solutions, and/or governing equations) of the potentially relevant subsystem multi-physics processes in the form of codes (including legacy codes) or code objects. Depending on the complexity of the process, these codes may represent anything from an integrated multi-physics (THCMBR) modeling and simulation capability to a simple non-grid numerical algorithm. The identification of a set of process models from the library and their integration into a disposal system model is facilitated by the System Analysis Workflow (integrated system model implementation). Depending on the integration approach (linked or coupled, as described in Section 2.3), the integration of the codes may also involve the Computational Capabilities (numerical solution techniques and mesh generation). The integration of the codes should not require modification of the process model source codes, but may involve the use of a code wrapper (a layer of code between the process model code and the integrated system model code, with defined inputs and outputs, such that the process code can be executed and pass inputs and output, without manual scripting and without requiring the assistance of a computer analyst, domain expert, or programmer).

Configuration Management: Configuration management supports the System Analysis Workflow by controlling the movement of files associated with the development, execution, and reproducibility of the integrated disposal system model. In addition, configuration management contributes to QA and V&V associated with the system model and the component subsystem models. Configuration management functions include:

- input data and file management – access and traceability to parameter database and uncertainty quantification parameters, input file access, transfer, and storage,
- code execution and workflow management – access and traceability to process model library and multi-physics code integration, access and traceability to numerical solution parameters, data transfer between codes and databases, access to and distribution of computational workload across available computing platforms/environments,
- output data and file management – transfer of output data for post-processing, output file access, transfer, and storage,
- QA and V&V support – version control, simulation reproducibility, backup services, security/user authentication

2.3.4. Graphical User Interface

The GUI supports the entire PA model framework by providing a user interface for implementing the functions of the other multi-physics model and computational model components. The PA model framework GUI must provide users, who have knowledge of the physics being modeled, the ability to construct disposal system models. The user creates a particular disposal system model by identifying the model components, the integration between models, and assembling them into a system model. The PA model framework supports configuration of the system by facilitating the selection of the multi-physics component models and the specification of how those models are coupled. Users should be able to easily use the GUI to construct disposal system models without the use of specialized programming languages or scripting or specialized knowledge of how the computational framework controls the flow of information or execution of the calculations.

The function of the GUI is to facilitate the following:

- Construction of integrated disposal system model – selection of representations of process models and coupling (from process model library), specification of model execution settings and parameters,
- Construction of input files – specification of spatial and temporal discretization (using mesh generation utility), specification of input parameter values (from parameter database and using uncertainty quantification utility)
- Post-processing and analysis of results – compilation, analysis, and storage of model results (using sensitivity analysis, visualization, and configuration management utilities)

3. ADVANCED PA MODEL FRAMEWORK REQUIREMENTS

The advanced modeling capability will provide a PA model framework that facilitates PA model development, execution, and evaluation. A number of desirable attributes for a PA model framework were outlined in Section 2. These high-level attributes collectively describe the desired capabilities of the two components of PA model framework: the generic multi-physics model framework (described in Section 2.2) and the computational framework (described in Section 2.3). These desired capabilities provide a basis for requirements for the multi-physics model framework (see Section 3.1) and computational framework (see Section 3.2) components. These requirements support the development and integration of the disposal system PA model within the context of the PA methodology (described in Section 2.1).

3.1. Generic Multi-Physics Model Framework Requirements

The multi-physics conceptual model is the basis for the mathematical and numerical representation of a specific disposal system option. No matter how efficient and elegant a computational framework is, it cannot produce a defensible model result if the conceptual model is flawed. Therefore, the computational model requirements (outlined in Section 3.2) are only useful if the multi-physics conceptual model satisfies the following high-level requirements (based on the functions discussed in Section 2.2):

- All potentially relevant FEPs and scenarios shall be included.

- The representation of the potentially relevant FEPs (e.g., as process or subsystem models) shall be based on fundamental models, wherever possible, rather than on highly-abstracted models.

- The integration of the process/subsystem models into a disposal system model shall adequately represent the important THCMBR multi-physics and their couplings. A simple THC representation (e.g., time-dependent radionuclide source term to fluid flow and radionuclide transport, with some capability for temperature and chemistry to affect the source, flow, and/or transport) is necessary.

- The mathematical models of the FEPs and their couplings shall adequately capture the necessary geometry, initial, and boundary conditions representing the source term, EBS, geosphere, and biosphere regions and the interfaces between regions.

- The numerical implementation of the mathematical models shall accommodate:
  - a spatially discretized geosphere region with 3D multiphase fluid flow and radionuclide transport (e.g., using Eulerian, Lagrangian, or hybrid methods), including the capability to represent the effects of fractures,
  - an EBS region surrounded by (embedded within) the geosphere region, that provides a time-dependent, and possibly spatially-variable, radionuclide source term at the EBS boundary with the geosphere, due to degrading waste forms, waste packages, and other engineered components in the EBS,
  - a biosphere region for calculating dose to a receptor,
  - radionuclide decay and ingrowth.

These high-level requirements provide a general indication of the FEPs that need to be represented. Examples of specific mathematical representation (e.g., the governing equations) of the FEPs and their couplings are presented in DOE (2010b), Freeze et al. (2011b, Section 4), Clayton et al. (2011, Section 4.1.1), Wang et al. (2011, Section 3), Arnold et al. (2012, Section 3), and Hardin (2012, Sections 3.3 and 3.4).

3.2. Computational Framework Requirements

In an advanced PA model, the computational framework provides the numerical efficiency to solve the mathematical representations of the conceptual model. Specific requirements for each of the computational framework components are identified in the following subsections. These requirements are specified to address the desired code functions of the computational framework components (as outlined in Section 2.3) and are augmented by the technical judgments of subject matter experts who have been involved in the development and use of disposal system PA and by software requirements identified in PA model framework planning documents developed for the NEAMS Waste IPSC (SNL 2009; Freeze et al. 2011b; Wang et al. 2011; and Edwards et al. 2011b).

3.2.1. System Analysis Workflow Requirements

Specific requirements for the System Analysis Workflow component are listed in Table 3-1, organized around the component functions presented in Section 2.3.1.

Table 3-1. System Analysis Workflow Requirements

Integrated System Model Implementation	
	Provide the capability to select from a range of multi-physics process models of relevant FEPs (e.g., select codes and/or code objects from the Process Model Library)
	Provide the capability to modularly integrate selected process models into a disposal system model of relevant scenarios (e.g., link or couple process codes and/or code objects into an integrated set of codes that provides a numerical representation of the disposal system)
	Provide options for the selection of discretization schemes, solution techniques, and code couplings as part of the creation of the integrated disposal system code(s) to maximize runtime efficiency (e.g., to take advantage of HPC capabilities).
	Support the transparency and traceability of the integrated numerical model represented by the disposal system code(s) (e.g., propagate initial and boundary conditions consistently, clearly define model interfaces, document model assumptions and interactions)
Pre-Processing	
	Provide an extensible capability (leveraging existing utilities and a user interface, where possible) for pre-processing including spatial and temporal discretization, input parameter specification, uncertainty quantification sampling, and input file generation
	Interface with the parameter database, process model library, and supporting computational capabilities (e.g., mesh generation, uncertainty quantification)
Integrated System Model Execution	
	Interface with configuration management to control, and provide traceability and versioning for: input data and files; integrated disposal system models and codes and the component models and codes; and output data and files
	Provide the capability to run on a variety of local and remote computing environments (e.g., Windows, Unix, or HPC).
	Interface with computational capabilities (uncertainty quantification and sensitivity analysis) to control iterative, multi-realization simulations
	Control execution of the integration disposal system code(s) including: translating, transferring, and tracking input and output data between computational codes and resources; managing restarts and use of previous results
	Control distribution of computational workload among available computational resources (e.g., remote servers, HPC clusters)
	Satisfy run time and solution precision limits (numerous aspects of the system model and computational environment impact numerical performance including: number of radionuclides, number and complexity of processes simulated, degree of coupling between component models, heterogeneity of the system, grid resolution, time step size, numerical solution algorithm, error limits, and convergence criteria).
	Produce outputs that are exportable in common formats to facilitate external use.
Post-Processing	
	Provide an extensible capability (leveraging existing utilities and a user interface, where possible) for post-processing including statistical reductions, sensitivity analysis, plotting, visualization and animation, and reporting.
	Interface with the supporting computational capabilities (e.g., sensitivity analysis, visualization)
	Support analysis of both system and subsystem results without re-execution of a simulation.

3.2.2. Computational Capabilities Requirements

Specific requirements for the Computational Capabilities component are listed in Table 3-2, organized around the component functions presented in Section 2.3.2.

