Amanzi: An Open-Source Multi-process Simulator for Environmental Applications

ASCEM

Environmental Management — safety ❖ performance ❖ cleanup ❖ closure

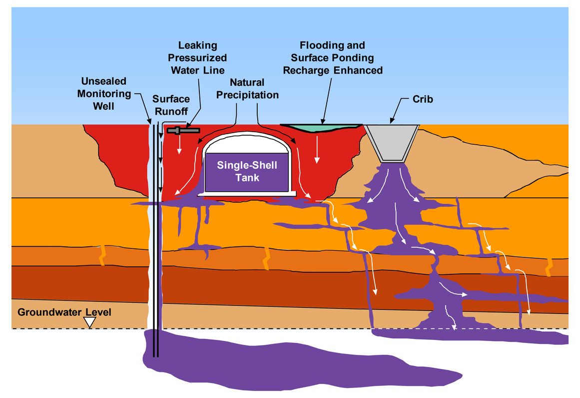
J. D. Moulton[1], S. Molins[2], J. Johnson[2], E. Coon[1], K. Lipnikov[1], M. Day[2], E. Barker[3]

[1] Los Alamos National Laboratory [2] Lawerence Berkeley National Laboratory [3] Pacific Northwest National Laboratory

Contact: David Moulton (moulton@lanl.gov)

1. Advanced Simulation Capability for Environmental Management (ASCEM)

The Office of Environmental Management (EM) is responsible for the cleanup and closure of legacy nuclear waste sites across the Department of Energy (DOE). To meet this challenge the Advanced Simulation Capability for Environmental Management (ASCEM) program is developing an integrated suite of open-source tools that will enable a graded and iterative approach to risk and performance assessments at these waste sites.



ASCEM activities are supported by three thrusts:

- *Platform and Integrated Toolsets* develops **Akuna**, the UI and supporting workflow tools.
- *The Multi-Process HPC Simulator* develops **Amanzi**, the flow and reactive transport simulator.
- *Site Applications* develops the phased demonstrations at the sites, and works with potential site users.

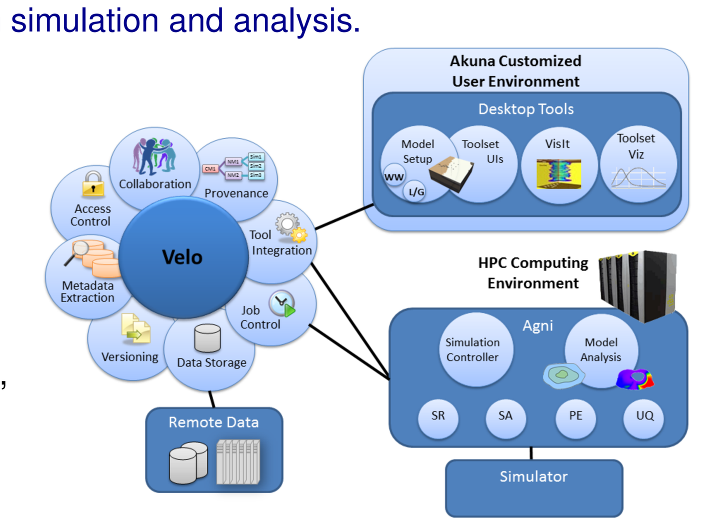
Additional information and documentation is available at http://ascemdoe.org.

Akuna: The Platform and Integrated Toolsets

Akuna is an open-source Java-based user environment that supports a complete modeling workflow, from model setup through simulation and analysis.

Current capabilities include,

- basic model setup,
- sensitivity analysis,
- parameter estimation,
- uncertainty quantification,
- simulation launching and monitoring,
- visualization of setup and simulation results.

