Advanced Simulation Capability for Environmental Management, Integrated Toolsets and Simulator to Enhance Public Communication – 15186

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ABSTRACT

The U.S. Department of Energy (US DOE) Office of Environmental Management (EM), Office of Soil and Groundwater Remediation, is supporting multi-laboratory development of the Advanced Simulation Capability for Environmental Management (ASCEM). ASCEM is an open source and modular computing framework that incorporates new advances and tools for predicting contaminant fate and transport in natural and engineered systems. ASCEM facilitates transparent, efficient and integrated approaches to modeling and site characterization, and provides robust and standardized assessments of performance and risk for EM cleanup and closure activities. Site subsurface simulation modeling and performance assessments are complex and involve sensitivity evaluations and uncertainty quantification to better understand the risks at a site. The ASCEM toolset was designed in close collaboration with the sites and other potential end-users (both the public and regulators) to allow better communication and understanding of these complex modeling efforts.

ASCEM's integrated toolsets provide a user interface and tools for managing workflows, including conceptual model development, management of data and metadata for model input, sensitivity analysis, model calibration and uncertainty analysis, model execution on diverse computational platforms, and processing of model output, including visualization. The hierarchical and modular design of ASCEM HPC simulator Amanzi easily lends itself to translating this conceptual model of a site into a numerical model that can easily be spatially and temporally discretized to run on the HPC simulator. Together this integrated workflow allows for a seamless and integrated analysis tracking all provenance information and modeling uncertainties.

INTRODUCTION

ASCEM is a state-of-the-art modeling framework with a workflow that seamlessly integrates toolsets to understand and predict contaminant fate and transport in natural and engineered systems. ASCEM is modular and open source software development project that is divided into three thrust areas: Multi-Process High Performance Computing (HPC), Platform and Integrated Toolsets, and Site Applications. ASCEM is designed to 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 toolset is being used to provide technical underpinnings for regulatory analyses at several US DOE sites and a NNSA site and is working toward deployment across the EM complex. In addition, ASCEM is being pursued to address a number of challenges related to modeling in the US DOE complex, for example:

- Move toward more standardized and consistent analyses using an integrated toolset that is open source (i.e., available at no cost to the user community),

- Improve model support for decision-making and demonstrations of regulatory compliance during and at the conclusion of assessment efforts, and
- Provide tools that can present complex information in an easily understandable manner and provide the capability to explore challenging remediation and disposal problems in greater detail.

ASCEM is being developed to not only have an impact on the decision making at the end of a modeling effort, but it will also provide support for decision-making during the modeling process through tools that prioritize data collection and model refinements expected to have the greatest influence on a decision. US DOE National Laboratories are actively contributing to the project, including: Los Alamos National Laboratory, Pacific Northwest National Laboratory, Lawrence Berkeley National Laboratory and Savanna River National Laboratory. This broad participation of scientists and engineers enables ASCEM to benefit from experience gained from related activities conducted in a wide variety of different programs. The ASCEM team recognizes the benefits from a close integration with on-going efforts such as the US DOE-EM Applied Field Research Initiatives (AFRIs) and related projects (i.e., Cementitious Barriers Partnership and Landfills Partnership) for an efficient approach to test the tools and show relevance for different problem sets across the US DOE complex. ASCEM activities are also leveraging advances in other US DOE programs, including the Offices of Science (Basic Energy Research, Advanced Scientific Computing Research), Nuclear Energy (Advanced Modeling and Simulation, Used Fuel Disposition), and Fossil Energy (National Risk Assessment Partnership).

In addition to leveraging previous and on-going development efforts, the ASCEM team has sought to engage end-users in the development process to ensure that user needs are incorporated into the ASCEM program and its user interface. End-user engagement has been a key element of the ASCEM initiative from its inception. Frequent and consistent engagement is seen as critical to developing user acceptance and eventual deployment and application of the ASCEM toolsets at US DOE sites. End-users include performance assessment (PA) and risk assessment practitioners, decision-makers, oversight personnel, and regulators who are engaged in the US DOE cleanup mission. User engagement is implemented in a number of different ways [refer to Seitz WM15 paper]. Direct engagement with the management team is conducted via a User Steering Committee and broader interactions with the user community are implemented through a variety of mechanisms throughout the project. Expanded user involvement working directly with and testing the tools began to be implemented via the Site Applications Thrust in fiscal year 2014. This outreach served as a showcase for the first limited user release (Version 1.0) of the ASCEM integrated toolsets and modeling workflow. Hands-on outreach to introduce the ASCEM tools was conducted at US DOE-EM HQ, PNNL and SRNL.

