Computing at scale:
From laptop to cloud and HPC

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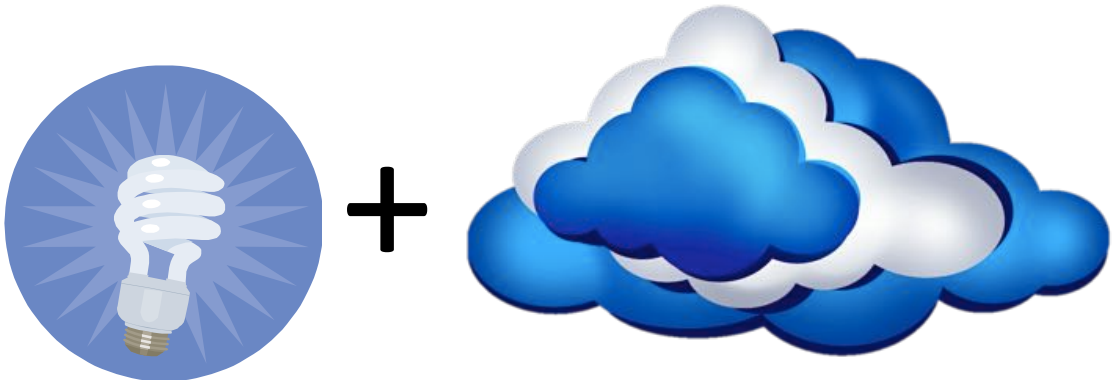
Topic Coverage

- General Innovation Lifecycle
- Why “computational thinking”
- NSF Infrastructure
- Technology landscape (cloud and containers)
- Hands on

Simple Formula for Success



The Reality

Excel R PERL
Python (Jupyter)
Java Ruby
Fortran C C# C++
MATLAB
etc.

Amazon
Azure
Google Cloud
Campus HPC
XSEDE
Etc.

Your favorite ML methods and lots of glue…..

+

More demand on your time

- Open innovation, science and collaboration
- Complexity of infrastructure
- Evolving landscape of technology
- Do you know where your data (and metadata) is ?
- We are in the age of extreme information technology
- You have to be willing to change your computational platform every 3 years !


Service Providers
rackspace
IBM
OPENSHIFT
Microsoft Azure
Yandex
Google
Quay.io
linode
Operating Systems
redhat
CoreOS
ubuntu
debian
fedora
CentOS
Configuration Management
puppet
Chef
Jenkins
SALTSTACK
Packer
ANSIBLE
docker
Big Data
syncsort
Dev Tools
Fig
VAGRANT
heroku
drone.io
Service Discovery
Eureka
SkyDNS
Official Repositories
MySQL
mongoDB
redis
NGINX
node
Orchestration
Shipper
Marathon
fleet
System Integrators
OpDemand
Wiredcraft
CentOS

Infrastructure every where

- NSF XSEDE invests $121M every 5 years
- UofA HPC invests $2.4 M every 3 years
- What is common between these offerings ?

We are data rich and knowledge poor

How do we change that ?

Computational thinking for Scalable Science

- Facilitating the **4A's** of "**Computational Thinking**" approaches: **A**bstraction, **A**utomation, **A**bility and **A**udacity
- Allowing researchers and educators to **establish and manage data driven collaborations**: Supporting distributed teams and virtual organizations (VO) at global scale
- Making **efficient and coordinated** use of CI resources from national, regional, institutional and commercial providers: NSF XSEDE, iPlant, campus HPC and high bandwidth connections to commercial cloud providers
- **Adopting best practices** from science domains where key CI challenges have been solved: HEP, Life science etc.
- Community driven, **self-provisioning, extensible** and open source: Development and prioritization driven through community engagement, active engagement with CISE communities

XSEDE: Resources for Science and Engineering

Slides from: Jeremy Fischer – jeremy@iu.edu

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What is XSEDE

- Virtual organization
- Distributed cyberinfrastructure
- Support
- Expertise
- Funded by the NSF

XSEDE supports a breadth of research

Some examples:

- **Earthquake Science and Civil Engineering**
- **Molecular Dynamics**
- **Nanotechnology**
- **Plant Science**
- **Storm modeling**
- **Epidemiology**
- **Particle Physics**
- **Economic analysis of phone network patterns**
- **Brain science**
- **Analysis of large cosmological simulations**
- **DNA sequencing**
- **Computational Molecular Sciences**
- **Neutron Science**
- **International Collaboration in Cosmology and Plasma Physics**
- **Social Sciences**
- **Humanities**

XSEDE supports thousands of such projects – these are sample domains.

