Introduction to XSEDE

Ben Lynch and Drew Gustafson
Aug 29, 2017

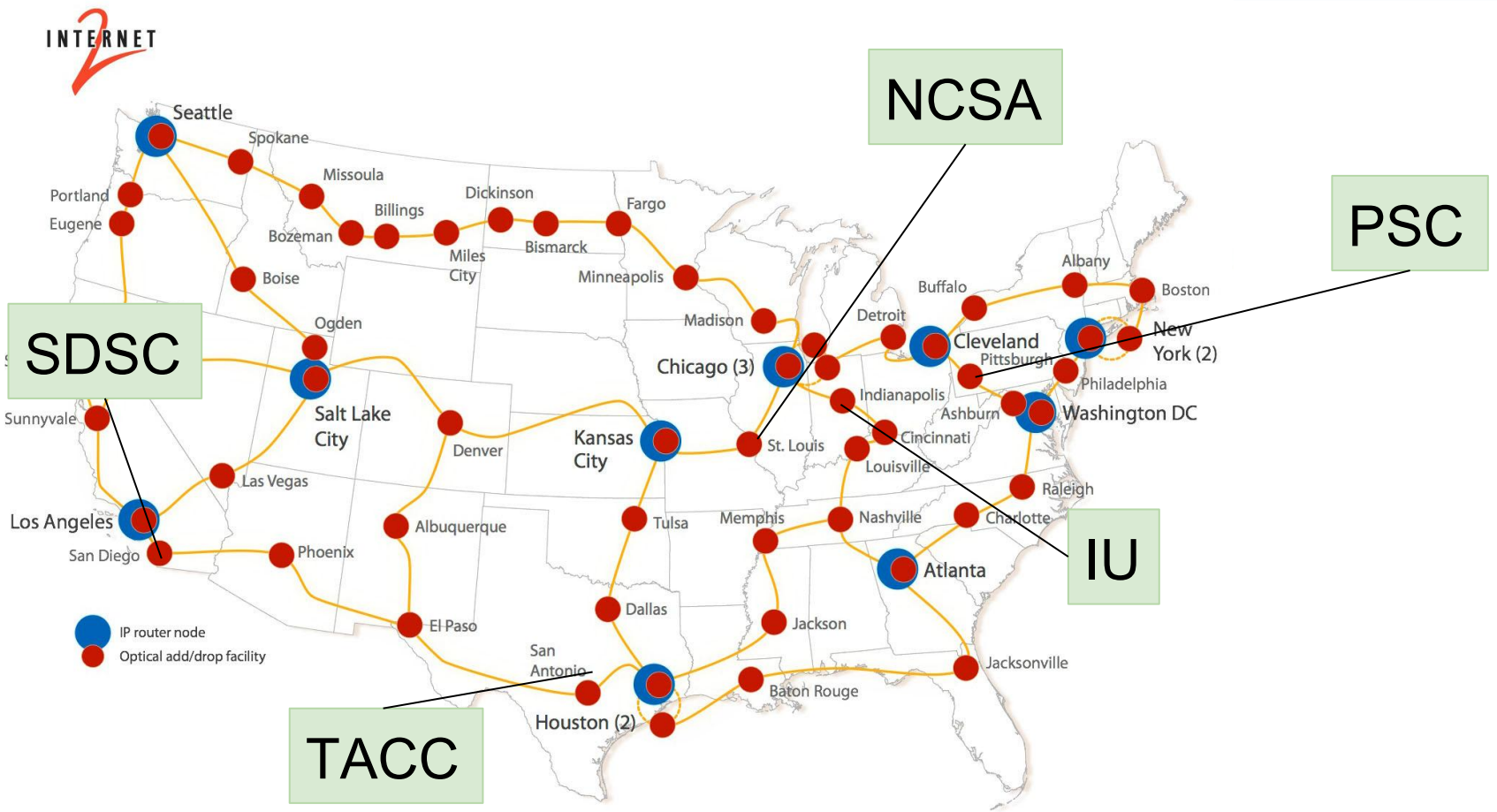
https://goo.gl/ARWMqw

Outline

- Overview of XSEDE
- Getting your account
- TACC
  - Running jobs on Stampede 2
- Globus data transfer
- JetStream
  - Creating Virtual Machines

XSEDE

- Available to investigators in the U.S. and their collaborators.
- Larger allocation are available to those with NSF funding
- Resources at Several sites including
  - Texas Advanced Computing Center (TACC)
  - Indiana University (IU)
  - Pittsburgh Supercomputing Center (PSC)
  - National Center for Supercomputing Applications (NCSA)
  - San Diego Supercomputing Center (SDSC)


INTERNET 2
NCSA
PSC
SDSC
IU
TACC
Seattle
Spokane
Portland
Eugene
Missoula
Billings
Dickinson
Fargo
Bozeman
Miles City
Bismarck
Minneapolis
Boise
Ogden
Madison
Albany
Buffalo
Boston
Detroit
Cleveland
New York (2)
Pittsburgh
Philadelphia
Chicago (3)
Indianapolis
Ashburn
Washington DC
Sunnyvale
Salt Lake City
Denver
Kansas City
St. Louis
Cincinnati
Louisville
Las Vegas
Raleigh
Los Angeles
Albuquerque
Tulsa
Memphis
Nashville
Charlotte
San Diego
Phoenix
Atlanta
Dallas
Jackson
El Paso
San Antonio
Jacksonville
Baton Rouge
Houston (2)
IP router node
Optical add/drop facility

