

AGNI: Coupling Model Analysis Tools and High-Performance Subsurface Flow and Transport Simulators for Risk and Performance Assessments

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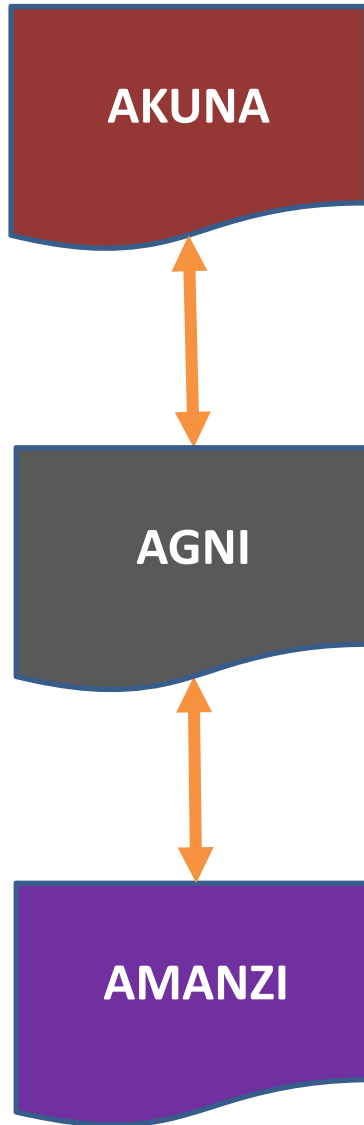
ASCEM=Advanced Simulation Capability for Environmental Management (<http://ascemdoe.org>)

- Consortium of five national laboratories



- Develop transformational, high performance computer modeling (simulation and model analysis) capabilities to better meet the challenge of waste disposal and cleanup.
- Bring together:
 1. supercomputing capabilities,
 2. new and open source HPC modeling (simulation and model analysis) tools, and
 3. improved understanding of subsurface hydrogeological-biogeochemical processes.
- Improve our ability to simulate and predict the fate and transport of subsurface contaminants.
- Provide scientifically defensible decision making, reduced risk, and increased safety throughout the DOE nuclear complex (Hanford, Savannah River).

ASCEM Simulation Modules



Akuna (“no worries”): Graphic User Interface (GUI; resides on user’s desktop) (*Karen Schuchardt, PNNL*)

- Open Source Eclipse/Java based
- Incorporates data management, visualization, and model development tools

Agni (“fire”): Simulation controller and Toolset driver (resides on remote server) (*George Pau, LBNL, Velimir Vesselinov, LANL*)

- Open Source C++ object oriented
- Provides coupling between **Akuna** and **Amanzi**
- Performs various model analyses (SA, UQ, PE, ...)

Amanzi (“water”): High Performance Flow and Transport Simulator (resides on remote server) (*David Moulton, LANL*)

- Open Source C++ object oriented
- Saturated / unsaturated groundwater flow, ...
- Structured / unstructured / adaptive gridding
- ...

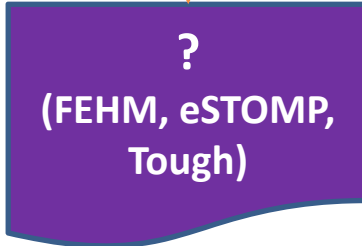
ASCEM Simulation Modules



Akuna: Graphic User Interface (GUI)



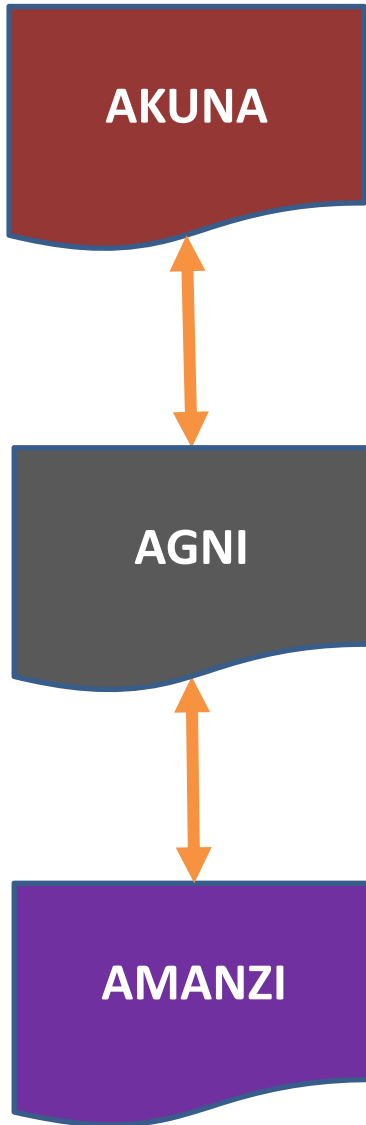
Agni: Simulation controller and Toolset driver



