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 RES T 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:

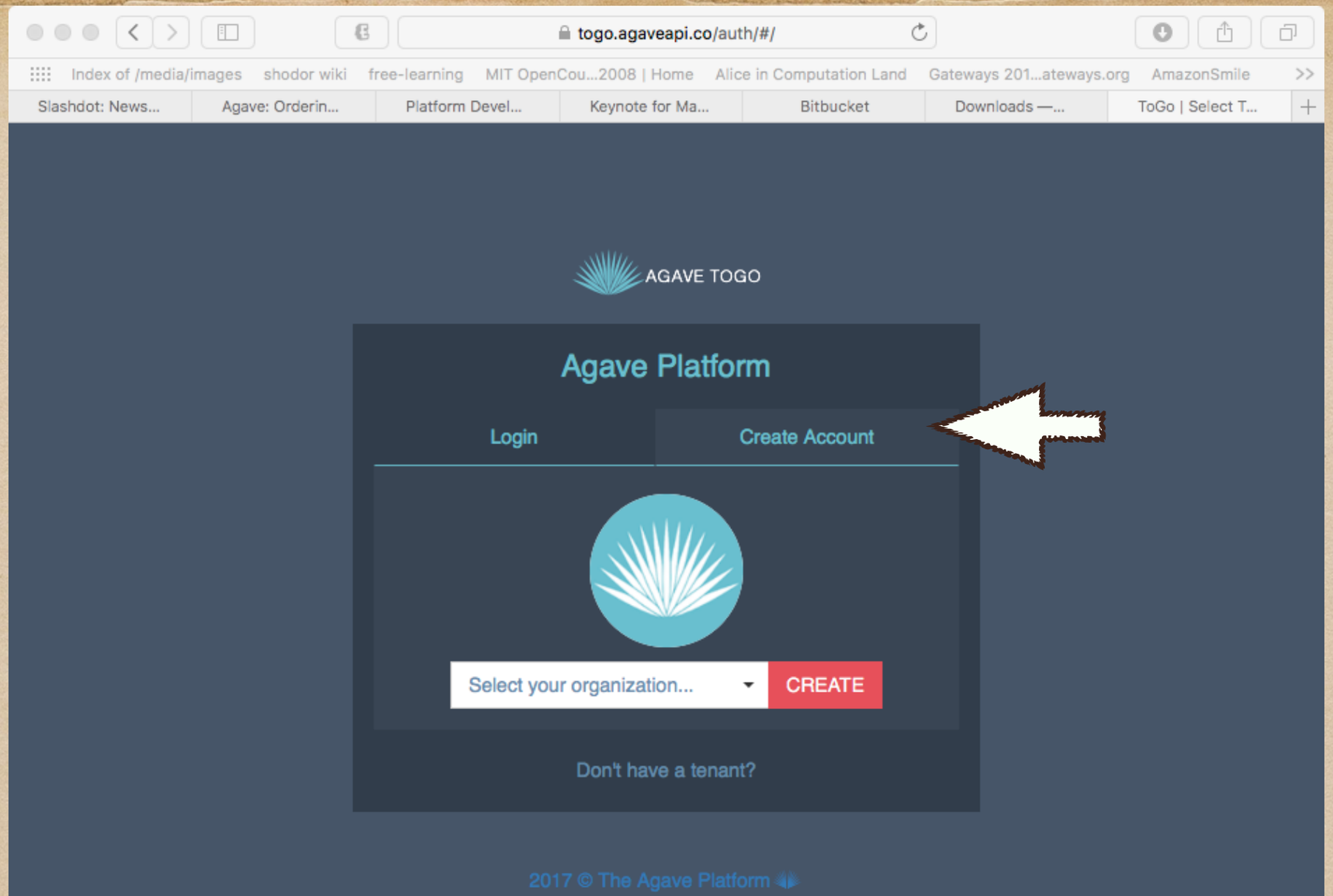
- mpic++ -o drawgau -std=c++11 drawgau.cpp