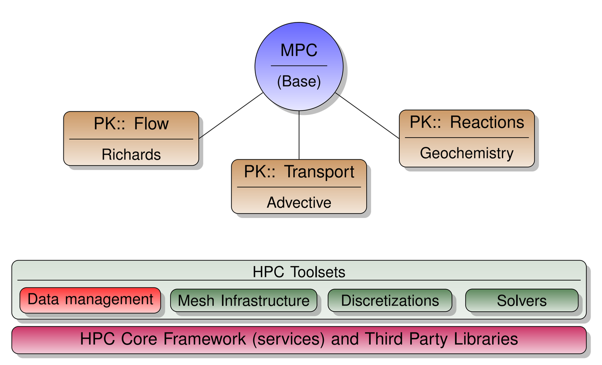


Amanzi: The Multi-Process HPC Simulator

Amanzi uses a hierarchical and modular design that reflects the steps in mapping a conceptual model to a numerical model and producing output for analysis.

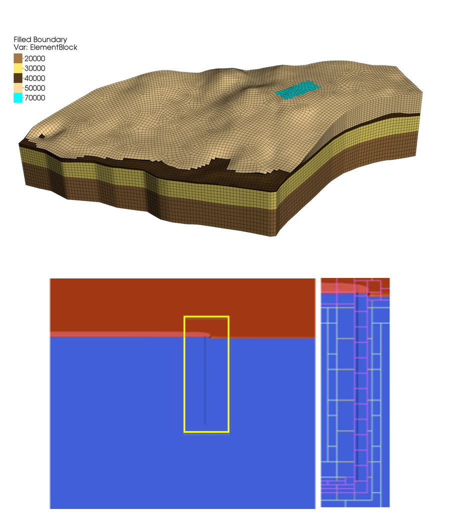
Current capabilities include,

- transient unsaturated flow (Richards) and single-phase flow (specific storage/yield),
- unstructured meshes with polyhedral cells,
- volume based sources (e.g., wells),
- reactive-Transport, with operator splitting,
- dispersion with non-grid aligned flow,
- a wide range of chemical reactions.



Leveraging Advances from across DOE and Academia

Akuna and Amanzi leverage a wide variety of algorithms, capabilities and open-source technologies developed across DOE, as well as the academic community.



Unique unstructured/structured AMR mesh capability leverages,

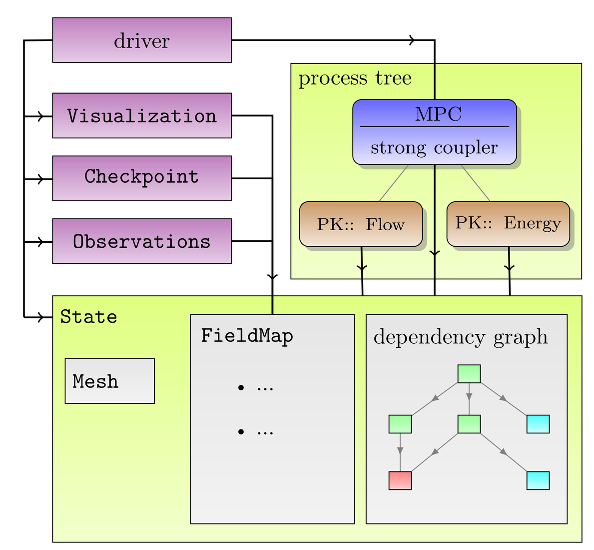
- general unstructured mesh frameworks (MSTK)
- structured AMR techniques and libraries (BoxLib)
- the Trilinos framework and supporting tools/solvers.
- advances in Mimetic Finite Difference (MFD) methods to support
  - complex geometries (e.g., pinch outs)
  - anisotropic coefficients on unstructured grids.

