

DISCLAIMER: This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

AKUNA – INTEGRATED TOOLSETS SUPPORTING ADVANCED SUBSURFACE FLOW AND TRANSPORT SIMULATIONS FOR ENVIRONMENTAL MANAGEMENT

Karen L. Schuchardt^{*}, Deborah A. Agarwal[†], Stefan A. Finsterle[†], Carl W. Gable[§], Ian Gorton^{*}, Luke J. Gosink^{*}, Elizabeth H. Keating[§], Carina S. Lansing^{*}, Joerg Meyer[†], William A.M. Moeglein^{*}, George S.H. Pau[†], Ellen A. Porter^{*}, Sumit Purohit^{*}, Mark L. Rockhold^{*}, Arie Shoshani[†], Chandrika Sivaramakrishnan^{*}

^{*} Pacific Northwest National Laboratory
902 Battelle Blvd, Richland, WA 99352 USA
e-mail: karen.schuchardt@pnnl.gov

[†] Lawrence Berkeley National Laboratory
1 Cyclotron Rd, Berkeley, CA 94720 USA

[§] Los Alamos National Laboratory
30 Bikini Atoll Rd, Los Alamos, NM 87545 94720 USA

Key words: user interface, data management, uncertainty quantification, parameter estimation, visualization, and modeling software

Summary. A next generation open source subsurface simulator and user environment for environmental management is being developed through a collaborative effort across Department of Energy National Laboratories. The flow and transport simulator, Amanzi, will be capable of modeling complex subsurface environments and processes using both unstructured and adaptive meshes at very fine spatial resolutions that require supercomputing-scale resources. The user environment, Akuna, provides users with a range of tools to manage environmental and simulator data sets, create models, manage and share simulation data, and visualize results. Underlying the user interface are core toolsets that provide algorithms for sensitivity analysis, parameter estimation, and uncertainty quantification. Akuna is open-source, cross platform software that is initially being demonstrated on the Hanford BC Cribs remediation site. In this paper, we describe the emerging capabilities of Akuna and illustrate how these are being applied to the BC Cribs site.

1 INTRODUCTION

Remediation and management of legacy wastes associated with DOE sites across the United States

is challenging for many reasons. Many of the sites are geologically complex and sparsely sampled. The nature of the waste streams and their disposal history are also often highly uncertain. Decisions regarding the management and remediation of these sites are therefore typically expensive and fraught with uncertainties. As the custodian of these legacy waste sites, DOE is entrusted with making the best possible decisions about remediation and monitoring activities.

Many of the DOE national labs have developed subsurface flow and transport simulators. Scientists have been trained in their use to support waste site remediation and management decisions. Examples include STOMP [1] PFLOTRAN [2], and TOUGH2 [3]. This multiplicity of simulators fosters competition, broadens capabilities, enables benchmarking, and drives creativity, but it can also lead to inefficient use of resources and lack of standardization in applications. Standardization is necessary to develop effective decision support tools that are broadly applicable to sites across the DOE complex. To this end, the development of a community-based subsurface flow and transport simulation model, Amanzi, and a supporting user environment, Akuna, is intended to provide novel, high-performance simulation capabilities, as well as standardization to applications and decision support.

Akuna is an open-source, platform-independent user environment that includes features for basic model setup, sensitivity analysis, inverse parameter estimation, uncertainty quantification, launching and monitoring simulations, and visualization of both model setup and simulation results. Features of the model setup tool include visualizing wells and lithologic contacts, generating surfaces or loading surfaces produced by other geologic modeling software (e.g., Petrel [4], earthVision [5]), and specifying material properties, initial and boundary conditions, and model output. The model setup tool utilizes LaGrit [6]) for generation of both structured and unstructured model simulation grids. Integrating with WorldWind [7] also allows a user to develop a model based on the initial visualization of their site in its actual geographic context, with displays of surface topography and geomorphic features.

