

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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<https://togo.agaveplatform.org>

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- ◆ If you want a tutorial for your group, etc. just call and we'll set it up

What is a Science Gateway?

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

Designing a GUI or web interface to resources and making it robust is a long complex process that can take many hours.

Today we are going to learn how to make a science gateway from your application in an hour!

More formally:

<https://www.xsede.org/gateways-overview>

What is Agave?

- ◆ The Agave Platform (LINK: <http://agaveplatform.org>) 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

Under the hood, Agave works by using a REST api and 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.
- 2 What is REST? REST stands for REpresentational State Transfer. REST is a stateless, cacheable, uniform way of using URL's to communicate between a client and server.

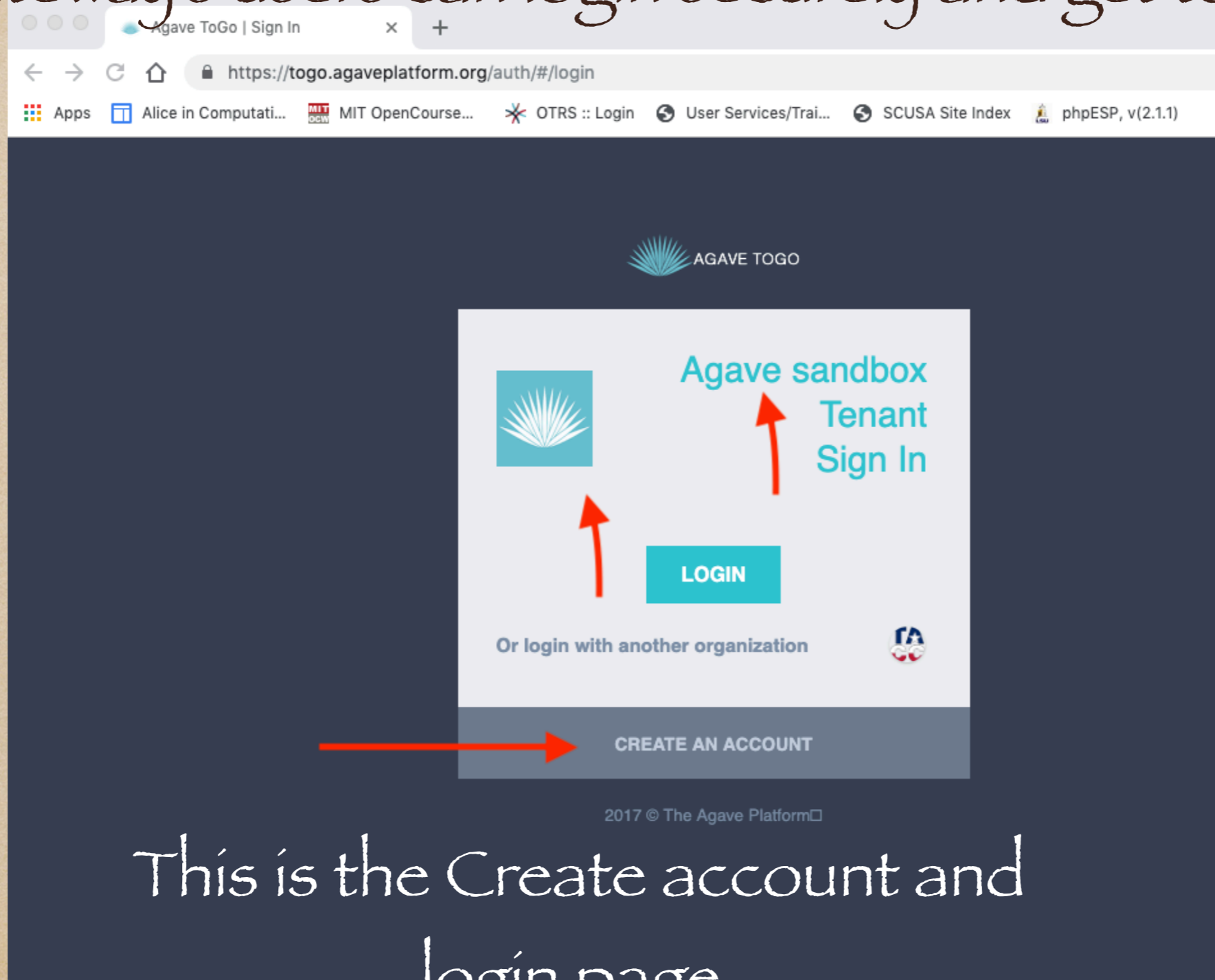
What Capabilities does Agave provide?

- ◆ Run code
- ◆ Manage data
- ◆ Collaborate meaningfully
- ◆ Integrate anywhere
- ◆ Provenance chain

<https://togo.agaveplatform.org>

- ◆ This is the URI you will use after the tutorial is over
- ◆ To use this you must have an Agave account and an HPC account

Everything on this screen if you were to create it from scratch would be a HUGE job requiring hours of coding. With ToGo your Gateway's users can login securely and get to work



This is the Create account and login page.

Finish Agave Account

- ◆ Finish creating your account by filling in required information and submitting
- ◆ Go to the email app you use for the email address you gave Agave and click on the link to verify and activate your account.

Setup HPC Account

- ◆ Already have an XSEDE or other supercomputer center (HPC) account? You are set.
- ◆ No HPC account? You must get one before you can proceed. Ask your group leader, major professor or other researchers around you where to get your account. HPC account: https://accounts.hpc.lsu.edu/login_request.php
- ◆ After acquiring your account and password you are ready to go.

Get the code and wrapper files

- ◆ To follow along with this tutorial you need several files. These files will be downloaded from my web page in the following slides.
 - ◆ `input.txt` (input parameter file)
 - ◆ `drawgau.cpp` (source code)
 - ◆ `drawgau-wrapper` (batch file script to run the job)

```
#!/bin/bash
echo 'Executing Draw Gau Code'
# Setting the x flag will echo every
# command onto stderr. This is
# for debugging, so we can see what's
# going on.
set -x
echo ==ENV=====
# The env command prints out the
# entire execution environment. This
# is also present for debugging purposes.
env > env.txt
echo ==PWD=====
# We also print out the execution
# directory. Again, for debugging purposes.
pwd > pwd.txt
echo ==JOB=====
EXE_DIR=/home/$USER/agave-deployment
if [ "${PBS_NODEFILE}" = "" ]
then
    # When running on a system managed by Torque
    # this variable should be set. If it's not,
    # that's a problem.
    echo "The PBS_NODEFILE was not set"
    exit 2
fi
# Strip off the .par from the end of the parfile name.
# Create a directory with the name of the parfile.
```

```
# More debugging.
echo PARFILE=$parfile
echo NODEFILE=$PBS_NODEFILE

# By default, the PBS_NODEFILE lists nodes multiple
# times, once for each MPI process that should run
# there. We only want one MPI process per node, so
# we create a new file with "sort -u".
LOCAL_NODEFILE=nodefile.txt
sort -u < ${PBS_NODEFILE} > ${LOCAL_NODEFILE}
PROCS=$(wc -l < ${LOCAL_NODEFILE})

echo "${xmin} ${xmax} ${deltax}" > input.txt

# Execute our MPI command.
mpirun -np ${PROCS} -machinefile ${LOCAL_NODEFILE} ${EXE_DIR}/drawgau input.txt

# Create a plot
python ./drawgau.py drawgau[0-9]*.txt
[ktraxler@shelob1 ~]$
```

