

A New Initiative for Developing Advanced Simulation Capabilities for Environmental Management (ASCEM) - 10470

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ABSTRACT

The United States Department of Energy (DOE), Office of Environmental Management (EM), in collaboration with other DOE offices, is leading a multi-institution, multi-disciplinary team of geoscientists, material scientists, and computational scientists from Los Alamos, Lawrence Berkeley, Pacific Northwest, Oak Ridge, and Savannah River National Laboratories to launch a new modeling initiative for Advanced Simulation Capability for Environmental Management (ASCEM). ASCEM is a state-of-the-art scientific tool and approach for understanding and predicting contaminant fate and transport in natural and engineered systems. This modular and open source high performance computing tool will facilitate integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for EM cleanup and closure activities. The ASCEM program is aimed at addressing critical EM program needs to better understand and quantify the subsurface flow and contaminant transport behavior in complex geological systems and the long-term performance of engineered components including cementitious materials in nuclear waste disposal facilities, in order to reduce uncertainties and risks associated with DOE EM's environmental cleanup and closure programs. Building upon national capabilities developed from decades of R&D in subsurface geosciences, modeling and simulation, and environmental remediation, the ASCEM initiative will develop an integrated, high-performance, open-source computer modeling system for multiphase, multicomponent, multiscale subsurface flow and contaminant transport. In addition, the integrated model will incorporate capabilities for predicting releases from various waste forms, identifying exposure pathways and performing dose calculations, and conducting systematic uncertainty quantification. The model will be demonstrated on selected sites and then applied to support the next generation of performance assessments of nuclear waste disposal and decommissioning facilities across the EM complex.

INTRODUCTION

The mission of the U.S. Department of Energy (DOE) Office of Environmental Management (EM) is to complete the safe cleanup of the environmental legacy brought about from the nation's five decades of nuclear weapons development, production, and

nuclear energy research. This work represents some of the most technically challenging and complex cleanup efforts in the world, and requires investment in long-term remediation science and technology development. In response to a congressional request to sustain support for EM R&D funding, EM developed a roadmap that identifies the key engineering and technology gaps [1]. In their review of DOE Cleanup Technology Roadmap, the National Research Council (NRC) of the National Academies provided advice to DOE EM for addressing principal science and technology gaps in the roadmap [2]. Table I shows the principal technology gaps identified by DOE in their groundwater and soil remediation program and their R&D priority ranking by the NRC.

Table I. Principal Science and Technology Gaps and Their R&D Priorities

GS#	Gap	Priority
GS-1	Contaminant behavior in the subsurface is poorly understood.	high
GS-2	Site and contaminant source characteristics may limit the usefulness of baseline subsurface remediation technologies.	medium
GS-3	Long-term performance of trench caps, liners, and reactive barriers cannot be assessed with current knowledge.	medium
GS-4	Long-term ability of cementitious materials to isolate wastes is not demonstrated.	high

To address these gaps, the NRC advised DOE, among taking other measures, to use more sophisticated computational models that better incorporate understanding of site geohydrology and contaminant geochemistry, develop the scientific basis to support delaying remediation activities until there is an adequate knowledge base to proceed with the remediation (for addressing GS-1), and develop robust models of barrier behavior that can incorporate appropriate uncertainty and account for natural and anthropogenic spatial and temporal changes, together with field data to calibrate these models (for addressing GS-4).

Similarly, the need for developing predictive capabilities using high-performance computing technologies to understand contaminant behavior and to support developing and implementing effective and sustainable remediation approaches has also been identified in DOE internal workshops and reviews [3, 4, 5].

In response to the NAS and internal DOE review recommendations, DOE Office of EM has launched the Advanced Simulation Capability for Environmental Management (ASCEM) initiative to address key challenge areas including GS-1 and GS-4. ASCEM is a state-of-the-art scientific tool and approach for understanding and predicting contaminant fate and transport in natural and engineered systems. The modular and open source high performance computing tool will facilitate integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for EM cleanup and closure activities. Specifically, the ASCEM initiative is aimed at addressing these critical EM program needs to better understand and quantify the subsurface flow and contaminant transport behavior in complex geological systems

and the long-term performance of engineered components including cementitious materials in nuclear waste disposal facilities, in order to reduce uncertainties and risks associated with DOE EM's environmental cleanup and closure programs. Building upon national capabilities developed from decades of R&D in subsurface geosciences, modeling and simulation, and environmental remediation, the ASCEM initiative will develop an integrated, high-performance, open-source computer modeling system for multiphase, multicomponent, multiscale subsurface flow and contaminant transport. In addition, the integrated model will incorporate capabilities for predicting releases from various waste forms, identifying exposure pathways and performing dose calculations, and conducting systematic uncertainty quantification. An illustration of the environmental processes that ASCEM will simulate is given in Figure 1. The model will be demonstrated to selected sites and then applied to support the next generation of performance assessments of nuclear waste disposal and decommissioning facilities across the EM complex.