As part of the development process, ASCEM is being deployed at several sites to test and highlight ASCEM components, engage site end users in the use of the ASCEM tools, and provide feedback to software developers. The overall approach for ASCEM demonstrations consists of testing components and integrated capabilities at an increasing number of US DOE sites and with disparate data sets over time. In 2014/2015, the ASCEM deployments included examples from the deep vadose zone (DVZ) at Hanford, the F-Area Seepage Basins at the Savannah River Site (SRS), and a representative tank closure performance assessment at the Nevada National Security Site (NNSS). This structure of ASCEM's toolset components and capabilities and provides example (case study) results from ongoing deployments in Fiscal Year 2015 (FY15) are highlighted in this paper.

THE ASCEM MODELING WORKFLOW CAPABILITY DEVELOPMENT

ASCEM provides a workflow consisting of a set of pre- and post-processing tools for translating conceptual models to numerical models, and for performing analyses based on model simulations. It is designed to operate on cloud computing such that users have access to high-performance computing resources. Multiple toolsets including model setup, calibration, sensitivity analysis, and uncertainty quantification are available, and other capabilities (such as risk assessment and decision making toolsets) are planned. ASCEM promotes collaborative modeling through file access for multiple users on a shared server.

Significant development of capabilities occurred on both the Platform (Akuna) and simulator (Amanzi) since our program update at WM2014 [1] and [2]. In FY14, a focused effort resulted in release of a research version of the ASCEM and collecting valuable feedback [6].   In addition, ASCEM is being successfully deployed at several sites to technically underpin PA's at Hanford and Savannah River Site [3]. Continued development and capability enhancements are ongoing to support the Nuclear Quality Assurance-1 (NQA-1) Applied Phase level D non-safety software release at the end of FY15.

AKUNA UPDATE

The Platform Thrust Area focused development on new features and streamlined workflows that increased existing capabilities within the toolsets, while maintaining tight integration among the four primary ASCEM components: Akuna, Velo, Agni and Amanzi (see Figure 1). Key features added to the toolsets make ASCEM cloud-based integrated technologies more user-accessible, as well as augmenting capabilities for uncertainty and sensitivity analyses, grid generation, data imports, and visualization. In addition to capability development, user outreach activities were supported at Hanford and Savannah River, increasing the ASCEM user base. User feedback on design and future development was also a critical component of the outreach events. As part of these outreach efforts, tutorials were integrated directly into the Akuna User Interface (UI) and new views were created to make collaborative modeling more accessible.

A critical capability integrated into the Platform toolsets was a server-side job launching capability, which permits end users to launch jobs through the ASCEM server, rather than their client machine, which due to organizational security controls, may block access to super computing resources. Automated proxy configuration was also incorporated into the Platform software to ease local software installation and configuration.

Several prototype capabilities were developed for integration into the first public release of the ASCEM software. These include an efficient visualization tool for Model Setup that enables faster rendering as well as the ability to create new regions through the UI. A VisIt visualization toolset, to be used as a graphical analysis tool for viewing simulation output, was also developed for integration into the first public software release. Gridding capabilities were also enhanced, and included a feature for gridding stacked surfaces. Prototypes for the simulation toolsets were also developed, which included additional algorithms for UQ and SA toolsets, as well as direct linkages to the Database Toolset through the SR, SA, PE and UQ Toolset UIs.

The Platform Thrust Area continued to work with the HPC Thrust Area on integrating Amanzi capabilities into the Akuna UI, such as linear sorption and block-structured adaptive mesh refinement inputs. In addition, the Platform collaborated with HPC to develop a general strategy and use case scenarios for integrating geostatistical methods into ASCEM. Continued integration with HPC was also critical for integration testing, and the development of the automated UI testing.