After the model has been set up, Akuna facilitates launching a single forward run, performing formal sensitivity analyses, parameter estimation and uncertainty quantification, and visualization of results. Automated job launching and monitoring capabilities allow a user to submit and monitor simulation runs on high-performance, parallel computers. Visualization of large outputs can be performed without moving the data back to local resources. These capabilities makes high-performance computing accessible to the users who might not be familiar with batch queue systems and usage protocols on different supercomputers and clusters.

The remainder of this paper provides a summary of the modeling workflow necessary to facilitate remediation decisions, describes the Akuna architecture, and provides an example of current Akuna features as applied to the Hanford BC Cribs remediation site.

2 WORKFLOW

Akuna supports a common workflow for developing and applying a numerical model in support of

environmental management. Many elements of this workflow are repeatedly and iteratively performed as part of the modeling process. Figure 1 provides a simplified chart of this workflow. In general, a conceptual understanding of the system to be analyzed is gained from site characterization efforts and monitoring data. This conceptual understanding is then translated into a mathematical model and further implemented in a numerical model, which requires tools to describe the model domain with its salient hydrogeochemical features, associated material properties, initial and boundary conditions, forcing terms, as well as information on how space and time are discretized for numerical solution.

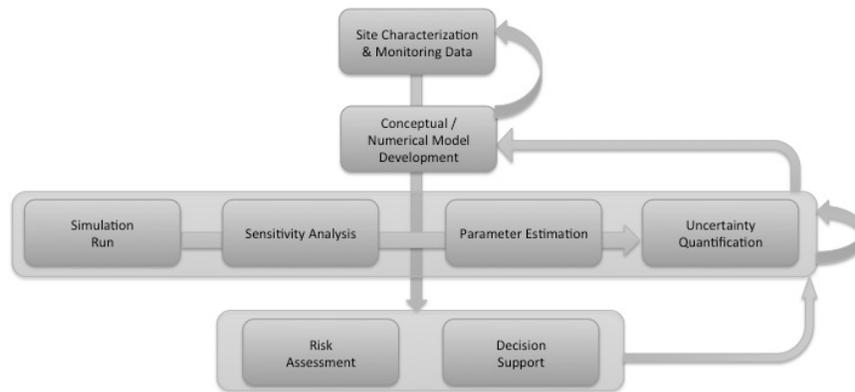


Figure 1: Schematic of analysis workflow and supporting Akuna toolsets

These functions are supported by Akuna’s Model Setup toolset. Once an initial numerical model has been developed, Akuna’s Simulation Run (SR) toolset can be used to launch and monitor a single simulation, the results of which can be analyzed and visualized. If this initial run is considered reasonable, a formal local or global sensitivity analyses can be performed (using Akuna’s Sensitivity Analysis (SA) toolset) to identify the parameters that most strongly influence the system behavior, and to examine output variables that are sensitive to (and – if measured in the field - contain information about) the parameters of interest. These parameters may include material properties, but also initial and boundary conditions, and generally any aspect of the conceptual model that can be suitably parameterized. If measurements of sufficient sensitivity and accuracy are available, the model can be automatically calibrated using Akuna’s Parameter Estimation (PE) toolset. This step not only provides effective parameter values that can be considered consistent with the data collected at the site; it also provides estimates of the uncertainty with which these parameters were determined. The latter can be used (along with other information) in Akuna’s Uncertainty Quantification (UQ) toolset to evaluate the uncertainty of model predictions and provide the basis for a subsequent assessment of environmental and health risks in Akuna’s Risk Assessment (RA) toolset. Finally, the information from these model analyses enter Akuna’s Decision Support (DS) toolset, which evaluates and optimizes performance measures that help manage DOE’s legacy sites.

In practical applications, the workflow is not as linear as described above. The toolsets integrated in Akuna are transparent and can be flexibly invoked to accommodate any application’s particular workflow.

3 ARCHITECTURE

There are several major components that comprise the Akuna architecture as shown in Figure 2. Each of these is briefly described in this section.

