Climate Modeling Workflow Automation

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AT OAK RIDGE NATIONAL LABORATORY

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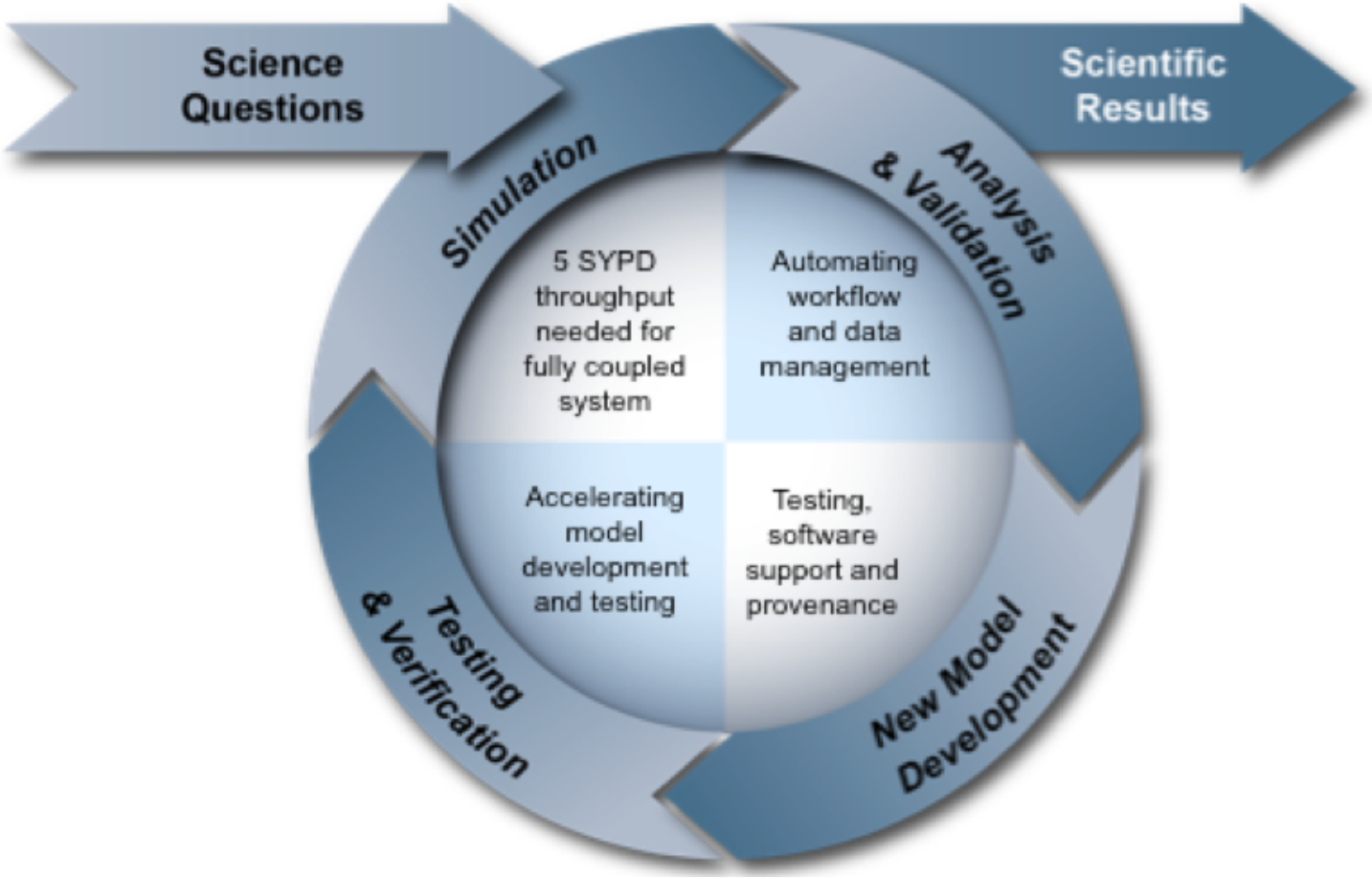
The Vision

- Scientific Discovery – The reason we are building workflow automation
  - Using the workflow tools along with the visualization tools also developed under the project to increase the ease and ability to discover
  - Using the reduced time to solution to increase the rate of discovery of new information.
- Reduce scientist effort to setup and run an experiment.
  - Web based front end, save previous configurations and their results (success, error), Rule engine to guide user away from broken configurations
- Increase amount of science completed per compute allocation by reducing and sometimes prevent configuration errors
  - Web based front end allows parties from each component to review proposed configuration for correctness.

