Connecting people and resources to accelerate discovery by empowering the science gateway community

Apache Airavata Open Source Framework

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Award Number
ACI-1547611
History of Airavata - LEAD
What Does Apache Airavata Do?

- Airavata runs computational experiments
- This means
  - Encoding how to run a wide range of scientific applications on a wide range of resources
  - Staging inputs and outputs to target resources
  - Monitoring long running applications
- And most importantly...
  - Managing all the data and metadata generated by these experiments
Job submission - API Server

- PHP Gateway
- Airavata API Service
- Registry Service
- Registry DB

- Thrift IDL
  - PHP
  - Java
  - C++
  - Py

createExperiment(AuthzToken, ExperimentModel)
launchExperiment(AuthzToken, experimentId)

Experiment Launch queue
Job submission - Orchestrator

Process
- Working directory
- Stage in
- Submit job
- Monitor
- Stage out

Orchestrator

Registry Service
- Registry DB

Experiment Launch queue

Process Launch queue
Job submission - GFac

- Process Launch queue
- Working directory
- Stage in
- Submit job
- Monitor
- Stage out

GFac

Update Experiment

Registry Service

Application Catalog

Registry DB

SSH

SCP

Compute Resources

Email Server
PGA – reference implementation
Security - Keycloak
Security – Keycloak + CILogon
Security – Credential Store

SSH Keys

Generate New SSH Key

Description: Generate

SimVascular Key for Comet

ssh-rsa AAAAB3NzaC1yc2EAAAADAQABAAQABQCBbarPpARgkLBywP8v2LIO7UrvK2MZ Copy Delete

stampede2 Key

ssh-rsa AAAAB3NzaC1yc2EAAAADAQABAAABAAQCAQ+bDeGrNlQHblUJH2L2kRmLTcN4In8 Copy Delete

New Gateway Key

ssh-rsa AAAAB3NzaC1yc2EAAAADAQABAAABAAQCFgLWSw6MftPbkeSyzPMxgT50cNe5 Copy Delete

Scratch Location

Allocation Project Number

Resource Specific Credential Store Token

Select a Credential Token from Store

SimVascular Key for Comet
stampede2 Key
New Gateway Key

DO-NO-SET
Sharing service

Entity

Sharing

Group

Permission
Scaling Airavata

- Multi-tenancy – can run several gateways on the same installation of Airavata services
- DevOps – Ansible scripts automate deployment and updates of gateways
Science Gateways built on Airavata
Some Gateway Types

Software as a Service Gateways
- Broaden access to your scientific software
- Simplify user support

Domain Gateways
- Provide access to many tools across a scientific domain
- Integrate many different computing resources

Campus Gateways
- Simplify and broaden access to campus resources
- Bridge between campus, regional, and national resources

Classroom Gateways
- Deliver scientific applications to students
- Create and share Airavata experiments

Apache Airavata provides a platform for these types of gateways
dREG: discriminative Regulatory Element detection from GRO-seq

- Prof. Charles Danko and Dr. Zhong Wang, Cornell
- dREG: Identification of the genomic regions that regulate transcription
  - Genetic basis of many diseases
- Code is actively developed
- You may not have local resources for running it.
  - Traditional MPI and GPU versions
dREG: Software as a Service

- Instead of requiring users to download and install the code, deliver it through a gateway.

And integrate third party Web tools
SEAGrid – Science Domain Gateway
University of South Dakota Campus Gateway

• Provide simplified access to campus computing resources
• Use campus identities all the way through (no community accounts)
• Simplify bridging between campus resources and XSEDE.

Welcome to research computing at the University of South Dakota!
SimVascular – Classroom Gateway

Welcome to SimVascular Supercomputing Gateway! Our gateway provides access to high performance computer clusters for SimVascular users who would like to run simulation with super computing (10x faster than desktop). The svSolver needed for running simulation is already setup and ready to use from the computer clusters. Through the gateway, SimVascular users just simply create simulation jobs, upload input/data files, launch simulation, and download results once the simulation is finished. There is no hassle for users to compile or setup svSolver. Detailed instructions about how to use the gateway are provided here.

SimVascular is an open source integrated software suite for image-based cardiovascular modeling and patient-specific simulation, providing a complete pipeline from medical image visualization/segmentation, 3D model construction, meshing, to blood flow simulation and hemodynamics analysis. It is recommended that new users to SimVascular first go through SimVascular Documentation Website to understand the workflow in SimVascular. With SimVascular, users can create input/data files for simulation and upload to the gateway.

Usage Policy
SimVascular Supercomputing Gateway is mainly for educational purpose. Only users from American institutions can be granted access after approval.

Contact us
SimVascular News Mailing List:
Sign up • Archive
SimVascular Public Forum
Suggest new features or report bugs
Make a Donation
Powered by Apache Airavata
Airavata as a Platform

- Django Portal
- Helix based task execution
- Group based authorization
Django Portal

Portal Page

Dynamic UI

Cust UI Comp

Django

REST API

Python High level API

Airavata API Client

Airavata Middleware

Web Browser

Web Server
Custom UI Components

Image credit: leafletjs.com website

Image credit: jmol.sourceforge.net website
Helix-based Task Execution
Group-based Authorization

• Currently, authorization based on statically defined roles

• Group-based authorization gives gateway admins more fine-grained control

• But also opens the door to allowing users to share resources and applications with other users
Conclusion

• Apache Airavata has been used as the basis for several kinds of gateways

• If you are interested in an Airavata gateway, we’re here to help

• Get involved! Help shape the future of Airavata by contributing feedback and code.
More Information

• Science Gateways Research Center
  • [https://sgrc.iu.edu/](https://sgrc.iu.edu/)

• Apache Airavata Open Source Science Gateway Software
  • Create a free demo account at [https://testdrive.airavata.org](https://testdrive.airavata.org)
  • Request a gateway at [https://scigap.org](https://scigap.org)

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