Akuna Desktop User Interface (UI): The Akuna UI provides a front end to the simulation workflow. The cross-platform UI is written in Java and is built on the Velo [8] knowledge management framework. The UI includes a data browser that provides access to all data, metadata, provenance, and tools associated with the workflow. Visit has been integrated to support remote visualization of large-scale outputs. A robust open-source content management system is used to manage workflow data and metadata [9]. Shared as well as private workspaces are supported to enable collaborative modeling.

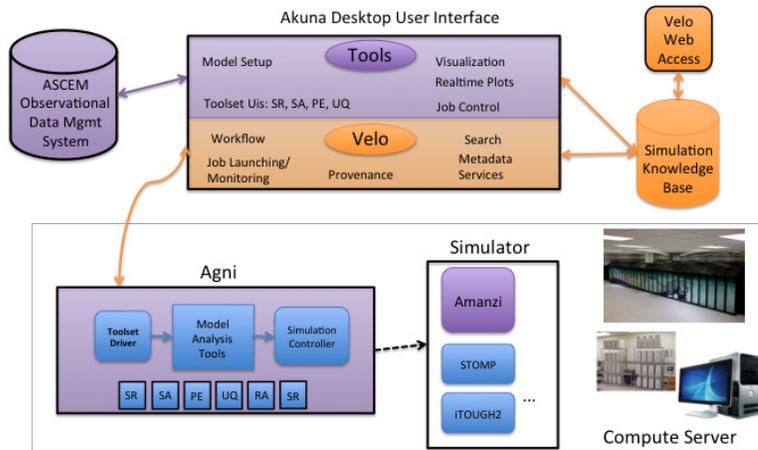


Figure 2: Akuna Architecture

Agni: Agni is software located on the compute server that takes modeling requests from the Akuna client, executes them and reports information back to the UI. Agni includes a component for controlling local execution of the simulator as well as the analysis toolsets for sensitivity analysis, uncertainty quantification, and parameter estimation. In the future, tools for risk assessment and decision support will be added.

Simulator: Amanzi is the main simulator supported by the Akuna platform. Akuna and Agni are however designed to accommodate other simulators that can be plugged in using a set of defined interfaces.

ASCEM Observational Data Management System: The ASCEM Observational Data Management System (AODMS) provides data management capabilities to import, organize, retrieve, and search across various types of observational datasets needed for environmental site characterization and

numerical modeling. The AODMS framework provides capabilities to organize, interactively browse on maps, search by filters, select desired data, plot graphs, and save selected data for subsequent use in the modeling process. Further description of this capability is beyond the scope of this paper, but readers are encouraged to view the AODMS site at <http://babe.lbl.gov/ascem/maps/SRDataBrowser.php>.

4 ILLUSTRATIVE EXAMPLE USING HANFORD BC-CRIBS

4.1 BC Cribs Description

The BC Cribs, located at the Hanford Site in southeastern Washington State, is serving as a driving use-case for the initial version of the Akuna platform and Amanzi simulator. The BC Cribs Area includes 6 relatively small cribs, which received waste from recovery processes from 1956 to 1958. Conceptual model uncertainties are largely attributed to two factors: site heterogeneity, and a lack of site characterization data. In this section, we will show how Akuna is being applied to the BC Cribs modeling effort. Due to space limitations, we will emphasize conceptual model definition and only briefly describe the toolsets and job management.

4.2 Conceptual / Numerical Model Development

Conceptual and numerical model development involves integrating numerous sub-tasks that focus on importing, creating, defining, and assigning definitions and properties to aspects of the model domain. Each task, therefore, cumulatively helps to build a well-defined domain that will eventually be used in numerical simulation. To support this process, Akuna's system divides these sub-tasks into a sequence of steps:

- Import and instantiate base domain definitions from site data;
- Define spatial attributes for the domain (e.g. volumes and surfaces);
- Define and assign property attributes (unique materials, solutes, fluids, initial and boundary conditions, sources, and sinks) to spatial regions;
- Specify a numerical grid that will be used for numerical simulation; and
- Specify output locations for observations, monitoring, and visualization.

