Scientific Computing Without the Command Line: Enabling Any HPC Code to Run Anywhere through a Web Interface with the Agave API

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What is a Science Gateway?

Normally, it means a web interface used to run a complex scientific application on a high performance computer.

More formally:

A Science Gateway is a community-developed set of tools, applications, and data that are integrated via a portal or a suite of applications, usually in a graphical user interface, that is further customized to meet the needs of a specific community. 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. Researchers can focus on their scientific goals and less on assembling the cyberinfrastructure they require. Gateways can also foster collaborations and the exchange of ideas among researchers. (quoted from https://www.xsede.org/gateways-overview)
What is Agave?

- The Agave Platform (http://agaveapi.co) is an open source, science-as-a-service API platform for powering your digital lab.

- Agave allows you to bring together your public, private and shared high performance computing (HPC), high throughput computing (HTC), cloud and Big Data resources under a single friendly REST API.
How does Agave work

Agave works by using a REST api and use JSON to format data.

What do the words JSON and REST mean?

1. What is JSON? JSON (JavaScript Object Notation) is a lightweight data-interchange format. It is easy for humans to read and write. It is easy for machines to parse and generate. It is based on a subset of the JavaScript Programming Language, Standard ECMA-262 3rd Edition - December 1999. JSON is a text format that is completely language independent but uses conventions that are familiar to programmers of the C-family of languages, including C, C++, C#, Java, JavaScript, Perl, Python, and many others. These properties make JSON an ideal data-interchange language (quoted from http://www.json.org/). Essentially, this is just a standard way to format data. You don't need to learn it, but you can.

2. What is REST? Representational state transfer (REST) or RESTful Web services are one way of providing interoperability between computer systems on the Internet. REST-compliant Web services allow requesting systems to access and manipulate textual representations of Web resources using a uniform and predefined set of stateless operations. (quoted from https://en.wikipedia.org/wiki/Representational_state_transfer)
What Capabilities does Agave provide?

- Run code
- Manage data
- Collaborate meaningfully
- Integrate anywhere
Setup Shelob Account

- Before we can run an Agave app we need to setup our Shelob training account.

- All training accounts begin with “hpctrn” and end in two numbers starting at “01” and ending with “14” inclusive

- I am using “hpctrn15”
Shelob setup

- To set your account up you need to copy the following files into your account.
- So login to Shelob using one of the SSH clients
- Type into your terminal window
  - `ssh hpctrn15@shelob.hpc.lsu.edu`
- You will see:
  - `hpctrn15@shelob.hpc.lsu.edu's password:`
- Type in `f=ma&one23four`
Shelob Setup

- There are three files we need to work with (already in your account:
  - input.txt
  - drawgau.cpp
  - drawgau-wrapper.txt
Shelob setup

- The C++ code has been compiled using the command:

- `mpic++ -o drawgau -std=c++11 drawgau.cpp`
Getting Started

- To get started go to the Agave web page and create an account.
- Visit https://togo.agaveapi.co/
- Then choose the “Create Account” link from the upper right corner of the “Agave Platform” box
Create an Agave App

- Back to working with Agave TOGO to run our job
This is the Create account and login page.
Be sure to choose the “Agave Public Tenant” by clicking on the logo.
Finish Account

- Finish creating your account by filling in required information
- Go to your dashboard
Introducing the new Agave ToGo!

Agave ToGo v2 is a full-featured web application designed to show off core functionality you are familiar with in the Agave Platform as well as demonstrate some of the advanced use cases which are possible leveraging the core Agave Core Science APIs.

This application is meant to serve as a reference from which you can build your own application. Feel free to fork this repository and edit as needed. To contribute back enhancement and bug fixes, please fork the repository and submit a pull request.
The left side of the dashboard

This is where we will do our work!
Explore Dashboard

- The left side of the dashboard is where you will find the links to the pages needed to create your own mini-gateway.