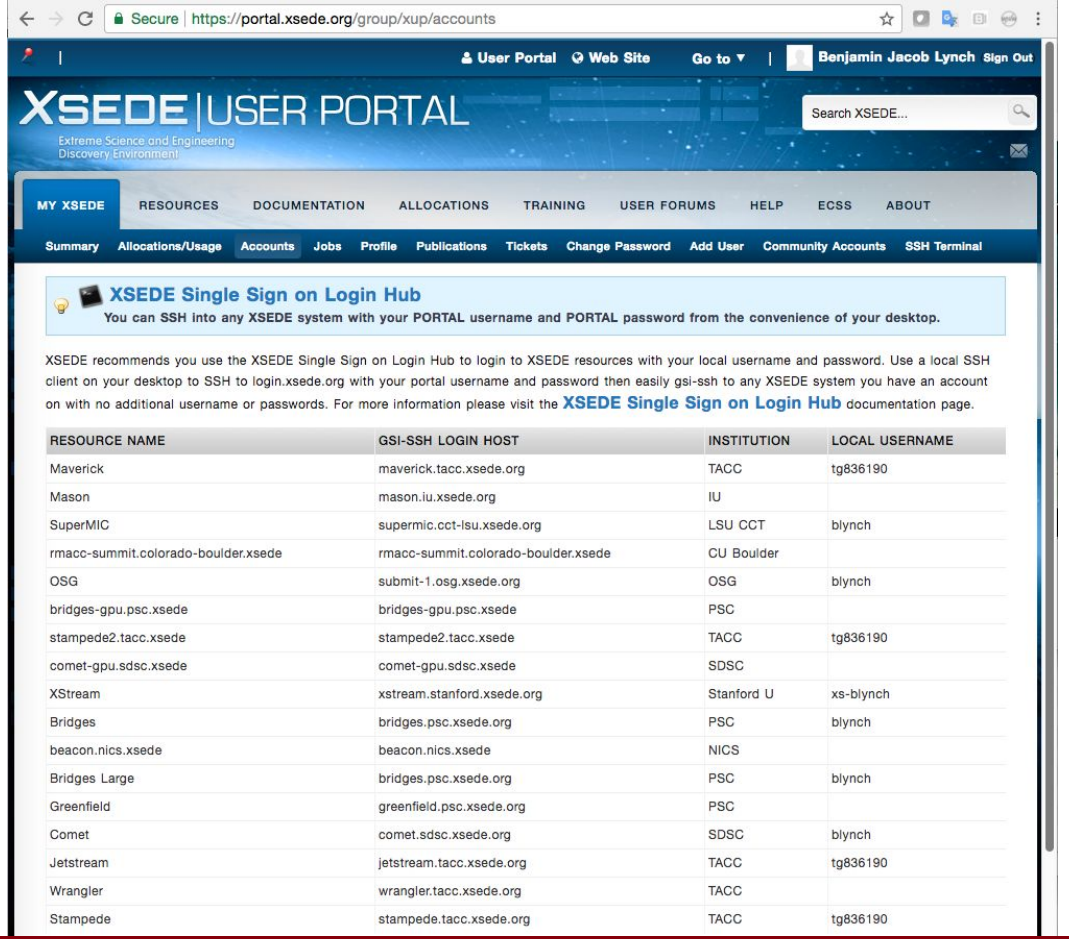
XSEDE - Why Would I Use It?

- When your jobs are waiting in the queue
  - Try Stampede 2 at TACC
- When you need more memory
  - Try Bridges at PSC
- When you need a VM to test something
  - Try Jetstream at IU

XSEDE Accounts

- Open a browser and go to xsede.org

XSEDE Accounts



RESOURCE NAME	GSI-SSH LOGIN HOST	INSTITUTION	LOCAL USERNAME
Maverick	maverick.tacc.xsede.org	TACC	tg836190
Mason	mason.iu.xsede.org	IU	
SuperMIC	supermic.cct-lsu.xsede.org	LSU CCT	blynch
rmacc-summit.colorado-boulder.xsede	rmacc-summit.colorado-boulder.xsede	CU Boulder	
OSG	submit-1.osg.xsede.org	OSG	blynch
bridges-gpu.psc.xsede	bridges-gpu.psc.xsede	PSC	
stampede2.tacc.xsede	stampede2.tacc.xsede	TACC	tg836190
comet-gpu.sdsc.xsede	comet-gpu.sdsc.xsede	SDSC	
XStream	xstream.stanford.xsede.org	Stanford U	xs-blynch
Bridges	bridges.psc.xsede.org	PSC	blynch
beacon.nics.xsede	beacon.nics.xsede	NICS	
Bridges Large	bridges.psc.xsede.org	PSC	blynch
Greenfield	greenfield.psc.xsede.org	PSC	
Comet	comet.sdsc.xsede.org	SDSC	blynch
Jetstream	jetstream.tacc.xsede.org	TACC	tg836190
Wrangler	wrangler.tacc.xsede.org	TACC	
Stampede	stampede.tacc.xsede.org	TACC	tg836190

Texas Advanced Computing Center (TACC)

- https://www.tacc.utexas.edu/
- Several systems available, primarily focused on large scale batch computing.
- The large supercomputer is named Stampede 2
- Stampede user guide: https://portal.tacc.utexas.edu/user-guides/STAMPEDE

Connecting to Stampede

- The first step is logging into the system.
- TACC uses two factor authentication.
- Configuring two factor authentication:
  - Easiest way is to use a phone app, or phone text messages.
  - A physical two factor device can also be mailed to you.

Connecting to Stampede

- SSH to Stampede:
  ssh username@stampede.tacc.xsede.org
- It will ask for your TACC password.
- It will then ask for the two factor code sent to your phone.

The Stampede Compute Environment

- Like MSI, Stampede uses the BASH shell by default.
- Like MSI, Stampede manages software using modules.
- The software visible via module depends on the currently loaded compiler/MPI configuration.

The Stampede Job Scheduler: SLURM

- SLURM is the job scheduler software used at TACC.
- SLURM job scripts are similar to PBS job scripts (the job scripts used at MSI).
- *sbatch* is the command that submits a job script.

Example SLURM Job Script

```
#!/bin/bash
#SBATCH -J myMPI           # job name
#SBATCH -o myMPI.o%j       # output and error file name (%j expands to jobID)
#SBATCH -n 32              # total number of mpi tasks requested
#SBATCH -p development     # queue (partition) -- normal, development, etc.
#SBATCH -t 01:30:00        # run time (hh:mm:ss) - 1.5 hours
#SBATCH --mail-user=username@tacc.utexas.edu
#SBATCH --mail-type=begin  # email me when the job starts
#SBATCH --mail-type=end    # email me when the job finishes

ibrun ./a.out              # run the MPI executable named a.out
```

Check on jobs using showq

login1$ **showq -u janeuser**

...

