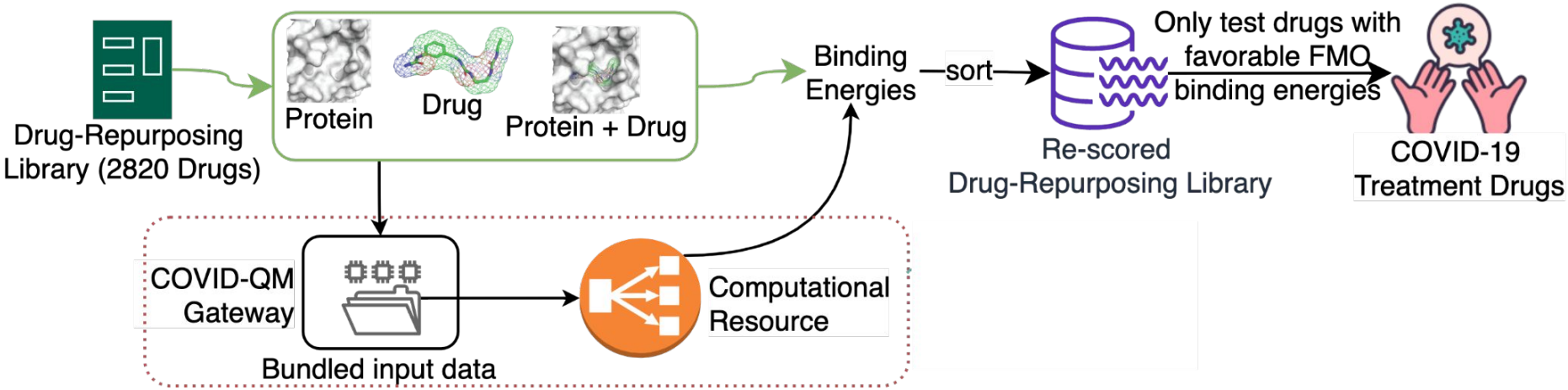
Overview

- Analysis of the computational challenge
- Testing and production computational resource identification
- Science Gateways and Airavata Framework
- Airavata Framework Extensions
- Results and observations
- Future outlook

Science Motivation



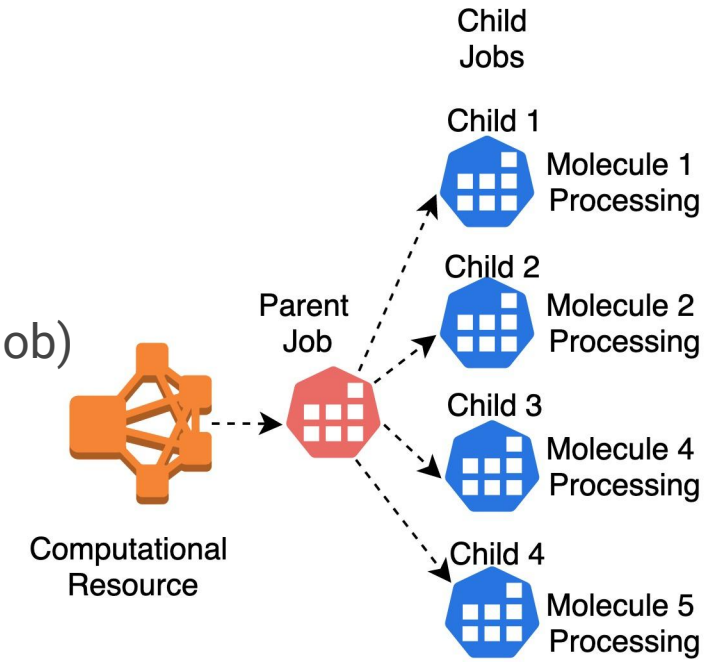
Nature of the computation

- Calculating FMO energies of drug molecules through GAMESS application

  2820 Ligands (Drugs) (48 cores, ~5 minutes / job)

  2820 Protein-ligand complexes (48 cores, ~7 hours / job)

- Solution - Static Parameter Sweeping on HPC



Jetstream

- Environment for initial testing
- Utilized SLURM job arrays to spin up child jobs
- Primarily used for debugging and trying out different GAMESS versions
- Running one job at a time with limited hardware resource
- 2820 Protein-ligand complexes
  - Best case runtime - 7h x 2820 = 19740 hours (823 days)
- 2820 Ligands
  - Best case runtime - 5m x 2820 = 14100 minutes (10 days)