- We will visit the Systems, Apps and Jobs pages as these pages are the ones we will use.
Create the Systems Needed

- We will first create the Storage System description
- Then create the Execution System description
- Use the Dashboard and choose the Systems item
The left side of the dashboard
Click on the “Systems” link
This will take you to the page where
you will create your execution and storage systems
# Systems

Manage your collection of systems

## System Management

- **ID**: condor.opensciencegrid.org
  - **Name**: Open Science Grid
  - **Type**: EXECUTION
  - **Actions**: View Actions

- **ID**: data.agaveapi.co
  - **Name**: Agave Cloud Storage
  - **Type**: STORAGE
  - **Actions**: View Actions

- **ID**: docker.tacc.utexas.edu
  - **Name**: Demo Docker VM
  - **Type**: EXECUTION
  - **Actions**: View Actions

- **ID**: ktrashler-qb
  - **Name**: QB at LONI
  - **Type**: EXECUTION
  - **Actions**: View Actions

- **ID**: qb-ktrashler
  - **Name**: qb (ktrashler)
  - **Type**: EXECUTION
  - **Actions**: View Actions

- **ID**: qb-storage-ktrashler
  - **Name**: qb storage (ktrashler)
  - **Type**: STORAGE
  - **Actions**: View Actions

- **ID**: shelob-sbrandt
  - **Name**: Shelob LSU (sbrandt)
  - **Type**: EXECUTION
  - **Actions**: View Actions

[+ New System button]
Choose storage from the window above.

Click on menu and choose storage for your system.
SYSTEM EDITOR WIZARD - STEP 2 OF 2

1. Type
   - shelob-storage-hpctrn20
2. Details
   - Name: Shelob at LSU
   - Status: UP
   - Description: The Shelob supercomputer at LSU
   - Site: hpc.lsu.edu
3. Connectivity
   - "owner": "ktraxler",
   - "available": true,
   - "description": "The Shelob supercomputer at LSU",
   - "storage": {
     "proxy": null,
     "protocol": "SFTP",
     "mirror": false,
     "port": 22,
     "auth": {
       "type": "PASSWORD"
     },
   },
   - "publicAppsDir": null,
   - "host": "shelob.hpc.lsu.edu",
   - "rootDir": "/",
   - "homeDir": "/home/hpctrn20",
   - "proxyTunnel": "NO"
### System Editor Wizard - Step 3 of 2

#### Storage

**Protocol**
- SFTP

**Host**
- shelob.hpc.lsu.edu

**System Auth Server Port**
- 22

**Root Directory**
- /

**Home Directory**
- /home/hpctmn20

**Proxy Tunnel**
- NO

```json
{
    "owner": "ktraxler",
    "available": true,
    "description": "The Shelob supercomputer at LSU",
    "storage": {
        "proxy": null,
        "protocol": "SFTP",
        "mirror": false,
        "port": 22,
        "auth": {
            "type": "PASSWORD",
            "username": "ktraxler",
            "password": "#SSdalejr#88amp2017"
        },
        "publicAppsDir": null,
        "host": "shelob.hpc.lsu.edu",
        "rootDir": "/",
        "homeDir": "/home/hpctmn20",
        "proxyTunnel": "NO"
    },
    "type": "STORAGE",
    "site": "hpc.lsu.edu",
    "default": false,
    "public": false,
    "globalDefault": false,
    "name": "Shelob at LSU",
    "id": "shelob-storage-hpctmn20",
    "status": "UP"
}
```
System Auth Server Port

22

Root Directory

/

Home Directory

/home/hpctrn20

Proxy Tunnel

NO

Storage Authentication

Type

PASSWORD

Username

hpctrn20

Password

**********
System Builder Wizard

You have successfully created your system

ID: shelob-storage-hpctm20
Name: Shelob at LSU
Status: UP
Type: STORAGE
Description: The Shelob supercomputer at LSU

