Open community software: Building science gateways and workflows

Marlon Pierce, Suresh Marru
Science Gateway Group
Research Technologies, UITS
November 16, 2012
Science Gateway Challenges

• Science Gateways are user environments for interacting with computing resources.
• Gateways can be built in many ways
  • Can run on desktops.
  • Can run in Web browsers.
  • Can use every Web technology known to humanity.
• Science Gateways need to do many things.
  • Run jobs on supercomputers.
  • Add value to online data collections.
  • Support collaborations
• Many gateways are powered by scientific workflows.
• Service oriented software allows us to work with many different gateways.
Apache Airavata

• Science Gateway software framework to:
  — Compose, manage, execute, and monitor 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
# Apache Airavata Components

<table>
<thead>
<tr>
<th>Component</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>XBaya</td>
<td>Workflow graphical composition tool.</td>
</tr>
<tr>
<td>Registry Service</td>
<td>Insert and access application, host machine, workflow, and provenance data.</td>
</tr>
<tr>
<td>Workflow Interpreter Service</td>
<td>Execute the workflow on one or more resources.</td>
</tr>
<tr>
<td>Application Factory Service (GFAC)</td>
<td>Manages the execution and management of an application in a workflow</td>
</tr>
<tr>
<td>Airavata API</td>
<td>Single wrapping client to provide higher level programming interfaces.</td>
</tr>
</tbody>
</table>
Can I Contribute to Apache Airavata?

• Absolutely…
• Join the mailing list and find out what needs to be done: dev@airavata.apache.org.
• Check out the Airavata Jira
• Learn the Apache Way.
• Get voted into the project as a committer and PMC member.
Apache Rave Overview

Rave is an Apache Top Level Project for building a Web portal on the Open Social and W3C Widget specifications.

- Initially, joint effort of Mitre, Hippo Software, SURFnet, and the OGCE project
- Several new members added to PMC

Goal 1: Provide a useable, packaged, downloadable OpenSocial portal.

- Get started with minimal hassle.

Goal 2: Provide a platform for non-invasive developer extensions, customizations

- Science gateways, for example
Rave Building Blocks

Rave is implemented in JavaScript, Java with Spring MVC

- Bean initialization specified in XML configuration files.
- Inversion of Control makes it easy to swap out implementations.
- Disciplined MVC through Java annotations

Builds on Apache Shindig and Wookie

- Provide layout management, user management, administration tools, production backend data systems, etc.
Open Source Software, Open Communities
Open Community Software and Governance

• Open source projects need governance.
• Incentives for projects to diversify their developer base.
• Govern how
  • Software is released
  • Contributions are handled.
  • Credit is shared.
• Our approach: Apache Software Foundation

Compete
Collaborate
Can I Get Some Help Building Gateways?