Stampede2

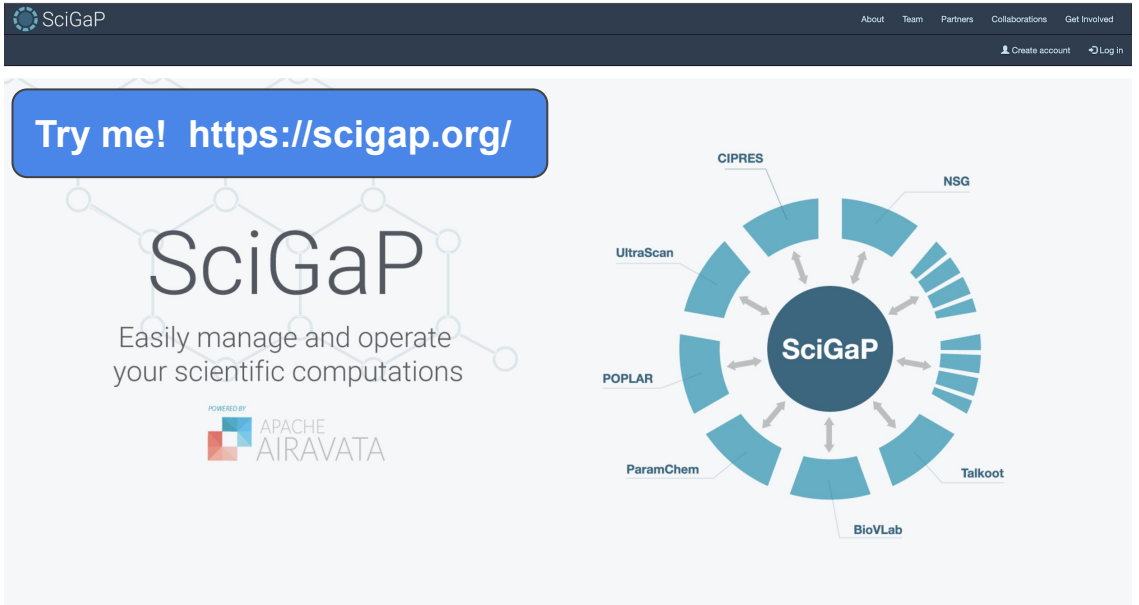
- Used SKX Normal Queue which has Skylake Intel Xeon Platinum 8160 nodes; GAMESS was compiled for SKX only
- One job for one node with all 48 cores used and 120 nodes (allowed by the allocation) at a time for maximum throughput
- Followed a **custom node binding mechanism** through a modified rungms script (in place of Slurm arrays which are not available in Stampede2) to spin up child jobs
- 2820 / 120 = 24 runs for Protein-ligand complexes
  - Best case runtime 7 x 24 = 168 hours (7 days)
- 2820 / 120 = 24 runs for Ligands
  - Best case runtime 5 x 24 = 120 mins
- Thanks to **Kent Milfeld, TACC,** for compiling Gamess and help with rungms modifications

Science Gateways for research

- Increased parallel computations = Increased complexity to handle HPC job submissions
- Science Gateway takes care of job submission, load balancing, fault tolerance, monitoring and data transfers
- PI works only on data preparation and submission through the Gateway

Airavata Gateway Framework and SciGap Platform

Registered SciGaP Gateways	45
Supported Applications	230+
Integrated Computing Resources	70+
Registered Users	4700+
Number of jobs run (3 years)	>270,000
Computing Hours (3 years)	> 22.8 M



We can be your “elevator”
Collaboratively we can nurture community gateways.