Table 3-2. Computational Capabilities Requirements

Mesh Generation	
	Provide the capability (using existing utilities and a graphical user interface, where possible) for geometry definition and spatial discretization.
	Provide options for different spatial domains (e.g., EBS and geosphere) and/or different physics component models to utilize differing meshes and time stepping.
Uncertainty Quantification	
	Provide the capability to represent and propagate uncertainty throughout the disposal system, considering both epistemic and aleatory uncertainty.
	Support deterministic and probabilistic analyses through the specification of, and sampling from, statistical distributions (using existing utilities, where possible). For deterministic analyses, provide the capability to select a value from a distribution of values (mean, median, or x-percentile) or enter user-specified values. For probabilistic analyses, provide the capability to sample from a distribution (using, at a minimum, a LHS Monte Carlo approach) and run multiple realizations.
Numerical Solution Techniques	
	Provide options for the selection of numerical solution techniques, based on the data structure, complexity and degree of coupling of the integrated processes, discretization, and desired numerical precision.
	Provide options for temporal discretization, including: dynamic time stepping (i.e., the automatic determination of appropriate time step size); and the use of different time stepping for different subsystem model components.
Sensitivity Analysis	
	Provide the capability to perform sensitivity and uncertainty analysis (using existing utilities, where possible). At a minimum, users must be able to perform scatter plots, pattern recognition, and stepwise regression among user-selected input and output. Users must be able to analyze, compare, and contrast results from different runs including the capability to import results generated externally or previously for the purpose of comparison.
Visualization	
	Provide the capability to display two- and three-dimensional data.

3.2.3. Configuration Management and Technical Bases Requirements

Specific requirements for the Configuration Management and Technical Bases component are listed in Table 3-3, organized around the component functions presented in Section 2.3.3.

Table 3-3. Configuration Management and Technical Bases Requirements

Parameter Database	
	Provide configuration management for an extensible set of physical parameter data including maintaining the integrity of data, and maintaining a historic log of data changes
	Provide the capability for user searches and queries of properties, parameters, source data and their usage.
	Provide traceability of physical parameter values and statistical distributions to underlying source information (e.g., credible references, experimental data)
Process Model Library	
	Provide configuration management for an extensible collection of codes and code objects representing mathematical models (e.g., numerical models, governing equations, analytic solutions) of potentially relevant multi-physics processes and couplings.
	Provide traceability of codes and code objects to source information (including V&V support)
Configuration Management	
	Develop and distribute codes in an open source environment
	Permit code access from multiple DOE sites
	Require user authentication to restrict unauthorized access
	Provide configuration management (file access, transfer, and storage) for input data, including an interface with the parameter database
	Provide configuration management (file access, transfer, and storage) for output data, including an archive for simulation results
	Provide configuration management (file access, transfer, and storage) for integrated disposal system code(s) and their component mathematical models, including an interface with the process model library
	Track code execution history including codes executed, execution environment, data input, data output, and resources used.
	Support quality assurance objectives
	Support V&V (e.g., provide configuration management for input and output files associated with test cases)
	Provide file backup services

3.2.4. User Interface Requirements

The user interface functionality and the functionality to integrate system component models permits the graphical plug and play building of disposal system PA models without the need for special computer skills or assistance of a computer programmer. This permits the user to focus on capturing the proper physics in the model and on analysis of results. Models can be assembled, linked, run, and results can be displayed graphically and analyzed all using a built in set of tools accessed through the user interface.

Specific requirements for the User Interface component are listed in Table 3-4, organized around the component functions presented in Section 2.3.4.

Table 3-4. User Interface Requirements

User Interface	
	Provide a graphical user interface to support the construction or modification of an integrated disposal system model from the process components available in the process model library
	Provide a graphical user interface to support the construction of input files including mesh generation, specification of input parameters and distributions, and specification of model execution settings and parameters
	Provide a graphical user interface to support the post-processing and analysis of model results including plotting and visualization, sensitivity analysis, and storage and/or export of output files

4. IDENTIFICATION OF POTENTIAL PA MODEL FRAMEWORK CODES

This section summarizes existing codes that have the potential to provide PA model framework capabilities, based on the requirements identified in Section 3. These existing codes can be divided into three groups, based on their primary function: codes that are focused on multi-physics modeling capabilities (and tend to address more of the requirements outlined in Section 3.1); codes that are focused on computational framework capabilities (and tend to address more of the requirements outlined in Section 3.2); and codes that address both multi-physics and computational framework requirements. Candidate codes are listed in the following subsections: integrated PA model framework codes (computational frameworks with multi-physics capabilities) are described in Section 4.1; multi-physics modeling codes are listed Section 4.2; and computational framework codes are listed in Section 4.3.

The lists of candidate codes were identified based on subject matter expert experience in the field of disposal system PA modeling, augmented by information available in open literature. It is recognized that the list of candidate codes, while comprehensive, may not be all-inclusive. Additional codes may be evaluated as they are identified. However, it is expected that any unidentified code would have similar capabilities to those already listed.

Even within the group of codes that provide both multi-physics and computational framework capabilities, there is no single code that addresses all of the requirements. However, the list of requirements in Section 3 is very comprehensive; a PA modeling capability that satisfies all of the requirements would represent a significant advancement in the state-of-the-art. Therefore, the approach to develop an advanced PA model framework capability will necessarily involve (1) an integration of multiple codes and/or code capabilities, rather than a single code, and (2) a phased implementation, where requirements are prioritized and iteratively re-evaluated as UFD program needs evolve. As a result, many of the codes listed here are candidates not because of their overall capabilities, but because of their perceived capability to (a) satisfy a few specific requirements, and (b) be easily integrated with other codes.

4.1. Computational Framework Codes with Multi-Physics Capabilities

There are a number of available codes that appear to address a reasonable subset of both the multi-physics model and computational framework requirements. These include research codes developed and maintained at universities and national laboratories and commercial codes available for purchase. Several of these candidate PA model framework codes, capable of providing both multi-physics and computational framework capabilities, are listed below with references:

Research Codes

- *ASCEM (Amanzi/Akuna/Agni)* – Advanced Simulation Capabilities for Environmental Management, DOE Office of Environmental Management and a consortium of national laboratories (esd.lbl.gov/research/projects/ascem/)

- *SIERRA Framework and Toolkit* – DOE Advanced Simulation and Computing (ASC) and Sandia National Laboratories (SNL) (Edwards and Stewart 2001; Notz et al. 2007; SIERRA Solid Mechanics Team 2010; www.trilinos.sandia.gov/packages/stk)

- *Albany* – DOE Advanced Simulation and Computing (ASC) and Sandia National Laboratories (SNL) (Parks et al. 2011, Sections 2 and 3)

- *MOOSE* – Multiphysics Object Oriented Simulation Environment, Idaho National Laboratory (INL) (www.inl.gov/research/moose/)

- *FRAMES* – Framework for Risk Analysis in Multimedia Environmental Systems, Pacific Northwest National Laboratory (PNNL) (mepas.pnnl.gov/FramesV2/index.stm)

- *OpenGeoSys* – Helmholtz Zentrum für Umweltforschung (UFZ) Centre for Environmental Research, Germany (Kolditz et al. 2012, www.ufz.de and www.ufz.de/index.php?en=18345)

Commercial Codes

- *GoldSim* – GoldSim Technology Group LLC (GoldSim Technology Group 2010a; 2010b; www.goldsim.com)

- *QPAC* – Quintessa General-Purpose Modelling Software, Quintessa Ltd. (Quintessa 2011; www.quintessa.org)

- *COMSOL 4* – COMSOL Group (www.comsol.com)

- *ANSYS Workbench and ANSYS Multiphysics* – ANSYS, Inc. (www.ansys.com)

- *ALGOR Professional Multiphysics* – ALGOR, Inc. (www.efunda.com/storefront/storefront.cfm?co=Algor%2C%20Inc%2E)

As noted in Section 4, there is no single PA model framework code that addresses all of the multi-physics and computational requirements. However, a logical starting point is to evaluate the status of several ongoing code development efforts that could be leveraged and/or integrated to develop an advanced PA modeling framework. Therefore, for each of the six research codes listed above, a brief description of capabilities (as outlined in the literature, but not confirmed by hands-on evaluation) is provided in a separate subsection. A description of the GoldSim capabilities is also included because it has been used for a number of disposal system PA models and has been used on the UFD project.

Two of the six candidate research codes, ASCEM and Albany, appear to offer the best combination of readily available open-source development, appropriate multi-physics capabilities, and HPC capabilities. Therefore, the ASCEM and Albany frameworks have been selected for further evaluation.

4.1.1. ASCEM

The Advanced Simulation Capabilities for Environmental Management (ASCEM) project is developing state-of-art computational and scientific tools and approaches for integrating data and scientific understanding to enable prediction of contaminant fate and transport in natural and engineered systems (Williamson et al. 2011). The ASCEM project includes development of both multi-physics model and computational framework capabilities. ASCEM multi-physics model and computational framework components and requirements are documented in DOE (2010b), DOE (2010c), DOE (2010d), Brown et al. (2011), DOE (2012), and Schuchardt et al. (2012). ASCEM codes include a multi-physics simulator (Amanzi) and supporting computational framework tools (Akuna, Agni, and Velo). An overview of the ASCEM multi-physics and computational capabilities is provided by Robinson (2012). The summary presented here is reproduced from the overview of Robinson (2012).