Getting Started

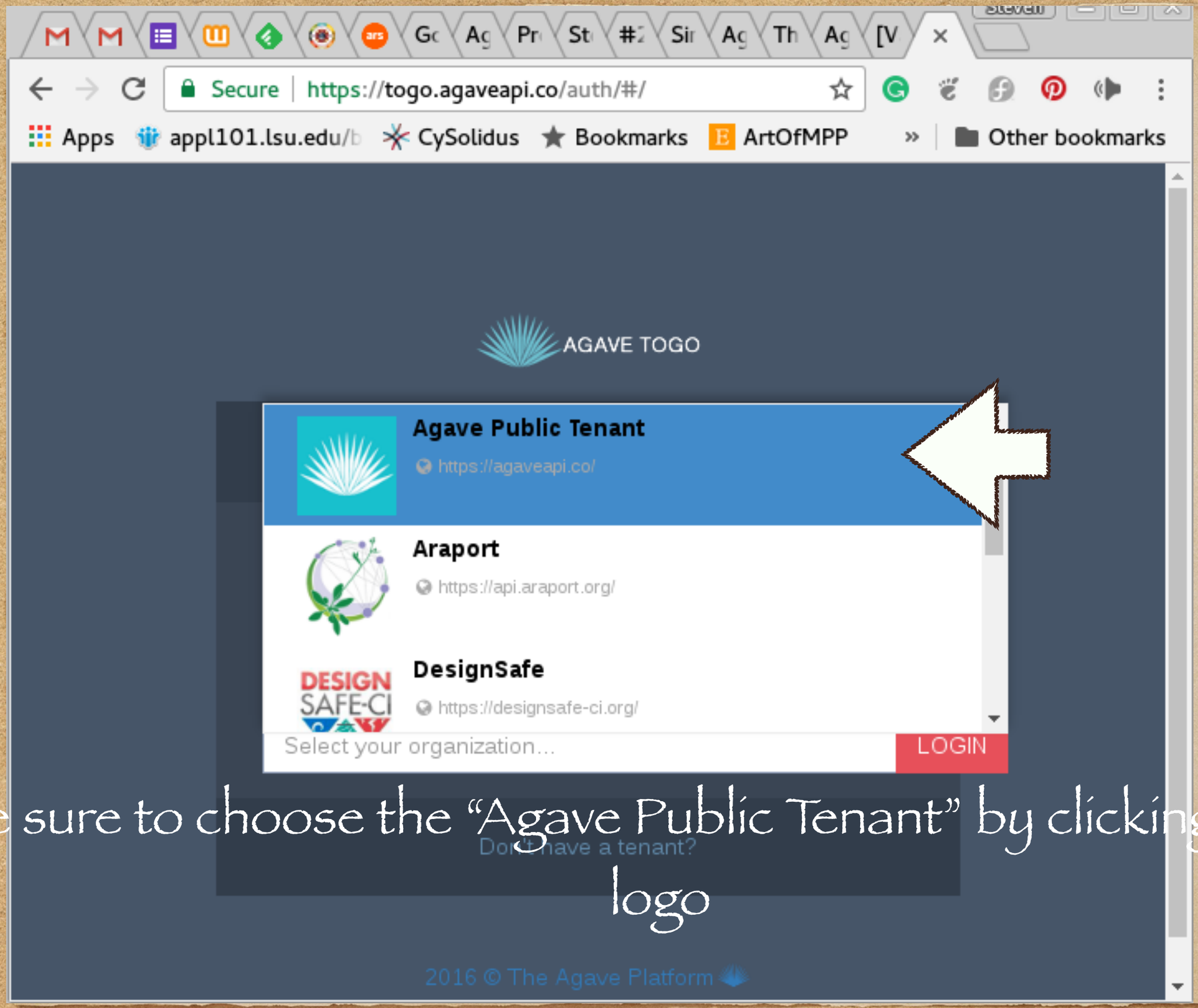
- To get started go to the Agave web page and create an account.
- Visit https://togo.agaveapi.co/
- Then choose the “Create Account” link from the upper right corner of the “Agave Platform” box

Create an Agave App

- Back to working with Agave TOGO to run our job



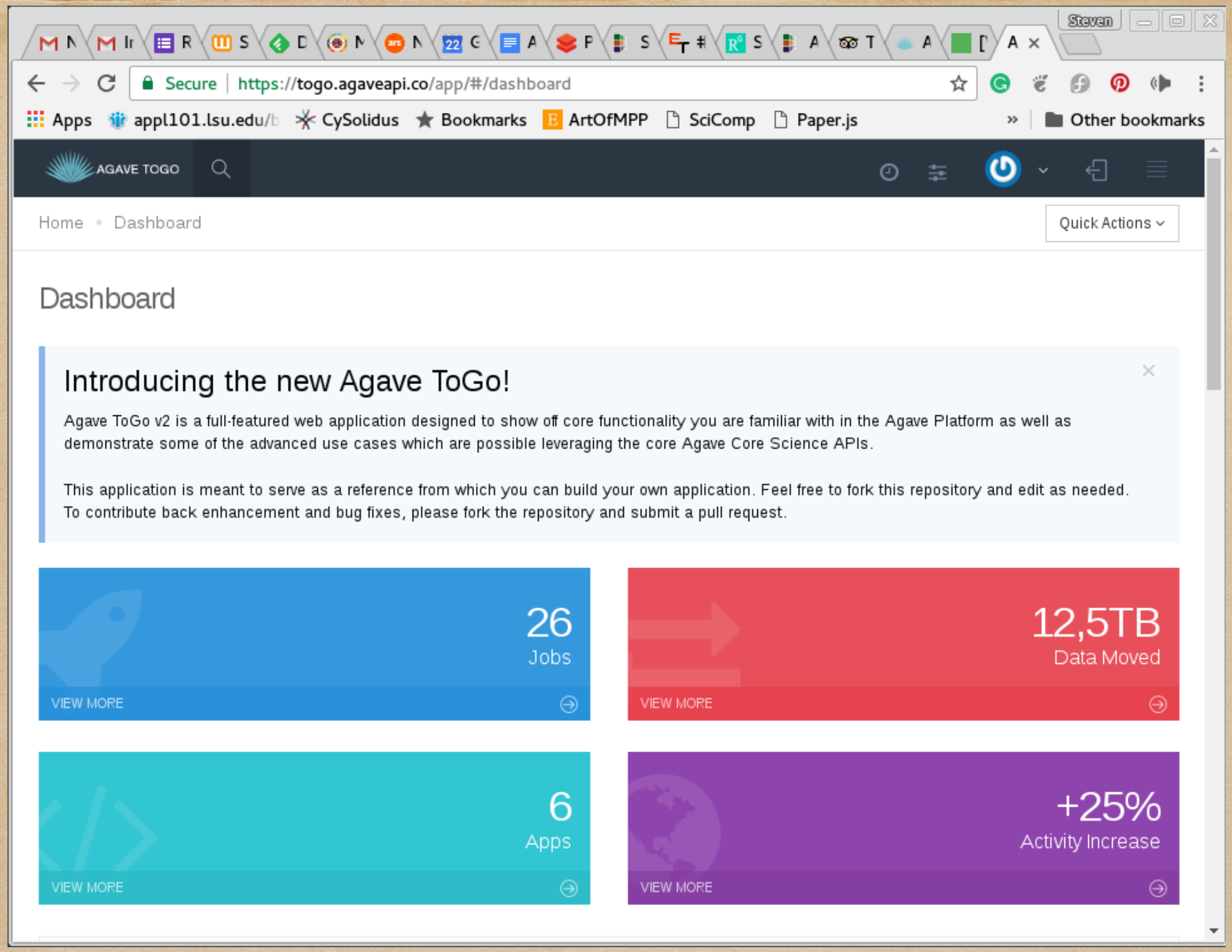
This is the Create account and login page.