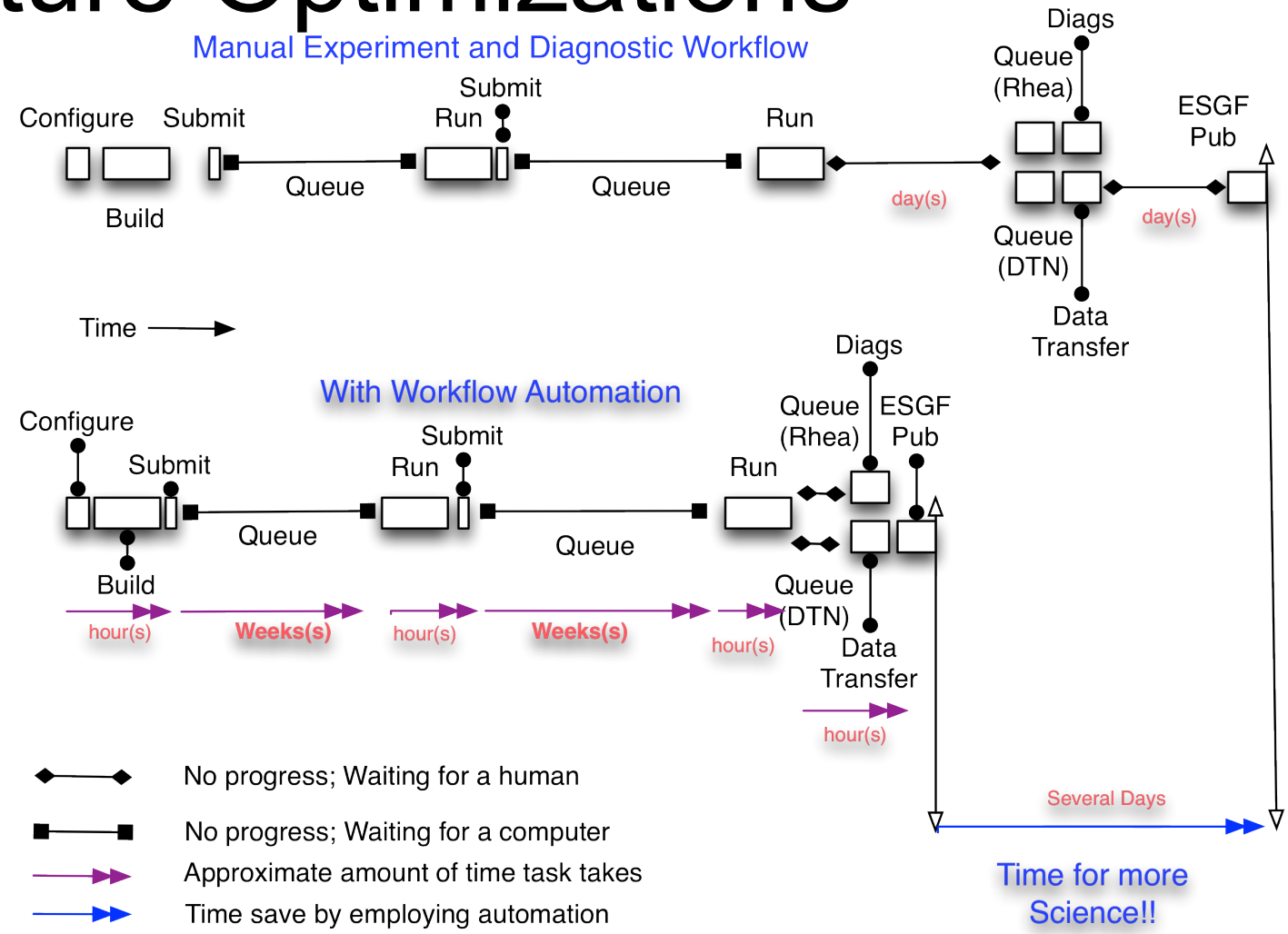
The Vision

- Reduce time to solution by automating the running of CESM, UQ, diagnostics, data movement and publishing. Potentially job size optimization.
  - Reduces delay of a human needing to submit follow on work
  - Reduces queue wait time
- Modular workflow components to allow quickly building new workflows and reusing existing best in practice methods
- Repeatability of experiments

Context


Science Questions
Scientific Results
Simulation
Analysis & Validation
New Model Development
Testing & Verification
5 SYPD throughput needed for fully coupled system
Automating workflow and data management
Accelerating model development and testing
Testing, software support and provenance