ANY Simulator



Coupling between the ASCEM Modules



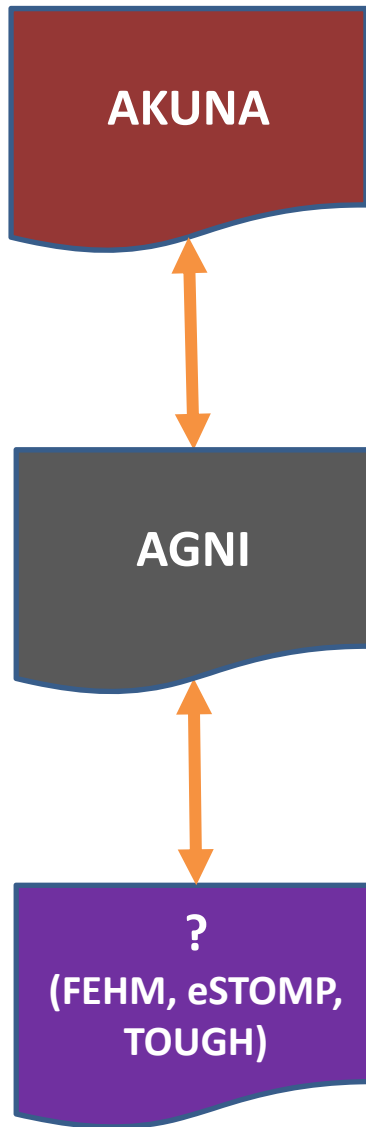
Akuna/Agni:

- External
- A series of input / output files in XML and Text formats
- Model analyses using Agni can be executed independently of Akuna through command-line options and manual changes of the input XML files

Agni/Amanzi:

- External or internal
- External coupling is performed by writing the Amanzi input XML files, and reading the Amanzi output files
- Internal coupling is performed by direct calling of Amanzi subroutines within Agni

Coupling of ASCEM Modules with other simulators



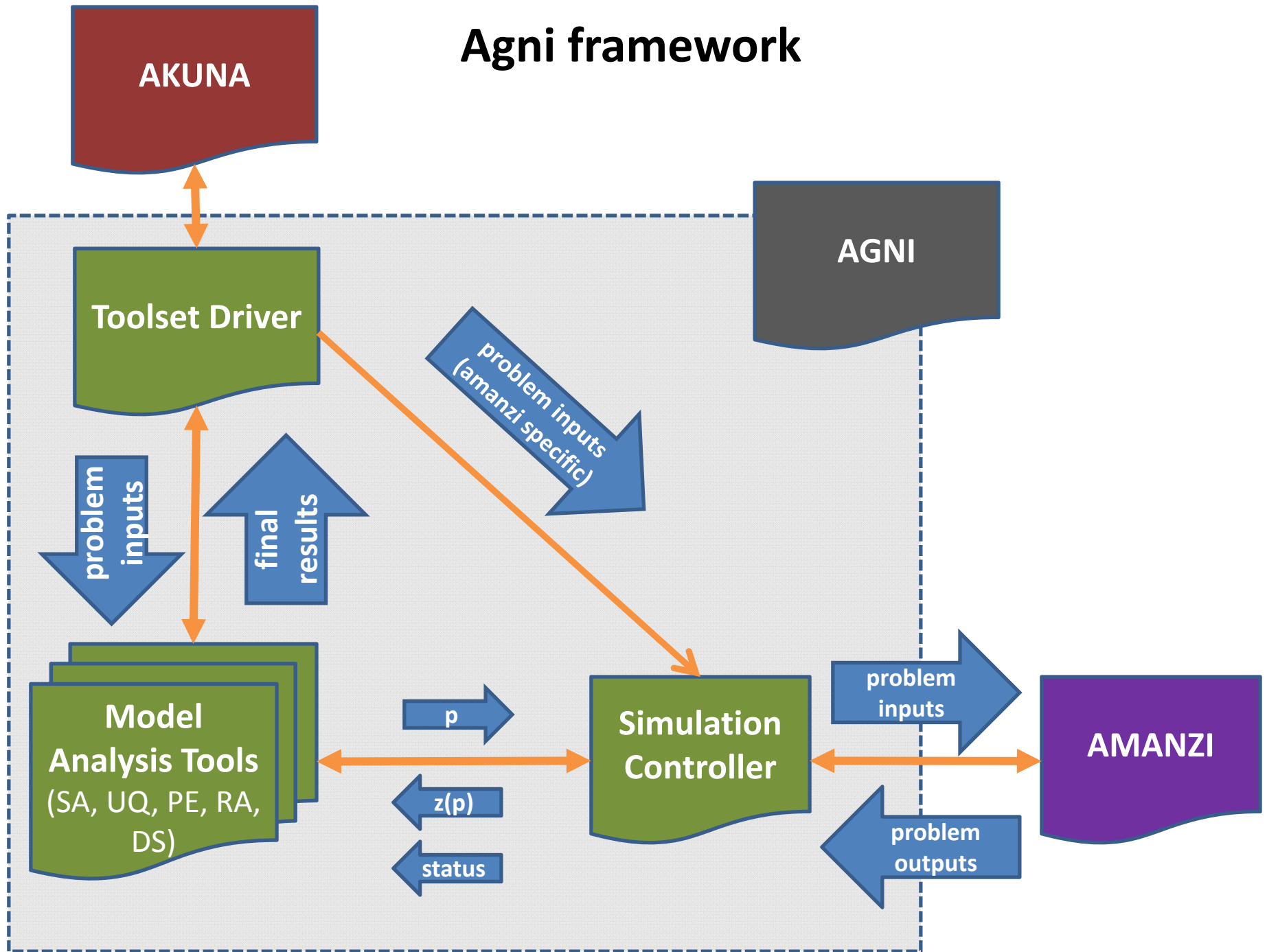
Akuna/Agni:

- External
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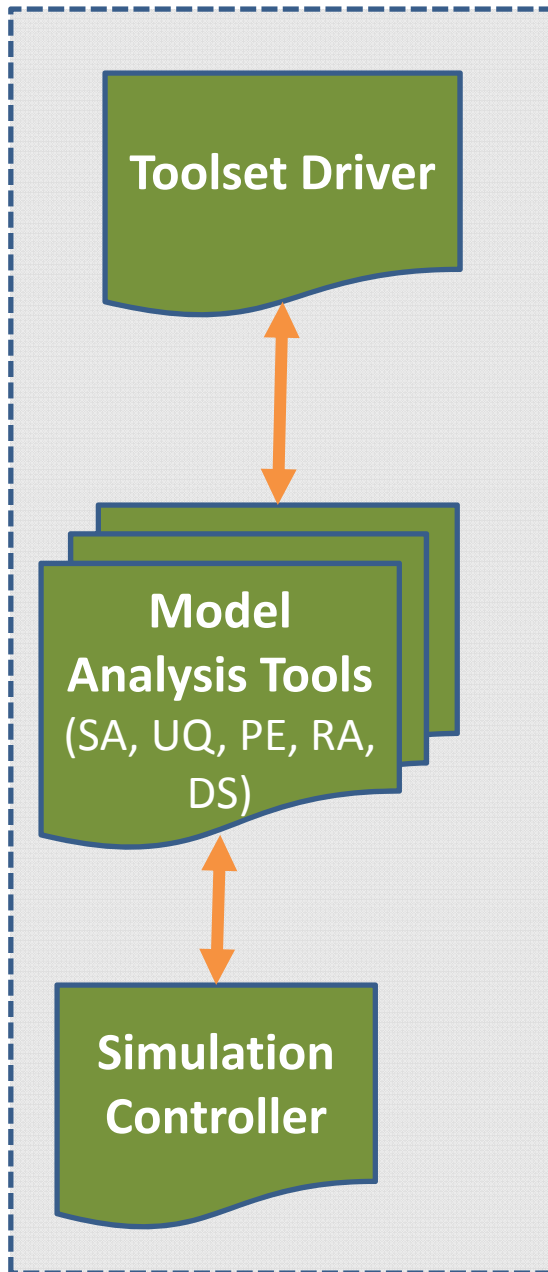
Agni/?:

- External only (at the moment)
- External coupling is performed by writing the simulator input files based on predefined template files, and reading the simulator output files based on predefined instruction files
- Supported template and instruction files are similar but more flexible and general than the format used by PEST
- Agni can work directly with existing PEST template and instruction files as well

Agni framework



Agni framework



Toolset Driver (TD):

- communication between **Akuna** and the **Model-Analysis Toolsets (MAT)**
- a series of libraries with flexible data structures for describing the model parameters and observations

Model-Analysis Toolsets (MAT):

- modules for **Sensitivity Analysis (SA)**, **Uncertainty Quantification (UQ)**, **Parameter Estimation (PE)**, **Risk Assessment (RA)** and **Decision Support (DS)**.
- designed to be extensible to add easily additional model-analyses methods and techniques

Simulation Controller (SC):

- communication between the simulator (**Amanzi/?**) and the **Model-Analysis Toolsets (MAT)**
- serial or parallel execution of simulations (MPI/Threading)
- dynamic job control, restarts and reruns (if needed)
- during the model executions, provides information to **MAT** and **Akuna** about the current status of the simulations (intermediate results, error messages, execution failures)

Model-Analysis Toolsets (MAT) in Agni:

Sensitivity Analysis (SA) (*Stefan Finsterle, Elizabeth Keating*):

- sensitivity of model predictions to conceptual model elements and model parameters;
- currently implemented: local (finite-difference based) and global (MOAT, Sobol's) techniques.