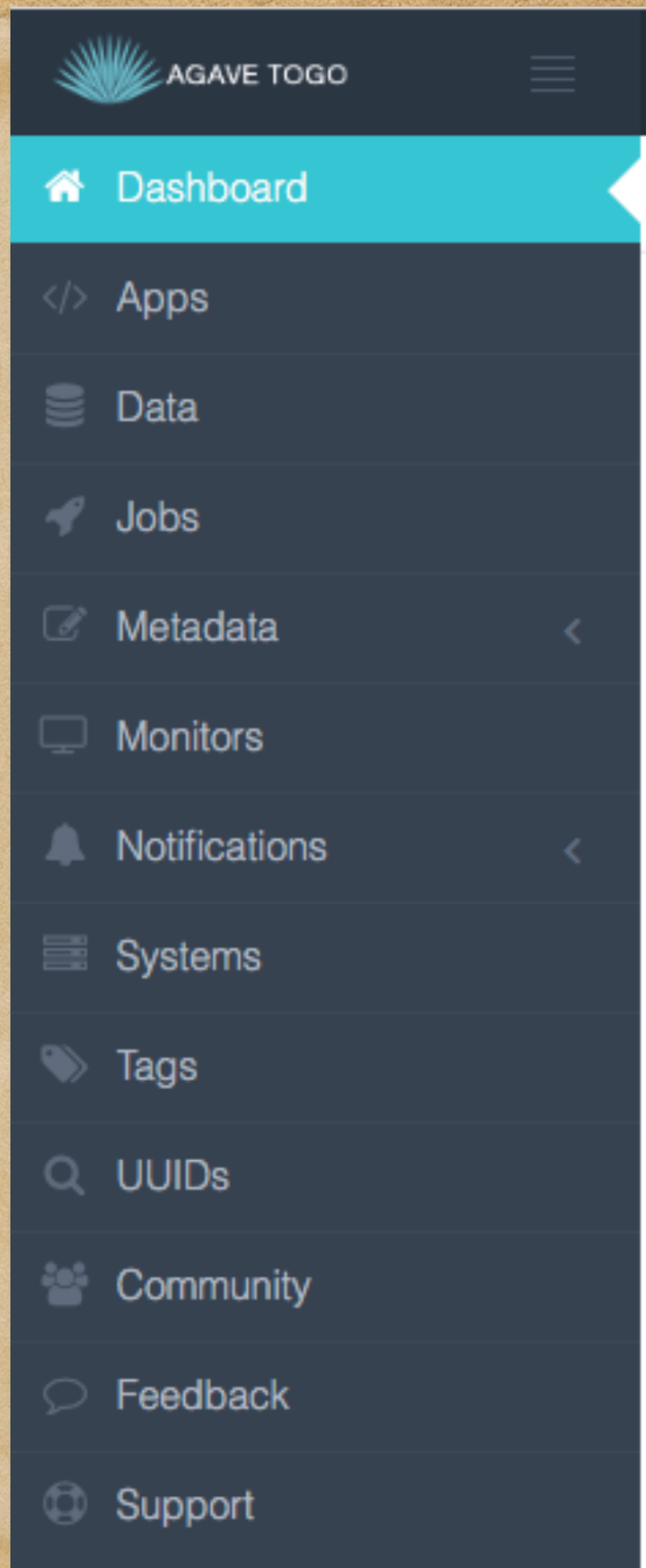
Be sure to choose the "Agave Public Tenant" by clicking on the logo

Finish Account

- Finish creating your account by filling in required information
- Go to your dashboard



The right side of the dashboard.