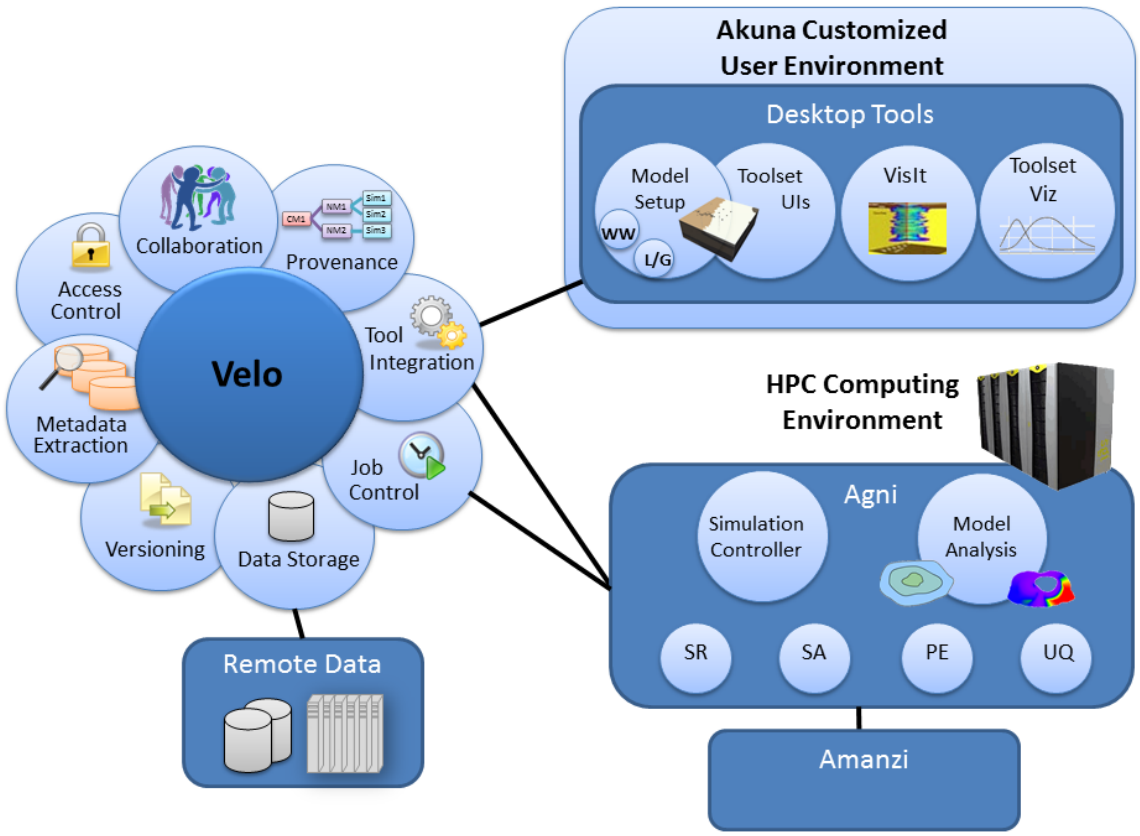

Figure 1. Overview of the four major ASCEM components: Akuna, Velo, Agni and Amanzi.