Get Files

- ◆ You need the files and the best way to get them is:
 - ◆ log into your personal hpc account and type the following statements:
 - ◆ `curl -LO https://cct.lsu.edu/~sbrandt/agave-deployment.tgz`
 - ◆ `tar xzvf agave-deployment.tgz`
 - ◆ `cd agave-deployment`
 - ◆ `make`

Setup Agave Storage
and Execution Systems

Steven

Secure | <https://togo.agaveapi.co/app/#/dashboard>

Apps appl101.lsu.edu/b CySolidus Bookmarks ArtOfMPP SciComp Paper.js Other bookmarks

AGAVE TOGO

Home > Dashboard Quick Actions

Dashboard

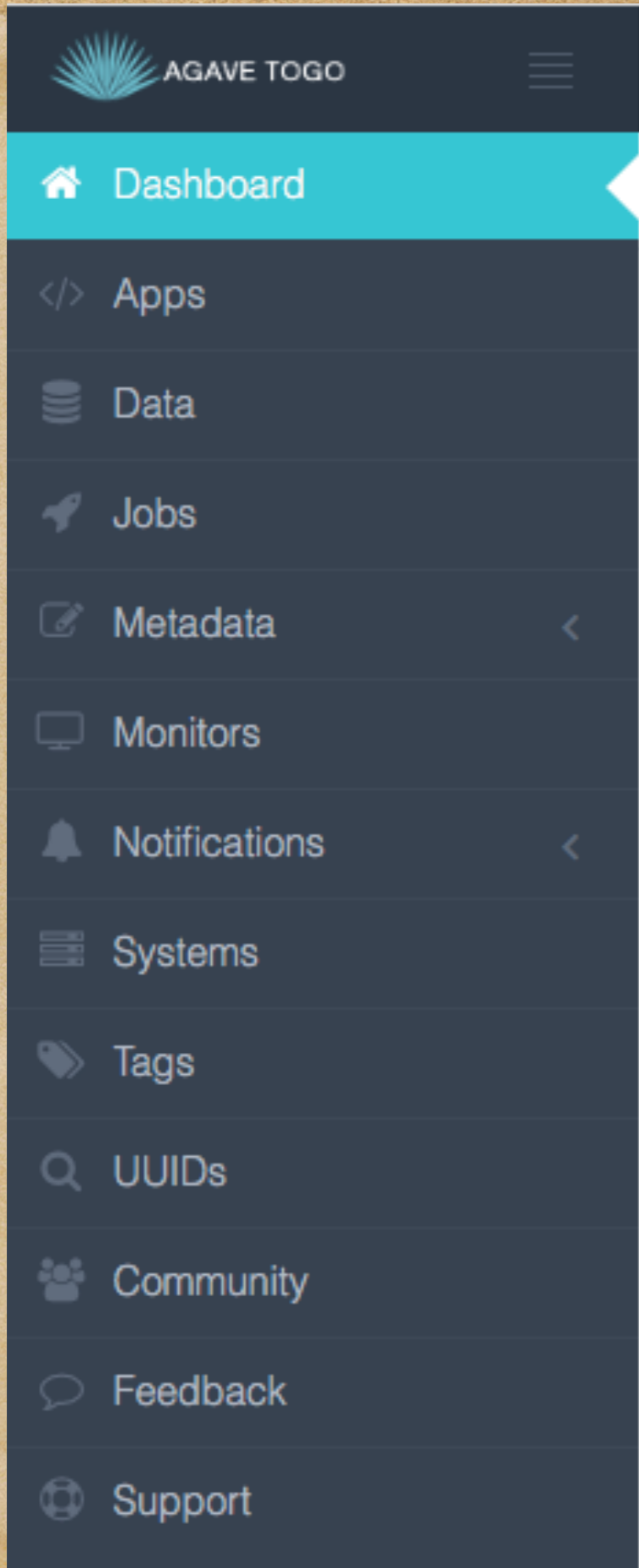
Introducing the new Agave ToGo!

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.

26 Jobs	12,5TB Data Moved
6 Apps	+25% Activity Increase

The right side of the dashboard.