2. Arcos: A Flexible Framework Prototype

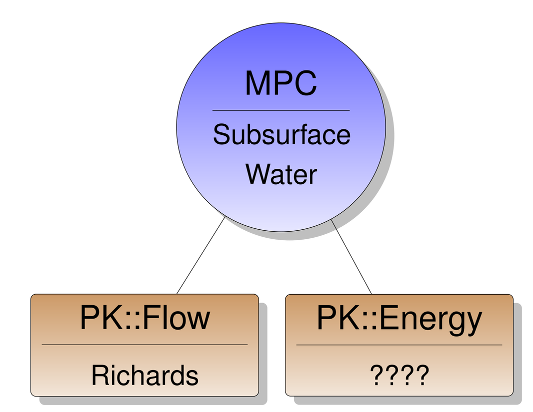
The increasing interest in the more complex models of remediation activities, a growing interest in climate impacts on terrestrial ecosystems, has created a need for lightweight frameworks that enable a flexbile hierarchical view of the model and its processes.

To support this flexible hierarchy of processes in the *Arctic Terrestrial Simulator (ATS)* we leveraged elements of the Amanzi Framework, and developed critical infrastructure, including dynamic data management and an abstract model representation as a direct acyclic graph (DAG). To demonstrate the flexibility of this hierarchical view consider three alternative models for the thermal energy.

A schematic showing the Arcos framework, which was developed for the Arctic Terrestrial Simulator (ATS) and is being prototyped in Amanzi in Amanzi (unstructured).



where ϕ is the porosity, ρ is the density as a function of pressure p and temperature T, s is the saturation as a function of pressure, and $|e|$ is the volume of cell e.



Flow:

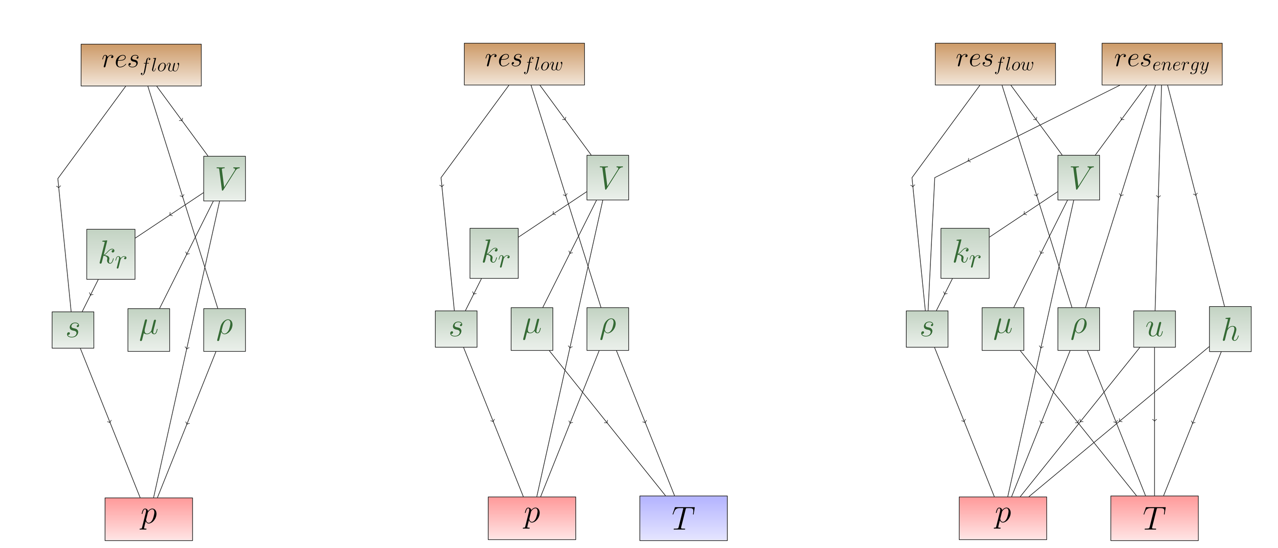
$$\frac{\partial}{\partial t}\left[\phi(\rho_l s + \rho_g(1-s)\right] = -\nabla\cdot(\rho \mathbf{V})$$

$$\mathbf{V} = -k(s)\frac{\mathcal{K}(\mathbf{x})}{\mu}\nabla p$$

Energy: ??

Constitutive Relations: ??