AMANZI UPDATE

The HPC Thrust balanced development activities for Amanzi across improvements in performance and robustness, advances in quality assurance, and enhancements to capabilities for the outreach sessions and working group collaborations. Enhancements in the XML input specification continued this year, improving the robustness of the Akuani/Amanzi interface and the readability of the Amanzi input files. This collaboration with the Platform developers also included the addition of several capability enhancements, such as the inclusion the block-structured Adaptive Mesh Refinement (AMR) framework, to the Akuna UI and XML writer. In this case, additional mesh and region definitions were added to enable flexible and rapid construction of AMR representations of cylindrical tanks with refined structural features for the Phase 3 Waste Tank demonstration. Improvements in the performance of lower level components of Amanzi were made as well. For example, the use of parallel performance analysis tools led to the development of an internal caching layer for the unstructured mesh interface, and exploration of design changes for emerging architectures led to refactoring the Mimetic Finite Difference discretizations. In contrast, other features of Amanzi were improved or added to support collaborations, including with ASCEM site applications working groups and outreach to the EM International programs. The meshing workflow for unstructured meshes with degenerate cells resulting from layers pinching out with the surface was completed and tested, as was support for prismatic cells. These cells are particularly flexible for gridding stacked surfaces, and are used in the new Savannah River Site F-Area seepage basin models, where the mesh is refined to capture the funnel and gate system. Flexibility of flow boundary conditions was enhanced to allow users to specify a polynomial fit to the water-table surface, which would typically be generated from well data. Finally, output of the flow field was added to support the use of the a particle tracking code to simulate contaminant transport in fractured rock typical of the Pahute Mesa at the Nevada National Security Site. Significant advances in Amanzi's reactive transport capabilities were made this year as well. First, performance of flow-aligned dispersion in an isotropic medium was improved. This unique capability supports the full tensor dispersion associated with non-grid-aligned flows, and was demonstrated on a benchmark test in which a sharp reaction front resides along a curved streamline cutting through several cells. This reactive transport test typically induces grid artifacts in the solution, but is captured cleanly by Amanzi. Second the geochemistry capabilities were enhanced with the initial support for the PFLOTRAN geochemistry engine, through the Alquimia interface library. Now, geochemical conditions (e.g., speciation reactions) defined and named in the PFLOTRAN input file, can be used to define boundary and initial conditions, as well as sources in Amanzi. Also, through work with the PFLOTRAN geochemistry engine, the robustness of our operator-splitting approach to hierarchically sub-cycle transport and reaction was significantly improved. Finally, the interfaces to linear Kd models, which can be defined for each material, and decay through Amanzi's original geochemistry engine were added to the XML input schema in Akuna and its UI.

The team continued to improve the Amanzi User Guide this year and its integration with the Sphinx documentation generation tools. The benefits of this integrated testing and document generation approach was demonstrated by the inclusion of additional verification tests by the NNSS working group in the User Guide, facilitating their addition to the suite of regression tests. In addition, the geochemistry benchmark tests were improved and enhanced to facilitate richer comparisons of unstructured and structured mesh frameworks, and testing of Amanzi with its native and Alquimia/PFLOTRAN engine.

The following capabilities for this release of Amanzi are available through Akuna:

1. Dual structured/unstructured mesh infrastructure:
    - Block-structured AMR meshes with internal generation of meshes on rectangular domains and swept polygonal regions (e.g. cylinders).
    - Unstructured meshes with polyhedral cells (i.e., prism, hexahedral, or more general shapes) and internal generation of hexahedral meshes in rectangular domains.
2. Transient unsaturated flow with Richards equation, and single-phase flow with specific storage/yield, including volume based sources for basins and wells.
3. Reactive Transport implemented through operator splitting:
    - Advection-dispersion transport of chemical species with flow-aligned dispersion tensors in steady state or transient, variably saturated or fully saturated, flow fields.
    - Reactions performed by PFLOTRAN through the Alquimia interface, or with Amanzi’s internal geochemistry engine.
4. Geochemical reactions including, equilibrium aqueous complexation and surface complexation, mineral precipitation–dissolution, and sorption isotherms (Kd, Langmuir, Freundlich).
5. Output flow fields for use in Walkabout particle tracking code.
6. Parallel input/output for visualization, restart, and checkpoints.
7. Flexible and easy to read XML input designed to integrate with Akuna model setup and toolsets.
8. Development in FY15 will enhance these capabilities and improve Amanzi’s quality assurance (QA).