Close | Browse Systems
<table>
<thead>
<tr>
<th>Name</th>
<th>Size</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>.gnome2</td>
<td>4KB</td>
<td>3 days ago</td>
</tr>
<tr>
<td>.mozilla</td>
<td>4KB</td>
<td>3 days ago</td>
</tr>
<tr>
<td>.pki</td>
<td>4KB</td>
<td>8 hours ago</td>
</tr>
<tr>
<td>.ssh</td>
<td>4KB</td>
<td>9 hours ago</td>
</tr>
<tr>
<td>.subversion</td>
<td>4KB</td>
<td>3 days ago</td>
</tr>
<tr>
<td>agave-deployment</td>
<td>4KB</td>
<td>2 hours ago</td>
</tr>
<tr>
<td>drawgau</td>
<td>4KB</td>
<td>7 hours ago</td>
</tr>
<tr>
<td>.bash_history</td>
<td>28.1KB</td>
<td>a few seconds ago</td>
</tr>
<tr>
<td>.bash_history3</td>
<td>364B</td>
<td>6 hours ago</td>
</tr>
<tr>
<td>.bash_logout</td>
<td>18B</td>
<td>3 days ago</td>
</tr>
<tr>
<td>.bash_profile</td>
<td>176B</td>
<td>3 days ago</td>
</tr>
<tr>
<td>.bashrc</td>
<td>124B</td>
<td>3 days ago</td>
</tr>
<tr>
<td>.emacs</td>
<td>500B</td>
<td>3 days ago</td>
</tr>
</tbody>
</table>
### System Management

- **ID**
- **Name**
- **Type**
- **Actions**

<table>
<thead>
<tr>
<th>ID</th>
<th>Name</th>
<th>Type</th>
<th>Actions</th>
</tr>
</thead>
<tbody>
<tr>
<td>condor.opensciencegrid.org</td>
<td>Open Science Grid</td>
<td>EXECUTION</td>
<td>Actions</td>
</tr>
<tr>
<td>data.agaveapi.co</td>
<td>Agave Cloud Storage</td>
<td>STORAGE</td>
<td>Actions</td>
</tr>
<tr>
<td>docker.tacc.utexas.edu</td>
<td>Demo Docker VM</td>
<td>EXECUTION</td>
<td>Actions</td>
</tr>
<tr>
<td>ktraxler-qb</td>
<td>QB at LONI</td>
<td>EXECUTION</td>
<td>Actions</td>
</tr>
<tr>
<td>qb-ktraxler</td>
<td>qb (ktraxler)</td>
<td>EXECUTION</td>
<td>Actions</td>
</tr>
<tr>
<td>qb-storage-ktraxler</td>
<td>qb storage (ktraxler)</td>
<td>STORAGE</td>
<td>Actions</td>
</tr>
<tr>
<td>shelob-sbrandt</td>
<td>Shelob LSU (sbrandt)</td>
<td>EXECUTION</td>
<td>Actions</td>
</tr>
</tbody>
</table>
Choose Execution this time
<table>
<thead>
<tr>
<th>ID</th>
<th>shelob-execu-hpctrn20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>Shelob supercomputer at LSU</td>
</tr>
<tr>
<td>Status</td>
<td>UP</td>
</tr>
<tr>
<td>Description</td>
<td>Shelob supercomputer at LSU</td>
</tr>
<tr>
<td>Site</td>
<td>hpc.lsu.edu</td>
</tr>
<tr>
<td>Execution Type</td>
<td>HPC</td>
</tr>
<tr>
<td>Scheduler</td>
<td>TORQUE</td>
</tr>
<tr>
<td>Maximum System Jobs</td>
<td>50</td>
</tr>
</tbody>
</table>

```json
{
    "maxSystemJobs": 50,
    "executionType": "HPC",
    "available": true,
    "description": "Shelob supercomputer at LSU",
    "storage": {
        "proxy": null,
        "protocol": "SFTP",
        "mirror": false,
        "port": 10,
        "auth": {
            "type": "PASSWORD"
        },
        "host": "shelob.hpc.lsu.edu",
        "rootDir": "/",
        "homeDir": "/home/hpctrn20",
        "proxyTunnel": "NO"
    }
}
```
Scheduler

TORQUE

Maximum System Jobs

50

Scratch Directory

/work/hpctrn20/

Work Directory

/work/hpctrn20/

Environment

Startup Script

Queues

Name

shelob

Arbitrary name for the queue. This will be used in the job submission process, so it should line up with the name of an actual queue on the execution system

Maximum Jobs

20
### Queues

<table>
<thead>
<tr>
<th>Name</th>
<th>shelob</th>
</tr>
</thead>
</table>

Arbitrary name for the queue. This will be used in the job submission process, so it should line up with the name of an actual queue on the execution system.