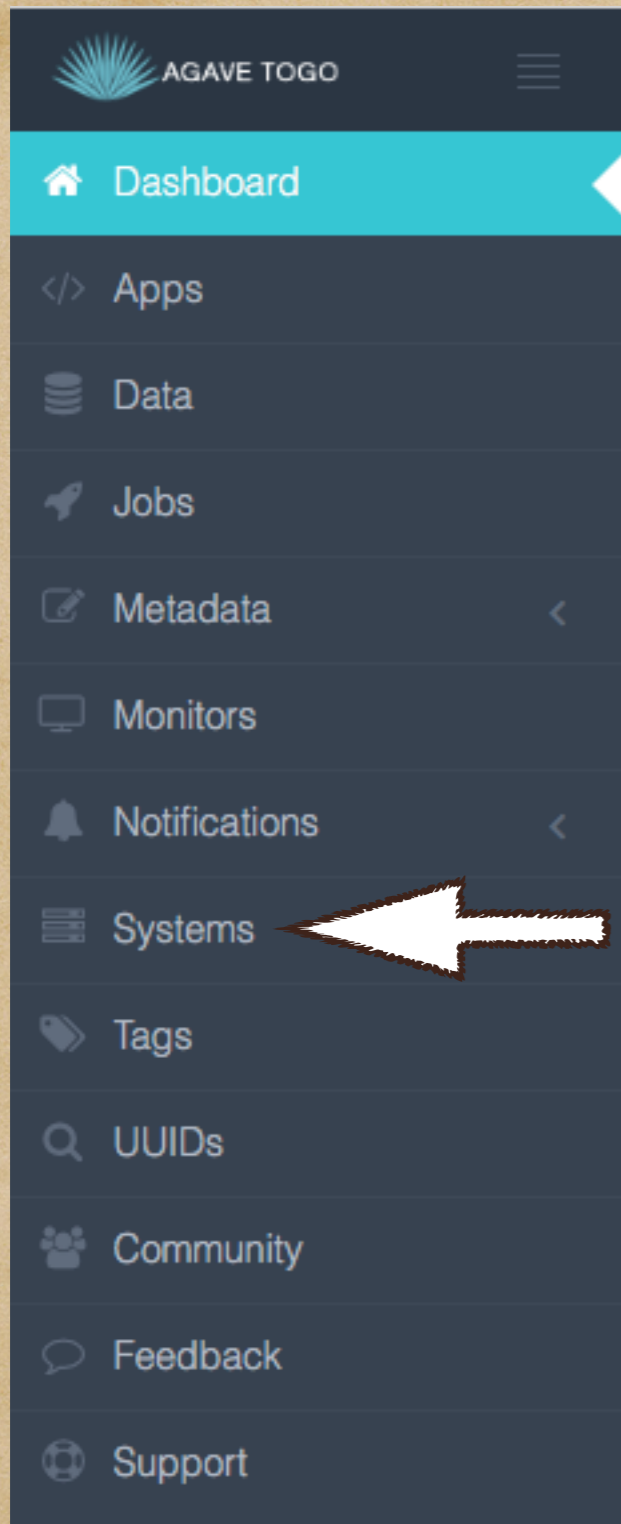


The left side of the dashboard

This is where we will do our work!

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

- AGAVE TOGO
- Dashboard
- Apps
- Data
- Jobs
- Metadata
- Monitors
- Notifications
- Systems**
- Tags
- UUIDs
- Community
- Feedback
- Support

Home • Systems

Systems

Manage your collection of systems

System Management

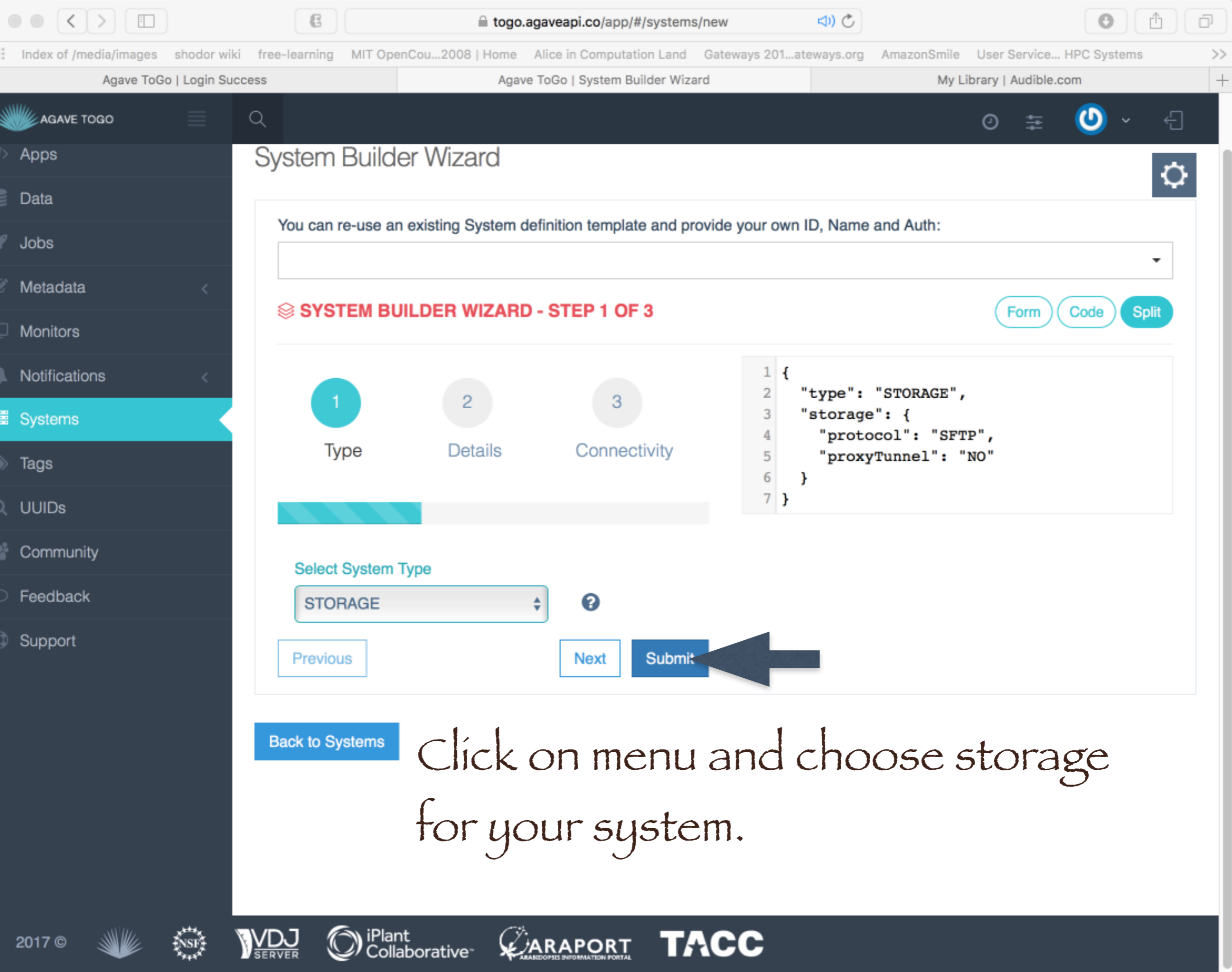


+ New System

Filter

Search Tools

ID	Name	Type	Actions
condor.opensciencegrid.org	Open Science Grid	EXECUTION	Actions
data.agaveapi.co	Agave Cloud Storage	STORAGE	Actions
docker.tacc.utexas.edu	Demo Docker VM	EXECUTION	Actions
ktraxler-qb	QB at LONI	EXECUTION	Actions
qb-ktraxler	qb (ktraxler)	EXECUTION	Actions
qb-storage-ktraxler	qb storage (ktraxler)	STORAGE	Actions
shelob-sbrandt	Shelob LSU (sbrandt)	EXECUTION	Actions



System Builder Wizard

You can re-use an existing System definition template and provide your own ID, Name and Auth:

SYSTEM BUILDER WIZARD - STEP 1 OF 3

Form Code Split

1

Type

2

Details

3

Connectivity

```
1 {
2   "type": "STORAGE",
3   "storage": {
4     "protocol": "SFTP",
5     "proxyTunnel": "NO"
6   }
7 }
```

Select System Type

STORAGE

Previous

Next

Submit

Back to Systems

Click on menu and choose storage for your system.