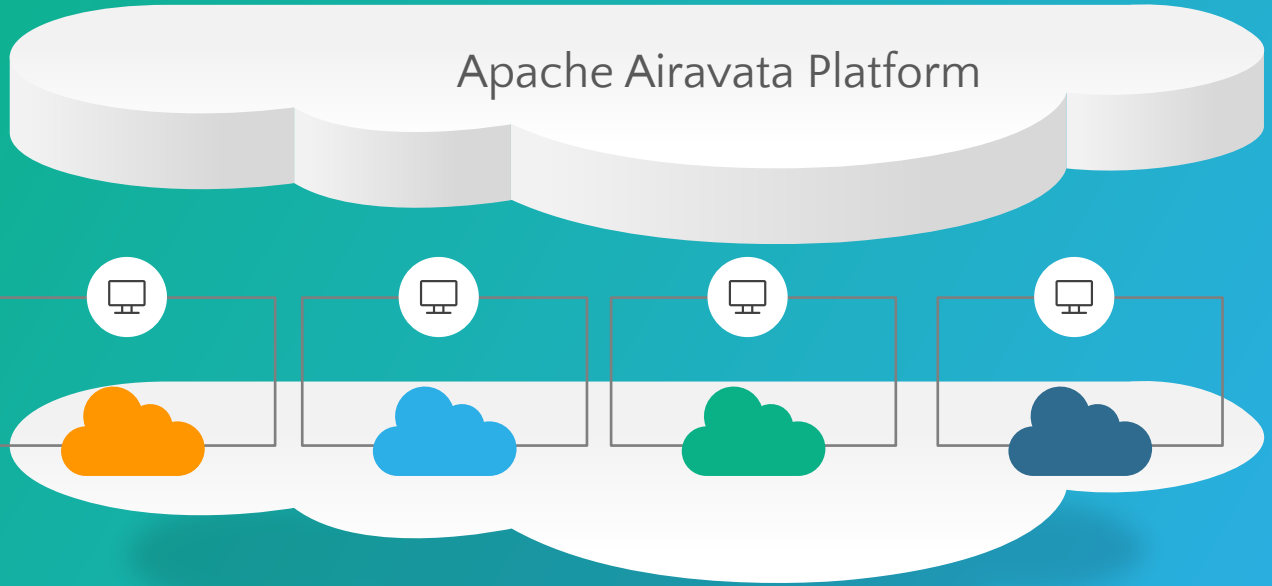
fMRI Data Management

Imagine Analysis Tools

Computational Models

Bring your own compute or storage or we can help you use IU, National and Cloud Computing

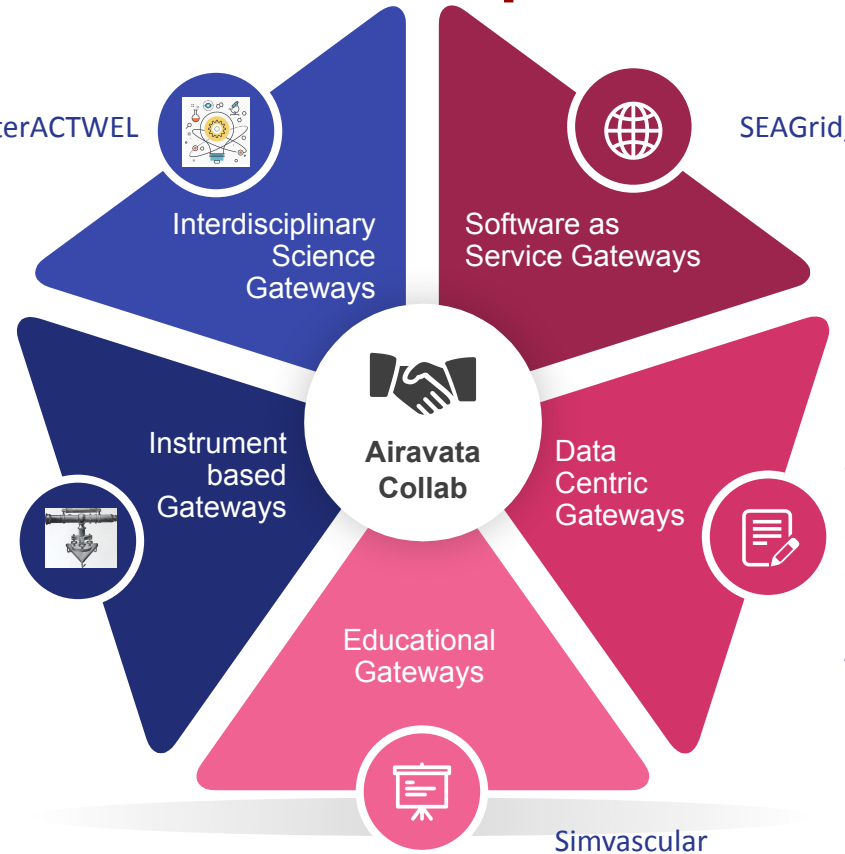
Your Data and Tools



We develop and operate the Platform

You administer your gateways but we have your back and operate them for you.

