Software Infrastructure
(Data Management L3 Area, WBS 1.09.03)

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Overview

- Establish key interfaces used by Simulation and Analysis L3 areas
- Enable Simulation and Analysis workflows to run on a wide range of computing platforms used by the project
- Indexing of data / metadata and provenance tracking of generated products
- Automation of both real-time processing and bulk reprocessing
Data Interfaces

- Formats on disk and in memory
  - SPT3G hand-off from DAQ, used for on-site computing and HTC platforms
  - TOAST used at HPC centers

- Indexing of data
  - Starting point is metadata from DAQ
  - Interfaces to Data Movement L3
  - Used for data selection and updated by data processing
Processing Interfaces

- API for simulation and analysis operations (G3Module / toast.Operator)
  - Minimize interface differences between frameworks (underway)
  - Copy / redistribute only when necessary
- Tools for constructing workflows for all our compute needs on HTC / HPC resources
  - Rapid data quality checks, transient detections, bulk reprocessing for data releases, Monte Carlo simulations, etc
- Optimizations sufficient to meet requirements on available compute resources
  - GPUs on Perlmutter (NVIDIA) and Aurora (Intel)
Deployment & Execution

● Software Deployment
  ○ Range of solutions, depending on target compute platform: containers (docker / singularity), Python packages, CVMFS
  ○ Most of the release process can be automated using existing practices

● Job Management
  ○ Need to run workflows on local, HTC, and HPC systems
  ○ Job tracking across all resources- separate but related to data provenance tracking
  ○ Automate as much as possible; Dedicated personnel resources for managing the execution of these systems

● Leverage upcoming Superfacility infrastructure for HPC work (next slide)
Superfacility Model

- Growing need to support workflows that can run across DOE/ASCR facilities (and institutional computing, cloud...)
  - Focus on connecting compute, network and experiment facilities - “superfacility” model

- A suite of tools for integrated use at multiple centers is being developed (at NERSC, and also at other ASCR/DOE facilities). This includes:
  - Federated Identity (i.e. using home institution as best source of identity)
  - Services gateway (typically K8-based, eg Spin/Slate) for databases, web portals, workflow management..
  - REST APIs for: Data movement / staging; System status; System reservations; Submitting / managing compute jobs...

- This is being discussed/coordinated at an ASCR level - aim is to have a coherent set of best practices for running cross-facility workflows.
Summary

● Currently making progress on specific tasks that are needed immediately on the schedule (prior to CD-1 / PDR)
  ○ Data and processing formats and interfaces
  ○ Deployment to upcoming NERSC system (Perlmutter)

● In the design phase of the project (now through CD-2 / FDR) need to:
  ○ Create and refine system for data indexing
  ○ Create draft system for job / data provenance tracking

● Continue tracking progress on Superfacility tools and how they can guide some of our automation efforts which are needed later during construction