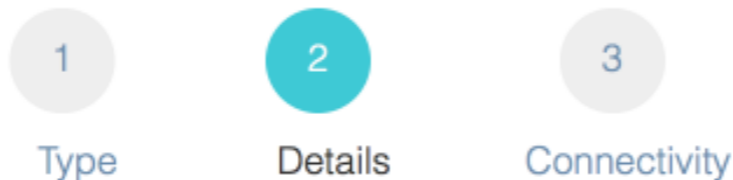


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System Editor Wizard

SYSTEM EDITOR WIZARD - STEP 2 OF 2

Form Code Split



ID

shelob-storage-hpctrn20 ✓



Name

Shelob at LSU ✓



Status

UP



Description

The Shelob supercomput ✓



Site

hpc.lsu.edu ✓



Previous

Next

Submit

```

1 {
2   "owner": "ktraxler",
3   "available": true,
4   "description": "The Shelob
supercomputer at LSU",
5   "storage": {
6     "proxy": null,
7     "protocol": "SFTP",
8     "mirror": false,
9     "port": 22,
10    "auth": {
11      "type": "PASSWORD"
12    },
13    "publicAppsDir": null,
14    "host": "shelob.hpc.lsu.edu",
15    "rootDir": "/",
16    "homeDir": "/home/hpctrn20",
17    "proxyTunnel": "NO"

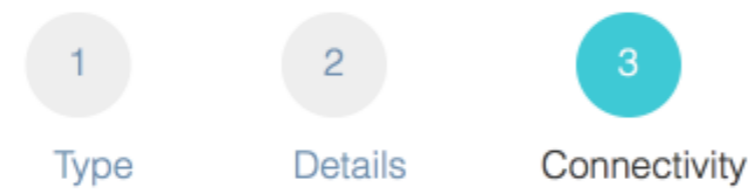
```

AGAVE TOGO

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SYSTEM EDITOR WIZARD - STEP 3 OF 2

Form Code Split



Storage

Protocol



Host



System Auth Server Port



Root Directory



Home Directory



Proxy Tunnel



```

1 {
2   "owner": "ktraxler",
3   "available": true,
4   "description": "The Shelob
supercomputer at LSU",
5   "storage": {
6     "proxy": null,
7     "protocol": "SFTP",
8     "mirror": false,
9     "port": 22,
10    "auth": {
11      "type": "PASSWORD",
12      "username": "ktraxler",
13      "password":
"#SSdalejr#88amp2017"
14    },
15    "publicAppsDir": null,
16    "host": "shelob.hpc.lsu.edu",
17    "rootDir": "/",
18    "homeDir": "/home/hpctrn20",
19    "proxyTunnel": "NO"
20  },
21  "type": "STORAGE",
22  "site": "hpc.lsu.edu",
23  "default": false,
24  "public": false,
25  "globalDefault": false,
26  "name": "Shelob at LSU",
27  "id": "shelob-storage-hpctrn20",
28  "status": "UP"
29 }

```



System Auth Server Port



Root Directory



Home Directory



Proxy Tunnel



```

20 },
21 "type": "STORAGE",
22 "site": "hpc.lsu.edu",
23 "default": false,
24 "public": false,
25 "globalDefault": false,
26 "name": "Shelob at LSU",
27 "id": "shelob-storage-hpctrn20",
28 "status": "UP"
29 }

```

Storage Authentication

Type



Username



Password



Previous

Next

Submit

Back to Systems

Use Definition





System Builder Wizard

You have successfully created your system

ID	shelob-storage-hpctrn20
Name	Shelob at LSU
Status	UP
Type	STORAGE
Description	The Shelob supercomputer at LSU

Close

Browse Systems

Previous

Next

Submit

Back to Systems

Use Definition



AGAVE TOGO

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Home • Data Explorer

QUICK ACTIONS ▾

File Browser



Shelob at LSU : /

+ CREATE FOLDER



<input type="checkbox"/>	Name ▾	Size	Date
<input type="checkbox"/>	📁 .gnome2	4KB	3 days ago
<input type="checkbox"/>	📁 .mozilla	4KB	3 days ago
<input type="checkbox"/>	📁 .pki	4KB	8 hours ago
<input type="checkbox"/>	📁 .ssh	4KB	9 hours ago
<input type="checkbox"/>	📁 .subversion	4KB	3 days ago
<input type="checkbox"/>	📁 agave-deployment	4KB	2 hours ago
<input type="checkbox"/>	📁 drawgau	4KB	7 hours ago
<input type="checkbox"/>	📄 .bash_history	28.1KB	a few seconds ago
<input type="checkbox"/>	📄 .bash_history3	364B	6 hours ago
<input type="checkbox"/>	📄 .bash_logout	18B	3 days ago
<input type="checkbox"/>	📄 .bash_profile	176B	3 days ago
<input type="checkbox"/>	📄 .bashrc	124B	3 days ago
<input type="checkbox"/>	📄 .emacs	500B	3 days ago


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Home • Systems

Systems

Manage your collection of systems

System Management

 [+ New System](#)

Filter

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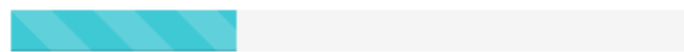
System Builder Wizard

You can re-use an existing System definition template and provide your own ID, Name and Auth:

SYSTEM BUILDER WIZARD - STEP 1 OF 3

Form Code Split

- 1**
Type
- 2
Details
- 3
Connectivity



Select System Type

EXECUTION

Previous Next Submit

```
1 {
2   "type": "EXECUTION",
3   "storage": {
4     "protocol": "SFTP",
5     "proxyTunnel": "NO"
6   },
7   "queues": [
8     {
9       "default": false
10    }
11  ]
12 }
```

Back to Systems

Choose Execution this time

Metadata <

Monitors <

Notifications <

Systems

Tags

UUIDs

Community

Feedback

Support

1 Type 2 Details 3 Connectivity

ID

shelob-execu-hpctrn20 ✓ ?

Name

Shelob supercomputer at ✓ ?

Status

UP ?

Description

Shelob supercomputer at ✓ ?

Site

hpc.lsu.edu ✓ ?

Execution Type

HPC ?

Scheduler

TORQUE ?