Overview

The ASCEM modeling initiative is developing an open source, multi-phase, multi-component, multi-scale subsurface flow and contaminant transport simulation capability, including cementitious barrier and source-term degradation. These modeling tools incorporate capabilities for predicting releases from various waste forms, identifying exposure pathways, performing dose calculations, and conducting systematic uncertainty quantification. ASCEM is demonstrating these modeling tools on selected sites and applying them in support of the next generation of performance assessments of nuclear waste disposal and decommissioning facilities across the EM complex.

A major ASCEM goal is to provide a community code for DOE-EM and the greater scientific and engineering communities. To that end, the ASCEM modeling tools are being developed using an open source model, with involvement from the DOE Office of Science (DOE-SC) community. This approach allows ASCEM to leverage the considerable scientific investment that has already been made both within and outside of DOE-EM in the areas of subsurface geosciences, modeling and simulation, and environmental remediation. Through integration of these efforts, the project is facilitating development of more accurate site models, allowing for predictive simulation of proposed remediation methods. This is anticipated to enable scientists to avoid the implementation of overly conservative and unnecessarily expensive remediation strategies. Wherever appropriate, ASCEM is using and building upon results and models developed through its associated DOE initiatives.

Within DOE-SC, DOE-NE, and DOE Office of Fossil Energy (DOE-FE), there are several efforts related to the development of advanced HPC capabilities, as well as scientific investigations of groundwater flow and transport, source term degradation and release, and mechanical degradation of structures and barriers. By leveraging these investments, ASCEM is

developing a toolset for use not only within DOE-EM, but one also potentially suitable for use by the greater DOE community in many areas including geologic carbon sequestration and high-level waste repository performance.

The ASCEM project is organized into three technical thrust areas: the Site Applications Thrust; the Platform and Integrated Toolsets Thrust, which provides the user interfaces; and the Multi-Process HPC Simulator Thrust, which provides the computational engine. Detailed descriptions of the three thrust areas are contained in the ASCEM Implementation Plan (DOE, 2010d).

Site Applications Thrust Area

Engaging the user community is particularly important in the early stages of the ASCEM development, and the Site Applications Thrust area incorporates a "user interface" task focused on establishing contact with end users, soliciting their input about ASCEM development plans, and conveying the feedback to members of the HPC and Platform Thrust areas responsible for code development.

The Site Applications Thrust also engages the end user community through a series of site demonstrations of the ASCEM capabilities. This is an iterative process implemented through working groups of development staff, Site Applications staff, and end users at the DOE sites. The working groups encompass two of the DOE-EM Applied Field Research Initiatives for (1) enhanced attenuation of metals and radionuclides in the subsurface at the Savannah River Site F Area, and (2) the deep vadose zone at the Hanford Site. An additional working group is focused around a waste tank performance assessment demonstration. Another working group is now being formed around the Oak Ridge Reservation and the mercury contamination problem.

Through the Site Applications Thrust, the ASCEM modeling capability is being made available to DOE-EM site users through training and technology transfer. It will also be made available to the greater scientific community for use in subsurface and risk analysis research and for creating additional modules incorporating scientific advances and new research areas.

Platform and Integrated Toolsets Thrust Area

The Platform and Integrated Toolset Thrust is being designed to provide a standardized user interface enabling end users to create inputs, analyze outputs, manage data associated with running simulations, and conduct performance and risk assessments. The ASCEM Platform provides both subsurface modelers and site management with tools to interact with the Amanzi simulator and the models, data, and results created throughout the site modeling lifecycle. The software design comprises a number of major components, as described below:

- *Desktop Platform:* The Akuna platform is the primary user interface that modelers utilize to create and analyze Amanzi simulations. It comprises a collection of tightly integrated toolsets for model setup, parameter estimation, uncertainty quantification, and decision support and risk analysis.

- *Data Management:* This provides the necessary user interfaces and underlying databases to manage and access the ASCEM database, which holds a wide variety of site and model specific data.

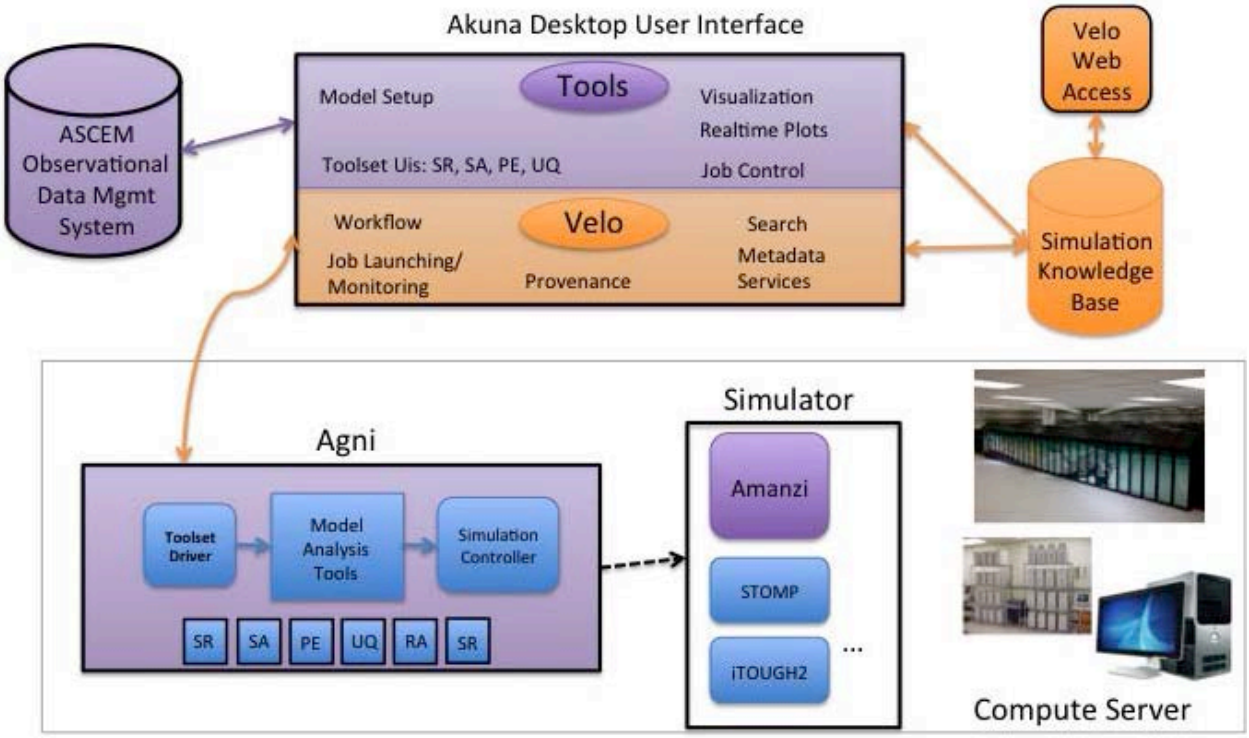
- *Knowledge Management Platform:* The Velo knowledge management platform provides web-based access through the ASCEM Web Interface to ASCEM data. For example, data related to modeling activities is tracked in Velo, providing access to project work through a browser interface.

- *Visualization:* The ASCEM platform provides primary support for VisIT-based visualizations, which can be launched from the desktop platform. Paraview and GMV will be supported in future versions of ASCEM.

- *Toolset Driver:* The toolset driver provides the interface between the Platform and the Amanzi simulator. It is responsible for communicating inputs from the Platform to Amanzi running on a remote HPC resource. It can execute a single forward run and/or multiple realizations of Amanzi as required, for example, in uncertainty quantification analyses, and specify the outputs that Amanzi should produce.

Under this thrust area, ASCEM is using a modular design approach by developing programming "interfaces" for each module (where an interface defines access to a module while hiding the details of its implementation). This methodology is broadly used in similar advanced software engineering approaches, for example, within the Scientific Discovery through Advanced Computing (SciDAC) program.

The architecture of the platform is illustrated in Figure 4-1. The two components depicted are the Desktop User Interface, called Akuna, and Agni, the underlying software on the compute server that translates instructions from Akuna and executes them. Thus, Akuna controls the modeling workflow on the front end of the process, passes instructions to Agni, which executes the model runs, and delivers model results back to the Desktop User Interface.