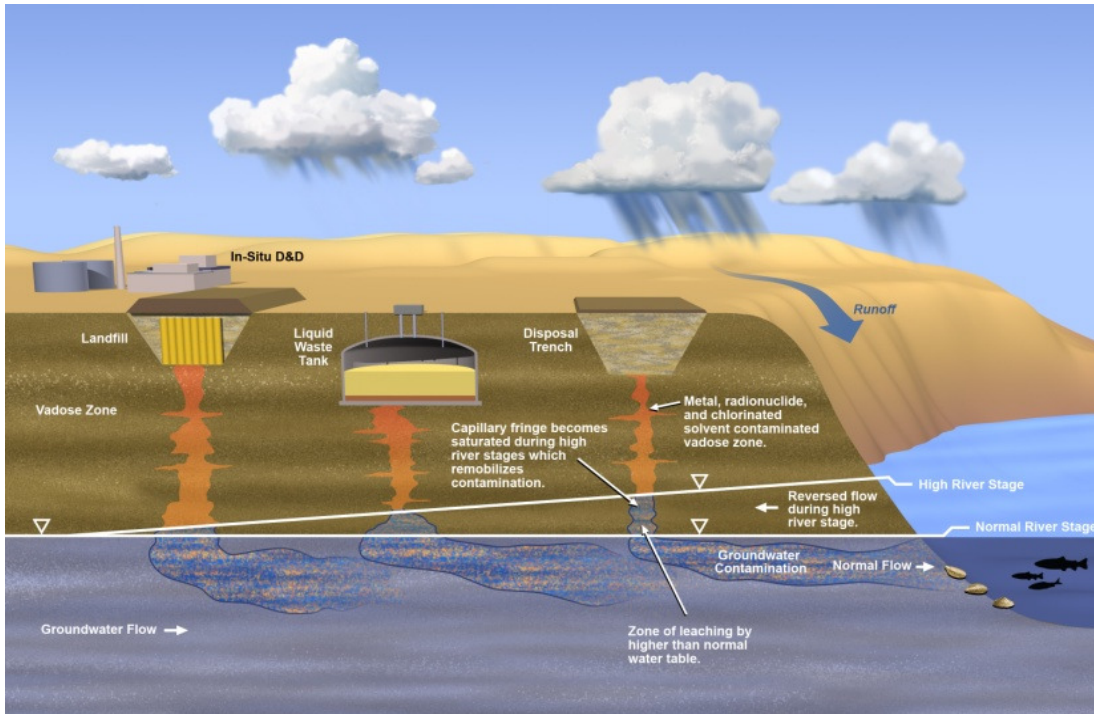


Fig. 1. Typical environmental processes to consider in ASCEM.

The following sections provide a description of the technical approach to developing this integrated model, followed by a more detailed description of ASCEM technical work activities which will be organized into three thrust areas: High Performance Computing (HPC) Simulator for Multi-Process Models, Integrated Platform and Toolsets, and Site Applications (see Figure 2), and by a summary of the preliminary plan for developing and deploying the toolsets in the next 5-10 years.