Our collaborations – some examples



Our Collaborators and Clients

Domain and Application Gateways

Title	Field of Science
SEAGrid Gateway	Chemistry & Engineering
Ultrascan Gateway	Biophysics
TestDrive Portal	Computer & Information Science & Engineering
dREG Gateway	Genetics & Nucleic Acids
Phasta Gateway	Mechanical Engineering
SimCCS Gateway	Geology Survey
Computational Systems Biology Group(CSBG) Gateway	Biological Science
SimVascular Gateway	Cardiovascular Simulation
IU Nano Confinement Gateway	Materials Research
Searching-SRA Gateway	Bio-informatics and Biology
InterACTWEL Science Gateway	Natural Resources Management Decisions Support
NextGen Thermodynamics Database Gateway	Geochemistry & Environmental Science
Atomic and Molecular Physic Gateway	Atomic, Molecular, and Optical Physics
Distant Reader Gateway	Library Science
Electron-Phonon-Wannier (EPW) Gateway	Material Science
Single Cell RNA Sequencing Gateway	Genetic Science
Indiana Future Water Gateway	Hydrology
Colorado School of Mines QUSP Gateway	Quantum Simulation
Data Discovery Studio	Geoscience
Delta (Descriptors of Energy Landscapes using Topological Analysis) Gateway	Geoscience
TopPIC Gateway	Health Science
Alzheimer's disease drug discovery (AD3) Center Gateway	Health Science
LROSE Gateway	Atmospherical Science

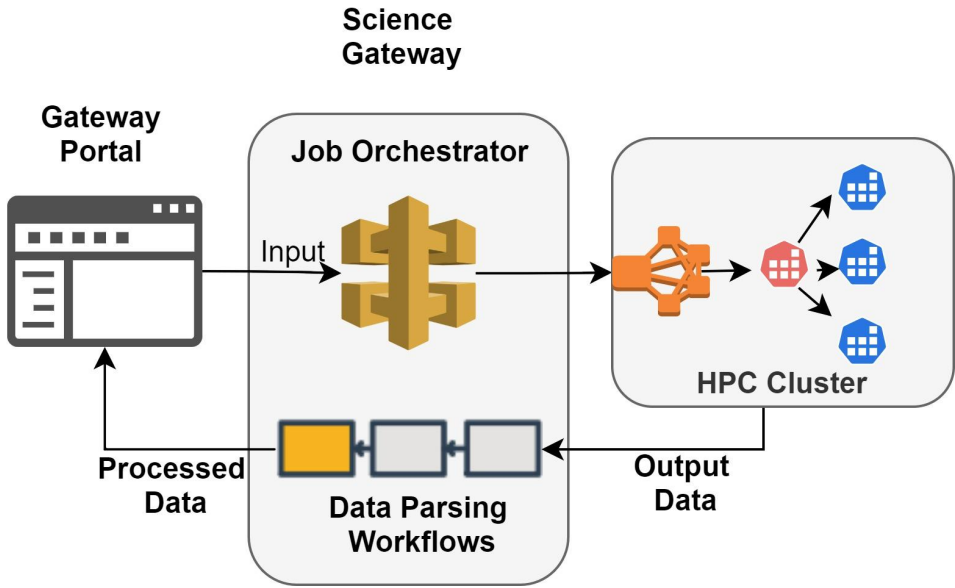
Campus Gateways

Title	Field of Science
University of South Dakota	Chemistry & Bio
Indiana University Bloomington	Generic Applications
Georgia Tech HIVE Gateway	Generic Applications
Oklahoma University	Chemistry & Engineering
Georgia State University	Generic Applications
University of Alabama Birmingham	Generic Applications
New Mexico State University	Generic Applications
West Virginia State University	Generic Applications
University of Kentucky Science Gateway	Generic Applications
South Dakota State University Gateway	Generic Applications