Source: http://esd.lbl.gov/research/projects/ascem/thrusts/platform/

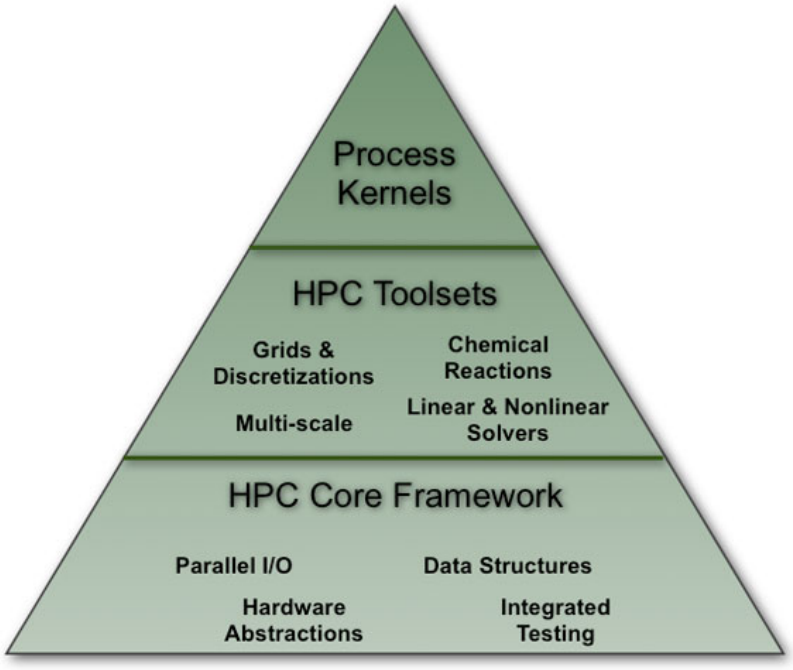
Figure 4-1. Architecture of the ASCEM Akuna Platform and Integrated Toolsets

Multi-Process HPC Simulator Thrust Area:

The third thrust area, the Multi-Process HPC Simulator, provides the core simulation capabilities necessary for modeling DOE-EM sites. The graded and iterative approach to assessments naturally generates a suite of conceptual models that span a range of process complexity, potentially coupling hydrological, biogeochemical, geomechanical, and thermal processes. The HPC Simulator provides a flexible and extensible computational engine to simulate the coupled processes and flow scenarios described by the conceptual models developed using the ASCEM Platform.

ASCEM has established a multi-disciplinary team of geoscientists, applied mathematicians, and computational scientists to leverage recent advances in these complementary fields, to develop Amanzi as a new open-source community code. While there is clear recognition that many problems will not require the highest-end computing capabilities, access to new computational power provides the option to use more complex models in lieu of, or to support, simplifying assumptions. Moreover, computer architectures on today's supercomputers may become commonplace on desktop computers in the near future. By developing the ASCEM modeling tools for HPC platforms today, this community code will be well-positioned to run on a range of platforms, including future desktops.

Figure 4-2 illustrates conceptually the hierarchy of different component levels in Amanzi, ASCEM's HPC core simulation capability.



Source: http://esd.lbl.gov/research/projects/ascem/thrusts/hpc/

Figure 4-2. Hierarchy of the Amanzi HPC Core Simulator

At the highest level, the process kernels are discrete representations of the physical and chemical models, derived from detailed mathematical process models. This concise mathematical description and use cases provides critical information for the requirements and design of Amanzi. For details on the multi-physics capabilities currently being built into Amanzi, see DOE (2010b). The middle layer, the HPC Toolsets, contains infrastructure that provides the building blocks for the process models. This includes the Multi-Process Coordinator (MPC) as well as the data management support for the system state necessary for the abstract interfaces to the process kernels. In addition, the HPC toolsets level contains the meshing, discretization, and solvers required to obtain accurate numerical solutions. The MPC approach allows new processes to be included simply by adding new process kernels, each of which takes advantage of the lower-level infrastructure in the HPC Core Framework level. These include data structures, input file specification and utilities, parallel input/output capabilities, and HPC related visualization support. Existing open source HPC Frameworks, such as Trilinos, and supporting libraries, such as the Hierarchical Data Format version 5 are leveraged here.

4.1.2. SIERRA

SIERRA is an object-oriented framework of software services and tools, developed by SNL with funding from the DOE ASC program, that supports a large, diverse set of complex, massively parallel, multi-physics application codes. The SIERRA framework consolidates complex physics-independent capabilities into a single software infrastructure that is shared by these application codes and is supported by software tools for configuration management and porting and distribution services on a variety of hardware platforms. The SIERRA framework, also referred to as the SIERRA Mechanics code suite (Edwards and Stewart, 2001), includes both multi-physics model and computational framework capabilities. An overview of the SIERRA Mechanics capabilities as they apply to disposal system PA modeling is provided by Wang et al. (2011, Section 5). The summary presented here is reproduced from the overview of Wang et al. (2011, Section 5).

SIERRA Mechanics was designed and developed to run on the latest and most sophisticated massively parallel computing hardware; spanning the hardware computing space from a single workstation to computer systems with 1000's of processors. The foundation of SIERRA Mechanics is the SIERRA Toolkit which provides finite element application code services such as: (1) mesh and field data management, both parallel and distributed, (2) transfer operators for mapping field variables from one mechanics application to another, (3) a solution controller for code coupling, and (4) included third party libraries (e.g. solver libraries, Message Passing Interface communications package, etc.). The two SIERRA Mechanics multi-physics codes which have been applied in the THMC coupling for repository systems modeling are Aria (Notz et al., 2007) for fluid flow and species transport and Adagio (SIERRA Solid Mechanics Team, 2010) for solid mechanics.

Aria is a Galerkin finite-element based program for solving coupled THC problems described by systems of partial differential equations (PDEs) and is capable of solving nonlinear, implicit, transient and direct-to-steady state problems in two and three dimensions on parallel architectures. The suite of physics currently supported by Aria includes: the incompressible Navier-Stokes equations, the energy transport equation, and species transport equations, as well as generalized scalar, vector and tensor transport equations. Both a saturated porous flow capability and a multiphase porous flow capability are recent additions to Aria (Martinez and Stone, 2008). Aria has basic geochemistry functionality available through existing chemistry packages such as Cantera (see Section 4.2). Additionally, Aria includes support for arbitrary Lagrangian-Eulerian (ALE) and level set based free and moving boundary tracking (Notz et al. 2007). Different regions of the physical domain (i.e., the input mesh) may have different materials and/or different collections of physics (i.e., PDEs) defined on them. These systems of equations may be solved alone, in a segregated but coupled algorithm ("loosely coupled") or as a single, fully-coupled system. Currently, Aria's loose coupling capabilities are handled by the Arpeggio application which also allows Aria to couple (loosely) to the Adagio mechanics code.

Adagio is a Lagrangian, three-dimensional, implicit finite element code for the analysis of solids and structures. It solves for the quasi-static, large deformation, large strain behavior of nonlinear solids in three-dimensions. Adagio has some discriminating technology that has been developed at Sandia for solving solid-mechanics problems. This technology involves the use of matrix-free

iterative solution algorithms that allow extremely large and highly nonlinear problems to be solved efficiently and lends itself to effective and scalable implementation on massively parallel computers. The implementation of Adagio with the SIERRA framework is sometimes referred to as SIERRA/Solid Mechanics (SM).

In summary, the coupling of the Aria and Adagio physics codes within the SIERRA Framework offers the following:

- an existing proven framework for coupled multi-physics (solution domains may be different for different physics),
- a finite-element based capability (which makes for more natural coupling),
- a massively parallel capability (scalability from 1 to 1000s of processors on a variety of platforms),
- various levels of coupling within the THC code (Aria) and loose coupling to the solid mechanics (M) capability (Adagio), and
- access to the SIERRA Toolkit for supporting computational capabilities.

4.1.3. Albany

The Albany Framework (Parks et al. 2011, Sections 2 and 3) employs a component-based scientific application code development strategy that is consistent with the current cutting edge approach to computational science software development. Albany Version 2.0 incorporates dozens of existing software libraries – ranging from input file parsers to multi-level pre-conditioning algorithms to uncertainty quantification methods – derived from the collective expertise of the computational science community. By leveraging existing technology (e.g., from the Trilinos, DAKOTA, and SIERRA Toolkit projects), the development burden of producing a new application code is reduced to adding the physics and models specific to that problem. A distinguishing aspect to the approach is the use of automatic differentiation technology integrated into a modular graph-based assembly engine, so that all new codes are born with transformational analysis capabilities, including:

- sensitivity analysis,
- optimization,
- calibration, and
- uncertainty propagation.

The development of a multi-physics modeling capability within the Albany Framework leverages development activities funded by ASC and DOE Office of Science. This is a prime example of leveraging work done for other customers to benefit UFD. Because large parts of the software engineering and numerical methods are already in place the repository system subject matter experts can focus on implementing the relevant multi-physics models into the software. Once this is done, the full range of Albany numerical capabilities is available to be utilized.