WAITING JOBS------------------------

JOBID	JOBNAME	USERNAME	STATE	CORE	WCLIMIT	QUEUETIME
1676351	helloworld	janeuser	Waiting	4096	15:30:00	Wed Sep 11 11:59:53
1676352	helloworld	janeuser	Waiting	4096	15:30:00	Wed Sep 11 12:00:07
1676354	helloworld	janeuser	Waiting	4096	15:30:00	Wed Sep 11 12:00:09

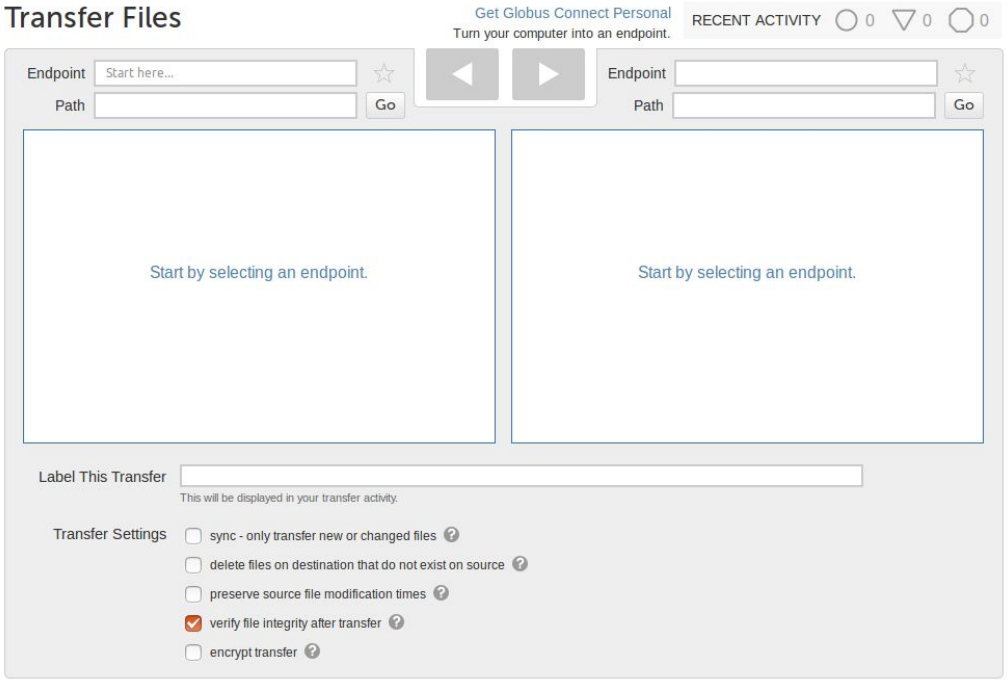
Stampede job queues

- Like MSI, Stampede uses job queues.
- The *development* queue is good for testing.
- The *normal* queue is good for many job types.
- Full queue list: https://portal.tacc.utexas.edu/user-guides/STAMPEDE#sandy-bridge-cluster-production-queues

Transferring data

- The scp command works, but requires two factor authentication.
- Globus is a user friendly transfer tool that allows transfers to be made from a convenient web interface.

Globus


Transfer Files
Get Globus Connect Personal
Turn your computer into an endpoint.
RECENT ACTIVITY 0 0 0
Endpoint
Start here...
Path
Go
Endpoint
Path
Go
Start by selecting an endpoint.
Start by selecting an endpoint.
Label This Transfer
This will be displayed in your transfer activity.
Transfer Settings
sync - only transfer new or changed files
delete files on destination that do not exist on source
preserve source file modification times
verify file integrity after transfer
encrypt transfer

Jetstream

- https://jetstream-cloud.org/

Secure https://jetstream-cloud.org

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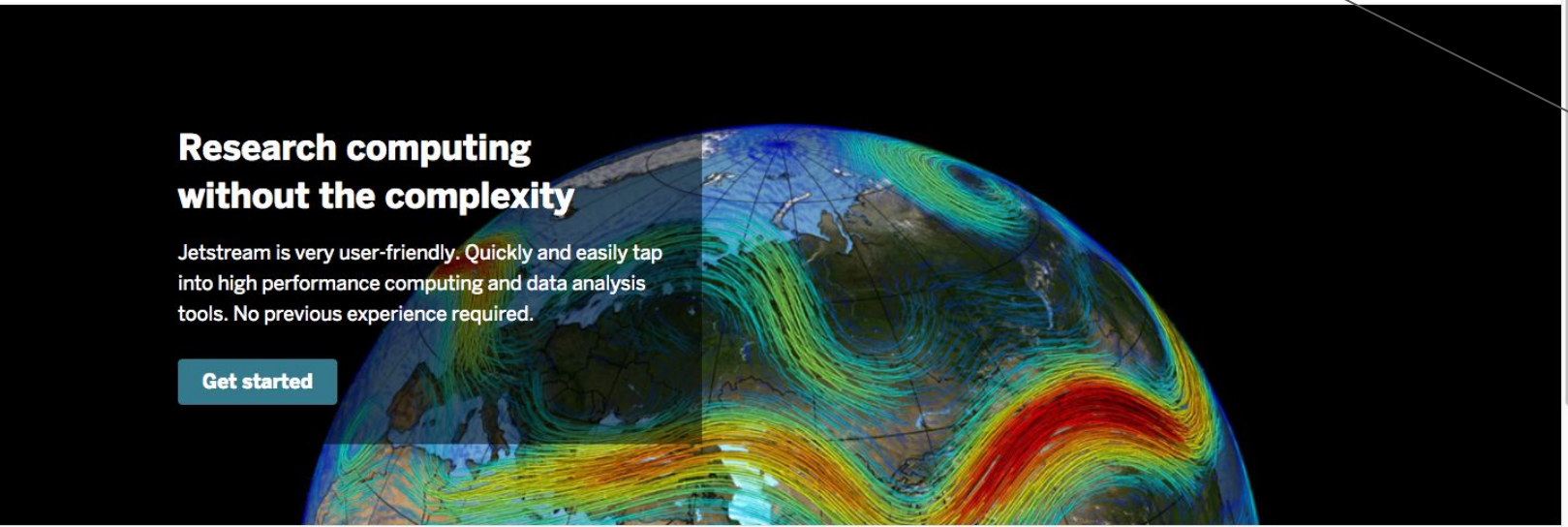

Cloud-based and on-demand, the 24/7 system includes discipline-

Tweets by @iu_pti

IU PTI @iu_pti

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community-contributed | Featured | m1_large | Ubuntu

R with Intel compilers (CentOS ...
Jul 14th 17 11:54 by jfischer

R with Intel compilers built on CentOS 7 (7.3)

** Requires m1.small or greater sized VM * ...

CentOS | desktop | development | Featured | gui | Intel | m1_small | vnc

Intel Development (CentOS 7)
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Intel compilers and development environment

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Centos 7 (7.3) Development GUI
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Centos 7 (7.3) Development GUI

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Getting Started

Launch New Instance

Browse Atmosphere's list of available images and select one to launch a new instance.