CASE STUDIES OF HOW ASCEM IS DEPLOYED TO TECHNICALLY UNDERPIN PUBLIC AND SCIENTIFIC UNDERSTANDING OF REMEDIAL DECISIONS

Working group efforts were performed in close collaboration with the site contractors, which allowed the ASCEM developers and site contractors to focus on advances needed to meet specific remediation objectives of the site. The approach also allows each working group to build on previously developed capabilities. There are four areas that are the current focus of deployment of ASCEM capabilities:

1. Technical underpinning calculations for the performance assessment update of the Single-Shell Tank Waste Management Area C (WMA-C) Tank Farm
2. Development of an integrated flow-transport-geochemistry model for the Savannah River Site F-Area Seepage Basin to be used for remediation decision making (SRS F-Basin)
3. Technical support to the Waste Tank performance assessment working group at the Savannah River Site H Tank Farm in developing a tank degradation and radionuclide release model (HTF PA)
4. Modeling at the Nevada Nuclear Security Site (NNSS) to bench mark and highlight the uncertainty quantification and parameter estimation (UQ/PE) capabilities of ASCEM using Pahute Mesa pump test data

The suite of ASCEM deployments provides the opportunity to highlight a number of different capabilities and tools in the ASCEM modeling workflow. These deployments of ASCEM will now be reviewed to look at the potential public communication impact of this work, which are highlighted and discussed in greater detail in several WM2015 papers and presentations discussed below.

The focus of the WMA-C performance assessment deployment is to provide technical underpinnings to their current modeling approach. Specifically, ASCEM is being deployed to investigate what impact small-scale heterogeneities in the geologic model may have on past tank leaks and future closure scenarios [3]. The baseline conceptual model to be used for the WMA-C PA is represented by the large-scale stratigraphy at the site. Results of simulations using an ASCEM created heterogeneous conceptual model can be compared to those from the baseline conceptual model used in the PA to fully evaluate the impact that heterogeneities have on long-term transport under rainfall-driven transport conditions.

The SRS F-Basin deployment is an ongoing multi-year effort. Efforts there continue to focus on implementing an integrated reactive flow and transport model in a well-characterized hydrological system with very complex geochemical conditions. This site provides an excellent opportunity to highlight and demonstrate the Amanzi simulator and Akuna toolsets. Complex and heterogeneous datasets available at the site have become a test bed for developing and showcasing the ASCEM visualization and data management capabilities. The advanced simulation and other capabilities, in turn, contribute to the US DOE-EM mission by enabling a systems-based approach that integrates laboratory and field measurements with modeling and decision-support toolsets for long-term management of remediation and monitoring of metals and radionuclides [4]. In particular, the SRS F-Basin working group has been and continues collaborating with the AFRI program for (1) evaluating the impact of engineering barriers on the tritium plume through visualizations and simulations, and (2) supporting the development of cost-effective long-term monitoring strategies based on the prediction of the plume evolution and the predictive understanding of correlations between contaminant concentrations and easily measurable variables (e.g., water table, electrical conductivity).

In the H Tank Farm PA deployment, the ASCEM toolsets are being used to address a longstanding technical concern expressed by the Nuclear Regulatory Commission (NRC). The specific concern is that the HTF PA "does not adequately assess waste release from the submerged and partially submerged tanks via a preferential pathway" (NRC Staff Request for Additional Information (RAI), 31 July 2013). The Nuclear Regulatory Commission is concerned about the possibility of 1) early formation of a preferential flow path due to material degradation and/or separation, as examples, grout shrinkage and steel corrosion, 2) the preferential flow path including residual waste layers in the tank annulus and/or sand/grout pads, and 3) significant advective flow through pathway due to hydraulic gradients in the aquifer/saturated zone. To adequately address this problem a fully coupled flow and transport reactive chemistry 3D model must be developed. The ASCEM integrated toolsets are ideally designed to solve such a problem by incorporating more efficient meshing capabilities, such as Adaptive Mesh Refinement (AMR) and flexible unstructured gridding, and utilizing high-performance computing numerical algorithms and hardware [3].

The ASCEM integrated toolsets are being applied to develop a test case that is relevant to the Underground Test Area (UGTA) at the Nevada Nuclear Security Site (NNSS) (former Nevada Test Site). Three benchmark test cases were run against UGTA-relevant analytical solutions to build confidence in Amanzi for potential UGTA uses. The benchmark problems entailed transient pumping scenarios using heterogeneous systems comprised of zones with contrasting aquifer properties. The Amanzi flow simulation results are benchmarked against analytical solutions and to analogous simulations run with the regulatory approved code for NNSS UGTA program modeling FEHM. The NNSS UGTA program will be choosing a code to model and evaluate the Pahute Mesa CAU closure scenarios in FY16 [5].