Albany is open-source code created using the agile components philosophy: rapid development of production quality codes with transformational capabilities. Albany already exercises many of the capabilities available in Trilinos (trilinos.sandia.gov), such as automatic differentiation,

embedded UQ, discretization tools, multi-physics dependency management, and a complete suite of solvers, among other things. Albany also includes the functionality from the SIERRA Toolkit, such as mesh representation and input/output (I/O). The intention is further adoption of SIERRA components as they are practically available. Figure 4-3 illustrates the integration of computational toolsets (e.g., Trilinos and SIERRA Toolkit) and solid mechanics (e.g., the Library of Advanced Materials for Engineering (LAME) developed as part of the Laboratory for Computational Mechanics (LCM) and SIERRA/SM) within the Albany Framework.

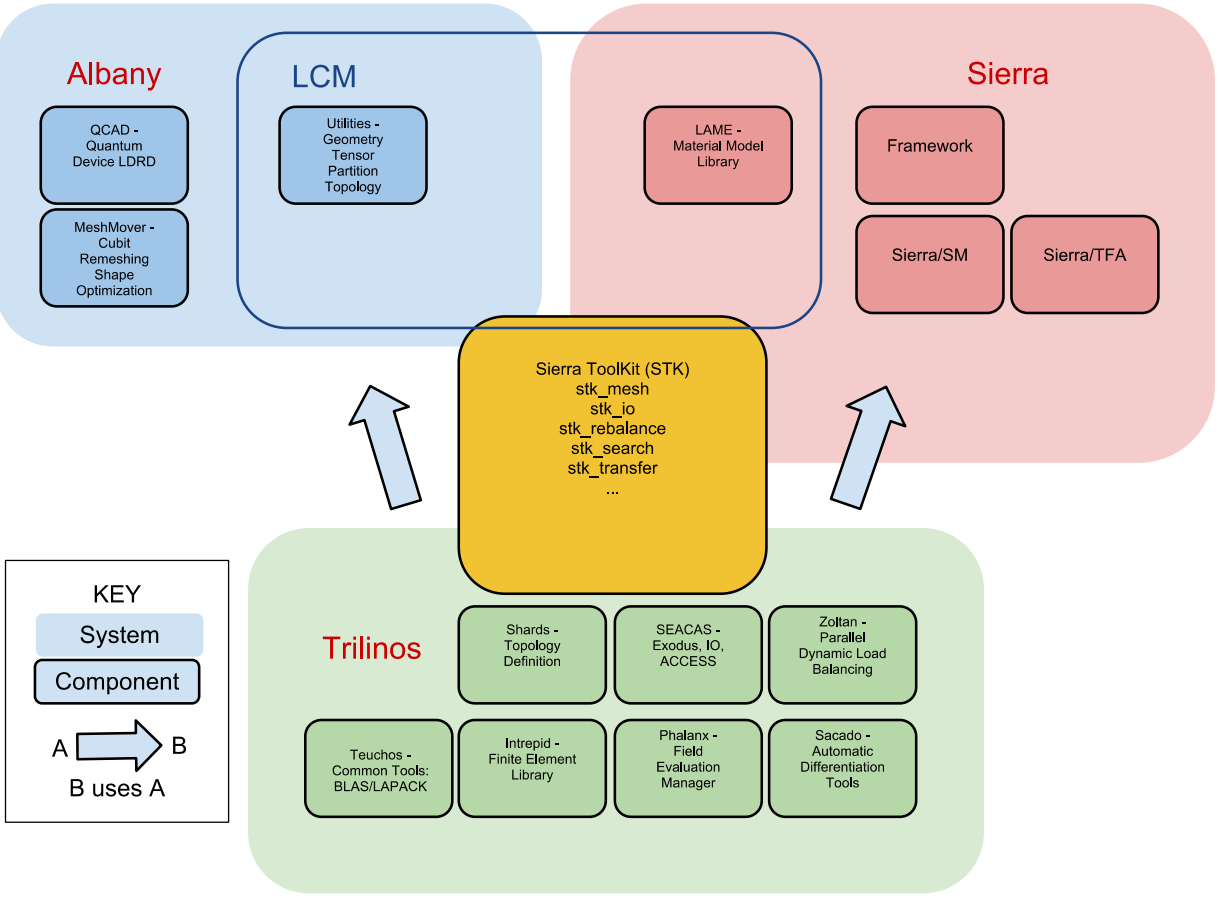


Figure 4-3. Integration of Toolsets within the Albany Framework

The Albany framework and its numerical methods are designed for multi-physics applications. Therefore it should be relatively straightforward to incorporate the necessary THCMBR multi-physics capabilities. There are already existing Albany examples of T, H, C, M, and R. In addition, Albany can easily be modified to meet any unexpected modeling challenges, and can benefit from multi-physics implementation experience from the SIERRA project.

4.1.4. MOOSE

The summary presented here is reproduced from the overview of Robinson (2012).

The Multiphysics Object Oriented Simulation Environment (MOOSE), developed by INL, is a parallel framework for solving systems of coupled partial differential equations relevant to many problems in nuclear engineering and other computational physics applications (Gaston et al., 2009). The framework is based on the Jacobian-Free Newton-Krylov method, using physics-based pre-conditioning to accelerate convergence and to achieve a more robust solution method capable of handling coupled physics problems that are tightly coupled or that operate on disparate time scales. This method facilitates the development of process kernels describing a variety of different physical and chemical processes in a streamlined fashion, opening the possibility of rapid development of new physics and chemistry modules for specific applications.

The MOOSE framework is designed for "engineering analysis applications" rather than as a computational research code. Thus, issues of computational speed, though important, are balanced against other priorities, such as: robust performance on a variety of computers, from desktops to mainframes; development using modern software engineering principles, using accepted software QA practices; integration of the framework with model setup and post-processing tools to facilitate the analysis; and comprehensive verification and validation specifications.

The MOOSE framework has formed the basis for a variety of applications. These include MOOSE-BISON, a nuclear fuel performance simulation code (Gaston et al., 2009), and Fracturing and Liquid Conservation (FALCON) and Reactive Transport (RAT), porous media codes designed to simulate geothermal reservoirs and general reactive chemical transport problems, respectively (Gaston et al., 2012). Two elements of these applications that are relevant to the development of an advanced disposal system PA modeling capability are the porous medium simulation capabilities represented in RAT and FALCON, and the thermal and solid mechanics physics modules in BISON. Elements of these capabilities could be incorporated into an advanced PA modeling capability for repositories.

4.1.5. FRAMES

The summary presented here is reproduced from http://mepas.pnnl.gov.

Framework for Risk Analysis Multimedia Environmental Systems (FRAMES) is a software platform developed by PNNL for selecting and implementing environmental software models for risk assessment and management problems. The purpose of FRAMES is to assist users in developing environmental scenarios and to provide options for selecting the most appropriate computer codes to conduct human and environmental risk management analyses. FRAMES allows legacy disparate models and databases to communicate in a plug and play atmosphere. FRAMES is a dynamic, reusable software interface structure that:

- Includes the Multimedia Environmental Pollutant Assessment System (MEPAS) and GENII modules.

- Establishes documented rule sets (which include as a criteria a minimum-set data transfer) to allow models to be added to the overall software structure.
- Provides a common Application Programming Interface (data protocols) to enable data transfer between models.
- Provides a way to perform sensitivity and uncertainty analysis on data from all kinds of deterministic models.
- Contains a suite of tools for integrating, analyzing, and visualizing data.
- Retains the model or database developer's choice of programming environment (languages, styles, tools) when inserting a software model into the FRAMES structure.

FRAMES has been used in applications for the DOE, U.S. Environmental Protection Agency, American Chemistry Council, U.S. Army Center for Health Promotion and Preventive Medicine, U.S. Army Corps of Engineers, NRC, and other federal and state agencies as well as private organizations.

One of FRAMES most popular applications is in the environmental arena, where it's multiple "medium-specific" models (for example: air, water, and human impacts) as well as a database of chemical properties with associated environmental parameters have proven an effective way to solve risk analysis problems.

4.1.6. OpenGeoSys

This overview is summarized from Kolditz et al. (2012). The OpenGeoSys (OGS) project is centered at Helmholtz Centre for Environmental Research (UFZ) in Germany, with collaborators form other European countries.

The OGS project is a scientific open source initiative for numerical simulation of thermo-hydro-mechanical-chemical (THMC) processes in porous media. The basic concept is to provide a flexible numerical framework (using primarily the Finite Element Method (FEM)) for solving multifield problems in porous and fractured media for applications in geoscience and hydrology. OGS is based on an object-oriented FEM concept including a broad spectrum of interfaces for pre- and post-processing. The OGS idea has been in development since the mid-eighties, as a continuous process of concept and software development evolving through FORTRAN, C, and C++ implementations. The idea behind OGS is to provide an open platform to the community, outfitted with professional software engineering tools such as platform-independent compiling and automated benchmarking. Benchmarking has been proven to be a valuable tool for cooperation between different developer teams, e.g. for code comparison and validation purposes (DEVOVALEX and CO2BENCH projects). On one hand, object-orientation provides a suitable framework for distributed code development; however the parallelization of object-oriented codes still lacks efficiency. HPC efficiency of object-oriented codes is subject to future research.