Browse Help Resources

View a video tutorial, read the how-to guides, or email the Atmosphere support team.

Change Your Settings

Modify your account settings, view your resource quota, or request more resources.

Resources Used

NEED MORE ?

Allocation Source

0 Instances

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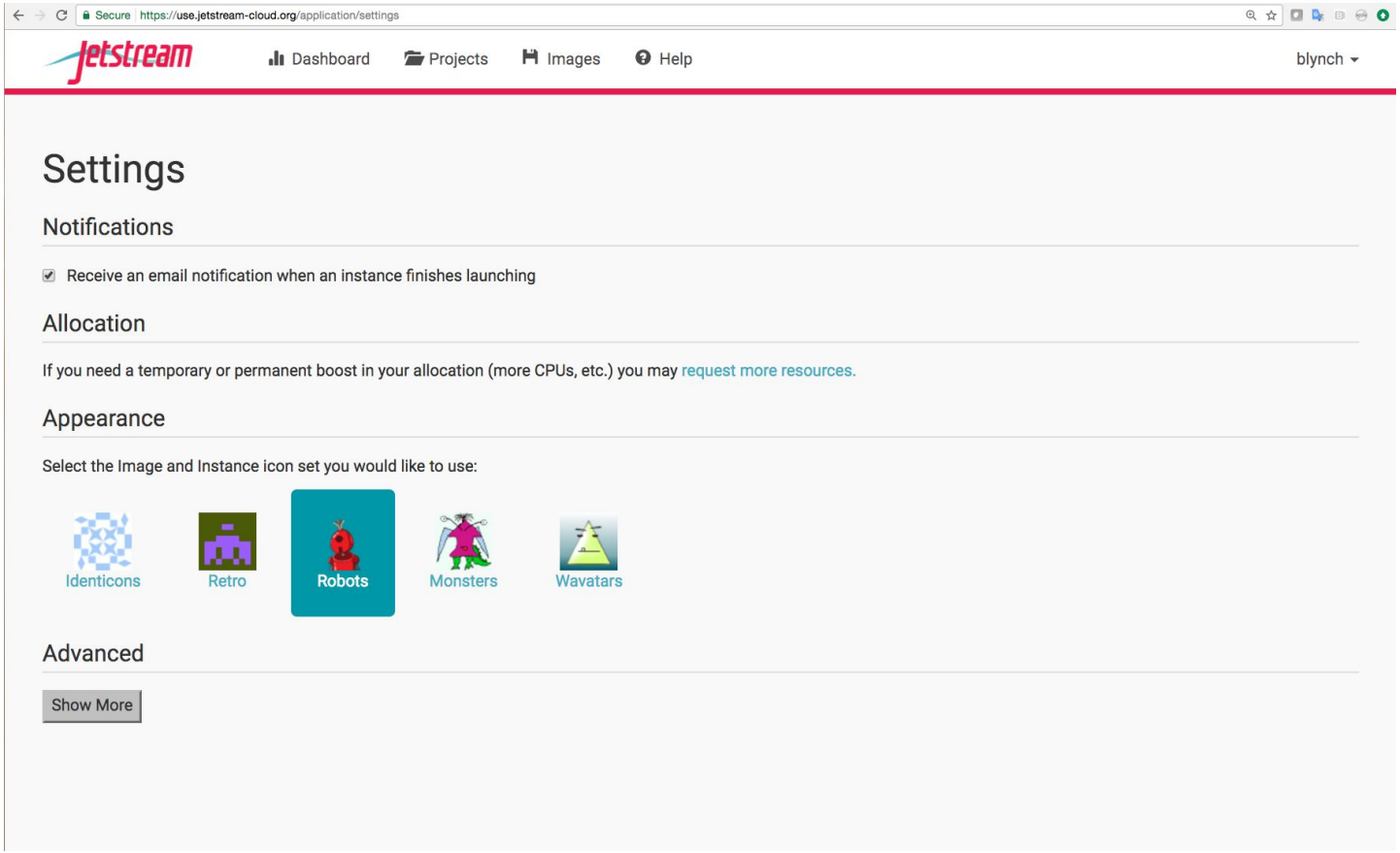
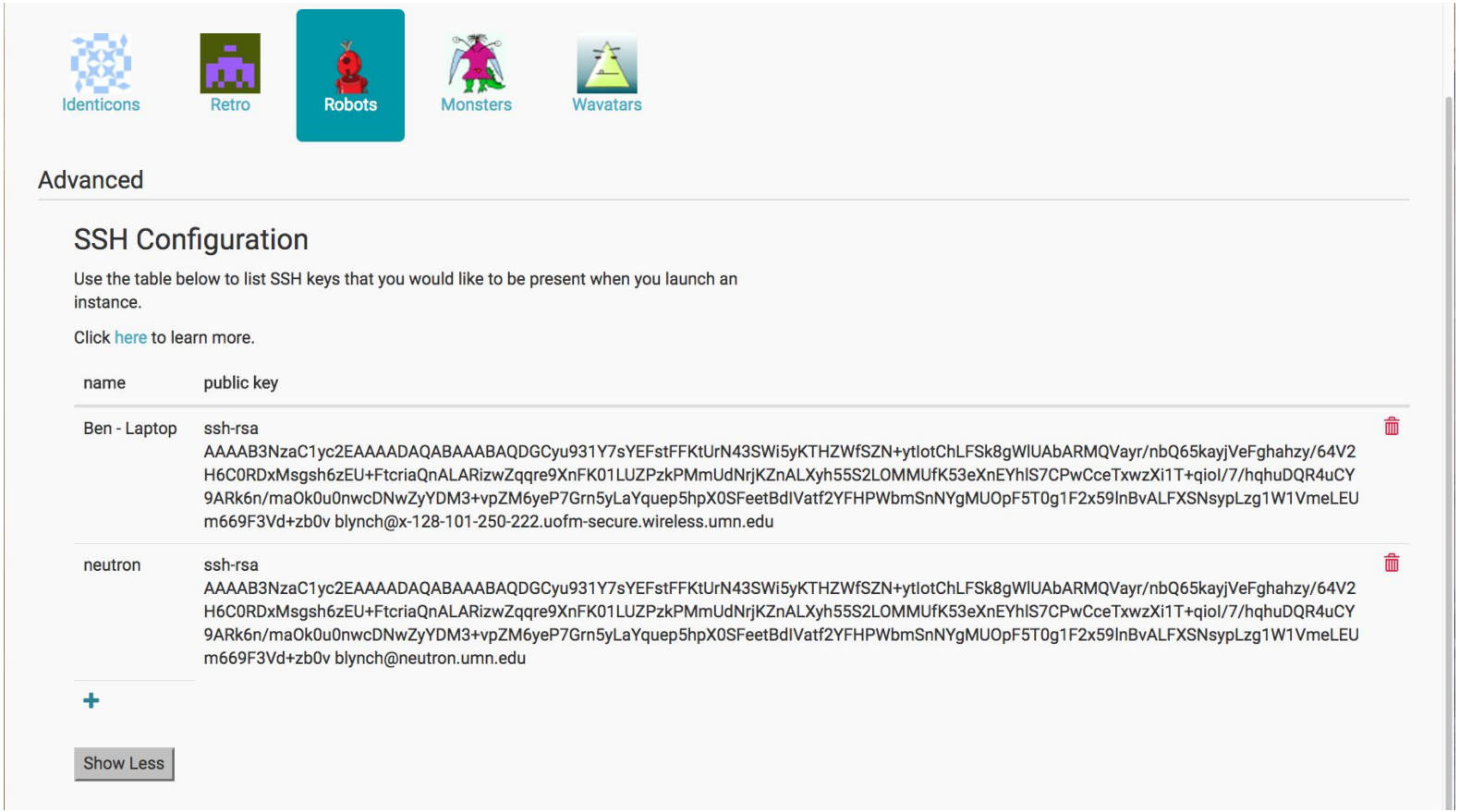
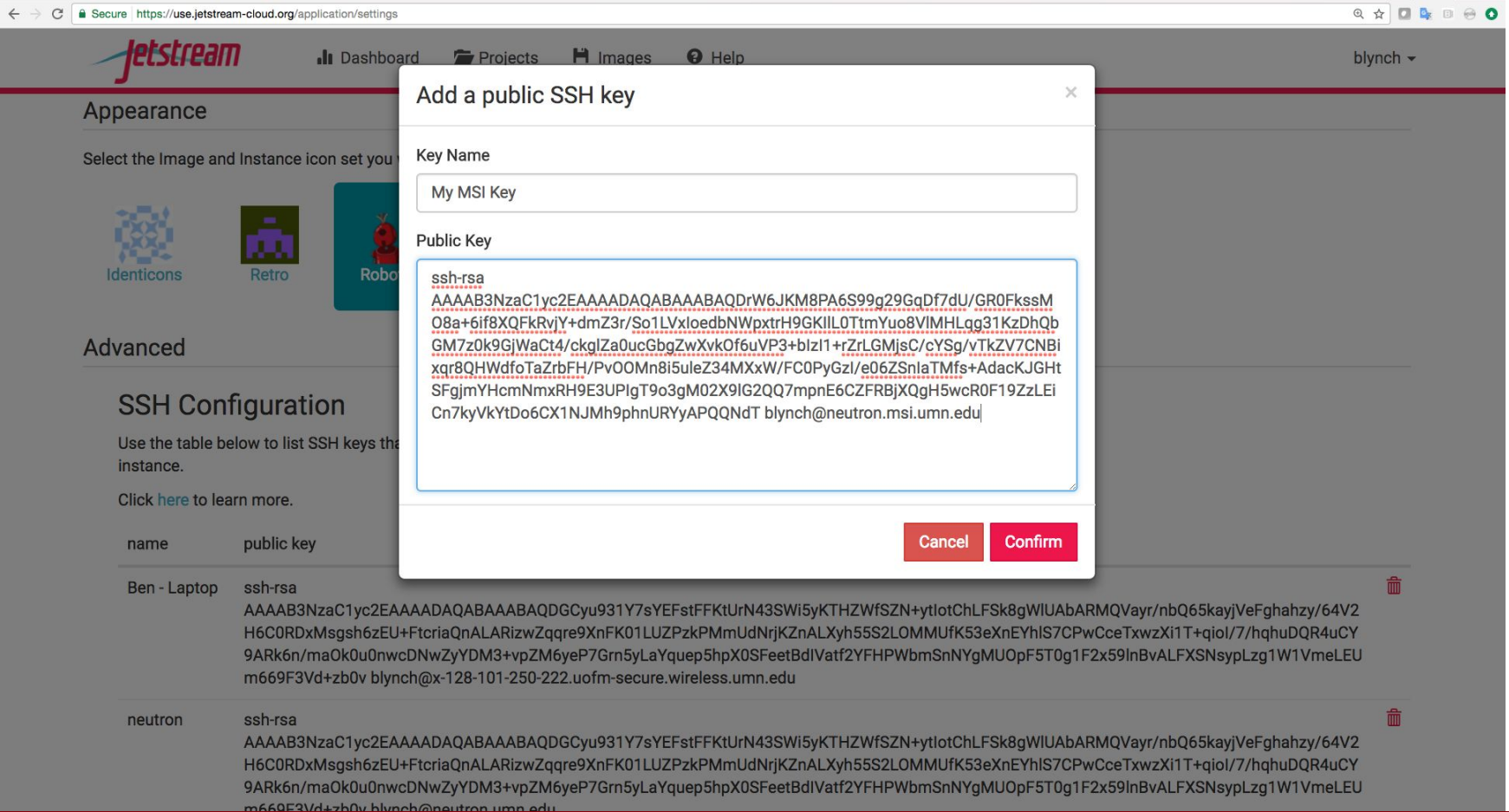

Secure https://use.jetstream-cloud.org/application/settings
jetstream
Dashboard
Projects
Images
Help
blynch
Settings
Notifications
Receive an email notification when an instance finishes launching
Allocation
If you need a temporary or permanent boost in your allocation (more CPUs, etc.) you may request more resources.
Appearance
Select the Image and Instance icon set you would like to use:
Identicons
Retro
Robots
Monsters
Wavatars
Advanced
Show More


