AMANZI: A PARALLEL OPEN-SOURCE FLOW AND REACTIVE-TRANSPORT SIMULATOR FOR ENVIRONMENTAL APPLICATIONS

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The Advanced Simulation Capability for Environmental Management (ASCEM) program is developing an approach, and the supporting open-source tools, to understand the fate and transport of contaminants in natural and engineered systems. The multi-process High Performance Computing (HPC) simulator, named Amanzi, provides a flexible and extensible simulation capability for ASCEM. Specifically, a wide range of conceptual models (scenarios) naturally arise in the graded and iterative approach to risk and performance assessment. The Platform toolsets (Akuna) generate these conceptual models and Amanzi provides the computational engine to perform the simulations, returning the results for analysis and visualization.

In this presentation we highlight key elements of our approach to developing Amanzi, including its design, algorithms, and software development practices. Specifically, we use a hierarchical and modular design that is aligned with the coupled processes being simulated, and hence, naturally supports a wide range of model complexity. Moreover, to model sites with complex hydrostratigraphy, as well as engineered systems, we are developing a dual unstructured/structured capability. To implement these capabilities in parallel with consideration for a range of modern architectures we leverage tools, expertise, and algorithms from several well established DOE programs. For example, we leverage the Trilinos framework to provide key infrastructure for general unstructured meshes, with recent advances in Mimetic Finite Difference methods to provide discretizations of flow models. Similarly, we leverage BoxLib to provide infrastructure for block structured adaptive mesh refinement.

To ensure that Amanzi is truly an open-source community code we require a completely open-source tool chain for our development. We will discuss our choices for developer tools, including version control, project management, testing, and documentation. Using these tools we have established a development and testing cycle that will provide a high-quality accessible and relevant code base. In particular, our hierarchical testing is motivated by a sequence of ASCEM capability demonstrations that is developed by the Site Applications thrust in ASCEM. We present simulation results from these demonstrations that highlight the capabilities of Amanzi.