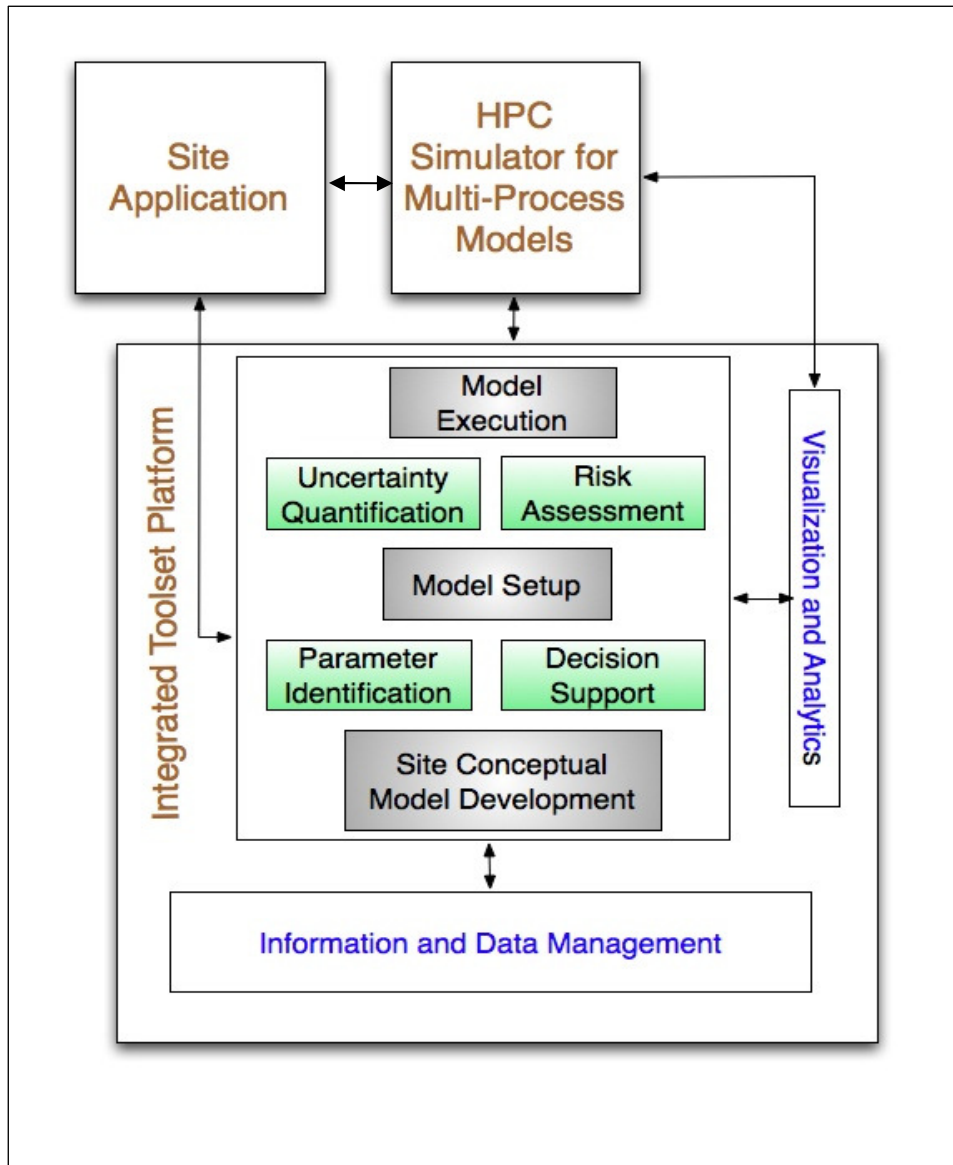


Fig. 2. Technical thrust areas of ASCEM.

GENERAL TECHNICAL APPROACH

The ASCEM computational framework will include a modular, open-source high performance capability for fate and transport modeling and systematic uncertainty analysis. It will be applicable to diverse natural and engineered systems and its modular design will be flexible to accommodate new advances as they become available. The framework will enable the use of disparate, multi-scale, and often sparse information for subsurface property and process parameterization. The platform and its interoperable structure will not require users to have extensive expertise with high performance computing tools and interfaces to utilize the tool. The platform interface will serve as a common, essential, and accessible scientific and engineering capability for Federal project directors and site contractors, allowing them to make transformational changes in

the way that science-based understanding is translated into products effectively used to guide remediation activities. An important goal is to develop a set of modeling and simulation tools that can be used on a wide range of computer platforms ranging from desktop computers to the largest computing facilities available within DOE.

The key idea behind the new HPC Simulator is to adopt a highly modular (or “interoperable”) approach to code development that will facilitate user accessibility and will create a platform that can be easily customized for specific applications by end users with minimal high-performance computational expertise. This can be accomplished through an approach that defines rigorous “interfaces” for each model; the interface defines access to a given module’s data and functionality while hiding the details of module implementation. Strict adherence to this approach allows specific functional components to be modified or added without touching or having to understand the rest of the code system. This will allow various modeling groups with different approaches and applications to join forces in development of a common platform. Also, much of the details of HPC (e.g., gridding methods, numerical solvers, parallel communications) can be implemented in modules by computational science experts and remain generally opaque to application domain scientists. This approach is broadly used in advanced software engineering approaches, for example within the DOE Scientific Discovery through Advanced Computing (SciDAC) program. In concept, various grid methods could be used in the HPC Simulator by simply plugging in different grid components (e.g., structured and unstructured grids, multi-scale grids, adaptive grids) as needed without modifying the remainder of the code. The new computational core will draw on tools and experience gained from the SciDAC program and other related efforts to facilitate broad community participation and utilization.