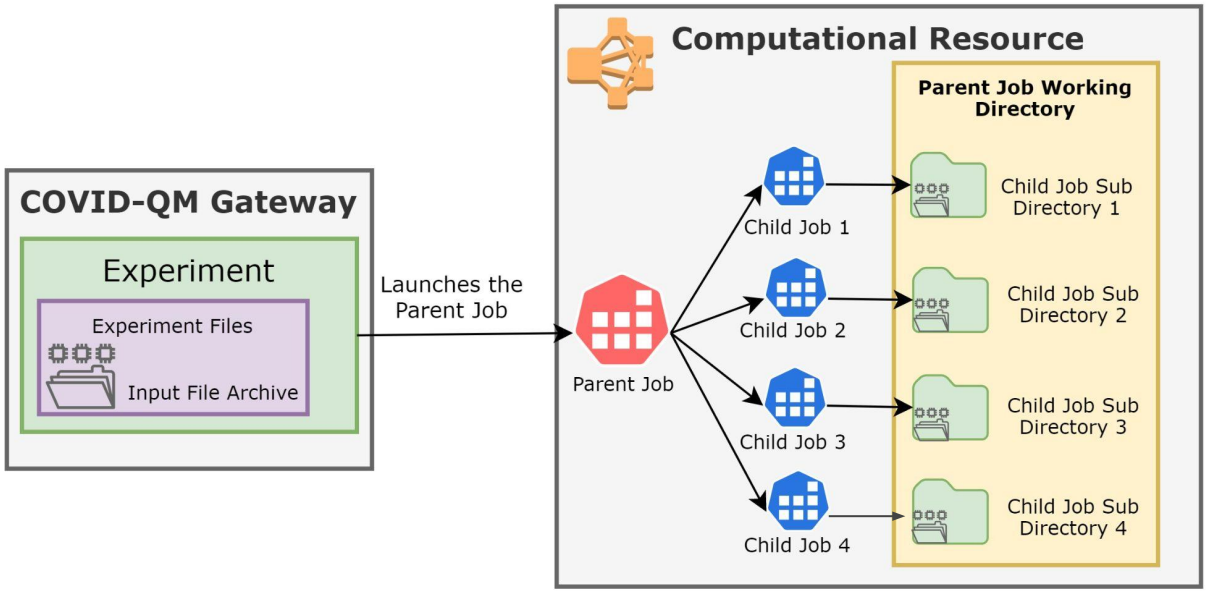
https://circ.iu.edu/collaborations.html

Required Extensions for Airavata

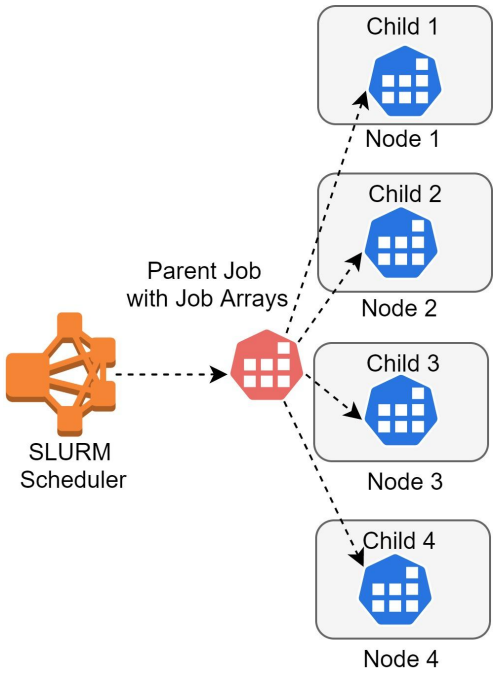
- One experiment but huge number of jobs
- Supporting multiple ways to scale jobs at HPC level (Job Arrays, Custom MPI)
- Preparing workspaces for jobs
- Monitoring sub jobs
- Parsing Output