**Maximum Jobs**

| Value | 20 |

Maximum number of jobs that can be queued or running within this queue at a given time. Defaults to 10. -1 for no limit.

**Maximum Nodes**

| Value | 203 |

Maximum number of nodes that can be requested for any job in this queue. -1 for no limit.

**Maximum Memory Per Node**

| Value | 64GB |

Maximum memory per node for jobs submitted to this queue in ###.[EIPITIG]B format.

**Maximum Processors Per Node**

| Value | |

Maximum Memory Per Node

64GB

Maximum memory per node for jobs submitted to this queue in ###.###EIPITIG format

Maximum Processors Per Node

16

Maximum number of processors per node that can be requested for any job in this queue. -1 for no limit

Maximum Requested Time

72:00:00

Maximum run time for any job in this queue given in hh:mm:ss format

Custom directive

Arbitrary text that will be appended to the end of the scheduler directives in a batch submit script. This could include a project number, system-specific directives, etc

Default

True if this is the default queue for the system, false otherwise.
can be requested for any job in this queue. -1 for no limit

Maximum Requested Time

72:00:00

Maximum run time for any job in this queue given in hh:mm:ss format

Custom directive

Arbitrary text that will be appended to the end of the scheduler directives in a batch submit script. This could include a project number, system-specific directives, etc

Default

True if this is the default queue for the system, false otherwise

+ Add

Previous  Next  Submit
System Auth Server Port
10
Root Directory
/
Home Directory
/home/hpctrn20
Proxy Tunnel
NO

Storage Authentication
Type
PASSWORD
Username
hpctrn20
Password

```
{  
  "maxNodes": 203,
  "maxProcessorsPerNode": 16,
  "mappedName": null,
  "maxUserJobs": -1,
  "customDirectives": null
  },
  "globalDefault": false,
  "name": "Shelob supercomputer at LSU",
  "status": "UP",
  "scratchDir": "/work/hpctrn20/"
}
```
System Builder Wizard

You have successfully created/updated your system

ID: shelob-execu-hpctrn20

Name: Shelob supercomputer at LSU

Status: UP

Type: EXECUTION

Description: Shelob supercomputer at LSU

Close  Browse Files  Create App
### File Browser

**Shelob at LSU**

<table>
<thead>
<tr>
<th>Name</th>
<th>Size</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>.gnome2</td>
<td>4KB</td>
<td>3 days ago</td>
</tr>
<tr>
<td>.mozilla</td>
<td>4KB</td>
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<td>.pki</td>
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</tr>
<tr>
<td>.subversion</td>
<td>4KB</td>
<td>3 days ago</td>
</tr>
<tr>
<td>agave-deployment</td>
<td>4KB</td>
<td>2 hours ago</td>
</tr>
<tr>
<td>drawgau</td>
<td>4KB</td>
<td>7 hours ago</td>
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<tr>
<td>.bash_history</td>
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</tr>
<tr>
<td>.emacs</td>
<td>500B</td>
<td>3 days ago</td>
</tr>
</tbody>
</table>
### Apps Management

Manage your collection of apps.