At the Helmholtz UFZ a new research platform TESSIN is available, which combines high-performance-computing (HPCLab) and high-end visualization facilities (VISLab). Post-processing becomes more and more important as more and more information becomes available, due to high-resolution measurement techniques and HPC itself.

4.1.7. GoldSim

GoldSim (GoldSim Technology Group 2010a) is a highly graphical, object-oriented computer program for carrying out dynamic, probabilistic simulations. GoldSim is like a "visual spreadsheet" allowing you to visually create and manipulate data and equations. GoldSim automatically indicates the influences and interdependencies between various objects in a model by visually connecting them in an appropriate manner. GoldSim also sets up and solves the equations represented by the objects and their interdependencies. GoldSim runs on personal computers using the Windows operating system and can also take advantage of distributed processing across multiple processors.

The following combination of features makes the GoldSim a unique simulation tool (GoldSim Technology Group 2010a, Chapter 2; GoldSim Technology Group 2010b, Chapter 1):

- **User friendly, highly graphical, and very flexible.** GoldSim can be applied to nearly any kind of system. Model building is performed in an intuitive, graphically-based manner by creating influence diagrams of a system. The software is designed in a modular manner such that model details can be added by directly entering functional relationships or linking user-defined functions or subroutines (e.g., finite difference flow models) into the program.

- **Specifically designed to quantitatively address the inherent uncertainty which is present in real-world systems.** GoldSim provides powerful tools for representing uncertainty in processes, parameters and future events, and for evaluating such systems in a computationally efficient manner. Uncertainty in processes and parameters can be represented by specifying model inputs as probability distributions. The impact of uncertain events can also be directly represented by specifying the occurrence rates and consequences of such "disruptive events".

- **Provides powerful capabilities for superimposing the occurrence and consequences of discrete events onto continuously varying systems.** This allows for the realistic simulation of discrete events such as accidents, system failures, earthquakes, floods, and sabotage.

- **Dimensional awareness through an extensive internal database of units and conversion factors.** Any units can be used to enter data and display results. Customized units can even be defined. GoldSim ensures dimensional consistency in models and carries out all of the unit conversions internally. As a result, it is never necessary to carry out (error-prone) unit conversions.

- **Highly extensible.** External programs or spreadsheets can be dynamically linked directly into a GoldSim model. In addition, GoldSim was specifically designed to support the addition of customized modules (program extensions) to address specialized applications.

- **Ability to create compelling presentations of a model.** GoldSim was specifically designed to allow a user to effectively document, explain and present a model. Graphics,

explanatory text, notes and hyperlinks can be added to a model, and it can be organized in a hierarchical manner such that it can be presented at an appropriate level of detail to multiple target audiences.

Because GoldSim is flexible and powerful enough to represent practically any aspect of a system, and because GoldSim provides unique capabilities for building a model in a hierarchical, modular manner, it acts as a system integrator. GoldSim facilitates the creation of a total system model – a consistent framework in which all aspects of the system, as well as the complex interactions and interdependencies between subsystems, can be represented.

The GoldSim Contaminant Transport Module (GoldSim Technology Group 2010b) is a program extension to the GoldSim simulation framework that allows dynamic modeling of mass transport within complex engineered and/or natural environmental systems. The fundamental output produced by the Contaminant Transport Module consists of predicted mass fluxes at specified locations within the system, and predicted concentrations within environmental media (e.g., groundwater, soil, air) throughout the system. If desired, concentrations in environmental media can be converted to doses and/or health risks to receptors by assigning appropriate conversion factors. The Contaminant Transport Module software allows the user to explicitly represent the following processes (GoldSim Technology Group 2010b, Chapter 1):

- **Release of mass (e.g., contaminants)** from specified sources, taking into account: 1) the failure of containers (if any) in which the contaminants are disposed; and 2) degradation of any materials in which the contaminants are bound (e.g., grout, metal, glass).

- **Physical transport of contaminants** through multiple transport pathways within an environmental system (e.g., aquifers, streams, atmosphere). The transport pathways can consist of any number of transport and storage media (e.g., water, air, soil), and a variety of transport mechanisms can be directly simulated, including 1) fluid advection; 2) solid advection (e.g., erosion and transport of contaminated soil); 3) diffusion through fluids; 4) advection and diffusion of contaminated particulates suspended in fluids; and 5) diffusion across boundary layers associated with adjacent fluids (e.g., transport across the air-water interface). Transport processes incorporate solubility constraints and partitioning of contaminants between the media present in the system, and can include the effects of chemical reactions and decay processes.

- **Biological transfer of contaminants within or between organisms**. Like physical transport pathways, biological transport pathways can consist of any number of transport and storage media (e.g., blood, tissue) which can be linked by a variety of transport mechanisms.

The GoldSim software has been used to implement complex PA models of radioactive waste disposal systems, such as the YMP Total System Performance Assessment Model for the License Application (TSPA-LA) (SNL 2008), and has also been used within the UFD project to implement simplified generic PA models (Clayton et al. 2011).

4.2. Multi-Physics Modeling Codes

As outlined in Section 2.2, a generic disposal system can be represented by the multi-physics phenomena that describe fluid flow and radionuclide transport through a 3D geosphere, driven by a radionuclide source term in an EBS embedded within the geosphere. Therefore, existing flow and transport simulation codes have the potential to contribute the multi-physics capabilities required by a PA model framework.

Wang et al. (2011) provides a comprehensive review of available flow and transport codes that combine conservation laws for mass, momentum, and energy, together with phenomenological or experimentally based equations of state, kinematic conditions, transport laws, rate expressions, and other constitutive relations to represent the linkages or couplings between various THCMBR multi-physics processes. Flow and transport code capabilities can be differentiated by such factors as dimensionality, number of fluid phases, number of components, and number of and degree of coupling between multi-physics processes. Flow and transport codes are most commonly grouped according to multi-physics capabilities. These include (ranging from simplest to most complex): isothermal flow (H), non-isothermal flow (TH), chemical equilibrium/reaction (TC), isothermal or non-isothermal flow and transport (H or TH with simplified C), and reactive transport (THC). Biological (B) and radiological (R) effects can generally be added to any of these groups through a reaction term. Fully coupled mechanical (M) effects are computationally intensive to model; however, mechanical effects can often be screened out or treated in a simplified fashion. As noted in Section 2.2.2, mechanical coupling is not likely to be considered in the disposal system PA model at this time or in the foreseeable future.

Specific codes reviewed by Wang et al. (2011, Section 4) include:

Chemical Equilibrium/Reaction (TC) Calculation Codes

- *EQ3/6* – performs geochemical modeling of fluid-mineral interactions and/or solution-mineral-equilibria in aqueous systems by combining EQ3NR, a speciation-solubility code, and EQ6 a reaction path modeling code (Wang et al. 2011, Section 4.1.1; Wolery 1992, ipo.llnl.gov/?q=technologies-software-browse_software-app&s=EQ3/6)

- *Cantera* – general purpose object-oriented constitutive modeling package (Wang et al. 2011, Section 4.1.2; Moffat and Jove-Colon 2009; code.google.com/p/cantera)

- *GEMS* – Gibbs energy minimization selector (GEMS) performs thermodynamic modeling of heterogeneous aquatic (geo)chemical systems (Wang et al. 2011, Section 4.1.3; gems.web.psi.ch/)

- *PHREEQC* – performs a wide range of ion-association aqueous geochemical calculations (Wang et al. 2011, Section 4.1.4; Parkhurst and Appelo 1999; wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/)

Thermal-Hydrologic-Chemical (THC) Codes

- *HYDROGEOCHEM* – comprehensive model of coupled fluid flow, thermal, and reactive chemical processes (Wang et al. 2011, Section 4.2.1; Yeh et al. 2004)

- *PFLOTRAN* – reactive flow and transport code for modeling subsurface processes, designed to run efficiently on machines ranging from supercomputers to laptops (Wang et al. 2011, Section 4.2.2; Hammond et al. 2011)

- *TOUGH2* – (TH only) non-isothermal multi-component, multi-phase flow in porous and fractured media (Wang et al. 2011, Section 4.2.3; Pruess et al. 1999)

- *TOUGHREACT* – 3D non-isothermal multi-component reactive fluid flow, heat flow, and solute transport simulator for saturated and unsaturated porous media (Wang et al. 2011, Section 4.2.4; Xu et al. 2004; esd.lbl.gov/TOUGHREACT/index.html)