The left side of the dashboard

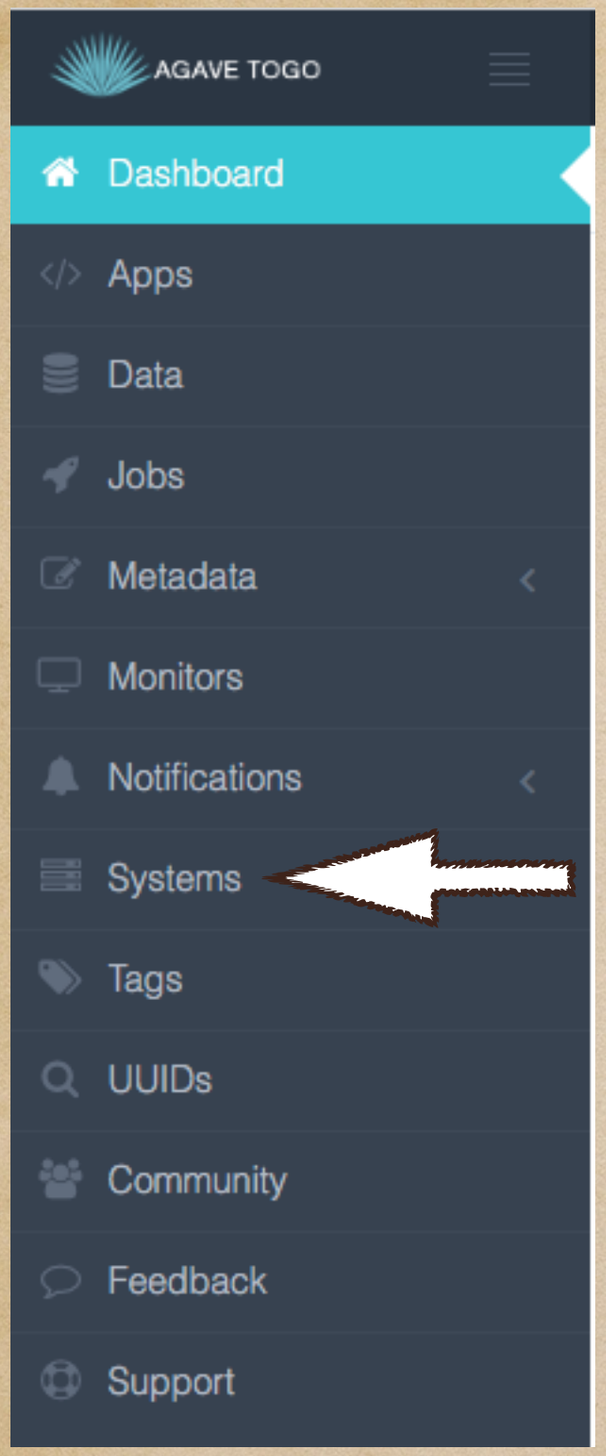
This is where we will do our work!

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

togo.agaveapi.co/app/#/systems

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System Management

+ New System

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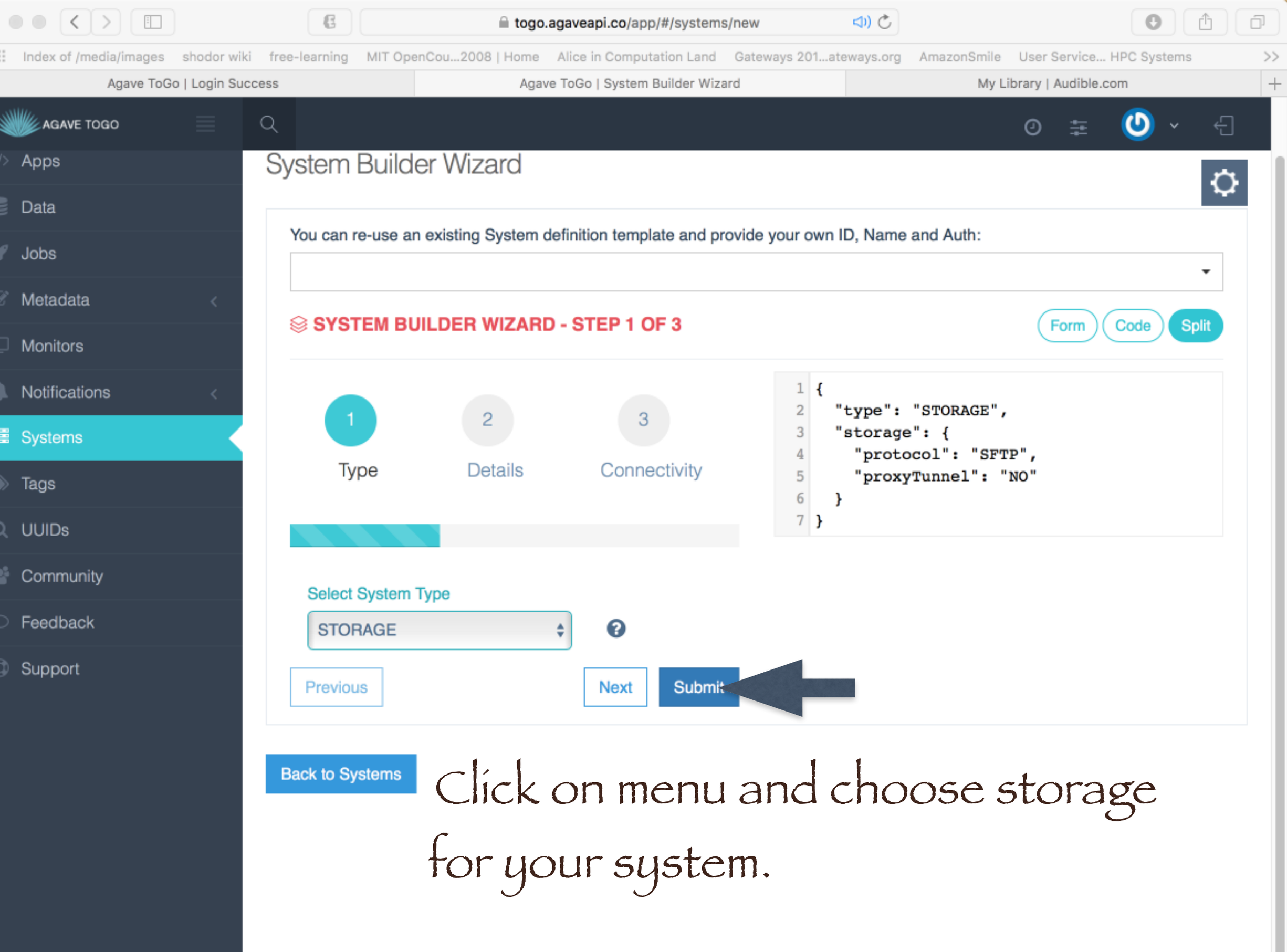
Search Tools