Maximum System Jobs

```
1 {
2   "maxSystemJobs": 50,
3   "executionType": "HPC",
4   "available": true,
5   "description": "Shelob
supercomputer at LSU",
6   "storage": {
7     "proxy": null,
8     "protocol": "SFTP",
9     "mirror": false,
10    "port": 10,
11    "auth": {
12      "type": "PASSWORD"
13    },
14    "host": "shelob.hpc.lsu.edu",
15    "rootDir": "/",
16    "homeDir": "/home/hpctrn20",
17    "proxyTunnel": "NO"
18  },
19 }
```



Scheduler

TORQUE



Maximum System Jobs

50



Scratch Directory

/work/hpctrn20/



Work Directory

/work/hpctrn20/



Environment



Startup Script



Queues

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

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



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

203



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

Maximum Memory Per Node

64GB



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

Maximum Processors Per Node





Maximum Memory Per Node

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

Maximum Processors Per Node

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

Maximum Requested Time

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



Type following lines into the "Custom Directives" box

Table 1

#PBS	-A	hpc_cmr (your allocation)
#PBS	-q	checkpt
#PBS	-l	nodes=\${AGAVE_JOB_NODE_COUNT}:ppn=16



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

[Empty text box]

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

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Submit

Back to Systems

Use Definition





Login Authentication

Type
 ?

Username
 ✓ ?

Password
 ✓ ?

Storage

Protocol
 ?

Host
 ✓ ?

System Auth Server Port
 ✓ ?

Root Directory
 ✓ ?

Home Directory
 ✓ ?

Proxy Tunnel
 ?

```

27     type: PASSWORD,
28     "username": "hpctrn20",
29     "password": "f=ma&one23four"
30   },
31   "host": "shelob.hpc.lsu.edu",
32   "proxyTunnel": "NO"
33 },
34 "startupScript": null,
35 "scheduler": "TORQUE",
36 "default": false,
37 "public": false,
38 "maxSystemJobsPerUser": 10,
39 "id": "shelob-execu-hpctrn20",
40 "workDir": "/work/hpctrn20/",
41 "owner": "ktraxler",
42 "site": "hpc.lsu.edu",
43 "environment": "",
44 "queues": [
45   {
46     "maxJobs": 20,
47     "maxMemoryPerNode": "64GB",
48     "default": false,
49     "maxRequestedTime": "72:00:00",
50     "name": "shelob",
51     "description": null,
52     "maxNodes": 203,
53     "maxProcessorsPerNode": 16,
54     "mappedName": null,
55     "maxUserJobs": -1,
56     "customDirectives": null
57   }
58 ],
59 "globalDefault": false,
60 "name": "Shelob supercomputer at
61 LSU",
62 "status": "UP",
63 "scratchDir": "/work/hpctrn20/"

```





System Auth Server Port



Root Directory



Home Directory



Proxy Tunnel



Storage Authentication

Type



Username



Password



Previous

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Submit

```

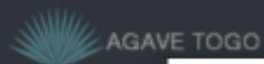
52     "maxNodes": 203,
53     "maxProcessorsPerNode": 16,
54     "mappedName": null,
55     "maxUserJobs": -1,
56     "customDirectives": null
57   }
58 ],
59 "globalDefault": false,
60 "name": "Shelob supercomputer at
LSU",
61 "status": "UP",
62 "scratchDir": "/work/hpctrn20/"
63 }

```

Back to Systems

Use Definition





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

Username

hpctrn20 ✓



Password

..... ✓



Previous

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Submit



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Home ● Data Explorer Quick Actions ▾

File Browser



Shelob at LSU : /

[+ Create folder](#)

<input type="checkbox"/>	Name ▼	Size	Date
<input type="checkbox"/>	📁 .gnome2	4KB	3 days ago
<input type="checkbox"/>	📁 .mozilla	4KB	3 days ago
<input type="checkbox"/>	📁 .pki	4KB	8 hours ago
<input type="checkbox"/>	📁 .ssh	4KB	9 hours ago
<input type="checkbox"/>	📁 .subversion	4KB	3 days ago
<input type="checkbox"/>	📁 agave-deployment	4KB	2 hours ago
<input type="checkbox"/>	📁 drawgau	4KB	7 hours ago
<input type="checkbox"/>	📄 .bash_history	28.5KB	a few seconds ago
<input type="checkbox"/>	📄 .bash_history3	364B	7 hours ago
<input type="checkbox"/>	📄 .bash_logout	18B	3 days ago
<input type="checkbox"/>	📄 .bash_profile	176B	3 days ago
<input type="checkbox"/>	📄 .bashrc	124B	3 days ago
<input type="checkbox"/>	📄 .emacs	500B	3 days ago

Create an Agave App

- ◆ Back to working with Agave TOGO to run our job

Apps Management Manage your collection of apps



</> Apps Management



[+ New App](#)

Filter

ID	Name	Version	Label	Short Description	Exec. System	Public	Revision	Last Modified	Actions
drawgau-ktraxler-0.1.0	drawgau-ktraxler	0.1.0	draw curve	gaussian curve	qb-exec-ktraxler	false	1	2 days ago	Actions ▾
shell-runner-0.1.0	shell-runner	0.1.0	Execute a command at a shell	This will execute whatever command you give in the command parameter	qb-exec-ktraxler	false	4	2 days ago	Actions ▾
cloud-runner-0.1.0u1	cloud-runner	0.1.0	Run your code in the cloud	Generic template for running arbitrary code in Agave's Dockerized cloud.	docker.tacc.utexas.edu	true	1	5 months ago	Actions ▾
jfonner-fork-1.0	jfonner-fork	1.0	Remote command execution script	Simple app for running a user-defined command on a remote system	stampede-fonner	false	1	5 months ago	Actions ▾
cactus-	cactus-	1.0	Cactus	Solves PDEs	shelob-	false	3	5 months	Actions ▾

App Builder Wizard

You can re-use an existing App definition template and provide your own Name and Dependencies:

APP BUILDER WIZARD - STEP 1 OF 6

Form Code Split



Name

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

Version

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

Label for use in forms generated by the jobs service

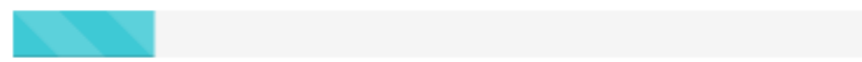
```
1 {
2   "name": "shell-runner",
3   "version": "0.1.0",
4   "helpURI": "http://developer.agaveapi.co/",
5   "label": "Execute a command at a shell",
6   "defaultNodeCount": 1,
7   "defaultMaxRunTime": "01:00:00",
8   "shortDescription": "This will execute
9   whatever command you give in the command
10  parameter",
11  "longDescription": "This will execute
12  whatever command you give in the command
13  parameter",
14  "executionSystem": "",
15  "executionType": "CLI",
16  "parallelism": "SERIAL",
17  "deploymentPath": "ktraxler/apps/shell-
18  runner-0.1.0",
19  "deploymentSystem": "storage.example.com",
20  "templatePath": "wrapper.sh",
21  "testPath": "test/test.sh",
22  "tags": [
23    "execute",
24    "awesome",
25    "demo"
26  ],
27 }
```