Setting up working environments for jobs

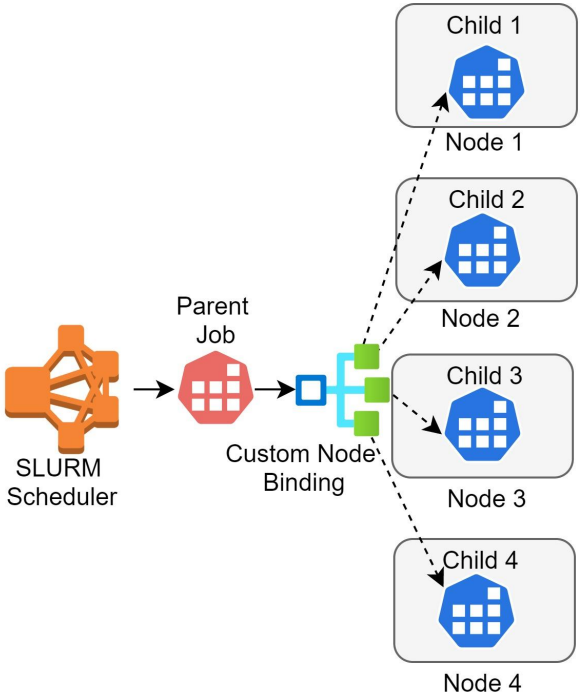


Static parameter sweeping using SLURM Job Arrays - Jetstream




```
#SBATCH --array=0-<n-1>
#SBATCH  -o <working directory>/%a/stdout
#SBATCH  -e <working directory>/%a/stderr
cd <working directory>/${SLURM_ARRAY_TASK_ID}
<execute the application logic>
```

Static parameter sweeping using node binding scripts - Stampede 2



Job Script pseudo code

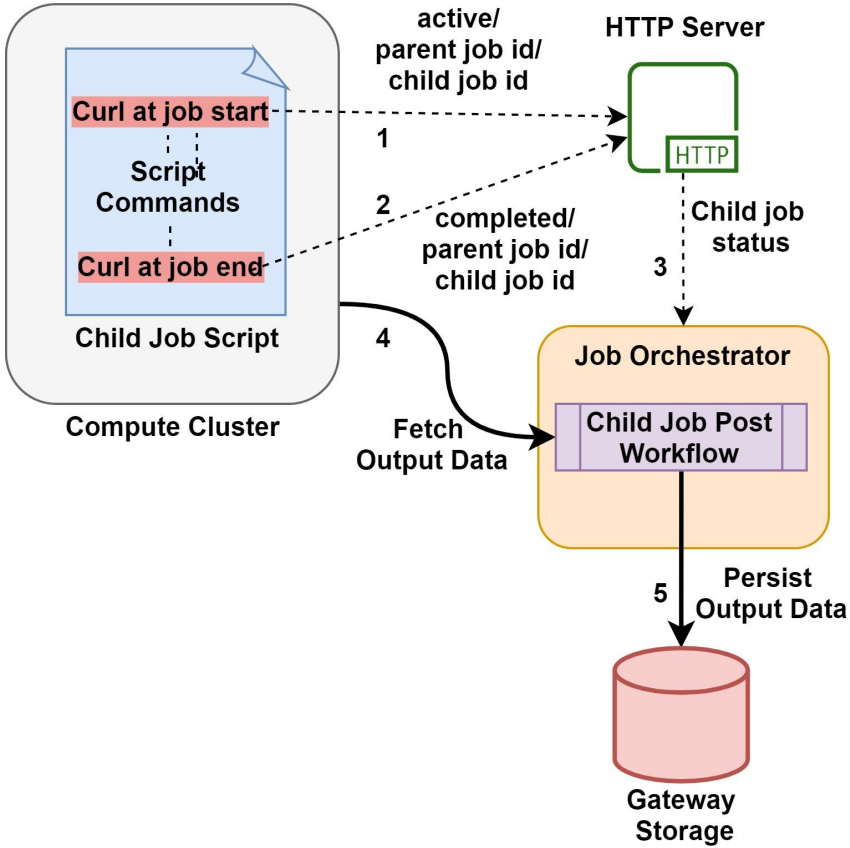
```
#SBATCH -p skx-normal
#SBATCH -N 120
module load intel/19.1.1  impi/19.0.7  gamess/2019.09.30R2; export RUNS_PER_NODE=1

array=(0 1 2 3)
NODES=( $(scontrol show hostnames $SLURM_JOB_NODELIST))
ncnt=0
for i in "${array[@]}"
do
(
  export SCRATCH_ID=${NODES[$ncnt]}
  export GMS_HOST=${NODES[$ncnt]}

  rungms_2019R02 gamess.inp 24  > Gamess.stdout 2>Gamess.stderr;
)&
ncnt=$ncnt+1;
```