XSEDE offers a variety of resources

- Leading-edge distributed memory systems
- Very large shared memory systems
- High throughput systems, e.g. OSG
- Visualization servers
- Accelerators and co-processors including NVIDIA GPUs and XEON Phi (MICs)
- Cloud services

Many scientific problems have components that call for use of more than one architecture.

Current XSEDE Compute Resources

- Stampede @ TACC *(soon to be Stampede II!)*
  - 10+ PFLOPS (PF) Dell Cluster w/ GPUs and Xeon PHIs
- Bridges @ PSC
  - Large memory, regular shared memory, GPUs
- Comet @ SDSC
  - 2 PFLOPS (PF) Dell Cluster
- Jetstream @ IU/TACC
  - .5 PF Distributed Cloud Compute Dell Cluster
- SuperMIC @ LSU, Xstream @ Stanford

https://www.xsede.org/web/xup/resource_monitor

Current XSEDE Visualization and Data Resources

- Visualization
  - Maverick @ TACC
    - 132 HP nodes, dual CPU, 20 cores per node, 1 K40 per node
    - 66 TB disk
- Storage
  - Pylon @ PSC
    - 4 PB disk
  - Wrangler @ TACC/IU
    - 10 PB disk per site
    - 4 TB FLASH @ TACC
  - Ranch @ TACC
    - 160 PB tape
  - Data Oasis @ SDSC
    - 4 PB disk

XSEDE User Services

XSEDE User Services are grouped into four main areas:

- Technical information
  - Always available via web site and XSEDE user portal
- Allocations
  - Request access to XSEDE systems
- Training
  - Sign up for classes to learn to use XSEDE resources
- User Engagement
  - Includes consulting support to answer questions
  - Also includes user interviews, focus groups, and surveys

Getting Started with XSEDE

It's **easy** to get started as an XSEDE user:

1. Go to the main web site: portal.xsede.org
2. Select 'Create account' on the left

XSEDE Allocations

- Resources at the right price…
  - HPC
  - High throughput computing
  - Remote visualization
  - Data storage
  - Etc.
- ECSS - Extended Collaborative Support Services
- Single Sign-On for most resources

XSEDE Allocations (2)

- Request allocations through the XSEDE User Portal
- It's **easy** to get a Startup allocation—best way to get started
- Education allocations for classroom/workshop use
- Larger year-long research allocations can be requested 4 times/year, are peer reviewed, and have a longer lead-time
- Quarterly webinars on writing allocations

XSEDE Training

- XSEDE provides extensive training
  - Covering every major resource
  - From beginner to advanced classes
  - At locations across the country
  - Online via
    - asynchronous technologies
    - Webcasts
- Signing up is **simple--**in the XSEDE User Portal!

Getting Help

- Getting help is **easy—again**, via the XUP
  - XSEDE Knowledge Base
  - User Guides
  - Campus Champion directory for local help
  - You can also call the helpdesk **1-866-907-2383** 24x7 to request assistance

Community Engagement Activities

- Student Programs
- Under-represented Community Engagement
- Champions Program
- XSEDE Community Infrastructure (XCI)
- Campus Visits
- Annual XSEDE/PEARC Conference

Student Programs

- XSEDE Scholars
  - engaging undergraduates and graduates in year-long series of webinars attend annual XSEDE Conference
- XSEDE/PEARC Annual Conference
  - travel support for students to attend the annual Conference
- HPC University
  - Lists other student engagement opportunities