Identicons
Retro
Robots
Monsters
Wavatars
Advanced
SSH Configuration
Use the table below to list SSH keys that you would like to be present when you launch an instance.
Click here to learn more.
name
public key
Ben - Laptop
ssh-rsa AAAAB3NzaC1yc2EAAAADAQABAAABAQDGCyu931Y7sYEFstFFKtUrN43SWi5yKTHZWfSZN+ytIotChLFSk8gWlUAbARMQVayr/nbQ65kayjVeFghahzy/64V2H6C0RDxMsgsh6zEU+FtcriaQnALARizwZqqre9XnFK01LUZPzkPMmUdNrjKZnALXyh55S2LOMMUfK53eXnEYhlS7CPwCceTxwzXi1T+qiol/7/hqhuDQR4uCY9ARk6n/maOk0u0nwcDNwZyYDM3+vpZM6yeP7Grn5yLaYquep5hpX0SFeetBdlVatf2YFHPWbmSnNYgMUOpF5T0g1F2x59lnBvALFXSNsypLzg1W1VmeLEUm669F3Vd+zb0v blynch@x-128-101-250-222.uofm-secure.wireless.umn.edu
neutron
ssh-rsa AAAAB3NzaC1yc2EAAAADAQABAAABAQDGCyu931Y7sYEFstFFKtUrN43SWi5yKTHZWfSZN+ytIotChLFSk8gWlUAbARMQVayr/nbQ65kayjVeFghahzy/64V2H6C0RDxMsgsh6zEU+FtcriaQnALARizwZqqre9XnFK01LUZPzkPMmUdNrjKZnALXyh55S2LOMMUfK53eXnEYhlS7CPwCceTxwzXi1T+qiol/7/hqhuDQR4uCY9ARk6n/maOk0u0nwcDNwZyYDM3+vpZM6yeP7Grn5yLaYquep5hpX0SFeetBdlVatf2YFHPWbmSnNYgMUOpF5T0g1F2x59lnBvALFXSNsypLzg1W1VmeLEUm669F3Vd+zb0v blynch@neutron.umn.edu
+
Show Less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name
public key
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ssh-rsa
AAAAB3NzaC1yc2EAAAADAQABAAABAQDGCyu931Y7sYEFstFFKtUrN43SWi5yKTHZWfSZN+ytIotChLFSk8gWIUAbARMQVayr/nbQ65kayjVeFghahzy/64V2
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m669F3Vd+zb0v blynch@x-128-101-250-222.uofm-secure.wireless.umn.edu
neutron
ssh-rsa
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9ARk6n/maOk0u0nwcDNwZyYDM3+vpZM6yeP7Grn5yLaYquep5hpX0SFeetBdIVatf2YFHPWbmSnNYgMUOpF5T0g1F2x59lnBvALFXSNsypLzg1W1VmeLEU
Add a public SSH key
Key Name
My MSI Key
Public Key
ssh-rsa
AAAAB3NzaC1yc2EAAAADAQABAAABAQDrW6JKM8PA6S99g29GqDf7dU/GR0FkssM
O8a+6if8XQFkRvjY+dmZ3r/So1LVxloedbNWpxtrH9GKIlL0TtmYuo8VlMHLqg31KzDhQb
GM7z0k9GjWaCt4/ckglZa0ucGbgZwXvkOf6uVP3+bIzI1+rZrLGMjsC/cYSg/vTkZV7CNBi
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SFgjmYHcmNmxRH9E3UPIgT9o3gM02X9lG2QQ7mpnE6CZFRBjXQgH5wcR0F19ZzLEi
Cn7kyVkYtDo6CX1NJMh9phnURYyAPQQNdT blynch@neutron.msi.umn.edu
Cancel
Confirm

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Centos 7 (7.3) Development GUI

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Ubuntu 16.04 Devel and Docker
Jun 21st 17 10:28 by jfischer

Ubuntu 16.04 LTS Development + GUI support + Docker

Based on Ubuntu cloud image for 16.04 ...

base | desktop | development | docker | docker-compose | Featured | Ubuntu | vnc | x2go

CentOS 6 (6.9) Development GUI
Jun 15th 17 03:52 by jfischer

Based on CentOS 6 (6.9) Development

- updated from 6.8 to 6.9

CentOS | desktop | development | Featured | gui | iRODS | vnc

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← Galaxy Standalone

☆ + ADD TO PROJECT | Launch

Created: 7/20/2017 11:34 am CDT

Created by: eafgan

Description: Galaxy Standalone - based on Ubuntu 14.04.4 LTS

This is a standalone Galaxy server that comes preconfigured with hundreds of tools and commonly used reference datasets: just launch and use.