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



Click on menu and choose storage for your system.

Apps
Data
Jobs
Metadata
Monitors
Notifications
Systems
Tags
UUIDs
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Feedback
Support

System Editor Wizard

SYSTEM EDITOR WIZARD - STEP 2 OF 2

Form | Code | Split

1 Type — 2 Details — 3 Connectivity

ID
shelob-storage-hpctrn20

Name
Shelob at LSU

Status
UP

Description
The Shelob supercomput

Site
hpc.lsu.edu

Previous | Next | Submit


```
{
  "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"
```

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SYSTEM EDITOR WIZARD - STEP 3 OF 2

Form | Code | Split

1 Type — 2 Details — 3 Connectivity

Storage

Protocol: SFTP

Host: shelob.hpc.lsu.edu

System Auth Server Port: 22

Root Directory: /

Home Directory: /home/hpctrn20

Proxy Tunnel: NO


```
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

22

Root Directory

/

Home Directory

/home/hpctrn20

Proxy Tunnel

NO

Storage Authentication

Type

PASSWORD

Username

hpctrn20

Password

••••••••••••••

Previous | Next | Submit


```
  },
  "type": "STORAGE",
  "site": "hpc.lsu.edu",
  "default": false,
  "public": false,
  "globalDefault": false,
  "name": "Shelob at LSU",
  "id": "shelob-storage-hpctrn20",
  "status": "UP"
}
```


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

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Home • Data Explorer

QUICK ACTIONS

File Browser

Shelob at LSU : /

+ CREATE FOLDER

	Name	Size	Date
	.gnome2	4KB	3 days ago
	.mozilla	4KB	3 days ago
	.pki	4KB	8 hours ago
	.ssh	4KB	9 hours ago
	.subversion	4KB	3 days ago
	agave-deployment	4KB	2 hours ago
	drawgau	4KB	7 hours ago
	.bash_history	28.1KB	a few seconds ago
	.bash_history3	364B	6 hours ago
	.bash_logout	18B	3 days ago
	.bash_profile	176B	3 days ago
	.bashrc	124B	3 days ago
	.emacs	500B	3 days ago

togo.agaveapi.co/app/#/systems

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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

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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

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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   },
```

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

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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

64GB

Maximum memory per node for jobs submitted to this queue in ###.#[E|P|T|G]B 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

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

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Back to Systems | Use Definition

Login Authentication

Type

PASSWORD

Username

hpctrn20

Password

••••••••••••••

Storage

Protocol

SFTP

Host

shelob.hpc.lsu.edu

System Auth Server Port

10

Root Directory

/

Home Directory

/home/hpctrn20

Proxy Tunnel

NO


```
      "type": "PASSWORD",
      "username": "hpctrn20",
      "password": "f=ma&one23four"
    },
    "host": "shelob.hpc.lsu.edu",
    "proxyTunnel": "NO"
  },
  "startupScript": null,
  "scheduler": "TORQUE",
  "default": false,
  "public": false,
  "maxSystemJobsPerUser": 10,
  "id": "shelob-execu-hpctrn20",
  "workDir": "/work/hpctrn20/",
  "owner": "ktraxler",
  "site": "hpc.lsu.edu",
  "environment": "",
  "queues": [
    {
      "maxJobs": 20,
      "maxMemoryPerNode": "64GB",
      "default": false,
      "maxRequestedTime": "72:00:00",
      "name": "shelob",
      "description": null,
      "maxNodes": 203,
      "maxProcessorsPerNode": 16,
      "mappedName": null,
      "maxUserJobs": -1,
      "customDirectives": null
    }
  ],
  "globalDefault": false,
  "name": "Shelob supercomputer at LSU",
  "status": "UP",
  "scratchDir": "/work/hpctrn20/"
}
```