- *FEHM* – Finite Element Heat and Mass Transfer Code (FEHM) is for simulating 3D, multi-phase, multi-component, non-isothermal reactive transport through porous and fractured media (Wang et al. 2011, Section 4.2.5; Zyvoloski 2007; fehm.lanl.gov)

- *MT3DMS* – The Modular 3-Dimensional Transport (MT3D) model with a Multi-Species (MS) structure for accommodating add-on reaction packages is compatible with any block-centered finite-difference flow model such as MODFLOW. MODFLOW / MT3DMS has been coupled with a number of different geochemical modules including RT3D (Clement 1997; Clement and Johnson 2011) and PHT3D (Prommer et al. 2003). RT3D is a finite difference, FORTRAN-based code for simulating 3D, multi-species, reactive transport of chemical compounds in groundwater. PHT3D is a 3D reactive transport model that couples the transport simulator MT3DMS to the geochemical modeling code PHREEQC. (Wang et al. 2011, Section 4.2.6; Zheng 1990; Zheng et al., 2001; hydro.geo.ua.edu/mt3d/)

- $CORE^{2D}$ – CORE is a C Ode for modeling partly or fully saturated water flow, heat transport and multi-component REactive transport (Wang et al. 2011, Section 4.2.7; Samper et al. 2003)

Thermal-Hydrologic-Mechanical (THM) Codes

- *SIERRA/Aria and Adagio* – these code capabilities are discussed in Section 4.1.2.

The THC and M capabilities in these codes could be leveraged and/or integrated into an advanced PA modeling framework.

As noted in Section 3.1, the initial multi-physics focus is on THC flow and transport. Of the THC codes listed above, PFLOTRAN appears to offer a useful combination of open-source development, appropriate multi-physics capabilities, and some HPC advantages (e.g., parallel processing). Therefore, PFLOTRAN has been selected for further evaluation. An overview of PFLOTRAN capabilities (as outlined in the literature, but not confirmed by hands-on evaluation) is provided in a separate subsection.

4.2.1. PFLOTRAN

PFLOTRAN is a multi-physics THC simulator that is designed to take advantage of some HPC capabilities. PFLOTRAN capabilities and applications are described in Mills et al. (2007), Lu and Lichtner (2007), and Hammond et al. (2007; 2008; and 2011). An overview of the PFLOTRAN capabilities is provided by Wang et al. (2011, Section 4.2.2) and Robinson (2012). The summary presented here is reproduced from the overview of Robinson (2012).

PFLOTRAN is a massively parallel, multi-phase, multi-component reactive transport code developed through the DOE-SC's SciDAC and Innovative and Novel Computational Impact on Theory and Experiment (INCITE) programs (Mills et al., 2007). The code, which uses the Portable Extensible Toolkit for Scientific Computation (PETSc) framework as the basis for performing the parallel computations, is a cutting edge research tool that has been demonstrated to be useful in tackling challenging subsurface modeling and simulation problems, including the Hanford site (Hammond et al., 2008), and carbon sequestration modeling (Lu and Lichtner, 2007).

The PFLOTRAN code employs an object-oriented design based mainly on the FORTRAN90 language. For any particular forward simulation, objects for the overall simulation, time stepping, solver, and other data structures are arranged in a fashion that facilitates code development and maintenance. In addition, a multiple realization object provides the low-level machinery for conducting multiple simulations as part of a simulation study. The multiple realization option is designed to take maximum advantage of multi-processor cores in the context of Monte Carlo simulations, which requires both parallelization of the individual model runs and simultaneously simulation of multiple realizations in parallel.

The flow and reactive transport capabilities in PFLOTRAN originally were implemented based on structured grids in the PETSc framework. However, recent development has been undertaken to employ structured Adaptive Mesh Refinement to provide high resolution where required, such as in an area in which a contaminant plume must be highly resolved within a large-scale flow and transport domain.

In keeping with its mission as a leading edge computational research code, PFLOTRAN has focused predominantly on computer science issues and performance on HPC machines. As such, it is a tool for performing simulations that cannot be performed by other codes due to problem size limitations. This allows research scientists to use PFLOTRAN as a testbed for developing the most efficient computational strategies for subsurface flow and transport simulations for current and future architectures. However, owing to its status as a research code, less emphasis is placed on elements that are required to place PFLOTRAN as the computational "center of mass" as a repository simulation tool. For example, data management, parameter estimation, sensitivity analysis, decision support, and model setup tools do not appear to be a focus. Furthermore, the QA requirements for a repository process- or PA-modeling code are onerous. Certification of PFLOTRAN for regulatory use would require a significant QA effort.

4.3. Computational Framework Codes

There are a number of commercial and research software tools available that address specific requirements outlined in Section 3.2 for the system analysis workflow, computational capabilities, and configuration management and technical bases functions. These software tools include computational frameworks and general purpose utilities; but none of them include any inherent multi-physics modeling capabilities.

Computational Framework Codes

- *PowerSim* – Powersim Software AS (www.powersim.com)
- *VenSim* – Ventana Systems, Inc. (www.vensim.com)
- *MatLab* – Mathworks, Inc. (www.mathworks.com)
- *SysML* – System Modeling Language (SysML), SysML Partners (www.sysml.org)
- *DeskTop PA* – SNL (Fewell et al. 2000)
- *SALOME* – Commission for Atomic Energy (CEA), EDF Group, and Open Cascade SAS, France (www.salome-platform.org)
- *SIMULIA* - Dassault Systemes, France (www.3ds.com/products/simulia/overview/)

Utility Codes (for uncertainty quantification, sensitivity analysis, optimization, and calibration)

- DAKOTA – Design Analysis toolKit for Optimization and Terascale Applications (Wang et al. 2011, Section 4.4.2; dakota.sandia.gov/)
- PEST – collaborative effort (www.pesthomepage.org/home.php)

Utility Codes (general)

- *Enthought Python Distribution and Tool Suite* – Enthought, Inc. (www.enthought.com)
- *Design Through Analysis Realization (DART) Workbench* – SNL (dta.ran.sandia.gov/)

A few other general purpose utility codes (e.g., Velo Knowledge Management, Trilinos, and SIERRA Toolkit) are incorporated in framework codes described in Section 4.1.

None of the computational framework codes are currently under consideration for further evaluation because they do not appear to offer open-source solutions beyond those already available in the framework codes that also offer some multi-physics capabilities (see Section 4.1). Some of the utility codes may be further evaluated as the need arises for their specific capabilities (e.g., DAKOTA).

5. FUTURE PLANS

The requirements for a PA model framework outlined in Section 3 are quite comprehensive. The acquisition, development, and/or integration of a suite of codes to satisfy all of the requirements would represent a significant advancement in PA modeling capabilities as compared to today's state-of-the-art. It would require a number of years and a multi-million dollar budget. Therefore, the approach to develop an advanced PA model framework capability will necessarily involve a phased implementation, where requirements are prioritized and iteratively re-evaluated as UFD program needs evolve. With proper prioritization of requirements, an integrated code suite can be developed that (a) satisfies a utile subset of the requirements, and (b) is extensible to address evolving needs.

In Section 4, the following three codes were selected for their potential to provide multi-physics modeling and computational capabilities desirable in an advanced PA model framework:

- ASCEM (Section 4.1.1) - Provides multi-physics modeling and computational framework capabilities. The framework supports a range of computational and configuration management functions and includes THC flow and transport capabilities. A representation of the source term multi-physics will need to be added. The source code is expected to become available for evaluation (i.e., be released as open source) in September 2012.

- Albany (Section 4.1.3) - Provides multi-physics modeling and computational framework capabilities. The framework supports a range of computational and configuration management functions and includes preliminary source term and flow and transport capabilities. Representations of the source term and THC flow and transport multi-physics will need to be enhanced. Open source code is currently available.

- PFLOTRAN (Section 4.2.1) – Provides THC flow and transport multi-physics modeling capabilities. A representation of the source term multi-physics will need to be added along with more comprehensive computational framework and configuration management capabilities. Open source code is currently available.

The multi-physics modeling and computational framework capabilities of these three codes will be further evaluated in Fiscal Year (FY) 2013. The evaluation will focus on the existing capabilities and necessary enhancements required to apply each code to solve a UFD-relevant demonstration problem. Specific details of the demonstration problem (e.g., included FEPs and scenarios) will be outlined in early FY2013. However, the demonstration problem is expected to be disposal of UNF and HLW in a salt formation and include, at a minimum, representations of the Source Term, EBS, and Geosphere. The selection of salt disposal system provides for integration with PA modeling being initiated as part of the UFD Salt R&D activity.

