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

Drug-Repurposing Library (2820 Drugs)

Protein

Drug

Protein + Drug

Binding Energies

sort

Re-scored Drug-Repurposing Library

Only test drugs with favorable FMO binding energies

COVID-19 Treatment Drugs
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
- \( \frac{2820}{120} = 24 \) runs for Protein-ligand complexes
  - Best case runtime \( 7 \times 24 = 168 \) hours (7 days)
- \( \frac{2820}{120} = 24 \) runs for Ligands
  - Best case runtime \( 5 \times 24 = 120 \) 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

Try me!  https://scigap.org/
We can be your “elevator”
Collaboratively we can nurture community gateways.

Apache Airavata Platform

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

- InterACTWEL
- SEAGrid, TOPPIC
- Interdisciplinary Science Gateways
- Software as Service Gateways
- Instrument based Gateways
- Data Centric Gateways
- Educational Gateways
- Ultrascan, IU Electron Microscopy Center
- SearchingSRA
- GeoGateway (NASA INSARS and GNSS joint image data analysis)
- AD3C Alzheimer's Disease Drug Discovery Center Data Sharing Platform (cf. https://osf.io/zcywr/)
- Simvascular
## Our Collaborators and Clients

### Domain and Application Gateways

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

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<tr>
<td>University of South Dakota</td>
<td>Chemistry &amp; Bio</td>
</tr>
<tr>
<td>Indiana University Bloomington</td>
<td>Generic Applications</td>
</tr>
<tr>
<td>Georgia Tech HIVE Gateway</td>
<td>Generic Applications</td>
</tr>
<tr>
<td>Oklahoma University</td>
<td>Chemistry &amp; Engineering</td>
</tr>
<tr>
<td>Georgia State University</td>
<td>Generic Applications</td>
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<tr>
<td>University of Alabama Birmingham</td>
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<tr>
<td>New Mexico State University</td>
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<td>West Virginia State University</td>
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<tr>
<td>University of Kentucky Science Gateway</td>
<td>Generic Applications</td>
</tr>
<tr>
<td>South Dakota State University Gateway</td>
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</tbody>
</table>

[https://circ.iu.edu/collaborations.html](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

```bash
#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

```bash
#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.