Working through these steps can be a straightforward process for simple models. However, more complicated designs may require several iterations to guarantee a model's design is correct. To help with this refinement, Akuna's model setup tool supports navigating these steps through an intuitive process tree. This tree allows the user to freely make changes to the domain's various spatial and property attributes at any time and see the results instantly updated in the visualization window. Additionally, as modelers complete tasks, these sub-stages are highlighted in the process tree.

Defining a Geologic Model The first step in defining a geological model is to initiate a base-definition for the domain. Akuna currently supports two general ways to perform this task: define a

simple layered system through the UI or import an existing data source (domains may be either two or three-dimensional). In the simple layered-system setup, the domain is created through a set of user-defined surface layers and bounding box. This case is illustrated in Figure 3 (left). In the latter case, data sources will either describe an initial geologic domain (e.g. through surfaces, regions, or a zonation mesh), or contain a collage of well data that record the depths of specific subsurface layers from which surfaces can then be generated.

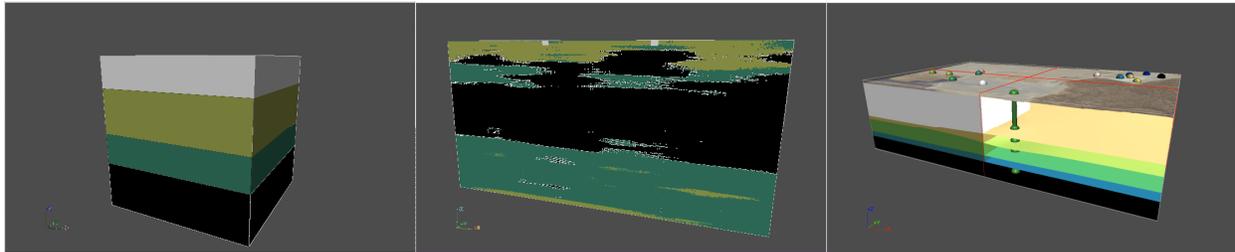


Figure 3: Three paths for defining the conceptual model: (left) manually defined layered model, (center) import geostatistical data, and (right) import well top data.

When importing existing data, modelers have two options for creating an initial domain. First, modelers can utilize data generated from external software that defines an initial geological model. In the BC Cribs example, geostatistical tools were used to generate a model based on three lithofacies. In loading this file, the initial domain can be seen in Figure 3 (center) using Akuna’s visualization viewer. A range of file formats are supported. A second option for importing data allows modelers to utilize existing well data contained in a well-tops file. This file, which is based on a simple spreadsheet (CSV) format, allows modelers to first load and observe their well data before selecting a set of the data to use for generating a geologic domain (see 4). Once this data has been selected, the user can import this data into the main viewer as shown in Figure 3 (right).

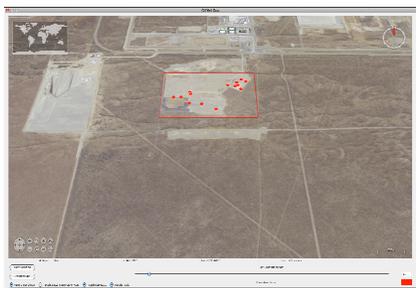
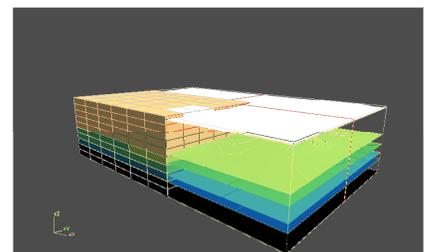


Figure 4: Visualizing well data and selecting the domain with geologic reference.

Defining Spatial and Property Attributes The next task for model development is to define the necessary material, solute, and fluid properties and assign these attributes to the appropriate spatial locations (e.g. regions, initial and boundary conditions, sinks, sources). Akuna facilitates these assignments easily through a simple collection of assignment tabs that lets modelers easily create and match properties to specific spatial locations.

Define Numerical Grid A final step in creating the model is to define the numerical grid that will be used to run the simulation. In Akuna, this task is straight forward as modelers can choose from a variety of grid types: uniform, irregular, and adaptively meshed.



