

CLM-Agni-Akuna Integration Demonstration: A Community Platform for Uncertainty Quantification

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The U.S. Department of Energy (DOE) office of Environmental Management (EM) is investing in development of a numerical modeling toolset called ASCEM (Advanced Simulation Capability for Environmental Management) to support modeling analyses at legacy waste sites. ASCEM is an open source and modular computing framework for predicting contaminant fate and transport in natural and engineered systems. The ASCEM toolset includes a data management and user interface platform (called Akuna) integrated with a simulation controller (called Agni), which work together to develop and execute simulations of subsurface flow and reactive transport using a high-performance computing multi-process simulator (called Amanzi). The Akuna-Agni platform provides the user interface and toolsets for managing workflows, including model development starting with definition of the conceptual model, 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.

Development of the ASCEM toolset has incorporated scientific advances developed by the Subsurface Biogeochemical Research (SBR) program, and SBR program managers and investigators have been actively involved in the ASCEM project since its inception. ASCEM components have been developed using advanced software development methodologies, with an emphasis on modularity, portability and extensibility to maximize utility by a broad user community. Although the ASCEM project is focused on the Amanzi subsurface reactive transport simulator, the Akuna-Agni platform can be customized to link to other simulation tools, facilitating reuse of system components such as data management, visualization, uncertainty quantification, sensitivity analyses, and parameter estimation that are useful to a wide range of earth systems modeling efforts.

This poster describes a collaborative demonstration project undertaken by members of the PNNL and LBNL SBR Scientific Focus Area projects and other key collaborators at those two institutions. We have customized the Akuna-Agni platform to integrate the Community Land Model (CLM) simulator, and are applying this system to several research sites to demonstrate its capabilities. Completed demonstrations include 1) 1D CLM simulations of the NGEE-Arctic site, with sensitivity analysis performed on several soil parameters (e.g., organic content, percent clay and sand), and 2) 1D CLM simulations of the ARM Southern Great Plains (SGP) site, with sensitivity analysis of ten parameters (with results compared to a previous publication using a different method) and application of the parameter estimation toolset. We are also working toward demonstrations of 3D CLM simulations at the NGEE-Arctic and Hanford 300 Area sites.