This computational engine will be developed by a multi-laboratory team, drawing on the various expertise embodied in the multiple existing reactive transport codes. Each applications group will contribute modules that implement the hydrology, geochemistry, geophysics, and/or biology of interest to that group’s application needs, and for which they have top-level expertise. The various application groups will work under the umbrella of the selected computational paradigm and will be fully integrated in teams with computational scientists having the requisite expertise to ensure consistency with system specifications and correct implementation of the best available techniques.

The modular, community-model approach will enable long-term applications of the new modeling system to actual site remediation work, as well as customization to meet future site needs and incorporate scientific developments. The modeling system will be made available to EM site users through the framework developed under the first stage described above. It will also be made available to investigators for use in subsurface research and for addition of modules incorporating new scientific advances.

An important component of the computational framework is developing mechanisms to ensure that the high performance tools will be used to guide DOE EM’s remediation and closure decisions and for performance assessment. Although the proposed architecture will be designed to permit access and use by practicing engineers and scientists in the

field, additional steps are needed to engage site personnel at an early stage in the development of the computational framework. To facilitate this engagement, working groups will be formed that are associated with key DOE EM sites that have significant legacy contamination and associated clean-up costs. Sites that will be the initial focus of the working groups will be focused on the Savannah River, Oak Ridge, and Hanford waste sites. These are a combination of field research sites designated by DOE EM and others being investigated in DOE SC Integrated Field-Research Challenge (IFRC) and Subsurface Focus Area (SFA) studies.

HIGH PERFORMANCE COMPUTING SIMULATOR AND PROCESS MODELS

The tool sets that make up the ASCEM Platform support and streamline the process of creating ensembles of conceptual models to quantify the associated uncertainty, sensitivity, and risk. These conceptual models may span a range of process complexity, potentially coupling hydrological, biogeochemical, and geomechanical processes. The High Performance Computing (HPC) Simulator provides a flexible and extensible computational engine that simulates the coupled processes and flow scenarios described by these conceptual models. It is composed of the HPC Core Framework and the HPC Toolsets. The HPC Core Framework provides the Multiprocess Coordinator (MPC) as well as underlying low-level services, such as parallel I/O and data structures. The HPC Toolsets provide the essential building blocks for the process models, including grids, advanced discretizations, multiscale techniques, and nonlinear/linear equation solvers.

Process Models:

At the highest level of the HPC Simulator design is a set of process models that mathematically represent the physical, chemical, and biological phenomena controlling contaminant release into, and transport in, the subsurface. These include process models for (1) source term behavior, i.e., to predict the performance of residual wastes in closed tanks, cribs, trenches, and landfills and degradation of waste forms and engineered barriers, and (2) subsurface flow and reactive transport, i.e., to predict the flow and reactive transport behavior of contaminants released from the engineered barrier into the vadose zone and groundwater. Based on the assessment of EM site applications and their characteristics, a preliminary list of EM-relevant process models was developed. Evolution of the list of processes is inevitable, and the modular design of the HPC Simulation Framework will accommodate easily the addition of new process implementations.

Source Term Processes - Source terms play a critical role in contaminant migration. We will focus on important source terms at selected sites, while identifying common characteristics of source terms across EM. Some source terms are easily modeled as isolated forcing terms in a model. However, complex source terms are themselves represented by a set of coupled processes (reaction, flow, transport, and geomechanical) to capture the source term accurately. Perhaps the most important of these are cementitious source terms, which involve a special set of coupled processes and thermodynamic, kinetic, and geomechanical parameters. In this case, ASCEM will

leverage source term work in related efforts, such as the EM-sponsored Cementitious Barrier Performance (CBP) project. We will explore weak and strong coupling of these source term models as localized or sub-grid sources in the HPC Simulator.

Infiltration Processes - Infiltration is a driving force for subsurface flow. A range of complexity will be available to represent infiltration processes in the HPC Simulator. The simplest representation is a uniform water flux over a model surface, whereas more mechanistic approaches account for transient precipitation, runoff, thermal- energy balance, weather conditions, plant physiology, soil moisture, and ground slope.

Flow and Transport Processes - Modeling of multiphase flow will be based on a set of conservation equations for individual components (e.g., water, oxygen, volatile organic compounds (VOCs), and other chemical components) tracked across multiple phases, i.e., the aqueous, gaseous, non-aqueous phase liquid (NAPL), and solid phase. The transport processes implemented in the HPC Simulator include advection, hydrodynamic dispersion, molecular diffusion, and electrochemical migration, and are all implemented within a multicomponent framework.