Both the coupling hierarchy (above-left) and dependency graphs (below) are formed and evaluated dynamically, enabling swappable physics.



energy not used — $s(p),\quad \mu,\quad \rho(p)$

prescribed temperature — $s(p),\quad \mu(T),\quad \rho(p,T)$

conservation of energy — $s(p), \mu(T), \rho(p,T), u(p,T), h(p,T)$

3. Alquimia

4. Amanzi XML Input Specification and Documentation

Amanzi input files use a custom XML schema that enables users to express complex models at a high level using a consitent well organized structure. A user or creates these files by hand, or through the Akuna UI, and the XML schema provides syntax checking of element structure and type, as well as some information about attributes. Major sections of the input file include

- ***Definitions*** (named times, constant, and macros)
- ***Execution Control*** - time evolution (e.g., distinct forcings and steady-state initalization)
- ***Numerical Controls*** - specialized parameters related to numerical algorithms
- ***Regions*** - subdomains of the mesh (e.g., box, point, logical polygon)
  - Amanzi-U supports regions defined as mesh blocks, face sets (for boundary conditions) or element sets (usually for wells) in the Exodus II mesh format.
  - Amanzi-S supports more grid generation options (e.g., swept polygon to generate cylinders enabling AMR).
- ***Geochemistry*** - Alquimia configuration and specifiation of the Geochemistry Engine (Amanzi, PFLOTRAN, or (coming soon) CrunchFlow.
- ***Process Kernels*** - active process kernels and their coupling
- ***Materials*** - material properties for all regions, and all PKs.
- ***Initial Conditions, Boundary Conditions, Source Terms*** - for all PKs, define conditions uses regions, material properties, etc.
- ***Output*** - Includes observations as well as parallel output for visualization

An example of a simple box region, named *Well* follows,

```
<regions>
  <box name="Well" low_coordinates="-2.0,-2.0,0.0"
                   high_coordinates="2.0,2.0,10.0"/>
</regions>
```

Logical operations with regions (e.g., union) make it possible to create complex with minimal effort. Then the source can use this region to define its spatial location. Here the source also prescribes a start time, with not end time (implying it will be on for the entire simulation)

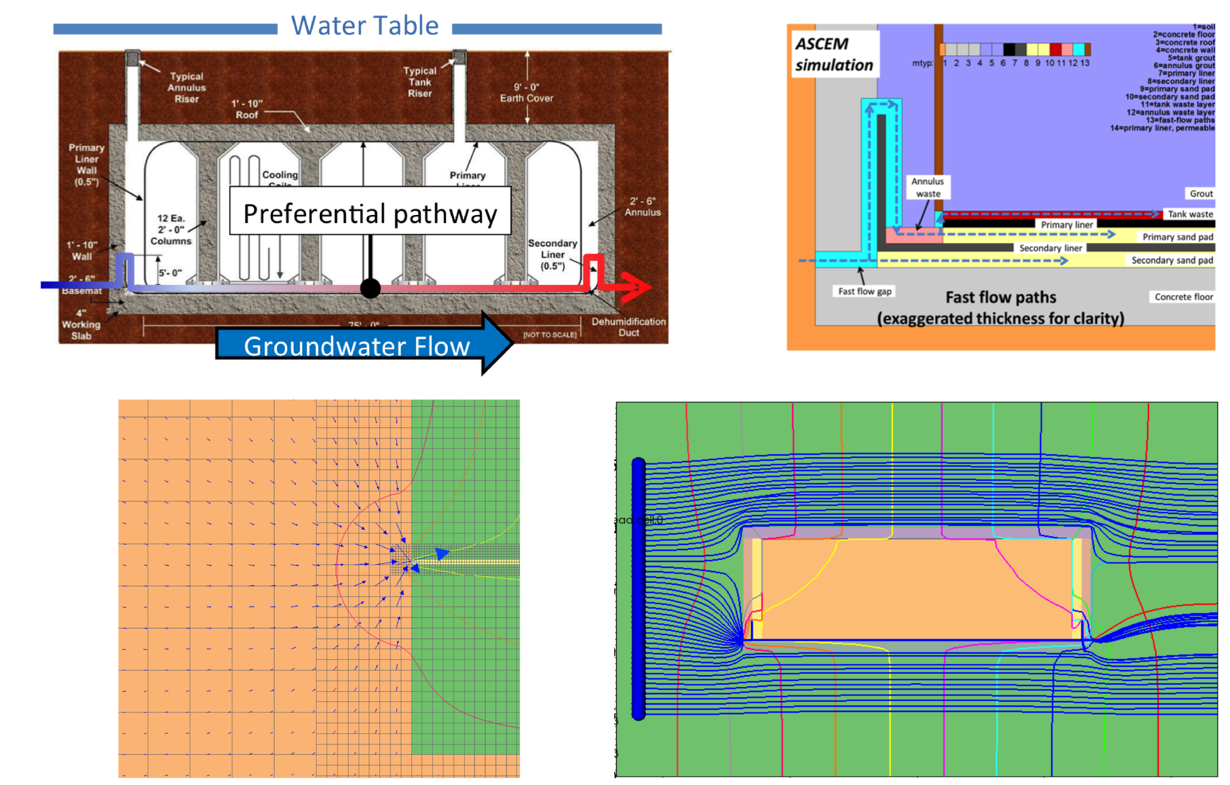
```
<sources>
   <source name="Pumping Well">
    <assigned_regions>Well</assigned_regions>
    <liquid_phase name="water">
        <liquid_component name="water">
            <volume_weighted start="0.0"
              function="constant" value="-11.5485"/>
        </liquid_component>
    </liquid_phase>
    </source>
</sources>
```