App Edit Wizard

</> Apps

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- Systems
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- UUIDs
- Community
- Feedback
- Support

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



Name

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

Version

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

Label for use in forms generated by the jobs service

Short description

Short description of this app

Long description

```

1 {
2   "id": "drawgau2-shelob-hpctrn20-0.1.0",
3   "name": "drawgau2-shelob-hpctrn20",
4   "icon": null,
5   "parallelism": "SERIAL",
6   "defaultProcessorsPerNode": 2,
7   "defaultMemoryPerNode": 64,
8   "defaultNodeCount": 1,
9   "defaultMaxRunTime": "00:10:00",
10  "defaultQueue": "shelob",
11  "version": "0.1.0",
12  "isPublic": false,
13  "helpURI":
14    "http://developer.agaveapi.co/",
15  "label": "Drawgau",
16  "owner": "ktraxler",
17  "shortDescription": "draw curve",
18  "longDescription": "Draw Gaussian Curve (points only)",
19  "tags": [
20    "execute",
21    "awesome",
22    "demo"
23  ],
24  "ontology": [
25    "execute",
26    "awesome",
27    "demo"
28  ],
29  "executionType": "HPC",
30  "executionSystem": "shelob-execu-hpctrn20",
31  "deploymentPath": "agave-deployment",

```



Short description

draw curve ✓

Short description of this app

Long description

Draw Gaussian Curve (points only) ✓

Full description of this app

Tags

tags ×
execute ✓

tags ×
awesome ✓

tags ×
demo ✓

+ Add

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

```
25     "awesome",
26     "demo"
27 ],
28 "executionType": "HPC",
29 "executionSystem": "shelob-execu-
hpctrn20",
30 "deploymentPath": "agave-
deployment",
31 "deploymentSystem": "shelob-
storage-hpctrn20",
32 "templatePath": "drawgau-
wrapper.txt",
33 "testPath": "test.txt",
34 "checkpointable": false,
35 "modules": [],
36 "inputs": [
37   {
38     "id": "parfile",
39     "value": {
40       "validator": "",
41       "visible": true,
42       "required": true,
43       "order": 0,
44       "enquote": false,
45       "default": "input.txt"
46     },
47     "details": {
48       "label": "input for the
program",
49     "description": null,
50     "argument": "input.txt",
51     "showArgument": false,
52     "repeatArgument": false
53   },
54   "semantics": {
55     "minCardinality": 1,
56     "maxCardinality": 1,
57     "ontology": [],
58     "fileTypes": []
59   }
60 }
```





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 x
execute ✓

ontology x
awesome ✓

ontology x
demo ✓

+ Add

An array of ontology terms describing this app.

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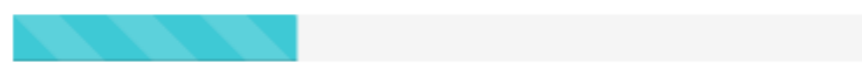
```
49     "description": null,  
50     "argument": "input.txt",  
51     "showArgument": false,  
52     "repeatArgument": false  
53   },  
54   "semantics": {  
55     "minCardinality": 1,  
56     "maxCardinality": 1,  
57     "ontology": [],  
58     "fileTypes": []  
59   }  
60 }  
61 ],  
62 "parameters": [],  
63 "outputs": [  
64   {
```

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Use Definition

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Deployment path

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

Deployment system

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

Wrapper script

The path to the wrapper script relative to the deploymentPath.

Test script

The path to the test script relative to the deploymentPath.

+ Add

```

1 {
2   "id": "drawgau2-shelob-hpctrn20-0.1.0",
3   "name": "drawgau2-shelob-hpctrn20",
4   "icon": null,
5   "parallelism": "SERIAL",
6   "defaultProcessorsPerNode": 2,
7   "defaultMemoryPerNode": 64,
8   "defaultNodeCount": 1,
9   "defaultMaxRunTime": "00:10:00",
10  "defaultQueue": "shelob",
11  "version": "0.1.0",
12  "isPublic": false,
13  "helpURI":
14    "http://developer.agaveapi.co/",
15  "label": "Drawgau",
16  "owner": "ktraxler",
17  "shortDescription": "draw curve",
18  "longDescription": "Draw Gaussian Curve (points only)",
19  "tags": [
20    "execute",
21    "awesome",
22    "demo"
23  ],
24  "ontology": [
25    "execute",
26    "awesome",
27    "demo"
28  ],
29  "executionType": "HPC",
30  "executionSystem": "shelob-execu-hpctrn20",
31  "deploymentPath": "agave-deployment",

```



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Deployment path

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

Deployment system

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

Wrapper script

The path to the wrapper script relative to the deploymentPath.

Test script

The path to the test script relative to the deploymentPath.

+ Add

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.

```

0.1.0",
3  "name": "drawgau2-shelob-hpctrn20",
4  "icon": null,
5  "parallelism": "SERIAL",
6  "defaultProcessorsPerNode": 2,
7  "defaultMemoryPerNode": 64,
8  "defaultNodeCount": 1,
9  "defaultMaxRunTime": "00:10:00",
10 "defaultQueue": "shelob",
11 "version": "0.1.0",
12 "isPublic": false,
13 "helpURI":
14 "http://developer.agaveapi.co/",
15 "label": "Drawgau",
16 "owner": "ktraxler",
17 "shortDescription": "draw curve",
18 "longDescription": "Draw Gaussian
Curve (points only)",
19 "tags": [
20   "execute",
21   "awesome",
22   "demo"
23 ],
24 "ontology": [
25   "execute",
26   "awesome",
27   "demo"
28 ],
29 "executionType": "HPC",
30 "executionSystem": "shelob-execu-
hpctrn20",
31 "deploymentPath": "agave-
deployment",
32 "deploymentSystem": "shelob-
storage-hpctrn20",
33 "templatePath": "drawgau-
wrapper.txt",
34 "testPath": "test.txt",
35 "checkpointable": false,

```

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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.

+ Add

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.