Future Optimizations



The Plan

- Working with scientists to define and iteratively implement
- Automate End-to-End science workflow including building and running CESM, running diagnostics and publishing (ESGF) computational science output for sharing and reference.
  - Not happening on a single HPC resource
  - Distributed workflow, but not Grid due to inability to symmetrically systematically access other machines (i.e. many communications are one way)
- Implement so automation “just happens” or can be used as helper scripts by hand

The Plan

- Workflow progress on compute resources is reported back by each workflow component (CESM, DTN, diags, etc.)
- Create central place to see progress of simulations
  - Current progress (23 / 50 years)
  - Current status of data (simulation progress, HPSS, ESGF)
  - Associated location on ESGF + HPSS
  - Direct link to diagnostics

The Plan

- Provenance can be extracted from status information if a configuration information is sent back
    - Not just the data, but the workflow as well
- Timing information of the Workflow Components.
- Also use above data to direct workflow optimization effort

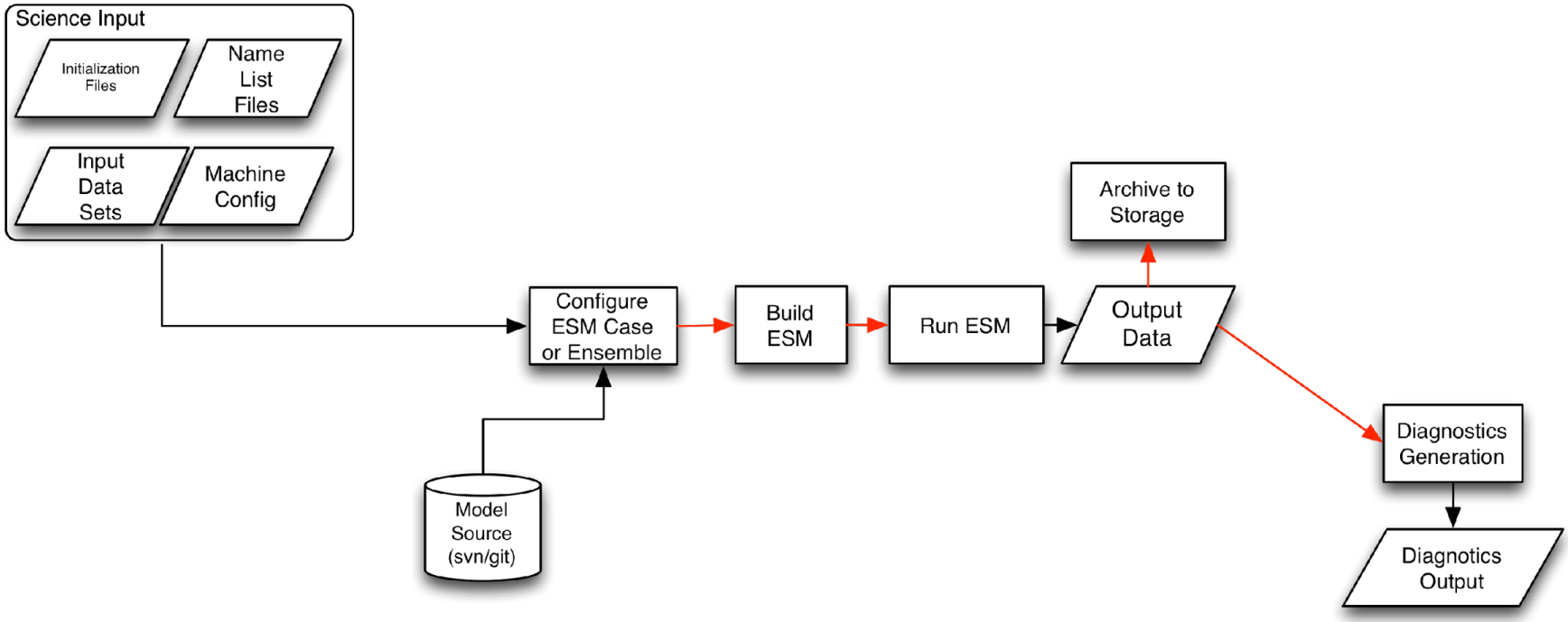
The Technology Plan

- Use of many DOE sponsored technologies
  - UV-CDAT
  - Globus GridFTP
  - Earth System Grid Federation (ESGF)
  - Akuna/Proven (?)