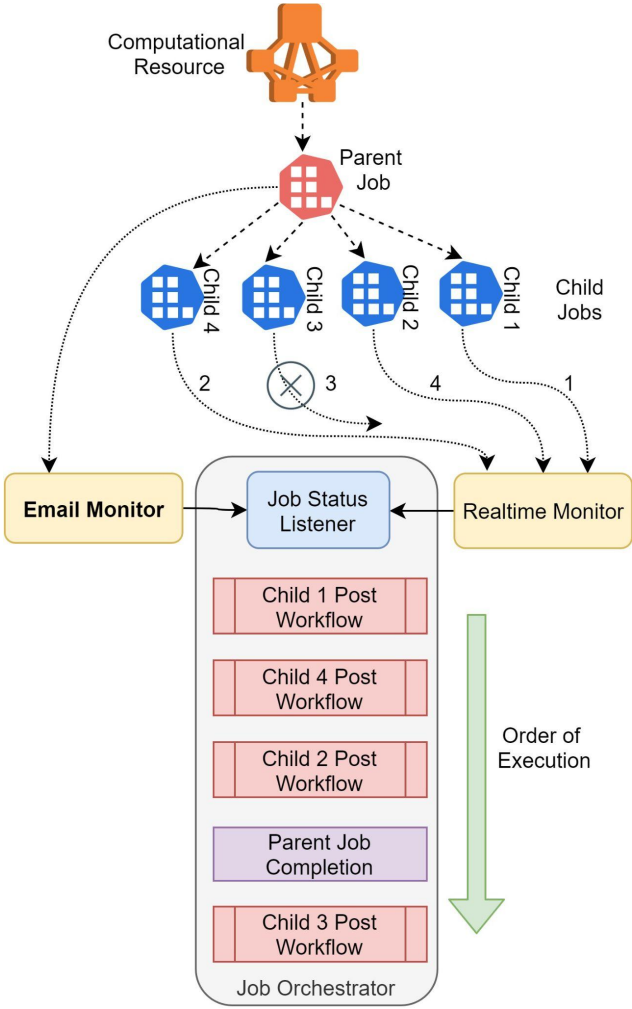
Monitoring Child Jobs

- We do not get emails for child job completions
- Programmatically entered curl commands to the SLURM script to get job status