Bio-Geochemical Processes - Transport processes may be coupled to a range of geochemical and microbiological processes of varying complexity. The design of the Platform interface and the HPC Simulator supports user-defined equilibrium and kinetic formulations of both homogeneous and heterogeneous reactions, enabling the simulation of any biogeochemical and even physical processes that can be expressed in the form of reactions. In addition, it may include models for aqueous complexation, dissolution and precipitation, sorption, as well as high ion activity models.

Geomechanical Processes - Geomechanical processes are important in engineered structures and waste forms. For example, the collapse of material associated with alteration of cementitious source terms may strongly affect the local flow field or the source term reactivity (and thus release rate). The geomechanical modeling in the HPC Simulator will focus on these critical scenarios first. We will pursue a full treatment of geomechanical effects, such as the effect of stress on mineral solubilities, if a selected site requires this additional complexity.

HPC Core Framework:

The HPC Core Framework provides a number of low-level services for the HPC Toolsets (the building blocks for the process models). These including data structures, parallel input/output capabilities, application programming interfaces and HPC related visualization support. In addition, it provides a unified hierarchical approach to testing, verification and validation, and benchmarking in order to ensure the reliability and robustness of the HPC Simulator. At the lowest level of the hierarchy, unit tests of individual models are used to verify the correctness of specific sub-modules. At higher levels various integrated tests are designed that span multiple couple processes. Finally, at the highest level, benchmarks are created based on real site applications.

The coupling of multiple processes, including flow, transport, geochemical and geomechanical processes, is both a technical and software engineering challenge. The HPC Core Framework provides a Multiprocess Coordinator (MPC) to face this challenge. In short, the MPC is responsible for coupling the physics and chemistry modules, or different "processes" more generally, for a given spatial and temporal discretization. The MPC will provide user options that will control the level of coupling necessary to preserve accuracy and attain computational efficiency. The MPC reduces complexity of the implementation, and results in more flexible, reliable, reusable software.

HPC Toolsets:

The HPC Toolsets provide the building blocks that transform the mathematical description of the process models into a discrete form suitable for simulation on a computer. The three HPC Toolsets are Meshing, Discretization, and Solvers.

Meshing - The mesh provides an essential and fundamental data structure that bridges the conceptual site model and the numerical methods, and is ultimately the building block that connects the resulting simulation with the computing hardware. ASCEM supports structured meshes that can be fit to the stratigraphy. Fully unstructured meshes to provide for geometric flexibility and adaptive refinement to improve fidelity of evolving features, such as propagating contaminant plumes, are also being explored.

Discretizations - The Discretization Toolset is composed of several modules, including spatial and temporal discretizations, geochemical reactions, and multiscale techniques. The importance of efficient and accurate discretization methods for multiprocess simulations has led to the overarching concept of compatible or mimetic discretizations. This concept provides a practical umbrella for the various methods that are used in existing subsurface flow and reactive transport simulators, while greatly improving their fidelity for complex sites. Geochemical and microbiological processes are localized processes, modeled within a single discretized control volume. The geochemical reaction module will capture these processes and be coupled to flow and transport processes through the Multiprocess Coordinator (MPC). Combining this view of spatial discretizations and localized processes with the traditional method of lines provides a flexible and robust capability for flow and reactive transport. To integrate with the ASCEM platform, additional features such as model gradients for optimization, adjoints for data assimilation, and augmented systems for direct evolution of parameter sensitivities are provided.

Solvers - Nonlinear systems of equations arise throughout Environmental Management applications, from the time evolution of discretizations to optimization and assimilation. The efficiency of nonlinear solvers is intimately connected with the spatial and temporal discretization schemes, the choice of the linear solvers used in the linearization, and in the preconditioners developed to accelerate the linear solvers. Thus, there will be strong coordination between the nonlinear solvers and these other areas. In ASCEM, we leverage established Newton-based nonlinear solvers with multilevel linear solvers, and

use the flexibility of the MPC to design effective preconditioners for tightly coupled processes.

INTEGRATED PLATFORM AND TOOLSETS

Creating models for understanding and predicting contaminant fate and transport in natural and engineered systems is a highly complex task. It requires the collection, management and analysis of large and diverse data sets, and a thorough understanding of modeling and simulation tools. The purpose of the Integrated Toolset Platform is to provide data management and model development and analysis tools that user's can utilize to exploit the advanced simulation capabilities for the solution of environmental management tasks.