The development and application of these three codes to the demonstration problem will facilitate a gap analysis relative to the PA model framework requirements. These requirements include the multi-physics modeling and computational framework requirements in Section 3. Specific details of the demonstration problem may provide clarification of some the multi-

physics modeling requirements. The gap analysis will be conducted against a set of metrics (to be defined in FY2013) designed to provide the following information for each code:

- Ability to address PA model framework requirements
- Code development necessary to address additional necessary requirements
- Ease of code development and expected level of effort and schedule to address requirement gaps

The results of the gap analysis will help to identify which of the three codes (or combination of capabilities from the codes) provides the most favorable path forward for further development of advanced disposal system PA modeling capabilities.

6. SUMMARY

This report describes the planning and initial development of an advanced disposal system PA modeling capability to facilitate the science-based evaluation of disposal system performance for a range of fuel cycle alternatives in a variety of geologic media and generic disposal system concepts. The advanced modeling capability will provide a PA model framework that facilitates PA model development, execution, and evaluation within a formal PA methodology. Desirable attributes of PA model framework, identified in Section 2, include:

- provide the flexibility to examine multiple generic and site-specific geologic disposal options at levels of complexity that are expected to increase as the UFD program matures,
- enable the evaluation of system- and subsystem-level performance,
- enable uncertainty and sensitivity analyses to isolate key subsystem processes and components,
- facilitate the modular integration of representations of subsystem processes and couplings, where the level of complexity of the representation may vary with intended use or relative importance to the total system,
- provide the capability to accommodate new or alternative subsystem process representations, including the use of legacy codes,
- provide data and configuration management functions,
- be developed and distributed in an open source environment,
- leverage existing utilities (e.g., meshing, visualization, matrix solvers, etc.), and
- facilitate implementation across a range of computing environments from laptops to HPC networks, including distributed code execution.

The PA model framework includes two main components: a multi-physics modeling capability (described in Section 2.2) and a computational framework capability (described in Section 2.3). These capabilities are implemented through integrated suites of computer codes. The multi-physics codes provide the conceptual and mathematical representations of the relevant FEPs. The computational framework codes provide the supporting functions to facilitate the numerical integration (coupling) and implementation of the multi-physics, computationally efficient code execution, and analysis and configuration management of results.

The challenge in developing an advanced disposal system PA modeling capability is one of allocating efforts toward these two components. An over-emphasis on computational framework development can result in a very robust framework code with extensive functionality, but may fail to provide adequate capabilities to address the range of multi-physics needed to represent the system being modeled. Conversely, an over-emphasis on the development of specific process modeling capabilities can result in very accurate conceptual and numerical representations of independent subsystem processes, but may fail to provide a mechanism to integrate those subsystem processes into a robust total system model or to integrate the multi-physics within or across subsystems. The initial development of an advanced disposal system PA modeling capability for UFD strives to balance these two efforts; it must provide an adequate range of process models and it must facilitate adequate multi-physics couplings across the entire disposal system.

Specific requirements for a multi-physics modeling capability and for a computational framework capability are outlined in Sections 3.1 and 3.2, respectively. Existing codes with the potential to address the multi-physics modeling and/or computational framework requirements are summarized in Section 4. The existing codes are organized into three groups, based on their primary function: codes that are focused on multi-physics modeling capabilities; codes that are focused on computational framework capabilities; and codes that address both multi-physics and computational framework requirements.

There is no single existing code that addresses all of the requirements. However, the list of requirements is quite comprehensive; a PA modeling capability that satisfies all of the requirements would represent a significant advancement in the state-of-the-art. Therefore, the approach to develop an advanced PA model framework capability will involve (1) an integration of multiple codes and/or code capabilities, rather than a single code, (2) a phased implementation, where requirements are prioritized and iteratively re-evaluated as UFD program needs evolve, and (3) leveraging relevant ongoing open-source code development efforts.

Three existing code development efforts were identified as having the best combination of readily available open-source development, appropriate multi-physics capabilities, and HPC capabilities. Two of these codes, ASCEM (Section 4.1.1) and Albany (Section 4.1.3), are computational framework codes that include multi-physics capabilities. The third code, PFLOTRAN (Section 4.2.1), is a THC multi-physics modeling code that includes some limited computational framework capabilities.

The multi-physics modeling and computational framework capabilities of these three codes will be further evaluated in FY2013. The evaluation will focus on the existing capabilities and necessary enhancements required to apply each code to solve a UFD-relevant demonstration problem. The development and application of these three codes to the demonstration problem will provide a gap analysis relative to the PA model framework requirements. The results of the gap analysis will help to identify which of the three codes (or combination of capabilities from the codes) provides the most favorable path forward for further development of advanced disposal system PA modeling capabilities.

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APPENDIX A: NUMERICAL CONSIDERATIONS FOR MULTI-PHYSICS COUPLING

The level of complexity of the mathematical models describing a specific disposal system may vary based on the representation and discretization of the geometry (e.g., 1D or 3D), representation of key THCMBR processes (ranging from simplified to very detailed), and degree of multi-physics process coupling. Simpler mathematical representations result in a reasonably linear numerical solution that can be easily solved on a desktop PC computing environment. More advanced mathematical representations lead to more complex governing equations that are likely to require advanced solution techniques and/or a HPC environment.

A discussion of multi-physics coupling, the resulting form of the governing equations, and effective solution strategies is presented in SNL (2009, Section 6.2). A summary of the key considerations relevant to the multi-physics coupling and the interface with the solution techniques is presented below.

The mathematical models that represent the FEPs are generally expressed as steady-state or transient partial differential equations (PDEs). These PDE models are discretized on a computational mesh often resulting in square sets of nonlinear equations (in the steady-state case), or sets of ordinary differential equations (ODEs) or differential algebraic equations (DAEs) (in the transient case) (SNL 2009, Section 6.2).

A transient[1] single-physics model is typically represented by a state equation as a function of a set of variables – in implicit ODE or DAE form. Coupled multi-physics models can be represented as either (a) a single state equation that contains the entire coupled set of variables, or (b) a set of single-physics state equations and a corresponding number of coupling equations. The multi-physics coupling required by the ADSM will generally involve the set of state and coupling equations. In the most general case, each of the single-physics models and their sets of variables can be represented on different meshes of the same physical domain or different domains. The coupling equations therefore can embody mesh transfer operations and mathematical equations needed to define the coupling.

The different physics models can vary in a number of important ways in a single physics or multi-physics setting. The different physics models may be strongly coupled or weakly coupled. The different physics models can represent dynamics on radically different type scales. The models may be representable as smooth continuous functions or may have significant discontinuities in the model functions. These and other factors affect how the discretization and the solution of these problems must be approached in order to be able to efficiently and accurately solve the underlying sets of multi-physics equations (SNL 2009, Section 6.2.1).

There are a range of strategies for solving transient multi-physics models, depending of the strength of the coupling (SNL 2009, Section 6.2.1):

[1] The discussion focuses on transient models because issues related to steady-state models are typically a subset of issues related to transient models (SNL 2009, Section 6.2.1).

- If the bi-directional coupling of the models is very weak, it may be possible to fully solve one set of physics over the entire time and space domain and then use the converged solution from the first physics to feed into the solution of the second physics model. This is referred to as "feed forward" coupling and is the easiest type of coupling to implement.

- If the models are weakly coupled or have radically different dynamic time scales and cannot be fully decoupled, it can be advantageous split up the different disparate models and solve them with different solution strategies and only keep the models in sync in less rigorous ways. This is known as the "operator split" approach where for example one set of physics models may be solved with an explicit time integration method and the other physics model may be solved with an implicit time integration scheme where the two models only exchanged updated state infrequently.

- If the models are very strongly coupled, any attempt to decouple them in the basic nonlinear and transient solution methods may result in divergence or in substantial degradation in the performance of the numerical method. In many of these cases, the more efficient approach to integrate the transient equations is to use a fully implicit time integration method. The classic problem with fully implicit methods is that off-the-shelf pre-conditioning approaches and software for solving the linear systems using iterative methods can be very inefficient when dealing with a challenging multi-physics problem. A growing trend in many research groups for addressing these multi-physics problems with fully implicit time integration methods is to use operator split ideas to instead build physics-based pre-conditioners. Such an approach has proven to be very computational efficient and yet very robust for many multi-physics problems.

The coupling equations may involve the transfer of data from one model to another where the models may use different computational meshes and/or may use different basis representations for the same or related qualities. It is desirable to implement these different-discretization couplings such that smoothness of the coupling equations is preserved and basic derivatives can be computed. However, if the coupling equations are not smooth, then it is not be possible to compute efficient and accurate sensitivities, impacting the embedded sensitivity and UQ capabilities. Considerations related to the calculation of forward and adjoint sensitivities, embedded sensitivity computation, and embedded UQ are described in SNL (2009, Sections 6.2.2, 6.2.3.1, and 6.2.3.2).

The strength of the coupling and the solution method selected impact the accuracy of the model results as well as the runtime resources (time and memory) required by the simulation. A computational framework that supports multi-physics coupling should accommodate the range of coupling options and solution strategies, and, ideally, also facilitate embedded sensitivity computations and embedded UQ.

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