#### Apps

<table>
<thead>
<tr>
<th>ID</th>
<th>Name</th>
<th>Version</th>
<th>Label</th>
<th>Short Description</th>
<th>Exec. System</th>
<th>Public</th>
<th>Revision</th>
<th>Last Modified</th>
<th>Actions</th>
</tr>
</thead>
<tbody>
<tr>
<td>drawgauktraxler-0.1.0</td>
<td>drawgauktraxler</td>
<td>0.1.0</td>
<td>draw curve</td>
<td>gaussian curve</td>
<td>qbe-exektraxler</td>
<td>false</td>
<td>1</td>
<td>2 days ago</td>
<td>Actions</td>
</tr>
<tr>
<td>shelle-runnerrunner-0.1.0</td>
<td>shelle-runnerrunner</td>
<td>0.1.0</td>
<td>Execute a command at a shell</td>
<td>This will execute whatever command you give in the command parameter</td>
<td>qbe-exektraxler</td>
<td>false</td>
<td>4</td>
<td>2 days ago</td>
<td>Actions</td>
</tr>
<tr>
<td>ccloud-runnerrunner-0.1.0u1</td>
<td>ccloud-runnerrunner</td>
<td>0.1.0</td>
<td>Run your code in the cloud</td>
<td>Generic template for running arbitrary code in Agave's Dockerized cloud</td>
<td>docker.tacc.utexas.edu</td>
<td>true</td>
<td>1</td>
<td>5 months ago</td>
<td>Actions</td>
</tr>
<tr>
<td>jfonner-forkjfonner-fork-1.0</td>
<td>jfonner-fork</td>
<td>1.0</td>
<td>Remote command execution script</td>
<td>Simple app for running a user-defined command on a remote system</td>
<td>stampedefonner</td>
<td>false</td>
<td>1</td>
<td>5 months ago</td>
<td>Actions</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>Cactus</td>
<td>Solves PDEs</td>
<td>shellob</td>
<td>false</td>
<td>3</td>
<td>5 months ago</td>
<td>Actions</td>
</tr>
</tbody>
</table>

Click the + New App button to add a new app.
You can re-use an existing App definition template and provide your own Name and Dependencies:

**APP BUILDER WIZARD - STEP 1 OF 6**

**1 Basics**

**Name**
- **shell-runner**

The name of the application. The name does not have to be unique, but the combination of name and version does.

**Version**
- 0.1.0

The version of the application in ### format. While the version does not need to be unique, the combination of name and version does have to be unique.

**Label**
- Execute a command at a shell

Label for use in forms generated by the jobs service
App Edit Wizard

Basics

Name

drawgau2-shelob-hpcptr20

The name of the application. The name does not have to be unique, but the combination of name and version does.

Version

0.1.0

The version of the application in `##.##` format. While the version does not need to be unique, the combination of name and version does have to be unique.

Label

Drawgau

Label for use in forms generated by the jobs service

Short description

draw curve

Short description of this app

Long description

Draw Gaussian Curve (points only)

Dependencies

Environment

Params


Short description

- draw curve

Short description of this app

Long description

- Draw Gaussian Curve (points only)

Full description of this app

Tags

- execute
- awesome
- demo

Array of terms you may associate with this app

Help URL

http://developer.agaveapi.co/

The URL where users can go for more information about the app.

Ontology

```json
{
  "awesome",
  "demo",
  "executionType": "HPC",
  "executionSystem": "shelob-exec-hpctrn20",
  "deploymentPath": "agave-deployment",
  "deploymentSystem": "shelob-storage-hpctrn20",
  "templatePath": "drawgau-wrapper.txt",
  "testPath": "test.txt",
  "checkpointable": false,
  "modules": [],
  "inputs": [
    {
      "id": "parfile",
      "value": {
        "validator": "",
        "visible": true,
        "required": true,
        "order": 0,
        "enquote": false,
        "default": "input.txt"
      },
      "details": {
        "label": "input for the program",
        "description": null,
        "argument": "input.txt",
        "showArgument": false,
        "repeatArgument": false
      },
      "semantics": {
        "minCardinality": 1,
        "maxCardinality": 1,
        "ontology": [],
        "fileTypes": []
      }
    }
  ]
}
```
Array of terms you may associate with this app

Help URL

http://developer.agaveapi.co/

The URL where users can go for more information about the app.

Ontology

- **ontology**: execute
- **ontology**: awesome
- **ontology**: demo

An array of ontology terms describing this app.

Previous  Next  Submit

```json
{
  "description": "Hello",
  "argument": "input.txt",
  "showArgument": false,
  "repeatArgument": false
}

"semantics": {
  "minCardinality": 1,
  "maxCardinality": 1,
  "ontology": [],
  "fileTypes": []
}

"parameters": [],
"outputs": [
  
}
```
Deployment path

```
agave-deployment
```

The path to the folder on the deployment system containing the application wrapper and dependencies.