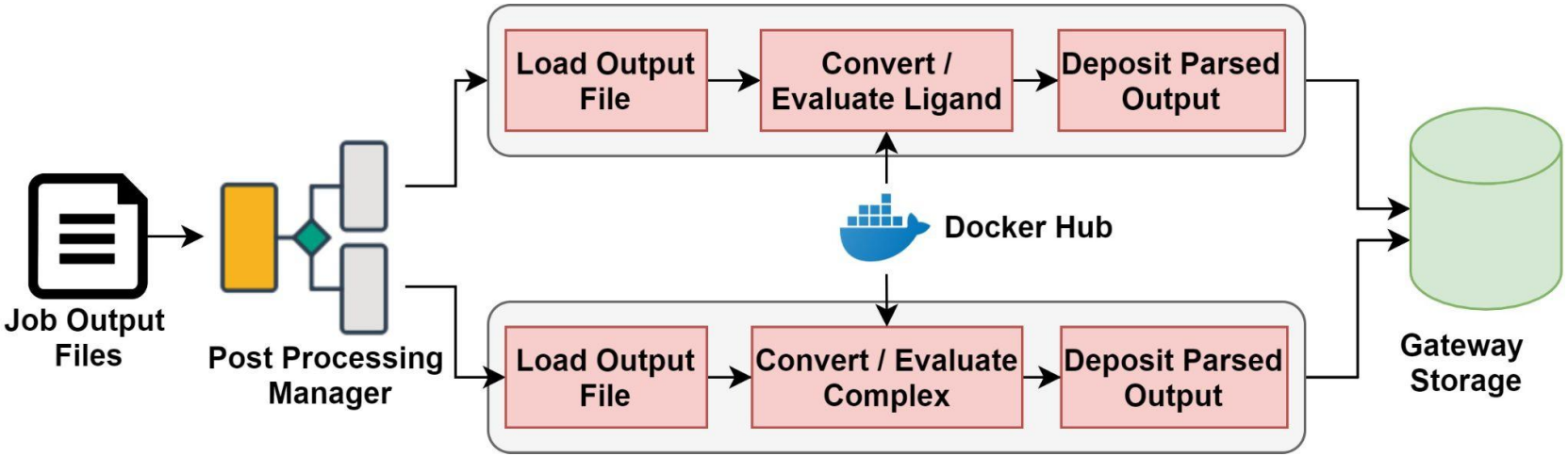
Recovering Missing Job Status

- It is possible to have lost child notifications due to network issues.
- Wait until the main job completes
- Get the remaining jobs that haven't notified through CURL monitoring
- Job Orchestrator checks statuses for those jobs and runs post workflows to fetch generated outputs



Post Processing Output

- Researchers needed to convert output files generated from GAMESS into a context specific format using their specific conversion scripts
- Airavata's data parsing framework can encapsulate those scripts into docker containers and run as a part of the post processing pipelines



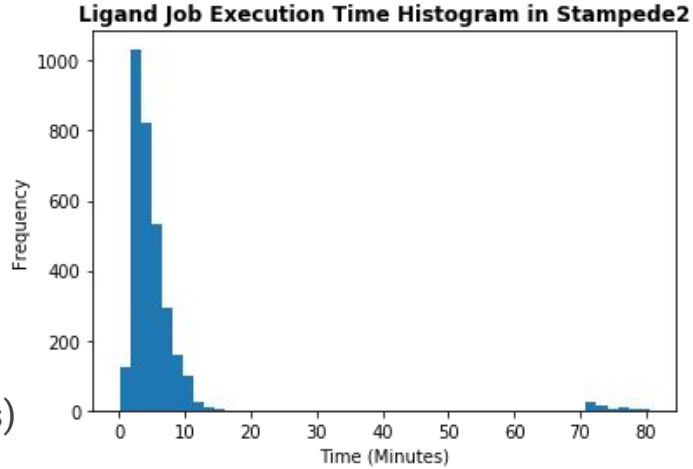
Observations

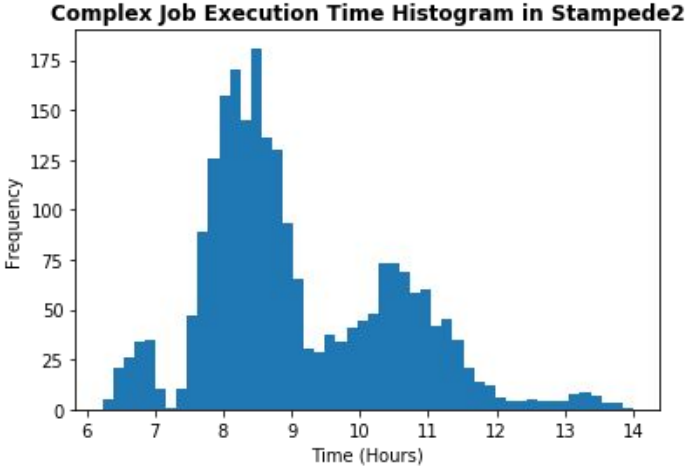
Stampede 2

- Ligands
  - 3224 Jobs
  - 29 Completed Experiments
  - 7 Failed Experiments (6 Queue size exceed, 1 SSH Errors)
- Complex
  - 2889 Jobs
  - 28 Completed Experiments
  - 8 Failed Experiments (4 SSH Errors, 4 Allocation issues)

Jetstream

- 30 Completed Experiments
- 19 Failed Experiments





Challenges

- Different GAMESS versions in different compute systems gave different FMO energies for the same input and required additional compilations
- Not having a standard mechanism (slurm arrays) to scale jobs at the scheduler level requiring modification of rungms explicitly

Future Outlook

- Seamlessly integrating “User” provided arbitrary parsers into post workflow.
- Diverse of computational job submissions distributed into multiple resources with fine control.
- Generalize the Data-Parallel parameter sweep workflow capability for other Apache Airavata framework based gateways.
- Make resource usage more efficient by using available nodes for additional computations during a reservation.