Essentially, the platform provides a computational environment that facilitates the complex process of code application to a given site and problem. The Integrated Platform and Toolset will provide a set of tools incorporated into a consistent user interface that permits a modeling approach that is flexible, maintains quality assurance procedures and data integrity, and increases user efficiency. Specific capabilities provided by the platform include toolsets for advanced information and data management, parameter identification, uncertainty quantification, decision support, risk assessment visualization. The platform will be designed to allow seamless interfacing with commercial and open source modeling tools that are in wide use at EM sites. We also anticipate supporting the simulation of site models by existing codes as well as the new HPC simulator that will be produced by ASCEM

Specifically, the capabilities and tools that the ASCEM platform will support include the following:

Site Data Integration and Access: The ASCEM Platform will enable site users to load heterogeneous site data sets and community databases so that the data can be easily search, queried and included in models. The Platform will also integrate with existing site data repositories, improving accessibility by allowing advanced search techniques.

Model Development: The Platform will integrate with commercial and freely available tools that are used to build site models. Additional advanced tools will be provided for tasks such as parameter estimation and import or generation of the computational grid, and the Platform will keep record of how models evolve over time as changes are made to reflect better understanding of site characteristics.

Visualization: The Platform will provide and integrate tools that meet the visual data integration, exploration, and analysis needs of site users. The primary types of visualizations will be for the site conceptual model, input parameter distributions, and simulation results. Additional visualizations will show quantities derived from EM simulation results (e.g., volume of a contaminant plume) and the results of sensitivity analyses or uncertainty quantification.

Data Provenance: The Platform will keep track of how model parameter values are derived and how model inputs relate to simulation outputs. This will allow provenance to be tracked and easily queried so that the basis for a given model and its outputs can be rapidly and accurately assessed.

Simulation: The Platform will enable users to launch simulations either locally on a workstation or remotely on a high-performance computing platform. The Platform will provide tools to simplify launching simulations, monitoring and visualizing the executions, and retrieving, storing and visualizing results.

Uncertainty Quantification: The Platform will implement approaches and provide the tools to quantify conceptual and parametric uncertainties in the ASCEM model predictions. Uncertainty quantification (UQ) of model predictions is critical to regulator decisions and therefore requires a high degree of consistency and defensibility. . HPC capabilities make possible the use of high-fidelity models for UQ without the need for model oversimplification. Given the acknowledged uncertain nature of model predictions, UQ provides a practical basis for framing simulation outputs in terms that are needed for regulatory and site management decisions, risk assessment, and prioritization of ongoing characterization and monitoring efforts.

Decision Support: This toolset will provide the capability to identify and address key uncertainties in model predictions and environmental risk and reduce costs by optimizing the level of modeling complexity as part of the iterative characterization and decision-making approach. Specific tools will support prioritization and optimization of data collection, optimal monitoring program design and optimization of facility design and remediation activities.

Risk Analysis: This integrating component is founded on and provides a synthesis of biokinetic, dosimetry, toxicology and risk experience and expertise available at DOE laboratories. This toolset will provide a comprehensive repository capability for parameters required for risk assessment, access to existing exposure pathway analysis and risk assessment models, and guidance to enhance the integration of ecological and human health risk in the EM decision process. Having an integrated set of risk tools available across the DOE complex will increase the consistency of approach in the decision process. The breadth of risk data and tools available on the ASCEM Platform will enable the flexibility to support all regulatory environments (or other basis for decisions), as well as synthesize the risk assessment with the other primary data and information components in support of more effective data-collection and decision-making processes.

SITE APPLICATIONS

Site application is a critical component for ensuring that the computational capabilities that are developed are relevant and ultimately can be used by DOE-EM. The main focus is to provide site data for model development and testing and a linkage between the computational capabilities and specific DOE-EM sites where cleaning up legacy wastes and managing disposal activities are ongoing. Early tasks involve identifying user needs to support establishing requirements and design of the user platform and computational

capabilities. Criteria will also be established that will form the basis of selecting one or more sites for demonstrations. Because of the need for early engagement with the sites to be paramount to the success of the initiative, working groups will be formed around the selected field sites at an early stage to engage end users, decision-makers, and regulators to test implementation of the platform and its components at selected DOE sites. The working groups will also be used to develop and document application protocols as well as best practices. To ensure an enduring product for EM, plans for long-term maintenance, application support, and training will be developed.