The Technology Plan

- Use of many DOE compute resources
  - CADES – Dynamic computational ability and openness to share data with collaborators
  - Titan's vast compute resources, as well as NERSC - Design general enough to work in almost all compute environments
  - Rhea - modern analysis hardware and software
  - ORNL HPSS (other site local HPSS is possible)

Component Dataflow



Legend

Monitoring & Provenance Dataflow (Simulation Manager)

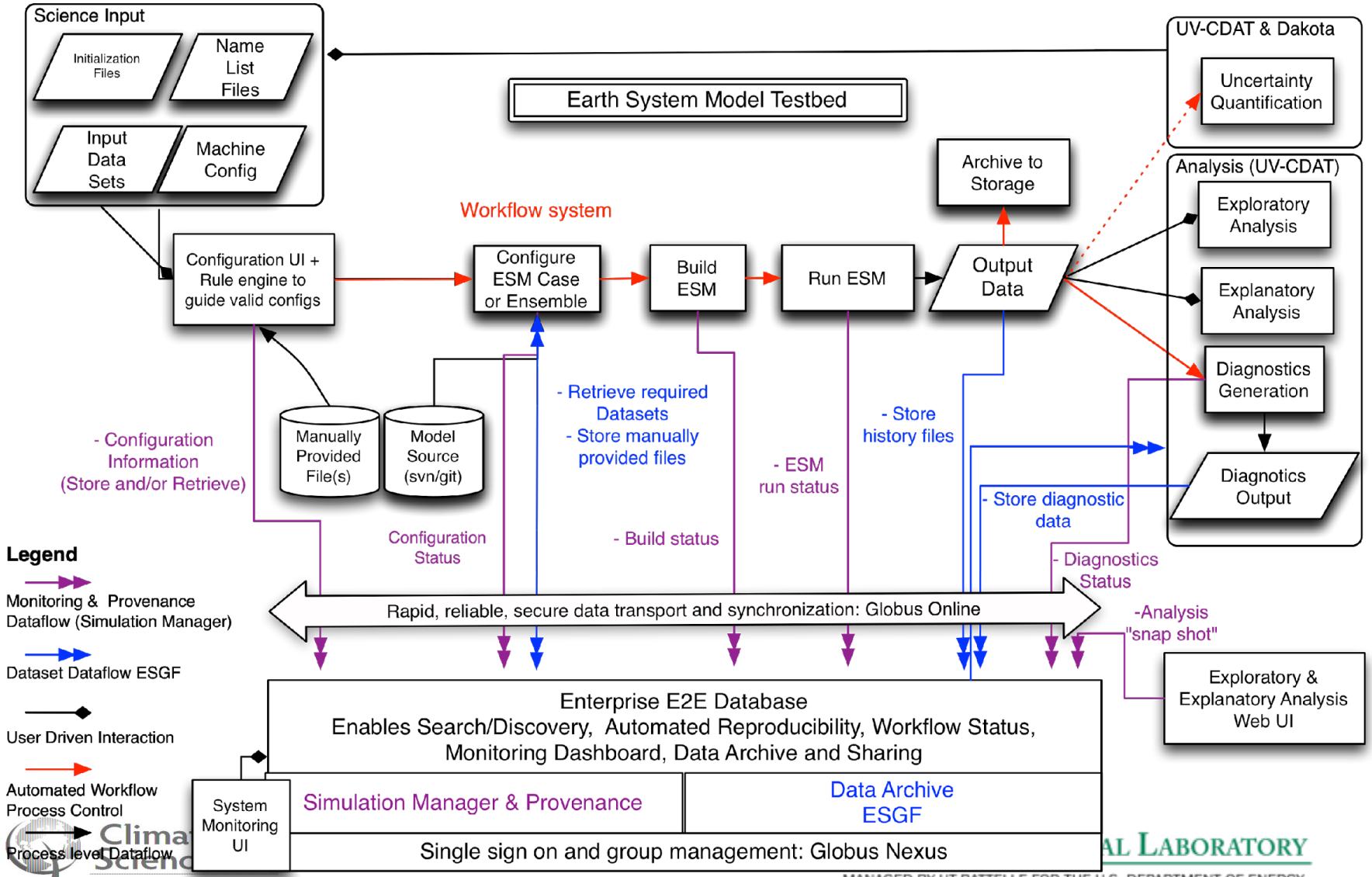
Dataset Dataflow ESGF

User Driven Interaction

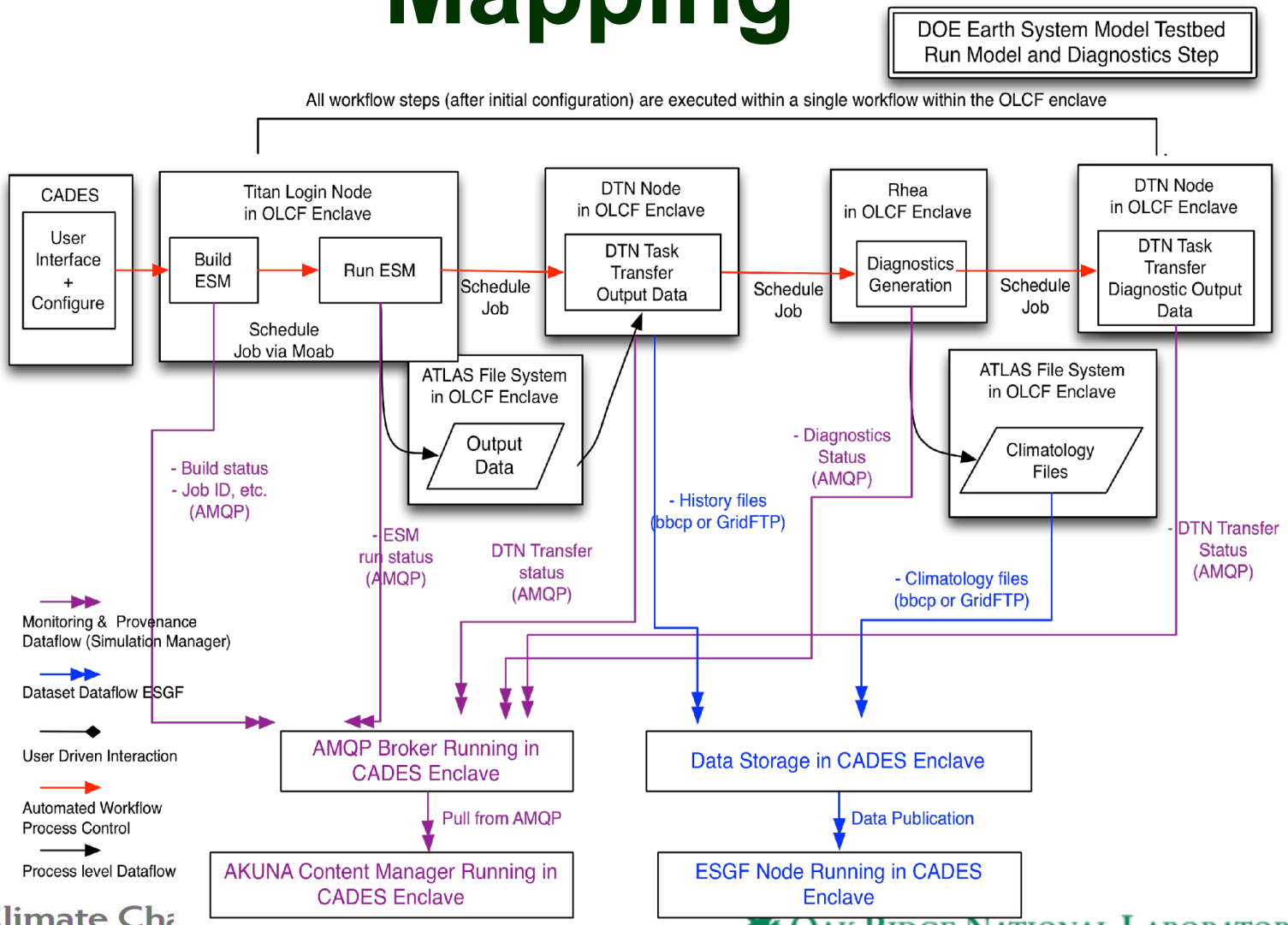
Automated Workflow Process Control

Process level Dataflow

Workflow Dataflow



WF Component to Machine Mapping



The Plan - Workflow

- Six months was building and configuring core infrastructure to demonstrate a distributed workflow would function in the DOE compute environment e.g. Open network ports, install and write software, getting software to talk to each other
- Next steps will involved:
  - Adding configuration ability to workflow (currently hard coded in scripts)
    - Continue to be scripts, but with metadata (consume, output, how to call)
    - Workflow engine (Open Source? Buy? Build?)
  - Adding advanced features (Provenance, integrated view of work performed)
  - Scientist requested features (changing requirements)

What is Working!

- Workflow launch
- Message and data transfer components functional (JSON/AMPQ and GridFTP)
- Scheduling of data transfer and HPSS archive jobs
  - Able to automate transfer using Globus GridFTP
- Scheduling diagnostics on simulation output
  - Waiting on diags that take command line parameters

What is Just About Working!

- Status Messages from each workflow component (not ESM component)
  - Add status messags for failures
- Software to take JSON/AMQP write to DB
- Publication to ESGF
  - Ability to call is in place, need publication script that takes command line input dataset to publish

End