Triggering Analysis Jobs Automatically

Robert D. French
Dr. Suzanne Parete-Koon
NCCS User Assistance

Triggering Analysis Jobs Automatically

- Normal workflow:
  - Log in to Titan
  - Submit Compute job
  - Wait
  - Log in to Rhea
  - Submit Analysis job
  - Make decision about next compute job

Oak Ridge National Laboratory

Triggering Analysis Jobs Automatically

- New workflow:
  - Log in to Titan
  - Submit Compute job
  - Submit Analysis job to Rhea at end of Compute Batch Script

Oak Ridge National Laboratory

Triggering Analysis Jobs Automatically

Batch Script 1 (from TITAN)

- Launch compute task
- Launch Batch Script 2 on Rhea

Batch script 2 (Rhea)

- Launch post-processing task

Oak Ridge National Laboratory

Triggering Analysis Jobs Automatically

- New workflow:
  - Log in to Titan
  - Submit Compute job
  - Submit Analysis job to Rhea at end of Compute Batch Script
- Reduces manual intervention
- Allows for many new forms of workflow

Oak Ridge National Laboratory

Batch DTN Workflow

Batch Script 1 (from TITAN)
- DTNs retrieve data from HPSS
- Launch Batch Script 2

Batch Script 2
- Launch compute job on Titan
- Launch Batch Script 3

Batch Script 3
- Launch viz job on Rhea
- Exit

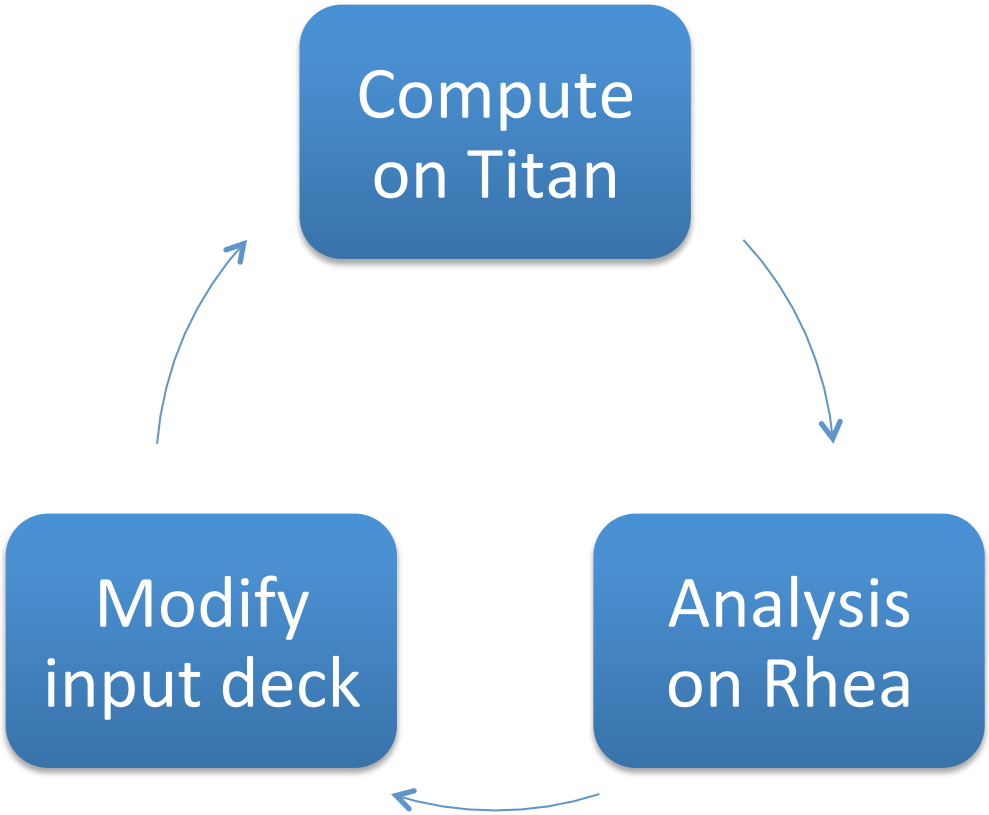
Oak Ridge National Laboratory

Caveats

- Make sure you submit to the right project (-A PRJ123)
- Beware of infinite loops

Oak Ridge National Laboratory

Potentially Dangerous Pattern



Caveats

- Make sure you submit to the right project (-A PRJ123)
- Beware of infinite loops
  - All workflows should have well-defined exits

Oak Ridge National Laboratory

Pro Tips

- Keep your workflow simple
  - Branching could make debugging hard
- Name scripts sequentially and meaningfully
  - monte_carlo1.prepare_initial_conditions.pbs
  - monte_carlo2.run_simulation.pbs
  - monte_carlo3.visualize_results.pbs
  - monte_carlo4.store_data.pbs

Oak Ridge National Laboratory

Availability

- Seeking volunteers (projects) for beta-testing
  - Email help@nccs.gov to request early access
- Will be available center-wide after a successful testing period

Oak Ridge National Laboratory

Thanks for your attention

QUESTIONS?

New software, Access for DD projects

OTHER RHEA NEWS

Newly Installed Software

- FFTW3-MPI
- SPRNG
- PETSc
- Dataspaces
- Adios
- NCO
- VisIt
  - https://www.olcf.ornl.gov/kb_articles/visit-profile-for-rhea/
- Many others!

Oak Ridge National Laboratory

Director's Discretion Access to Rhea

- As a reminder, DD Projects can request Rhea
  - Email: help@nccs.gov
  - Describe Intended use
  - Number of hours needed
    - Rhea uses "node-hours" (1 per node per hour) whereas Titan uses "core-hours" (30 per node per hour)

Oak Ridge National Laboratory

THANKS FOR YOUR TIME