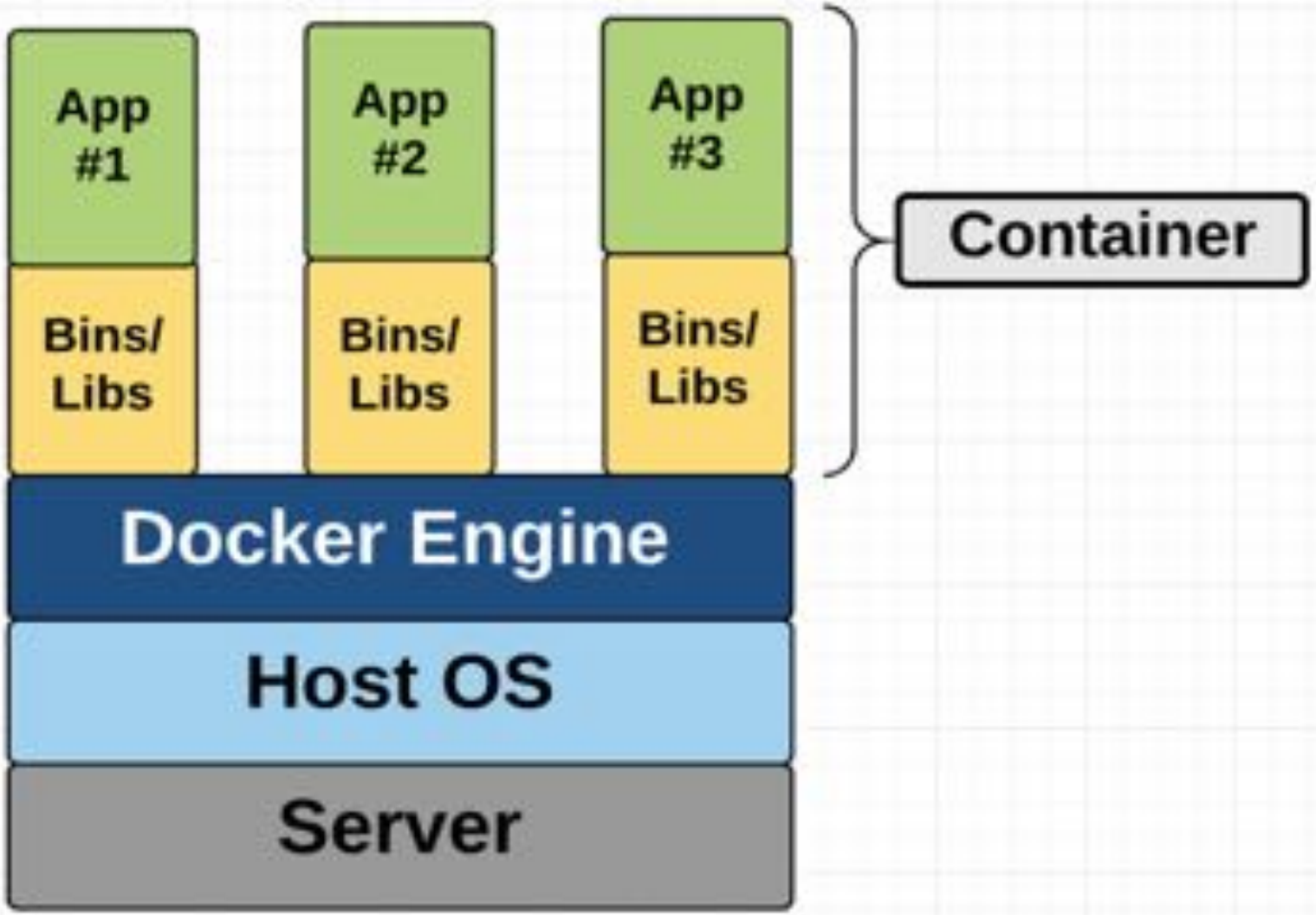
Under-represented Community Engagement

- Outreach to faculty and students at Minority Serving institutions
- Assist faculty with conducting their research using XSEDE resources
- Assist faculty with incorporating computational tools, resources and methods into the curriculum
- Minority Research Committee – faculty assisting one another
- Engaging students various programs

Campus Champions Role

- Raise awareness locally
- Provide training
- Get users started with access quickly
- Represent needs of local community
- Provide feedback to improve services
- Attend annual conference
- Share their training and education materials
- Build community among all Champions

Why and Why for Containers



What is Jetstream and why does it exist?