Deployment system

```
shelob-storage-hpctrn20
```

The ID of the storage system where this app's assets should be stored.

Wrapper script

```
drawgau-wrapper.txt
```

The path to the wrapper script relative to the deploymentPath.

Test script

```
test.txt
```

The path to the test script relative to the deploymentPath.
Deployment path

agave-deployment

The path to the folder on the deployment system containing the application wrapper and dependencies.

Deployment system

shelob-storage-hpctrn20

The ID of the storage system where this app's assets should be stored.

Wrapper script

drawgau-wrapper.txt

The path to the wrapper script relative to the deploymentPath.

Test script

test.txt

The path to the test script relative to the deploymentPath.

An array of modules to load prior to the execution of the application. This is only relevant when you use the unix Modules or LMOD utilities to manage dependencies on the app execution system.
agave-deployment

The path to the folder on the deployment system containing the application wrapper and dependencies.

Deployment system

shelob-storage-hpctrn20

The ID of the storage system where this app's assets should be stored.

Wrapper script

drawgau-wrapper.txt

The path to the wrapper script relative to the deploymentPath.

Test script

test.txt

The path to the test script relative to the deploymentPath.

An array of modules to load prior to the execution of the application. This is only relevant when you use the unix Modules or LMOD utilities to manage dependencies on the app execution system.

"version": "0.1.0",
"isPublic": false,
"helpURI": "http://developer.agaveapi.co/",
"label": "Drawgau",
"owner": "ktraxler",
"shortDescription": "draw curve",
"longDescription": "Draw Gaussian Curve (points only)",
"tags": [
  "execute",
  "awesome",
  "demo"
],
"ontology": [
  "execute",
  "awesome",
  "demo"
],
"executionType": "HPC",
"executionSystem": "shelob-exec-hpctrn20",
"deploymentPath": "agave-deployment",
"deploymentSystem": "shelob-storage-hpctrn20",
"templatePath": "drawgau-wrapper.txt",
"testPath": "test.txt",
"checkpointable": false,
"modules": [],
App Edit Wizard

Execution type

**HPC**

The execution type of the application. If you're unsure, it's probably HPC.

Execution system

**shelob-execu-hpcptrn20**

The ID of the execution system where this app should run.

Default queue

Default queue to use when submitting this job if none is provided in the job request. Can be left blank and a queue will be determined at run time.

Default node count

**1**

Default number of nodes to be used when running this app if no node count is given in the job request.

```
{
  "id": "drawgau2-shelob-hpcptrn20-0.1.0",
  "name": "drawgau2-shelob-hpcptrn20",
  "icon": null,
  "parallelism": "SERIAL",
  "defaultProcessorsPerNode": 2,
  "defaultMemoryPerNode": 64,
  "defaultNodeCount": 1,
  "defaultMaxRunTime": "00:10:00",
  "defaultQueue": "shelob",
  "version": "0.1.0",
  "isPublic": false,
  "helpURI": "http://developer.agaveapi.co/",
  "label": "Drawgau",
  "owner": "ktraxler",
  "shortDescription": "draw curve",
  "longDescription": "Draw Gaussian Curve (points only)",
  "tags": [
    "execute",
    "awesome",
    "demo"
  ],
  "ontology": [
    "execute",
    "awesome",
    "demo"
  ],
  "executionType": "HPC",
  "executionSystem": "shelob-execu-hpcptrn20",
  "deploymentPath": "agave-api2"
}
```
Default node count

1

Default number of nodes to be used when running this app if no node count is given in the job request

Default memory (GB)

64

Default memory in GB to be used when running this app if no memory is given in the job request

Default processor count

2

Default number of processors per node to be used when running this app if no processor count is given in the job request

Default run time

00:10:00

Default max run time to be used when running this app if no requested run time is given in the job request

Parallelism

SERIAL

The parallelism type of the application. If you're unsure, it's probably SERIAL.

Checkpointable

True False

Does this app support checkpointing?

