Climate Modeling Workflow Automation

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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

Diagram showing the cycle of science questions leading to simulation, new model development, testing and verification, analysis and validation, and finally scientific results.

- Science Questions
- Simulation
- New Model Development
- Testing & Verification
- Analysis & Validation
- Scientific Results

Key points:
- Accelerating model development and testing
- 5 SYPD throughput needed for fully coupled system
- Automating workflow and data management
- Testing, software support and provenance

Oak Ridge National Laboratory
Managed by UT-Battelle for the U.S. Department of Energy
Future Optimizations

Manual Experiment and Diagnostic Workflow

Configure Submit
Build

Queue Submit Run

Run

Queue

ESGF Pub

Diags

Queue (Rhea)

Queue (DTN)

Data Transfer

Several Days

Time for more Science!!

- No progress: Waiting for a human
- No progress: Waiting for a computer
- Approximate amount of time task takes
- Time save by employing automation

Future Optimizations

Time
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

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Earth System Model Testbed

UV-CDAT & Dakota
- Uncertainty Quantification
- Analysis (UV-CDAT)
  - Exploratory Analysis
  - Explanatory Analysis
  - Diagnostics Generation
  - Diagnostics Output

Workflow system
- Configure ESM Case or Ensemble
- Build ESM
- Run ESM
- Output Data

- Configuration Information (Store and/or Retrieve)
- Manually Provided File(s)
- Model Source (svn/git)
- Configuration Status
- Model Build Status
- ESM run status
- Store diagnostic data
- Store diagnostic history files

Rapid, reliable, secure data transport and synchronization: Globus Online

Enterprise E2E Database
Enables Search/Discovery, Automated Reproducibility, Workflow Status, Monitoring Dashboard, Data Archive and Sharing

Simulation Manager & Provenance
Data Archive ESGF

Single sign on and group management: Globus Nexus

System Monitoring UI
WF Component to Machine Mapping

All workflow steps (after initial configuration) are executed within a single workflow within the OLCF enclave.
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 messages 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