- NSF's first production cloud facility
- Based on project Atmosphere from CyVerse*
- Part of the NSF eXtreme Digital (XD) program
- Provides on-demand *interactive* computing and analysis
- Enables *configurable* environments and *programmable cyberinfrastructure*
- User-friendly, widely accessible cloud environment
- User-selectable library of preconfigured virtual machines

Jetstream
http://jetstream-cloud.org/

funded by the National Science Foundation
Award #ACI-1445604

What is Jetstream, continued…

- Focus on ease-of-use, broad accessibility
- Command line access for those who want it and GUI access for those who don't
- Will support persistent gateways (SEAGrid, Galaxy, GenApp NAMDRunner, CIPRES and others)
- Reproducibility: Share VMs and then store, publish via IU Scholarworks (DOI)

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Who uses Jetstream?

- The researcher needing a handful of cores (1 to 44/vCPU)
- Software creators and researchers needing to create their own customized virtual machines and workflows
- Science gateway creators using Jetstream as either the frontend or processor for scientific jobs
- STEM Educators teaching on a variety of subjects

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21st Century Workforce Development

- Specialized virtual Linux desktops and applications to enable research and research education at small colleges and universities
- HBCUs (Historically Black Colleges and Universities)
- MSIs (Minority Serving Institutions)
- Tribal colleges
- Higher-education institutions in EPSCoR States

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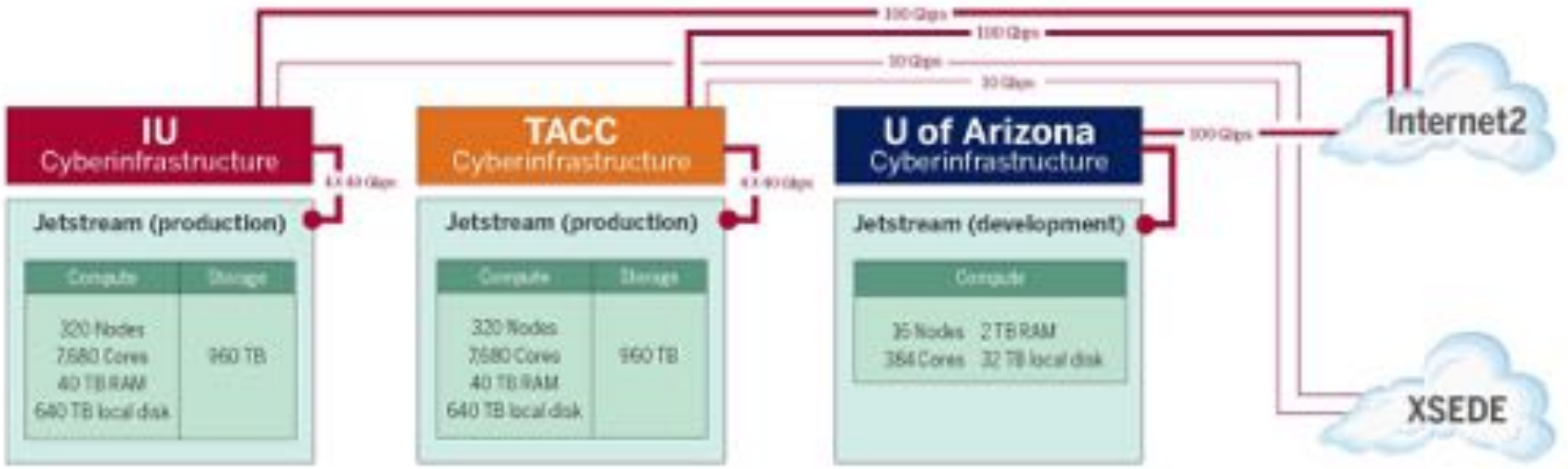
Jetstream System Overview