Previous Next Submit

"demo",
"executionType": "HPC",
"executionSystem": "shelob-exec-hptrn20",
"deploymentPath": "agave-deployment",
"deploymentSystem": "shelob-storage-hptrn20",
"templatePath": "drawgau-wrapper.txt",
"testPath": "test.txt",
"checkpointable": false,
"modules": []]
"inputs": [
  {
    "id": "parfile",
    "value": {
      "validator": "",
"...
App Edit Wizard

1. Basics
2. Dependencies
3. Environment
4. Parameters

id: "drawgau2-shelob-hpctrn20-0.1.0",
name: "drawgau2-shelob-hpctrn20",
icon: null,
paralleled: "SERIAL",
defaultProcessorsPerNode: 2,
defaultMemoryPerNode: 64,
defaultNodeCount: 1,
defaultMaxRunTime: "00:10:00",
defaultQueue: "shelob",
version: "0.1.0",
isPublic: false,
helpURI: "http://developer.agaveapi.co/",
label: "Drawgau",
owner: "xtraxler",
shortDescription: "draw curve",
longDescription: "Draw Gaussian Curve (points only)",
tags: [
  "execute",
  "awesome",
  "demo"
],
onontology: [
  "execute",
  "awesome",
  "demo"
],
executionType: "HPC",
executionSystem: "shelob-exec-hpctrn20"
App Edit Wizard

ID
parfile

The unique identifier for this input file. This will be referenced in the wrapper script.

Details

Descriptive details about this app inputs used in form generation.

Label
input for the program

The label displayed for this input.

Prepend command line argument?

Should this command line argument be injected into the workflow?

true  false

 parasal

The working directory, where the app will run.

// ...
Semantics

Semantic information about the input field.

Ontology

Array of ontology terms describing this input.

Min cardinality

1

Minimum number of instances of this input per job.

Max cardinality

1

Max number of instances of this input per job.

Values

Default value and validations for the input field.

Default value

input.txt

Validator regex

The regular expression used to validate this parameter value.

Visible

Yes

Prepend command line argument?

- True
- False

Should this command line argument be injected into the submit script preceding the input?

Semantics

Semantic information about the input field.

Ontology

Array of ontology terms describing this input

Min cardinality

| 1 |

Minimum number of instances of this input per job.

Max cardinality

| 1 |

Max number of instances of this input per job.

Values

Default value and validations for the input field.

Default value

input.txt

Validator regex


```json
{
  "id": "parfile",
  "value": {
    "validator": "",
    "visible": true,
    "required": true,
    "order": 0,
    "enquote": false,
    "default": "input.txt",
  },
  "details": {
    "label": "input for the program",
    "description": null,
    "argument": "input.txt",
  }
}
```
Default value and validations for the input field.

Default value

input.txt

Default value

Validator regex

The regular expression used to validate this parameter value.

Visible

Yes  No

Should this parameter be visible? If not, there must be a default and it will be required.

Required

Yes  No

Is this parameter required? If visible is false, this must be true.

Order

0

The order in which this parameter should be printed when generating an execution command for forked execution. This will also be the order in which parameters are returned in the response json.
App Edit Wizard

Basics

ID
drawgau0.txt

Add output

The unique identifier for this input file. This will be referenced in the wrapper script.

Details

Descriptive details about this app outputs used in form generation.

Label

drawgau0.txt

The label displayed for this input.

Prepend command line argument?

True  False

Should this command line argument be injected into the command line call?
Prepend command line argument?

True  False

Should this command line argument be injected into the submit script preceding the input?

Semantics

Semantic information about the output field.

Ontology

Array of ontology terms describing this input.

Min cardinality

1

Minimum number of instances of this input per job.

Max cardinality

-1

Max number of instances of this input per job.

Values

Default value and validations for the output field.

Default value

drawgau0.txt

Validator regex
Values

Default value and validations for the output field.

Default value

drawgau0.txt

Validator regex

The regular expression used to validate this parameter value.

Visible

Yes  No

Should this parameter be visible? If not, there must be a default and it will be required.

Order

1

The order in which this parameter should be printed when generating an execution command for forked execution. This will also be the order in which parameters are returned in the response json.