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```

11  "version": "0.1.0",
12  "isPublic": false,
13  "helpURI":
14  "http://developer.agaveapi.co/",
15  "label": "Drawgau",
16  "owner": "ktraxler",
17  "shortDescription": "draw curve",
18  "longDescription": "Draw Gaussian
19  Curve (points only)",
20  "tags": [
21    "execute",
22    "awesome",
23    "demo"
24  ],
25  "ontology": [
26    "execute",
27    "awesome",
28    "demo"
29  ],
30  "executionType": "HPC",
31  "executionSystem": "shelob-execu-
32  hpctrn20",
33  "deploymentPath": "agave-
34  deployment",
35  "deploymentSystem": "shelob-
36  storage-hpctrn20",
37  "templatePath": "drawgau-
38  wrapper.txt",
39  "testPath": "test.txt",
40  "checkpointable": false,
41  "modules": [],

```



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Execution type

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

Execution system

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

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

Default memory (GB)

```

1 {
2   "id": "drawgau2-shelob-hpctrn20-0.1.0",
3   "name": "drawgau2-shelob-hpctrn20",
4   "icon": null,
5   "parallelism": "SERIAL",
6   "defaultProcessorsPerNode": 2,
7   "defaultMemoryPerNode": 64,
8   "defaultNodeCount": 1,
9   "defaultMaxRunTime": "00:10:00",
10  "defaultQueue": "shelob",
11  "version": "0.1.0",
12  "isPublic": false,
13  "helpURI":
14    "http://developer.agaveapi.co/",
15  "label": "Drawgau",
16  "owner": "ktraxler",
17  "shortDescription": "draw curve",
18  "longDescription": "Draw Gaussian
19  Curve (points only)",
20  "tags": [
21    "execute",
22    "awesome",
23    "demo"
24  ],
25  "ontology": [
26    "execute",
27    "awesome",
28    "demo"
29  ],
30  "executionType": "HPC",
31  "executionSystem": "shelob-execu-hpctrn20",
32  "deploymentPath": "agave-
  
```





Default node count

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

Default memory (GB)

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

Default processor count

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

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

Parallelism

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

Checkpointable

 True False

Does this app support checkpointing?

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```
26     "demo"
27   ],
28   "executionType": "HPC",
29   "executionSystem": "shelob-execu-
hpctrn20",
30   "deploymentPath": "agave-
deployment",
31   "deploymentSystem": "shelob-
storage-hpctrn20",
32   "templatePath": "drawgau-
wrapper.txt",
33   "testPath": "test.txt",
34   "checkpointable": false,
35   "modules": [],
36   "inputs": [
37     {
38       "id": "parfile",
39       "value": {
40         "validator": "",
```



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```

1 {
2   "id": "drawgau2-shelob-hpctrn20-
3   0.1.0",
4   "name": "drawgau2-shelob-hpctrn20",
5   "icon": null,
6   "parallelism": "SERIAL",
7   "defaultProcessorsPerNode": 2,
8   "defaultMemoryPerNode": 64,
9   "defaultNodeCount": 1,
10  "defaultMaxRunTime": "00:10:00",
11  "defaultQueue": "shelob",
12  "version": "0.1.0",
13  "isPublic": false,
14  "helpURI":
15  "http://developer.agaveapi.co/",
16  "label": "Drawgau",
17  "owner": "ktraxler",
18  "shortDescription": "draw curve",
19  "longDescription": "Draw Gaussian
20  Curve (points only)",
21  "tags": [
22    "execute",
23    "awesome",
24    "demo"
25  ],
26  "ontology": [
27    "execute",
28    "awesome",
29    "demo"
30  ],
31  "executionType": "HPC",
32  "executionSystem": "shelob-execu-
33  hpctrn20",

```

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parfile

ID

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

The label displayed for this input.

Prepend command line argument?

True False

Should this command line argument be injected into the wrapper script?

```

1 {
2   "id": "drawgau2-shelob-hpctrn20-0.1.0",
3   "name": "drawgau2-shelob-hpctrn20",
4   "icon": null,
5   "parallelism": "SERIAL",
6   "defaultProcessorsPerNode": 2,
7   "defaultMemoryPerNode": 64,
8   "defaultNodeCount": 1,
9   "defaultMaxRunTime": "00:10:00",
10  "defaultQueue": "shelob",
11  "version": "0.1.0",
12  "isPublic": false,
13  "helpURI":
14    "http://developer.agaveapi.co/",
15  "label": "Drawgau",
16  "owner": "ktraxler",
17  "shortDescription": "draw curve",
18  "longDescription": "Draw Gaussian
19    Curve (points only)",
20  "tags": [
21    "execute",
22    "awesome",
23    "demo"
24  ],
25  "ontology": [
26    "execute",
27    "awesome",
28    "demo"
29  ],
30  "executionType": "HPC",
31  "executionSystem": "shelob-execu-
32    hpctrn20",

```

Semantics

Semantic information about the input field.

Ontology

+ Add

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

Default value

Validator regex

The regular expression used to validate this parameter value.

Visible

Yes No

```
deployment",
31  "deploymentSystem": "shelob-
storage-hpctrn20",
32  "templatePath": "drawgau-
wrapper.txt",
33  "testPath": "test.txt",
34  "checkpointable": false,
35  "modules": [],
36  "inputs": [
37    {
38      "id": "parfile",
39      "value": {
40        "validator": "",
41        "visible": true,
42        "required": true,
43        "order": 0,
44        "enquote": false,
45        "default": "input.txt"
46      },
47      "details": {
48        "label": "input for the
program",
49        "description": null,
50        "argument": "input.txt",
```



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

+ Add

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

Default value

Validator regex

```
26 "demo"
27 ],
28 "executionType": "HPC",
29 "executionSystem": "shelob-execu-
hpctrn20",
30 "deploymentPath": "agave-
deployment",
31 "deploymentSystem": "shelob-
storage-hpctrn20",
32 "templatePath": "drawgau-
wrapper.txt",
33 "testPath": "test.txt",
34 "checkpointable": false,
35 "modules": [],
36 "inputs": [
37 {
38 "id": "parfile",
39 "value": {
40 "validator": "",
41 "visible": true,
42 "required": true,
43 "order": 0,
44 "enquote": false,
45 "default": "input.txt"
46 },
47 "details": {
48 "label": "input for the
program",
49 "description": null,
50 "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 paramters are returned in the response json.

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drawgau0.txt [+ Add output](#)

ID
drawgau0.txt ✓

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
output file ✓

The label displayed for this input.

Prepend command line argument?