In addition, named constants for times or values could be used to simplify testing and reduce the number of conceptual errors made when adjusting/experimenting with the model.

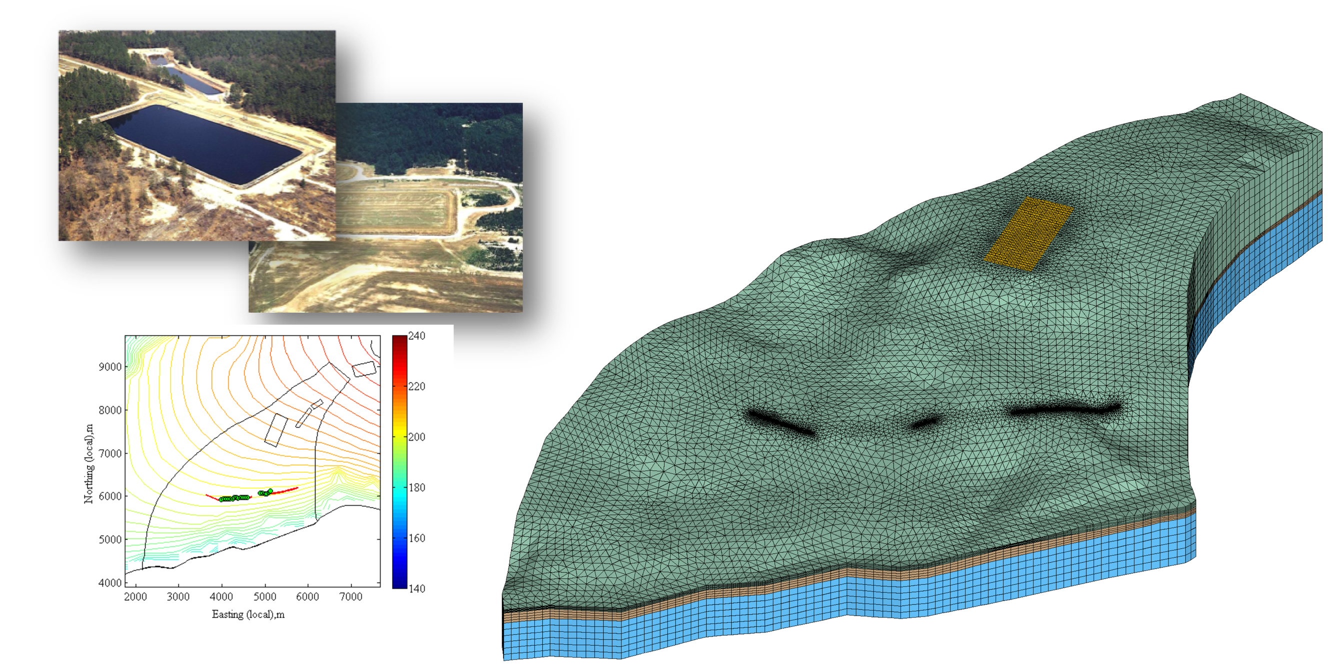
5. Site Application Demonstrations