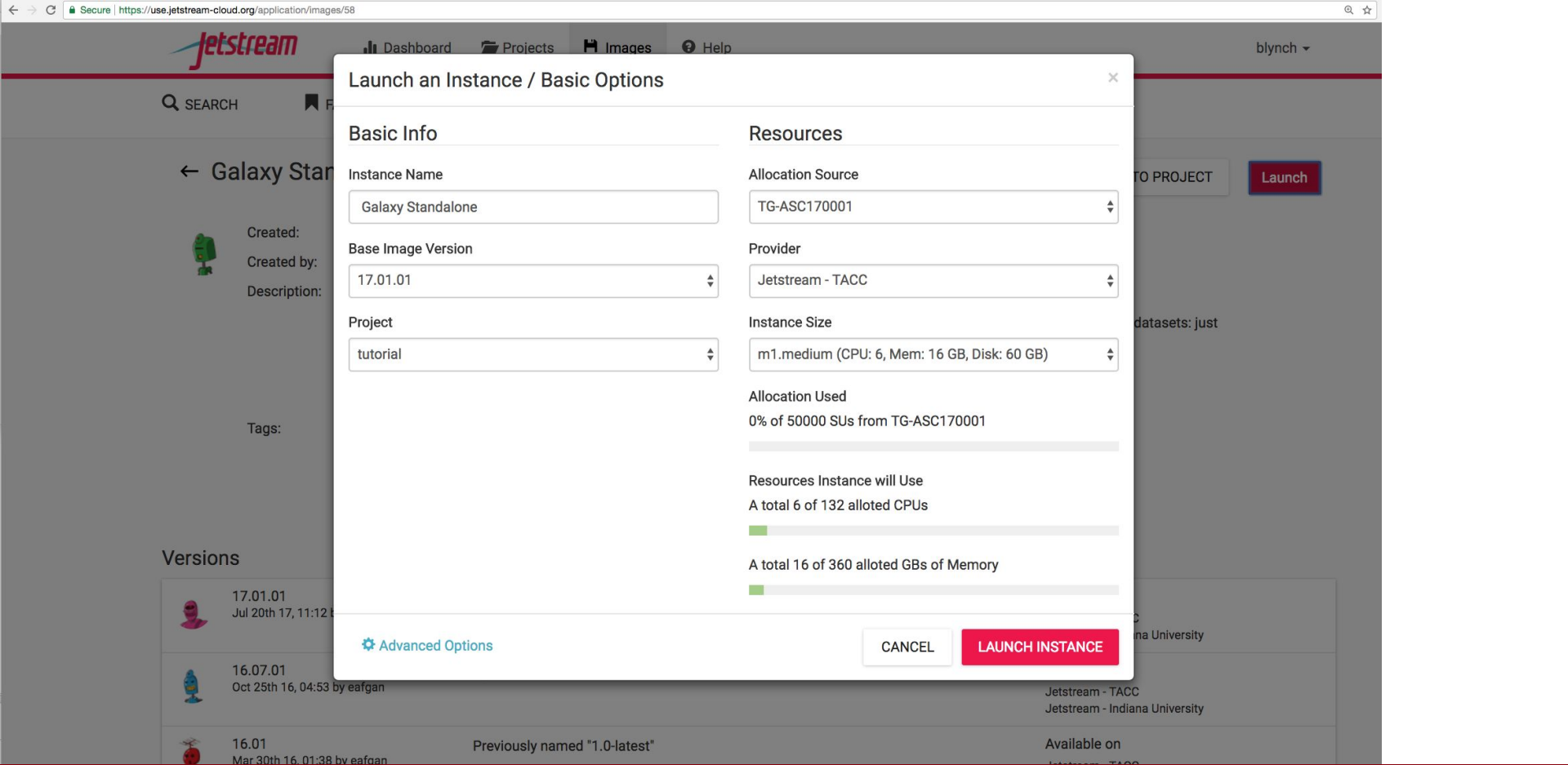
It is necessary to launch an instance type of Large or larger.

See https://galaxyproject.org/cloud/jetstream/ for information about this image and using it.

Tags: community-contributed | Featured | m1_large | Ubuntu

Versions

 17.01.01 Jul 20th 17, 11:12 by eafgan	Galaxy 17.01 with an updated toolset.	Available on Jetstream - TACC Jetstream - Indiana University
 16.07.01 Oct 25th 16, 04:53 by eafgan	Updated from 16.01 to 16.07	Available on Jetstream - TACC Jetstream - Indiana University
 16.01 Mar 30th 16, 01:38 by eafgan	Previously named "1.0-latest"	Available on Jetstream - TACC