True False

Should this command line argument be injected into the wrapper script?

```

1 {
2   "id": "drawgau2-shelob-hpctrn20-0.1.0",
3   "name": "drawgau2-shelob-hpctrn20",
4   "icon": null,
5   "parallelism": "SERIAL",
6   "defaultProcessorsPerNode": 2,
7   "defaultMemoryPerNode": 64,
8   "defaultNodeCount": 1,
9   "defaultMaxRunTime": "00:10:00",
10  "defaultQueue": "shelob",
11  "version": "0.1.0",
12  "isPublic": false,
13  "helpURI":
14  "http://developer.agaveapi.co/",
15  "label": "Drawgau",
16  "owner": "ktraxler",
17  "shortDescription": "draw curve",
18  "longDescription": "Draw Gaussian
19  Curve (points only)",
20  "tags": [
21    "execute",
22    "awesome",
23    "demo"
24  ],
25  "ontology": [
26    "execute",
27    "awesome",
28    "demo"
29  ],
30  "executionType": "HPC",
31  "executionSystem": "shelob-execu-
32  hpctrn20",

```





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

+ Add

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

Default value

Validator regex

```

26     "demo"
27   ],
28   "executionType": "HPC",
29   "executionSystem": "shelob-execu-
hpctrn20",
30   "deploymentPath": "agave-
deployment",
31   "deploymentSystem": "shelob-
storage-hpctrn20",
32   "templatePath": "drawgau-
wrapper.txt",
33   "testPath": "test.txt",
34   "checkpointable": false,
35   "modules": [],
36   "inputs": [
37     {
38       "id": "parfile",
39       "value": {
40         "validator": "",
41         "visible": true,
42         "required": true,
43         "order": 0,
44         "enquote": false,
45         "default": "input.txt"
46       },
47       "details": {
48         "label": "input for the
program",
49         "description": null,
50         "argument": "input.txt",
51         "showArgument": false,
52         "repeatArgument": false
53       },
54       "semantics": {
55         "minCardinality": 1,
56         "maxCardinality": 1,
57         "ontology": [],
58         "fileTypes": []
59     }
60   ]

```





Values

Default value and validations for the output field.

Default value

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.

Order

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 paramters are returned in the response json.

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```

48     label : input for the
program",
49     "description": null,
50     "argument": "input.txt",
51     "showArgument": false,
52     "repeatArgument": false
53   },
54   "semantics": {
55     "minCardinality": 1,
56     "maxCardinality": 1,
57     "ontology": [],
58     "fileTypes": []
59   }
60 }
61 ],
62 "parameters": [],
63 "outputs": [
64   {
65     "id": "drawgau0.txt",
66     "value": {
67       "validator": "",
68       "order": 1,
69       "default": "drawgau0.txt"
70   },
71   "details": {
72     "label": "output file",
73     "description": null
74   },
75   "semantics": {
76     "minCardinality": 1,
77     "maxCardinality": -1,

```





App Builder Wizard

You have successfully created/updated your app

Name	drawgau2-shelob-hpctrn20
Version	0.1.0
Label	Drawgau
Description	draw curve
Execution Type	HPC
Execution System	shelob-execu-hpctrn20
Parallelism	SERIAL
Deployment System	shelob-storage-hpctrn20
Deployment Path	agave-deployment

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77 "maxCardinality": -1,

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File Browser

Agave Cloud Storage : ktraxler/archive/jobs/job-964575848630709785-242ac11c-0001-007

[+ Create folder](#) [U](#)

[ktraxler](#) / [archive](#) / [jobs](#) / [job-964575848630709785-242ac11c-0001-007](#)

<input type="checkbox"/>	Name ▼	Size	Date
<input type="checkbox"/>	.agave.log	398B	2 minutes ago
<input type="checkbox"/>	drawgau-0612-0827-964575848630709785-242ac11c-0001-007.err	1.1KB	2 minutes ago
<input type="checkbox"/>	drawgau-0612-0827-964575848630709785-242ac11c-0001-007.out	5.8KB	2 minutes ago
<input type="checkbox"/>	nodefile.txt	10B	2 minutes ago

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ID	Name	Label	Short Description	Exec. System	Last Modified ▲	Actions
drawgau2-shelob-hpctrn20-0.1.0	drawgau2-shelob-hpctrn20	Drawgau	draw curve	shelob-execu-hpctrn20	a minute ago	<div style="border: 1px solid red; padding: 2px;">Actions ▾</div> <ul style="list-style-type: none"> ▶ Run ✎ Edit ✕ Disable 🗑 Delete ↪ Share 🔔 Notifications 📄 Clone 👁 Publish
drawgau-shelob-hpctrn20-0.10	drawgau-shelob-hpctrn20	draw curve	draw curve	shelob-execu-hpctrn20		
drawgau-shelob-hpctrn15-0.1.0	drawgau-shelob-hpctrn15	draw curve	draw curve	shelob-exec1-hpctrn15		
drawgau-lsu-tutorial-0.1.0	drawgau-lsu-tutorial	draw curve	gaussian curve	shelob-hpctrn14		

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DRAWGAU2-SHELOB-HPCTR20-0.1.0

Details **Run**

Drawgau

Draw Gaussian Curve (points only)

[Drawgau Documentation](#)

Inputs

input for the program

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

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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 *Uncheck the "Archive output" box*

Should the output be archived

Job output archive location (optional)

<username>/archive/jobs/\${YYYY-MM-DD}/\${JOB_NAME}-\${JOB_ID}

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

- AGAVE TOGO
- </> Apps
- Data
- Jobs
- Metadata
- Monitors
- Notifications
- Systems
- Tags
- UUIDs
- Community
- Feedback
- Support

Successfully submitted job

ID	964575848630709785-242ac11c-0001-007
Name	drawgau-0612-0827
Owner	ktraxler
Status	PENDING
Execution System	shelob-hpctrn20-exec
Archive	true
Archive System	data.agaveapi.co
Archive Path	ktraxler/archive/jobs/job-964575848630709785-242ac11c-0001-007
Batch Queue	shelob
Application ID	drawgau2-shelob-hpctrn20-0.1.0

[Details](#) [Exit](#)

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

A recognizable name for this job

Batch Queue

Output from Job Run

- ◆ Log into your HPC account
- ◆ `cd into /work/username`
- ◆ `ls -l`

Conclusion

- ◆ Once you define your storage system, execution system, and app you have a working science gateway!
- ◆ We have successfully run a job without logging into our hardware system and using the command line.
- ◆ Save development time by using Agave.

Final thoughts

- ◆ If you want a demo or hands on for your group let us know:
 - ◆ ktraxler@lsu.edu
 - ◆ sbrandt@cct.lsu.edu