On Enabling Hydrodynamics Data Analysis of Analytical Ultracentrifugation Experiments

Outline

- Background
- Ultrascan Application
- Ultrascan Software Components
- Airavata: Science Gateway Framework
- Current Architecture - Identified Limitations
- Integrated Architecture
- Conclusions
Science gateways have emerged as a lightweight layer for accessing distributed and heterogeneous computational and data resources.

They offer users with easy access to perform science without knowing underlying details of their remote application runs.

Many scientific communities are motivated for providing user-facing scientific gateways to their researchers.
EGI and XSEDE Impressions

“The most popular and most rapidly developing tools used by EGI communities to interact with the European Grid Infrastructure” [egi.eu]

“Gateways enable entire communities of users associated with a common discipline to use national resources through a common interface that is configured for optimal use.” [xsede.org]
The Scientific Case: Ultrascan 3 (US3)

- US3 interprets complex data coming from high resolution analytical ultracentrifugation (AUC) experiments using sedimentation velocity centrifugation methods.

- It provides better understanding of biological macromolecules and synthetic polymers that allows in the investigation of structural relationships of biological systems in many diseases such as different kind of cancers.

- Users can fit their experiments using a 2-dimensional spectrum analysis, genetic algorithm optimization and Monte Carlo analysis to obtain fine grained details and analyze noise components in the data.
Image Courtesy: Institute of Physical Biology, Universität Düsseldorf
Ultrascan Application – US3

- An open source analysis and modeling software suite for biophysicists, biochemists, and material scientists

- US3 is an OpenAUC based analysis environment for analytical ultracentrifugation (AUC) experiments

- US3 provides an interface to manage data before and after AUC analysis
US3 Software Components

- MPI Data analysis package
  - Installed on HPC resources
- US-LIMS (Laboratory Information and Management System)
  - Scientific Gateway to the Ultrascan3 deployments
  - A web-based interface for collaboration, analysis job submission to remote HPC resources
  - Manage all data related to AUC analysis
  - Manage users and roles
- Desktop visualization and analysis package
  - Client side visualization suite
  - Data editing (preprocessing/cleaning)
  - Package Optimization
  - Finite Element Modeling
US-LIMS Gateway Architecture
What Is Apache Airavata?

- Science Gateway software system to
  - Compose, manage, execute, and monitor distributed, computational workflows
  - Wrap legacy command line scientific applications with Web services.
  - Run jobs on computational resources ranging from local resources to computational grids and clouds

Courtesy: Marlon Pierce, OSG All Hands 2013
## Apache Airavata

<table>
<thead>
<tr>
<th>Domain</th>
<th>Description</th>
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<tbody>
<tr>
<td>Astronomy</td>
<td>Image processing pipeline for One Degree Imager instrument on XSEDE</td>
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<tr>
<td>Astrophysics</td>
<td>Supporting workflow of Dark Energy Survey simulations working group on XSEDE</td>
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<td>Bioinformatics</td>
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<td>Manage large scale data analysis of analytical ultracentrifugation experiments on XSEDE and campus resources</td>
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Apache Airavata Architecture

End Users

Gateway Developer

Scientific Application

Core Developer

Message Box

Workflow Interpreter

Registry

Application Factory (GFAC)

Computational Resources

 Courtesy: Marlon Pierce, OSG All Hands 2013
Current Architecture
Evolved Architecture
Integrated Architecture

1. AuthN: Username & Password (local login)
   US-LIMS (browser)

2. Manual end-user choice
   Instrument Input
   US-LIMS (PHP)

3. Apache Airavata System
   @ UoIndiana

4. Workflow Interpreter
   GridFTP Server & Staging File System

5. Credential Service
   Previously Created ID

6. ID retrieval
   data stagings

7. GridFTP Client
   UNICORE BES/JSIDL Client Classes Plugin

8. AuthN (X.509 SLC)
   UNICORE Gateway

9. MyProxy Protocol
   OAuth Protocol
   MyProxy (CA)
   Previously Created ID (IGTF Certificate)

10. AuthZ
    UNICORE/X
    OGSA-BES (JSIDL)

11. Ultrascan3 Application
    Module environment

12. GridFTP Client
    JUROPA File System

13. HPC Resource
    Grid access

Servers
@ JSC

Scientific Gateway
Client & User
JUROPA

- **JUROPA** (Jülich Research on Petaflop Architectures)
- Computing Power: 207 teraflops
- Processor Nodes: 2208 with two processors each
- Processor Type: Intel Xeon X5570 quad core, 2.93 GHz
- Batch System: Moab / Torque
- Middleware: UNICORE
Conclusions and Future Work

- Implementation is under production testing by Airavata Team
- Besides JUROPA deployment this implementation has also been proposed as a pilot activity in XSEDE
- Push based job status notifications to Gateway users
- Better integration with OAuth4MP to support individuals
- Improper handling of community (pooled) accounts
- Introduce UNICORE file transfer mechanisms (ByteIO, UFTP) - complimentary to GridFTP
- Enable other science gateways to use UNICORE through Apache Airavata framework (ParamChem, GridChem, CIPRES, NeroScience, etc.)
References

- Borries Demeler et al., *Ultrascan Gateway Enhancements*, Terarid ’11, Salt Lake City, Utah, USA
- Apache Airavata: [http://airavata.apache.org](http://airavata.apache.org)
Questions?