End users will be engaged to document simulation needs across the DOE EM complex and to identify considerations related to efficient implementation of simulation tools in performance assessments and to support site remediation. Experiences at relevant DOE sites will be evaluated and documented with respect to methodologies for performance and risk assessment analyses performed, level of data availability, source-term evaluations, remedial action assessments, regulatory preferences, and risk management issues. Continuing interactions will be maintained with end users at DOE EM sites through groups such as the DOE EM Low-Level Waste Disposal Facility Federal Review Group (LFRG), the EM Performance Assessment Community of Practice (PACoP), and other organizations involved in the conduct and review of risk assessments and performance assessments. This engagement of end users will continue throughout the project to provide continuous feedback regarding the tools being developed. The objective is to collect information that will contribute to efforts to develop requirements documents for the Platform and HPC Thrust Areas and to support identification of demonstration problems to be considered in subsequent tasks in the Site Applications Thrust. Consistent with the nature of tasks in the Platform and HPC Thrust Areas, two levels of information will be obtained:

- 1) Higher-level implementation-related information that will support key tasks in the Platform Thrust (e.g., regulatory and programmatic considerations, implementation of graded and iterative approach, user interface suggestions) and
- 2) More detailed technical information that will support conceptual model and data related tasks in the Platform Thrust and identification of modeling needs for the HPC Thrust (e.g., environmental conditions found at different sites, engineered features being used, data availability, conceptual models and modeling approaches, and specific processes that need to be considered).

Criteria will be established to enable selection of sites for demonstration of the platform and HPC core. Because hydrogeological, geochemical, and microbial conditions at sites play a significant role on contaminant fate and transport, a range of key site conditions will be examined (e.g., humid vs. arid; porous granular vs. fractured rock materials; saturated vs. unsaturated, pH, background and contaminant geochemistry, as well as other site conditions; subsurface contamination vs. waste behavior in tanks). In many cases, availability of such datasets and insights will heavily rely on investments by DOE EM and SC. Based on the established criteria, representative demonstration sites will be selected. As a preliminary step, a number of key DOE sites have been identified that are actively involved in modeling for site remediation and performance assessment.

Hanford – The Hanford Site is representative of a semi-arid Northwestern US climate with groundwater/river interactions at some locations and a relatively thick vadose zone composed of heterogeneous layers of sands and gravels at other locations. Several candidate sites have been identified including 1) the 300 Area Integrated Field Research Challenge (IFRC) Site, and 2) BC Cribs and Trenches in the Central Plateau.

Oak Ridge – The Oak Ridge Reservation is representative of a humid Southeastern US climate with relatively thin surface sediments and saprolite underlain by fractured rock and karst formations with groundwater - surface water interactions. Several candidate sites have been developed including 1) the ORNL IFRC in Bear Creek Valley, and 2) the Oak Ridge Integrated Facilities Disposition Program (IFDP) in Upper East Fork Poplar Creek Watershed.

Savannah River – The Savannah River Site is representative of humid Southeastern US sites with a relatively shallow water table in a mixture of sandy, clayey and silty soils and significant interactions with surface water. Several candidate sites have been identified including 1) the F-Area Seepage Basins, and 2) the T-Area VOC Groundwater Treatment plume.

Los Alamos – Los Alamos is representative of a semi-arid Southwestern US sites with a relatively thick vadose zone in fractured rock that is linked with surface water in canyons. At Los Alamos, chromium Contamination in Technical Area 03 has been selected as the candidate site.

At each of these DOE EM candidate sites, data sets from laboratory and field investigations are available that can be used to test and validate process models and components of ASCEM. Working groups will be formed associated with the selected demonstration sites to engage end users. The working groups will consist of key site technical personnel working with disciplinary environmental subsurface and computer scientists involved in the platform development and testing brought together in collaborative project teams.

As development of the ASCEM Platform and HPC Core proceeds, developers and site practitioners will apply the Platform to selected demonstration problems. Activity will occur throughout the development process, starting with problem specification, assembly and assessment of field and laboratory data currently available at each site, execution of model runs, interpretation of results, and assessment of model performance metrics. Computational analysis of the sites can begin and progress as relevant components of the ASCEM framework (e.g., Conceptual Model toolset, Uncertainty Quantification, reactive transport simulator in the HPC Core) become available for field testing by end users. Comprehensive site analyses will occur as development of the ASCEM framework matures.

Protocols for applications of ASCEM will be developed along with documentation of best practices for risk and performance assessments. Examples include the development of consistent approaches for performance assessment and best practices for site characterization and conceptual model development. The protocols and best practices

will be communicated to the broader DOE EM modeling community through workshops and training sessions. Workshops and training will be conducted at each of the major DOE EM sites across the complex toward the end of the project.

The Platform and HPC Core, and associated data will require periodic maintenance and renewal to remain current with new scientific, engineering, and computational advances, reflect the evolving nature and needs of the EM cleanup program, and incorporate lessons learned and data from DOE's most challenging legacy cleanup sites. A long-term maintenance plan will be developed for continued improvement of computational tools and incorporation of process understanding developed by other components of the DOE EM program as well as DOE SC.