System Auth Server Port

10

Root Directory

/

Home Directory

/home/hpctrn20

Proxy Tunnel

NO

Storage Authentication

Type

PASSWORD

Username

hpctrn20

Password

••••••••••••••

Previous | Next | 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 | Next | Submit

togo.agaveapi.co/app/#/data/explorer/shelob-storage-hpctrn20/

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Quick Actions

File Browser

Shelob at LSU : /

+ Create folder

	Name	Size	Date
	.gnome2	4KB	3 days ago
	.mozilla	4KB	3 days ago
	.pki	4KB	8 hours ago
	.ssh	4KB	9 hours ago
	.subversion	4KB	3 days ago
	agave-deployment	4KB	2 hours ago
	drawgau	4KB	7 hours ago
	.bash_history	28.5KB	a few seconds ago
	.bash_history3	364B	7 hours ago
	.bash_logout	18B	3 days ago
	.bash_profile	176B	3 days ago
	.bashrc	124B	3 days ago
	.emacs	500B	3 days ago

togo.agaveapi.co/app/#/apps

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Apps Management

+ New App

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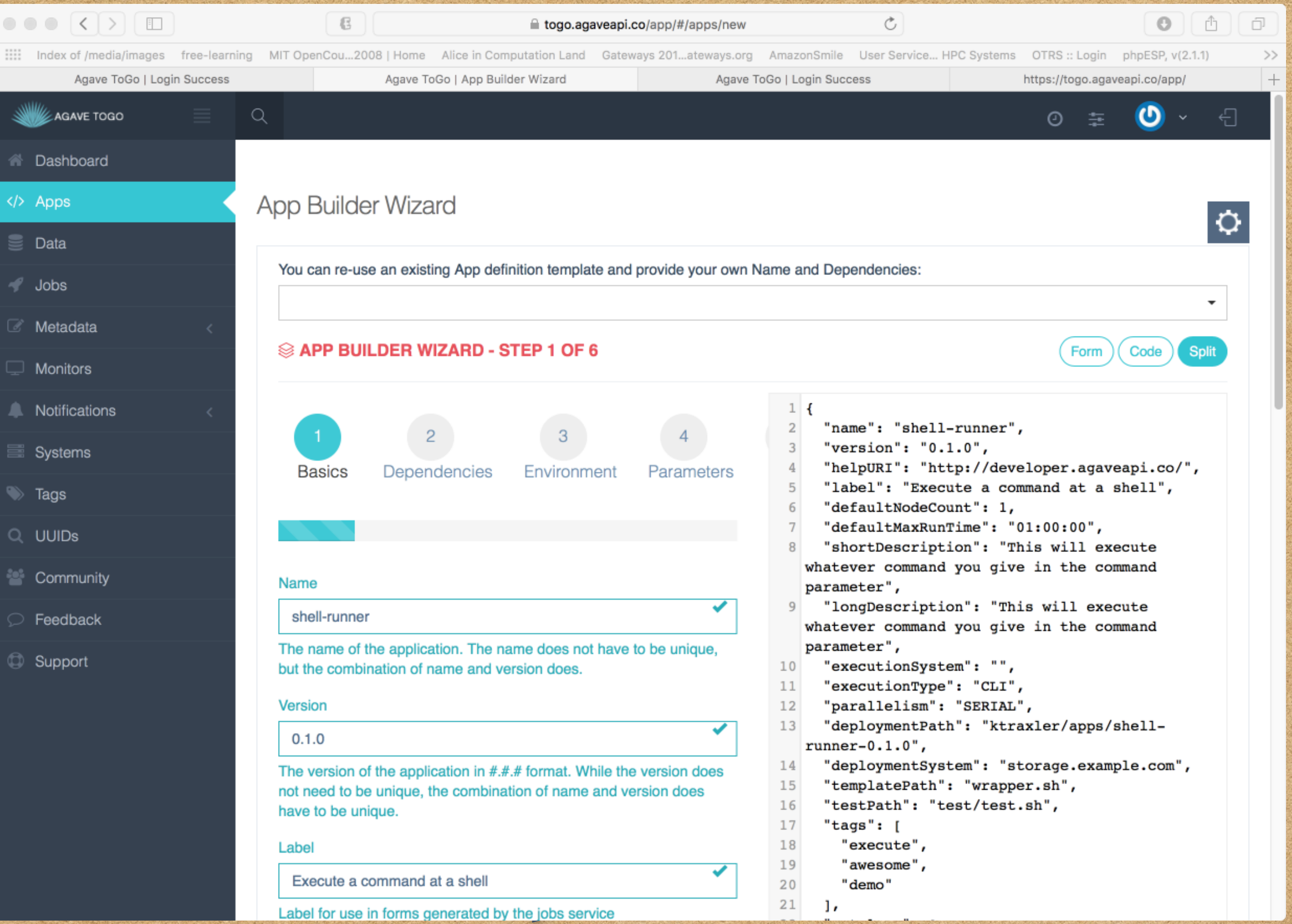
Search Tools