Parameter Estimation (PE) (*Stefan Finsterle, LBNL*):

- identification conceptual model elements and model parameters based on site observation data (calibration targets and performance criteria)
- currently implemented: local (LM) and global (PSO) techniques; stochastic inversion

Uncertainty Quantification (UQ) (*Elizabeth Keating, LANL*):

- uncertainty of model predictions due to uncertainties in conceptual model elements and model parameters
- currently implemented: local (Null Space Monte Carlo) and global (Monte Carlo and Bayesian based) techniques.

Risk Assessment (RA) (*Wilson McGinn, ORNL*):

- environmental risk based of existing data and model predictions
- currently implemented: ... still in development stage.

Decision Support (DS) (*Velimir Vesselinov, LANL*):

- decision support based on environmental risk and management goals: remedy selection, monitoring network optimization, selection of data acquisition and model analyses activities for reduction of environmental management uncertainties
- currently implemented: ... still in development stage.

Agni Third-Party Libraries (TPLs) and Subroutines

- Teuchos (part of Trilinos) – importing and exporting Extensible Markup Language (XML) files;
- Boost – portable C++ source libraries;
- Blas, LAPack and GSL – linear-algebra and mathematical subroutines;
- GSLib – geostatistical simulations;
- LevMar – Levenberg Marquardt optimization;
- Psuade – Uncertainty Quantification Project;
- MADS – external coupling and simulation control;
- Evolving Objects (EO) – an Evolutionary Computation Framework;
- ...

Agni execution:

- Coupled with Akuna (Agni execution is controlled by the GUI)
- Standalone (command-line execution)

```
> Agni --infile=agni.xml
```

Agni testing:

- NERSC's Hopper (Linux, peta-flop Cray XE6, with a peak performance of 1.28 Petaflops/sec, 153,216 Opteron 6172 12C 2.10GHz compute cores, 217 Terabytes of memory, and 2 Petabytes of disk; currently, #16 the Supercomputer list)
- **PE/UQ** analyses for a series of test and real world problems
- **Amanzi / eSTOMP / TOUGHREACT**

Example Agni input file (agni.xml):

```
<ParameterList name="agni.xml">
  <Parameter name="toolset" type="string" value="FR/UQ/PE/..." />
  <ParameterList name="parameter">
    <Parameter name="num of parameters" type="int" value="x" />
  </ParameterList>
  <ParameterList name="observation">
    <Parameter name="num of observations" type="int" value="x" />
  </ParameterList>
  <ParameterList name="simulator">
    <Parameter name="do_syscall" type="int" value="1" />
    <Parameter name="verbose" type="int" value="1" />
    <Parameter name="testing" type="int" value="1" />
    <Parameter name="prefix" type="string" value="s01" />
    <Parameter name="name" type="string" value="estomp" />
    <Parameter name="path" type="string" value="/bin/estomp.x" />
    <Parameter name="mpi_call" type="string" value="aprun" />
    <Parameter name="ncpu_total" type="int" value="48" />
    <Parameter name="ncpu_pertask" type="int" value="2" />
    <ParameterList name="external coupling">
      <Parameter name="num of template files" type="int" value="1" />
      <Parameter name="num of instruction files" type="int" value="1" />
      <ParameterList name="instruction 1">
        <Parameter name="out" type="string" value="model.output" />
        <Parameter name="ins" type="string" value="model.output.instruction" />
      </ParameterList>
      <ParameterList name="template 1">
        <Parameter name="inp" type="string" value="model.input" />
        <Parameter name="tmp" type="string" value="model.input.template" />
      </ParameterList>
    </ParameterList>
  </ParameterList>
```

Summary

- Agni is open source / community / multi platform framework for model-based analyses (SA, UQ, PE, RA, DS)
- Agni can be applied independently from other ASCEM modules.
- Agni will be (is) available as Mercurial repository (hg clone <https://akuna.labworks.org/hg/Platform>) including source code, manual, test and verification examples