Secure | https://use.jetstream-cloud.org/application/images/58
Jetstream
Dashboard
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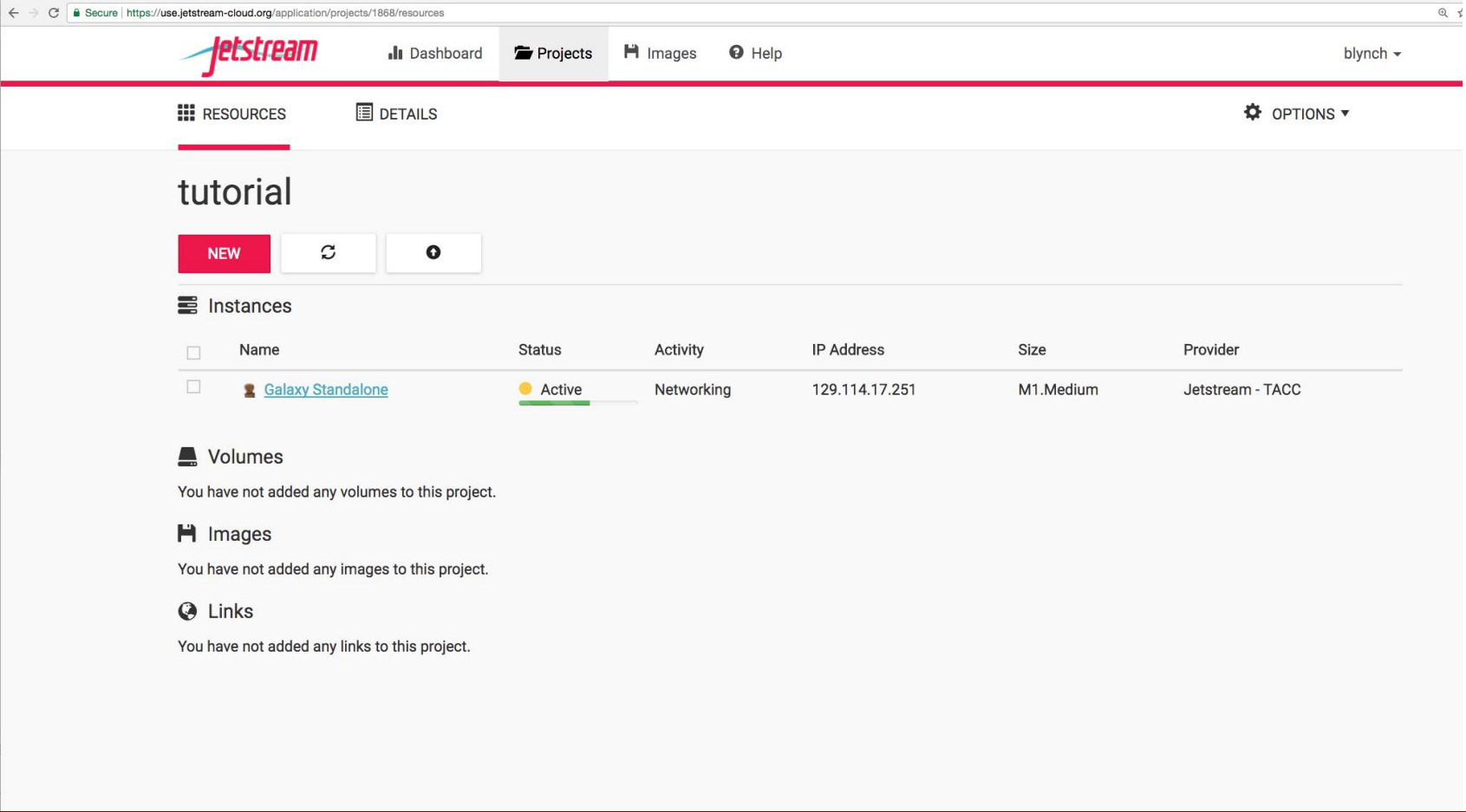
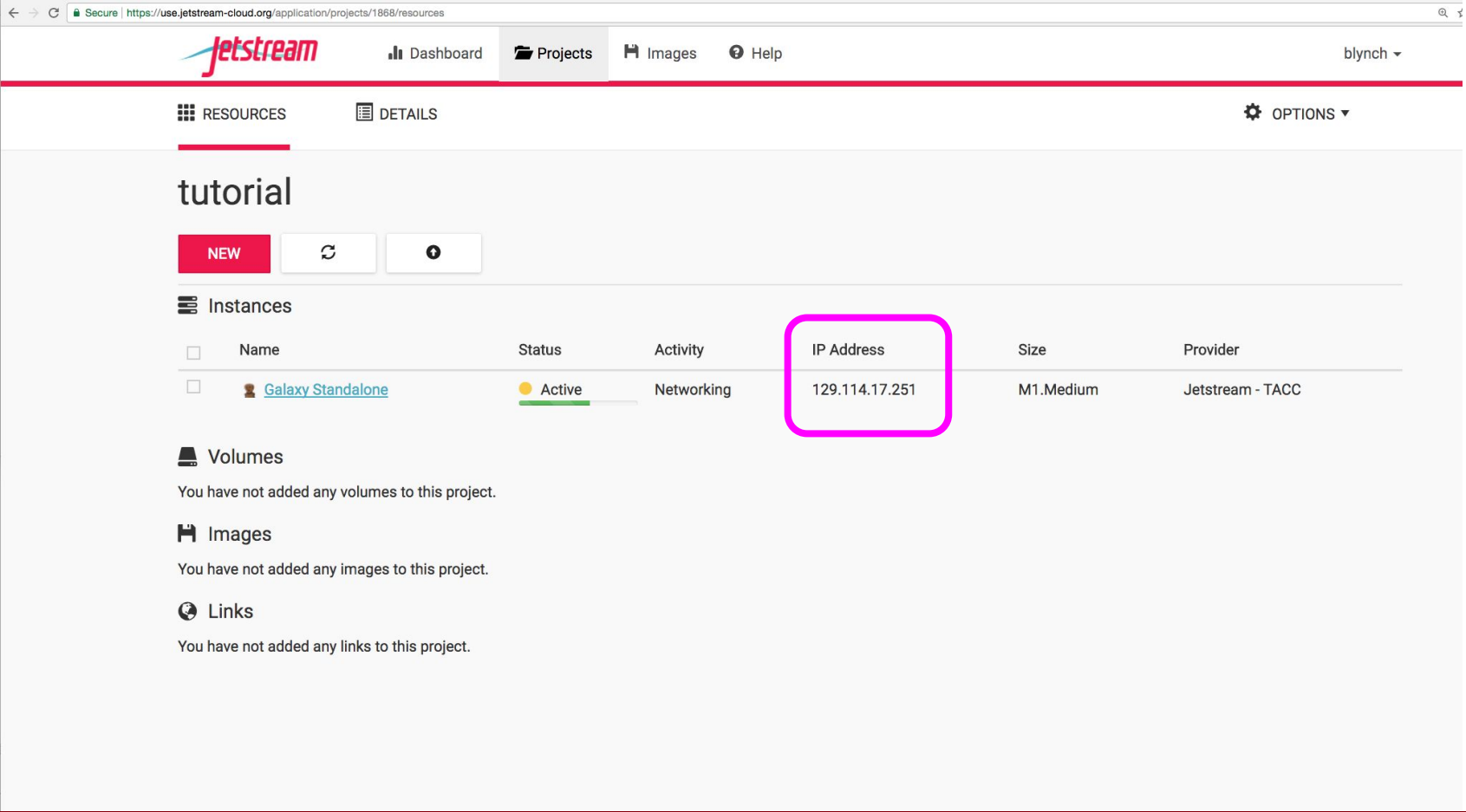
Images
Help
blynch
SEARCH
Launch an Instance / Basic Options
Basic Info
Instance Name
Galaxy Standalone
Base Image Version
17.01.01
Project
tutorial
Resources
Allocation Source
TG-ASC170001
Provider
Jetstream - TACC
Instance Size
m1.medium (CPU: 6, Mem: 16 GB, Disk: 60 GB)
Allocation Used
0% of 50000 SUs from TG-ASC170001
Resources Instance will Use
A total 6 of 132 alloted CPUs
A total 16 of 360 alloted GBs of Memory
Advanced Options
CANCEL
LAUNCH INSTANCE
Galaxy Star
TO PROJECT
Launch
Created:
Created by:
Description:
Tags:
Versions
17.01.01
16.07.01
Oct 25th 16, 04:53 by eafgan
16.01
Previously named "1.0-latest"
Jetstream - TACC
Jetstream - Indiana University
Available on


Secure | https://use.jetstream-cloud.org/application/projects/1868/resources
Jetstream
Dashboard
Projects
Images
Help
blynch
RESOURCES
DETAILS
OPTIONS
tutorial
NEW
Instances
Name
Status
Activity
IP Address
Size
Provider
Galaxy Standalone
Active
Networking
129.114.17.251
M1.Medium
Jetstream - TACC
Volumes
You have not added any volumes to this project.
Images
You have not added any images to this project.
Links
You have not added any links to this project.


Secure | https://use.jetstream-cloud.org/application/projects/1868/resources
Jetstream
Dashboard
Projects
Images
Help
blynch
RESOURCES
DETAILS
OPTIONS
tutorial
NEW
Instances
Name
Status
Activity
IP Address
Size
Provider
Galaxy Standalone
Active
Networking
129.114.17.251
M1.Medium
Jetstream - TACC
Volumes
You have not added any volumes to this project.
Images
You have not added any images to this project.
Links
You have not added any links to this project.

Next Steps

- Apply for your own allocation
- Discuss how you're able to move work between resources
  - https://groups.google.com/a/umn.edu/forum/#!forum/msi-epic
- Video tutorials for reference
  - z.umn.edu/msivideo