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-	fals	3	5 months	Actions


togo.agaveapi.co/app/#/apps/new
Agave ToGo | Login Success
Agave ToGo | App Builder Wizard
Agave ToGo | Login Success
https://togo.agaveapi.co/app/
AGAVE TOGO
Dashboard
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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
1 Basics
2 Dependencies
3 Environment
4 Parameters
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
{
"name": "shell-runner",
"version": "0.1.0",
"helpURI": "http://developer.agaveapi.co/",
"label": "Execute a command at a shell",
"defaultNodeCount": 1,
"defaultMaxRunTime": "01:00:00",
"shortDescription": "This will execute whatever command you give in the command parameter",
"longDescription": "This will execute whatever command you give in the command parameter",
"executionSystem": "",
"executionType": "CLI",
"parallelism": "SERIAL",
"deploymentPath": "ktraxler/apps/shell-runner-0.1.0",
"deploymentSystem": "storage.example.com",
"templatePath": "wrapper.sh",
"testPath": "test/test.sh",
"tags": [
"execute",
"awesome",
"demo"
],

togo.agaveapi.co/app/#/apps/edit/drawgau2-shelob-hpctrn20-0

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App Edit Wizard

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Name

drawgau2-shelob-hpctrn20

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)


```
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":
"http://developer.agaveapi.co/",
14   "label": "Drawgau",
15   "owner": "ktraxler",
16   "shortDescription": "draw curve",
17   "longDescription": "Draw Gaussian
Curve (points only)",
18   "tags": [
19     "execute",
20     "awesome",
21     "demo"
22   ],
23   "ontology": [
24     "execute",
25     "awesome",
26     "demo"
27   ],
28   "executionType": "HPC",
29   "executionSystem": "shelob-execu-
hpctrn20",
30   "deploymentPath": "agave-
deployment",
```

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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


```
    "awesome",
    "demo"
  ],
  "executionType": "HPC",
  "executionSystem": "shelob-execu-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

+ Add

An array of ontology terms describing this app.

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```
      "argument": "input.txt",
      "showArgument": false,
      "repeatArgument": false
    },
    "semantics": {
      "minCardinality": 1,
      "maxCardinality": 1,
      "ontology": [],
      "fileTypes": []
    }
  }
],
"parameters": [],
"outputs": [
  {
```


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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.

+ 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": "http://developer.agaveapi.co/",
14   "label": "Drawgau",
15   "owner": "ktraxler",
16   "shortDescription": "draw curve",
17   "longDescription": "Draw Gaussian Curve (points only)",
18   "tags": [
19     "execute",
20     "awesome",
21     "demo"
22   ],
23   "ontology": [
24     "execute",
25     "awesome",
26     "demo"
27   ],
28   "executionType": "HPC",
29   "executionSystem": "shelob-execu-hpctrn20",
30   "deploymentPath": "agave-deployment",
```

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Deployment path

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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.


```
0.1.0",
  "name": "drawgau2-shelob-hpctrn20",
  "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-
hpctrn20",
  "deploymentPath": "agave-
deployment",
  "deploymentSystem": "shelob-
storage-hpctrn20",
  "templatePath": "drawgau-
wrapper.txt",
  "testPath": "test.txt",
  "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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```
  "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-hpctrn20",
  "deploymentPath": "agave-deployment",
  "deploymentSystem": "shelob-storage-hpctrn20",
  "templatePath": "drawgau-wrapper.txt",
  "testPath": "test.txt",
  "checkpointable": false,
  "modules": [],
```

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Execution type

HPC

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

Execution system

shelob-execu-hpctrn20

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

Default memory (GB)


```
{
  "id": "drawgau2-shelob-hpctrn20-0.1.0",
  "name": "drawgau2-shelob-hpctrn20",
  "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-hpctrn20",
  "deploymentPath": "agave-
```

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?

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```
    "demo"
  ],
  "executionType": "HPC",
  "executionSystem": "shelob-execu-hpctrn20",
  "deploymentPath": "agave-deployment",
  "deploymentSystem": "shelob-storage-hpctrn20",
  "templatePath": "drawgau-wrapper.txt",
  "testPath": "test.txt",
  "checkpointable": false,
  "modules": [],
  "inputs": [
    {
      "id": "parfile",
      "value": {
        "validator": "",
```