The ASCEM site deployments are showcasing the ASCEM Akuna and Amanzi capabilities, educating the site contractors in the deployment of ASCEM into their modeling efforts, and assisting te public and regulators in their ability to ground truth the many simplifying assumptions in the existing risk and performance assessment models.

CONCLUSIONS

The ASCEM project has successfully implemented and is beginning to deploy different capabilities in the Platform and HPC toolsets. The ongoing deployments provide excellent examples of implementation of the ASCEM tools to typical US DOE modeling challenges. These deployments are also demonstrating how the ASCEM tools can be used to address detailed what if scenarios from both the public and regulators and build greater acceptance of the existing conservative PA models. Additional capabilities continue to be added to the tools, and the demonstrations are expected to continue to add complexity as to which capabilities are included in the tools. The first software fully qualified to NQA-1 level D standards will be available for user release in late 2015. Working group activities and interactions will continue with end users and will become the main focus of the Site Applications Thrust starting in 2015. Thus we are beginning to integrate ASCEM into the EM community and gaining broader feedback on needed performance and capability enhancements to make the ASCEM tools broadly applicable across the US DOE-complex. It is hoped that through these interactions, the public will become more informed and accepting of the technical decisions that are being proposed in remedial clean up decisions from the PA models.

The ASCEM capabilities are expected to help EM provide efficient and cost-effective transition to site closure end states with greater public acceptance. Through the working groups and end user engagement, ASCEM will sequentially test and demonstrate capabilities that will enable it to be used to guide US DOE site decision making to develop long-term paths to completing the US DOE cleanup mission.

REFERENCES

1. Freedman VL, X Chen, SA Finsterle, MD Freshley, I Gorton, LJ Gosink, E Keating, C Lansing, WAM Moeglein, CJ Murray, GSH Pau, EA Porter, S Purohit, ML Rockhold, KL Schuchardt, C Sivaramakrishnan, VV Vesselinov, and SR Waichler. 2014. "A high-performance workflow system

for subsurface simulation." *Environmental Modelling & Software* 55:176-189. doi:10.1016/j.envsoft.2014.01.030

2. Freshley, M. D., T. D. Scheibe, D. Moulton, V. L. Freedman, S. S. Hubbard, S. A. Finsterle, C. I. Steefel, H. Wainwright, G. P. Flach, R. Seitz, P. Dixon, and J. Marble, “Advanced Simulation Capability for Environmental Management Initial User Release,” Waste Management Symposia, Phoenix, AZ, March 2-6, 2014.

3. Freshley, M.D., V. Freedman, M. Rockhold, G. Flach, E. Barker, R. Seitz and P. Lee, Enhancing Performance Assessments using the ASCEM toolsets,” Waste Management Symposia, Phoenix, AZ, March 15-19, 2015.

4. Wainwright, H.M., S. Molins, J. Davis, B. Arora, B. Faybishenko, H. Krishnan, S. S. Hubbard, G. Flach, M. Denham, C. Eddy-Dilek, D. Moulton, K. Lipnikov, C. Gable, T. A. Miller and M. Freshley, “Using ASCEM Modeling and Visualization to Inform Stakeholders of Contaminant Plume Evolution and Remediation Efficacy at F-Basin Savannah River, SC,” Waste Management Symposia, Phoenix, AZ, March 15-19, 2015.

5. Dixon, P.R., B. Wilborn, D. Harp, Z. Lu, G. Srinivasan, E. Kwicklis and A. Wolfsberg, “Underground Test Area (UGTA) Activity Collaboration with the Advanced Simulation Capability for Environmental Management (ASCEM) Project – An example of leveraging federal resources,” Waste Management Symposia, Phoenix, AZ, March 15-19, 2015.

6. Seitz, R., P.R. Dixon, J. Marble, P. Lee, and M. D. Freshley, “Integrating Regulatory, Programmatic and Technical Needs for Modeling Tools to Support Decision-Making,” Waste Management Symposia, Phoenix, AZ, March 15-19, 2015.