Remove

Previous  Next  Submit

label: "input for the program",
"description": null,
"argument": "input.txt",
"showArgument": false,
"repeatArgument": false

"semantics": {
  "minCardinality": 1,
  "maxCardinality": 1,
  "ontology": [],
  "fileTypes": []
}

"parameters": [],
"outputs": [
{
  "id": "drawgau0.txt",
  "value": {
    "validator": "",
    "order": 1,
    "default": "drawgau0.txt"
  },
  "details": {
    "label": "output file",
    "description": null
  },
  "semantics": {
    "minCardinality": 1,
    "maxCardinality": -1,
You have successfully created/updated your app

<table>
<thead>
<tr>
<th>Name</th>
<th>drawgau2-shelob-hpctrn20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version</td>
<td>0.1.0</td>
</tr>
<tr>
<td>Label</td>
<td>Drawgau</td>
</tr>
<tr>
<td>Description</td>
<td>draw curve</td>
</tr>
<tr>
<td>Execution Type</td>
<td>HPC</td>
</tr>
<tr>
<td>Execution System</td>
<td>shelob-execu-hpctrn20</td>
</tr>
<tr>
<td>Parallelism</td>
<td>SERIAL</td>
</tr>
<tr>
<td>Deployment System</td>
<td>shelob-storage-hpctrn20</td>
</tr>
<tr>
<td>Deployment Path</td>
<td>agave-deployment</td>
</tr>
</tbody>
</table>
## Apps Management

Manage your collection of apps

### Apps Management

<table>
<thead>
<tr>
<th>ID</th>
<th>Name</th>
<th>Label</th>
<th>Short Description</th>
<th>Exec. System</th>
<th>Last Modified</th>
<th>Actions</th>
</tr>
</thead>
<tbody>
<tr>
<td>drawgau2-shelob-hpcrn20-0.1.0</td>
<td>drawgau2-shelob-hpcrn20</td>
<td>Drawgau</td>
<td>draw curve</td>
<td>shelob-execu-hpcrn20</td>
<td>a minute ago</td>
<td>Actions</td>
</tr>
<tr>
<td>drawgau-shelob-hpcrn20-0.10</td>
<td>drawgau-shelob-hpcrn20</td>
<td>draw curve</td>
<td>draw curve</td>
<td>shelob-execu-hpcrn20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>drawgau-shelob-hpcrn15-0.1.0</td>
<td>drawgau-shelob-hpcrn15</td>
<td>draw curve</td>
<td>draw curve</td>
<td>shelob-execu-hpcrn15</td>
<td></td>
<td></td>
</tr>
<tr>
<td>drawgau-lsu-tutorial-0.1.0</td>
<td>drawgau-lsu-tutorial</td>
<td>draw curve</td>
<td>gaussian curve</td>
<td>shelob-hpcrn14</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Drawgau

Draw Gaussian Curve (points only)

Drawgau Documentation

Inputs

input for the program

Select agave://data.agaveapi.co/ktraxler/agave/input.txt

Job details

Maximum job runtime

00:10:00

In HH:MM:SS format. The maximum time you expect this job to run for. After this amount of time your job will be killed by the job scheduler. Shorter run times result in shorter queue wait times. Maximum possible time is 48:00:00 (48 hours).

Job name

drawgau-0611-728

A recognizable name for this job

Batch Queue

System queue to which the job should be submitted

Archive output

Should the output be archived
Inputs

input for the program

Select agave://data.agaveapi.co/ktraxler/agave/input.txt

Job details

Maximum job runtime

00:10:00

In HH:MM:SS format. The maximum time you expect this job to run for. After this amount of time your job will be killed by the job scheduler. Shorter run times result in shorter queue wait times. Maximum possible time is 48:00:00 (48 hours).

Job name

drawgau-0811-728

A recognizable name for this job

Batch Queue

System queue to which the job should be submitted

Archive output

Should the output be archived

Job output archive location (optional)

Specify a location where the job output should be archived. By default, job output will be archived at:

<username>/archive/jobs/$(YYYY-MM-DD)/$(JOB_NAME)-$(JOB_ID)

Run