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+ Add parameter

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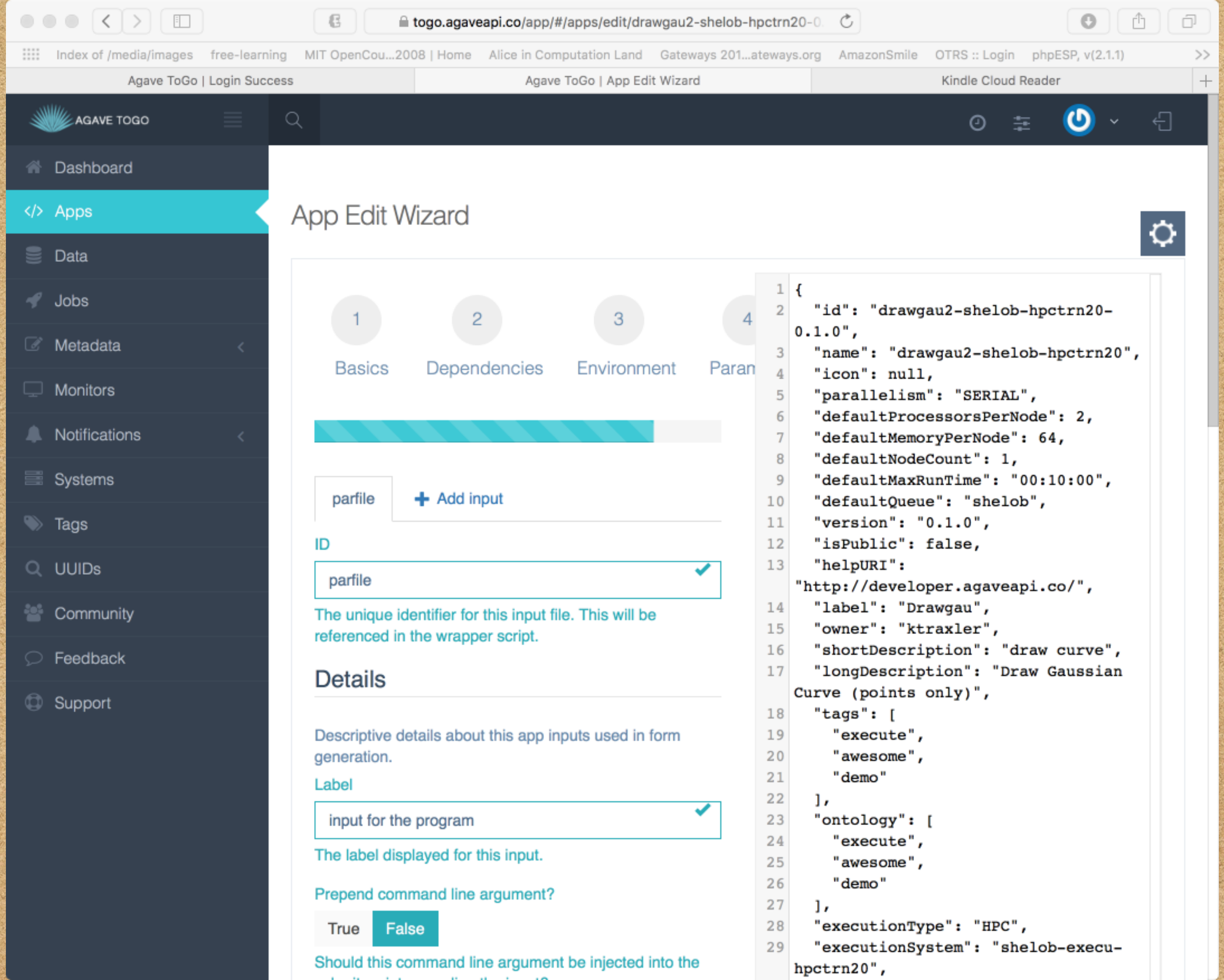
```
1  {
2    "id": "drawgau2-shelob-hpctrn20-
0.1.0",
3    "name": "drawgau2-shelob-hpctrn20",
4    "icon": null,
5    "parallelism": "SERIAL",
6    "defaultProcessorsPerNode": 2,
7    "defaultMemoryPerNode": 64,
8    "defaultNodeCount": 1,
9    "defaultMaxRunTime": "00:10:00",
10   "defaultQueue":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

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


```
    "demo"
  ],
  "executionType": "HPC",
  "executionSystem": "shelob-execu-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",
```

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.

Remove

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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


```
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": "http://developer.agaveapi.co/",
14  "label": "Drawgau",
15  "owner": "ktraxler",
16  "shortDescription": "draw curve",
17  "longDescription": "Draw Gaussian Curve (points only)",
18  "tags": [
19    "execute",
20    "awesome",
21    "demo"
22  ],
23  "ontology": [
24    "execute",
25    "awesome",
26    "demo"
27  ],
28  "executionType": "HPC",
29  "executionSystem": "shelob-execu-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


```
    "demo"
  ],
  "executionType": "HPC",
  "executionSystem": "shelob-execu-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": []
      }
```

Values

Default value and validations for the output field.

Default value

drawgau0.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.

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 paramters are returned in the response json.

Remove

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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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Apps Management

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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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togo.agaveapi.co/app/#/apps/drawgau2-shelob-hpctrn20-0.1.0/
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Agave ToGo | Login Success | Agave ToGo | | Kindle Cloud Reader

AGAVE TOGO

- Jobs
- Metadata
- Monitors
- Notifications
- Systems
- Tags
- UUIDs
- Community
- Feedback
- Support

DRAWGAU2-SHELOB-HPCTRN20-0.1.0

Details | Run

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 submited

☑ Archive output

Should the output be archived

AGAVE TOGO

- Tags
- UUIDs
- Community
- Feedback
- Support

Inputs

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drawgau-0611-728

A recognizable name for this job

Batch Queue

System queue to which the job should be submited

☑ Archive output

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