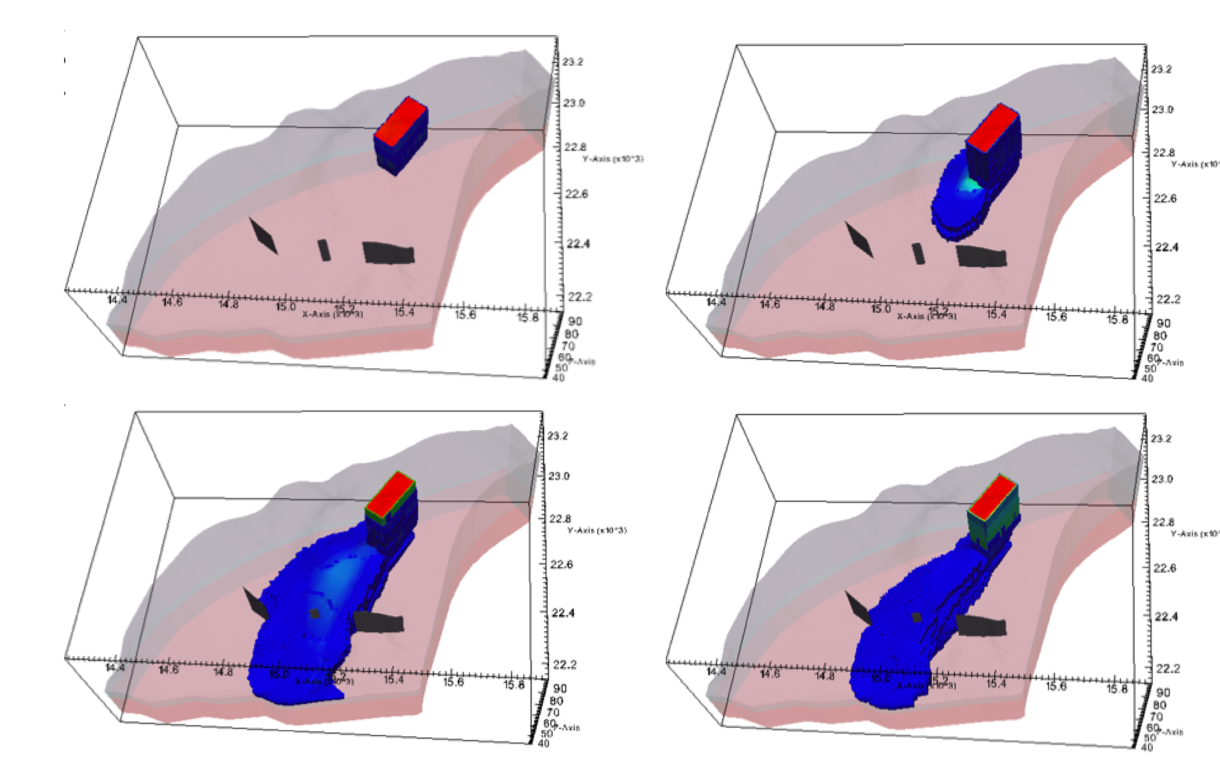
5.1 Savannah River Tank

Some words about the problem



5.2 F-Area Seepage Basins at Savannah River Site





6. Conclusions and Future Work

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