XSEDE Extended Collaborative Support Services
<table>
<thead>
<tr>
<th>RESOURCE NAME</th>
<th>SITE</th>
<th>MANUFACTURER</th>
<th>MACHINE</th>
<th>PEAK TERAFLIPS</th>
<th>DISK SIZE (TB)</th>
<th>LINKS</th>
<th>AVAILABILITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wispy</td>
<td>Purdue U</td>
<td>HP DL140g3</td>
<td>Cluster</td>
<td>0.0</td>
<td>0.0</td>
<td>User Guide</td>
<td>Production through 2013-07-31</td>
</tr>
<tr>
<td>Gordon</td>
<td>SDSC</td>
<td>Appro</td>
<td>Cluster</td>
<td>0.0</td>
<td>4000.0</td>
<td>User Guide</td>
<td>Production through 2015-03-01</td>
</tr>
<tr>
<td>Ranger</td>
<td>TACC</td>
<td>Sun Constellation System</td>
<td>Cluster</td>
<td>579.3</td>
<td>1730.0</td>
<td>User Guide</td>
<td>Production through 2013-02-04</td>
</tr>
<tr>
<td>Kraken-XT5</td>
<td>NICS</td>
<td>Cray XT5</td>
<td>MPP</td>
<td>1174.0</td>
<td>2400.0</td>
<td>User Guide</td>
<td>Production through 2014-04-01</td>
</tr>
<tr>
<td>Lonestar4</td>
<td>TACC</td>
<td>Dell PowerEdge Westmere Linux Cluster</td>
<td>Cluster</td>
<td>302.0</td>
<td>1000.0</td>
<td>User Guide</td>
<td>Production through 2014-01-31</td>
</tr>
<tr>
<td>Keeneland KIDS</td>
<td>Georgia Tech</td>
<td>HP and NVIDIA</td>
<td>Cluster</td>
<td>0.0</td>
<td>0.0</td>
<td>User Guide</td>
<td>Production through 2014-08-31</td>
</tr>
<tr>
<td>Steele</td>
<td>Purdue U</td>
<td>Dell 1950</td>
<td>Cluster</td>
<td>66.59</td>
<td>130.0</td>
<td>User Guide</td>
<td>Production through 2013-07-31</td>
</tr>
<tr>
<td>Gordon Compute Cluster</td>
<td>SDSC</td>
<td>Appro</td>
<td>Cluster</td>
<td>341.0</td>
<td>4000.0</td>
<td>User Guide</td>
<td>Production through 2015-03-01</td>
</tr>
<tr>
<td>Trestles</td>
<td>SDSC</td>
<td>Appro</td>
<td>Cluster</td>
<td>100.0</td>
<td>140.0</td>
<td>User Guide</td>
<td>Production through 2014-06-30</td>
</tr>
<tr>
<td>Quarry</td>
<td>Indiana U</td>
<td>Dell AMD</td>
<td>SMP</td>
<td>0.0</td>
<td>335.0</td>
<td>User Guide</td>
<td>Production through 2016-06-30</td>
</tr>
<tr>
<td>Stampede</td>
<td>UT Austin</td>
<td>Dell Power Edge C8220 Cluster with Intel Xeon Phi coprocessors</td>
<td>Cluster</td>
<td>9000.0</td>
<td>14336.0</td>
<td>Typing Soon</td>
<td></td>
</tr>
<tr>
<td>Blacklight</td>
<td>PSC</td>
<td>SGI UV 1000 cc-NUMA</td>
<td>SMP</td>
<td>36.0</td>
<td>150.0</td>
<td>User Guide</td>
<td>Production through 2013-06-30</td>
</tr>
<tr>
<td>Keeneland</td>
<td>Georgia Tech</td>
<td>HP and NVIDIA</td>
<td>Cluster</td>
<td>615.0</td>
<td>0.0</td>
<td>User Guide</td>
<td>Production through 2014-08-31</td>
</tr>
</tbody>
</table>
XSEDE ECSS Science Gateways Program

Mission/purpose

- Science Gateways enable communities of users associated with a common discipline to use computational resources through a familiar and simpler interface.
- The missions of the Extended Support for Science Gateway (ESSGW) Group is to provide Extended Collaborative Support to existing and new Scientific Communities in developing, enhancing and maintaining Science Gateways in effectively using XSEDE Computational Resources.
- Outreach to potential communities and help fostering new gateways.
- Engage the gateway community through forums & discussions.
ECSS Gateway Examples

- Implementation of new workflows for automation of scientific processes
- Incorporation of new visualization methods
- Innovative scheduling implementation
- Integration of XSEDE resources into a portal or Science Gateway
- Move data from gateway to XSEDE resources
- Bridge Campus Resources with XSEDE through a gateway
Contact Information

- Marlon Pierce: marpierc@iu.edu
- Suresh Marru: smarru@iu.edu
- Science Gateway Group Website: http://pti.iu.edu/sgg
- Apache Airavata: http://airavata.apache.org
- Apache Rave: http://rave.apache.org
Indiana University Science Gateway Group