: Conceptual model showing block mesh.

As with all of the user interface components, the changes made to the domain are readily updated in the visualization window as shown in 5.

4.3 Toolsets

Once the conceptual model has been defined and mapped to a numerical mesh, the Akuna toolsets can be used to run forward simulations, estimate parameters, perform sensitivity analysis and uncertainty quantification. The toolsets can be run in any order and are designed to make it easy to re-use options from previously defined toolset configurations. Each of the toolsets includes a common panels to override model parameters, define simulation observations, and set execution control parameters. In addition, each may have an analysis panel for specifying algorithms and associated inputs for sensitivity analysis, parameter estimation (PE), or uncertainty quantification respectively. In the case of PE, measured data must also be assigned. Once the simulations for the toolsets are complete, they can easily be run on any computer through a job launching and monitoring UI. Real-time, and post-run analysis capabilities are also available. These capabilities are shown in Figure 6.

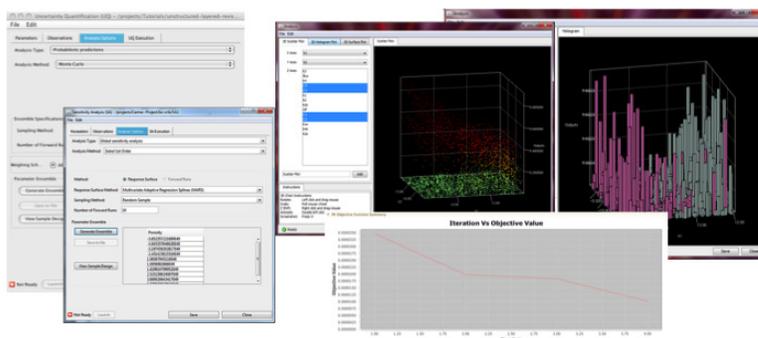


Figure 6: Collage of toolset UIs and output analysis.

5 CONCLUSIONS

Akuna provides an integrated set of tools that will support the full workflow of subsurface flow and transport modeling. It is open-source, cross-platform, and designed to support multiple simulators. It has numerous capabilities that support seamless exploitation of supercomputing resources and yet runs on the user's desktop. A robust content store provides complete tracking of the workflow and supports collaborative modeling. The first release of Akuna is expected in late 2012 upon completion of testing against both the Hanford and Savannah River remediation sites.

6 ACKNOWLEDGEMENTS

This work was funded by the DOE EM-32 Office of Technology Innovation and Development under Contract No. DE-AC05-76RL01830.

REFERENCES

- [1] White M.D., and M. Oostrom. 2006. *STOMP - Subsurface Transport Over Multiple Phases, Version 4.0, User's Guide*. Rep. PNNL-15782, Pac. Northwest Natl. Lab., Richland, WA.
- [2] Hammond G.E., and P.C. Lichtner. 2010. *Field-scale model for the natural attenuation of uranium at the Hanford 300 Area using high-performance computing*. Water Resoures. Res. 46, W09527, doi:10.1029/2009WR008819.
- [3] Pruess, K., C. Oldenburg, and G. Moridis, *TOUGH2 User's Guide, Version 2.0*, Report LBNL-43134, Lawrence Berkeley National Laboratory, Berkeley, Calif., 1999.
- [4] <http://www.slb.com/services/software/geo/petrel.aspx>, February 2012.
- [5] <http://www.dgi.com/earthvision/evmain.html>, February 2012.
- [6] <https://lagrit.lanl.gov/>, February 2012.
- [7] <http://worldwind.arc.nasa.gov/> February 2012.
- [8] I. Gorton, C. Sivaramakrishnan, G. Black, S. White, S. Purohit, M. Madison, K. Schuchardt, Y. Liu, C. Lansing, "Velo: A Knowledge Management Framework for Modeling and Simulation," *Computing in Science and Engineering*, 21 Nov. 2011. IEEE Computer Society Digital Library. IEEE Computer Society.