Akuna: An Open Source and High-Performance Workflow System for Simulation

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Akuna

- Pre- and post-processing toolsets, job launching and monitoring
- Promotes collaborative modeling as users access files on shared server
- Job launching through the server makes for easy access to high-performance computing resources
  - Environmental Molecular Sciences Laboratory (EMSL) user access
- Open source, platform independent user environment written in Java
- Simulator agnostic
  - Amanzi
  - STOMP/eSTOMP
  - GEOSIM
Why Use Akuna?

• User interface for integrating conceptual site model
• Communication enhancement of model configuration and results
• Workflow streamlining
  ▪ Model setup, grid generation, conceptual model viewing, multiple simulation staging
  ▪ Ease of access to high performance computation
    ✓ Simulation controller(s) performs all job launching and reports run completion back to UI (Agni [Pau 2015] and MADS [Vessillnov et al. 2012])
  ▪ Ease of setting up geochemical reactive transport simulations
  ▪ Management of simulation and data provenance
• Linkange of multiple codes, where outputs from one code serve as inputs to the next code
Getting Started

Advanced Simulation Capability for Environmental Management (ASCEM) is a state-of-the-art approach that uses integrated toolsets for understanding and predicting contaminant fate and transport in natural and engineered systems. The Akuna platform is a powerful and flexible environment for modeling, simulation and analysis that enables users to easily:

- Setup conceptual and numerical models
- Execute simulations on laptops or supercomputers
- Visualize and analyze simulation results
- Full lifecycle data management, from site data to modeling results

Getting Started

- Take a Tutorial
- Browse My Projects
- Create a Team
- Report a Problem
- Get More Information on Akuna
My Workspace
Model Setup Toolset
Geochemistry Interface
Simulation Toolsets

- Single-Run (SR)
- Sensitivity Analysis (SA)
  - Local Method
  - Morris-One-At-a-Time (MOAT)
- Parameter Estimation (PE)
- Uncertainty Quantification (UQ)
  - Monte Carlo
  - Markov Chain Monte Carlo
UQ Toolset – Parameter Selection

Parameter Selection Interface:
- Analysis Specifications
  - Analysis method: Monte Carlo
  - Parameter(s) 1: perm1
    - Prior value: 1.9876E-13 m²
    - Initial value: 1.9E-13
    - Type: Logarithm
    - Distribution: Normal
  - Parameter(s) 2: perm2
    - Prior value: 6.9365E-12 m²
    - Initial value: 6.9E-12
    - Type: Logarithm
    - Distribution: Normal
  - Parameter(s) 3: perm3
    - Prior value: 2.0706E-10 m²
    - Initial value: 1.9E-10
    - Type: Logarithm
    - Distribution: Normal

Summary:
- Geo-logic Domain
- Domains
- Mesh
- Specify Uniform
- Number of blocks
- Block size
- Transport Schemes Patankar
- Reactions
- Solve Tc-99
- Initial Conditions
- Initial Saturation Aqueous Pressure - G

Status:
If you select any reference node variables, you must also specify the regions.
Analysis – Akuna Plotting Toolset

• Quick 2D plots of multiple simulations
  ▪ JFreeChart
  ▪ Line plots, histograms, scatter plots
  ▪ Parameters, simulated and measured data
Visualization Access

- Option available for downloading plot files to local machine
- Selection of visualization software
  - VisIt
  - Paraview
  - Tecplot
GEOSIM
Model Linkages (GEOSIM + eSTOMP)

• Describes channel belts of abandoned braided rivers [Scheibe and Freyberg (1995), Ramanathan et al. (2010) and Guin et al. (2010)]

• Described in terms of
  ▪ Shapes of discrete bed forms
  ▪ Trends in grain size
  ▪ Spatial relationships of defined geologic facies

• Geologically realistic distributions of heterogeneity
  ▪ Size of model domain and spatial resolution of heterogeneous features are controlled by user
  ▪ Useful as numerical testbeds to evaluate the potential impacts of multiscale heterogeneity on subsurface flow and reactive transport
GEOSIM

• Compound Bar Generation
  ▪ Serial determination of number of compound bars
  ▪ Creates locations of compound bars and cross-bar channel fills

• Unit Bar and Cross Strata Generation
  ▪ Generates hierarchical stratigraphic units within each compound bar
  ▪ Execution is embarrassingly parallel

• Domain construction
  ▪ Integrates individual compound bars and subunits into cohesive domain using domain decomposition
  ▪ User specifies domain boundary and voxel size
  ▪ Each voxel is assigned an indicator based on location and textural class

• Post-processors
  ▪ Ind2vtk
    ✓ Processes output for visualization 28 “material types”
  ▪ ind2STOMP
    ✓ Translates Ind2vtk output to textural classes for eSTOMP/STOMP

5 realizations resulting from the same GEOSIM input
Compound Bars
Unit Bars
Cross-Stratified Deposits
Indicator Mapping
Job Control Panel
Results Visualization
GEOSIM Transition to eSTOMP
Heterogeneity Example Simulation

- Import files into eSTOMP model setup
  - Auto-generation of materials file and grid description
Simulation Description

• Fully saturated
• Groundwater flow is from west to east
• Homogenous property distributions for like-textural classes
• Conservative tracer applied as a 100-day boundary condition (concentration 10 molar) in the upper central region of the western boundary
• 3000 days of simulation

Region definition visualization using Akuna Model Setup Visualization Tool
Tracer Transport

Time = 5 day
Summary

- Akuna is open-source, cross-platform, and designed to support multiple simulators
- Akuna framework provides complete tracking of workflow for subsurface flow and transport simulation
- Supports seamless exploitation of supercomputing resources
- Web page: akuna.labworks.org