LEVERAGING

To allow the most rapid deployment of ASCEM, the project is leveraging the efforts of other science and computing initiatives to strengthen and enhance the project. The following is a listing of the leveraging efforts and collaborations that are currently underway. All of these efforts will allow the ASCEM team to quickly advance a PA/RA tool for use in EM leveraging the investments that DOE and other Federal and state agencies have made in HPC and environmental modeling.

- 1) One of the most important leveraging efforts is with the DOE Office of Science's Subsurface Environmental System Science Program (SESP). Leveraging efforts with SESP are tied to ongoing research in the areas of modeling and high performance computing, geohydrology, geochemistry, geophysics, microbiology, and remediation. The data rich SFAs and IFRCs are being heavily leveraged to allow testing and demonstration of the ASCEM toolset with high quality data.
- 2) The SciDAC (Scientific Discovery through Advanced Computing) efforts are being leveraged to capitalize on the HPC software infrastructure development, numerical libraries, data management and visualization efforts.
- 3) Since one of the major goals of ASCEM is to produce the next generation of performance and risk assessment tools for DOE EM, the ASCEM team is working closely with the DOE Office of Health, Safety and Security (HSS) to make sure the performance and risk tools being developed are internally consistent with the ongoing regulatory practices being overseen by DOE. In addition, the ASCEM team is working closely with former Yucca Mountain PA specialists to leverage lessons learned and expertise to support the next generation EM PA toolset.
- 4) The Nuclear Energy Advanced Modeling and Simulation (NEAMS) efforts led by the DOE Office of Nuclear Energy in the area of source term and waste form modeling are being leveraged to reduce duplication of efforts between these two DOE efforts.
- 5) Much work has been accomplished over the past ten years on the DOE National Nuclear Security Administration's Accelerated Strategic Computing (ASC) Initiative. The ASCEM project is leveraging existing experience on UQ (uncertainty quantification), V&V (verification and validation), model development, and large-scale simulation. These efforts strengthen ties to research

- efforts on HPC multi core computer architecture, modeling and advanced numerical methods that are being developed at the nations national laboratories.
- 6) Through participations in the Federal Interagency Steering Committee on Multimedia Environmental Models (ISCMEM) and Interstate Technology and Regulatory Council (ITRC), the ASCEM team is collaborating with other Federal and state agencies in i) developing requirements for ASCEM; ii) reviewing of ASCEM workscope, approach, and products; and iii) leveraging of relevant HPC and environmental modeling work that is performed by the other agencies.
 - 7) The ASCEM team is also looking to team with international collaborators on HPC modeling and new programming models for the emerging multicore computer architectures.

PATH FORWARD

The ASCEM project has set aggressive goals to get user buy-in and acceptance from both the EM site users and their regulatory federal and state oversight agencies. To accomplish these goals a detailed plan is being developed by the multi-national laboratory team. First, the ASCEM team will engage EM site users in development of this integrated, open source performance assessment/risk assessment capability with user stake holder input. Year one will entail the development of detailed requirements and design documents and prototyping of capabilities. Then, the first prototype of the platform utilizing enhanced fate and transport HPC modules will be developed and used at a selected field site to demonstrate the new UQ and decision support capability of this tool. This phase will also highlight demonstrations of remote visualization and analysis of these simulations on the integrated toolset platform. In the next phase, Version 1.0 of an integrated, open source simulation capability PA/RA capability will be released and demonstrated at a second field site. Version 1.0 will highlight the HPC flow and reactive transport/geochemistry modules, have an initial prototype of multiscale modeling capabilities for flow processes and be supported by utilization of a selected set of high-priority integration platform components. Training of the end users will begin and continue throughout the remainder of lifecycle of the tools development. Following that, Version 2.0 of platform will be released to limited set of site user groups for demonstration. Version 2.0 of the platform will integrate all existing HPC modules and be benchmarked against a comprehensive set test case at the demonstration sites. Advances in the HPC core will include and initial prototype and demonstration of weakly coupled non-isothermal and geomechanical processes, as well as enhance multiscale modeling capabilities to include geochemical processes. This version of the platform in 2.0 will fully implement platform decision support and risk assessment tools, and integrate user community databases to make them accessible for a broad range of inner site applications. In the final phase of the development, Version 3.0 of the tool will be released that will have full platform and modular HPC with full capabilities. To highlight the tools capabilities, demonstrations of the full UQ capability at two selected sites will be conducted. The training materials for Version 3 will be distributed and end users, the end user support infrastructure will be finalized and training sessions on tool use will be expanded across the EM community.

Once developed, the integrated, general-purpose model may also find wide applications to other subsurface studies such as high-level nuclear waste disposal and carbon sequestration.

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