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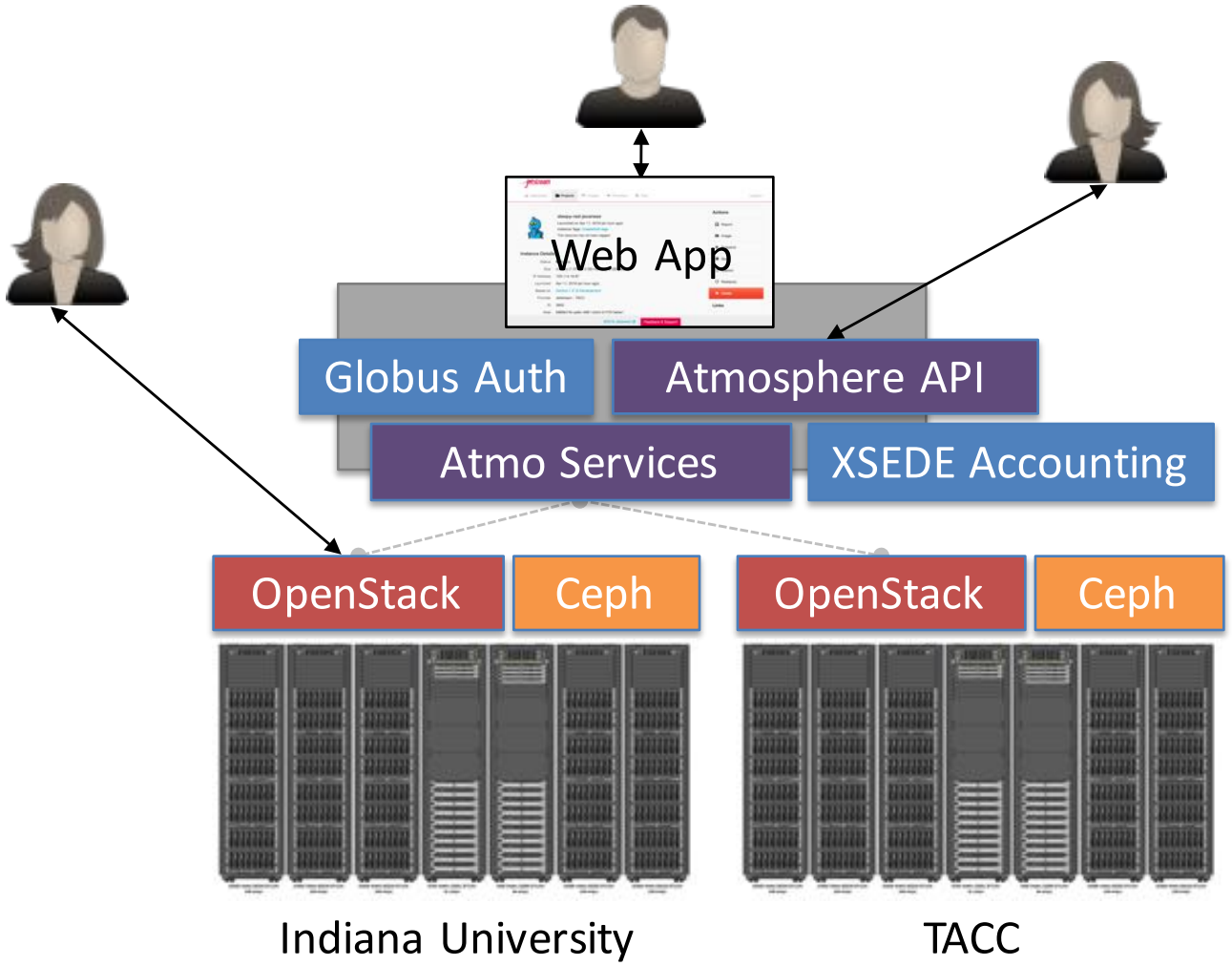
Platform Overview



Hardware and Instance "Flavors"

VM Host Configuration

- Dual Intel E-2680v3 "Haswell"
- 24 physical cores/node @ 2.5 GHz (Hyperthreading on)
- 128 GB RAM
- Dual 1 TB local disks
- 10GB dual uplink NIC
- Running KVM Hypervisor

- Short-term *ephemeral* storage comes as part of launched instance
- Long-term storage is XSEDE-allocated
- Implemented as OpenStack Volumes
- Each user can get 10 volumes up to 500GB total storage*

Flavor	vCPUs	RAM	Storage	Per Node
m1.tiny	1	2	8	46
m1.small	2	4	20	23
m1.medium	6	16	60	7
m1.large	10	30	60	4
m1.xlarge	24	60	60	2
m1.xxlarge	44	120	60	1
s1.large**	10	30	120	4
s1.xlarge**	24	60	240	2
s1.xxlarge**	44	120	480	1

** s1.* based instances are not eligible to be saved into a customized image

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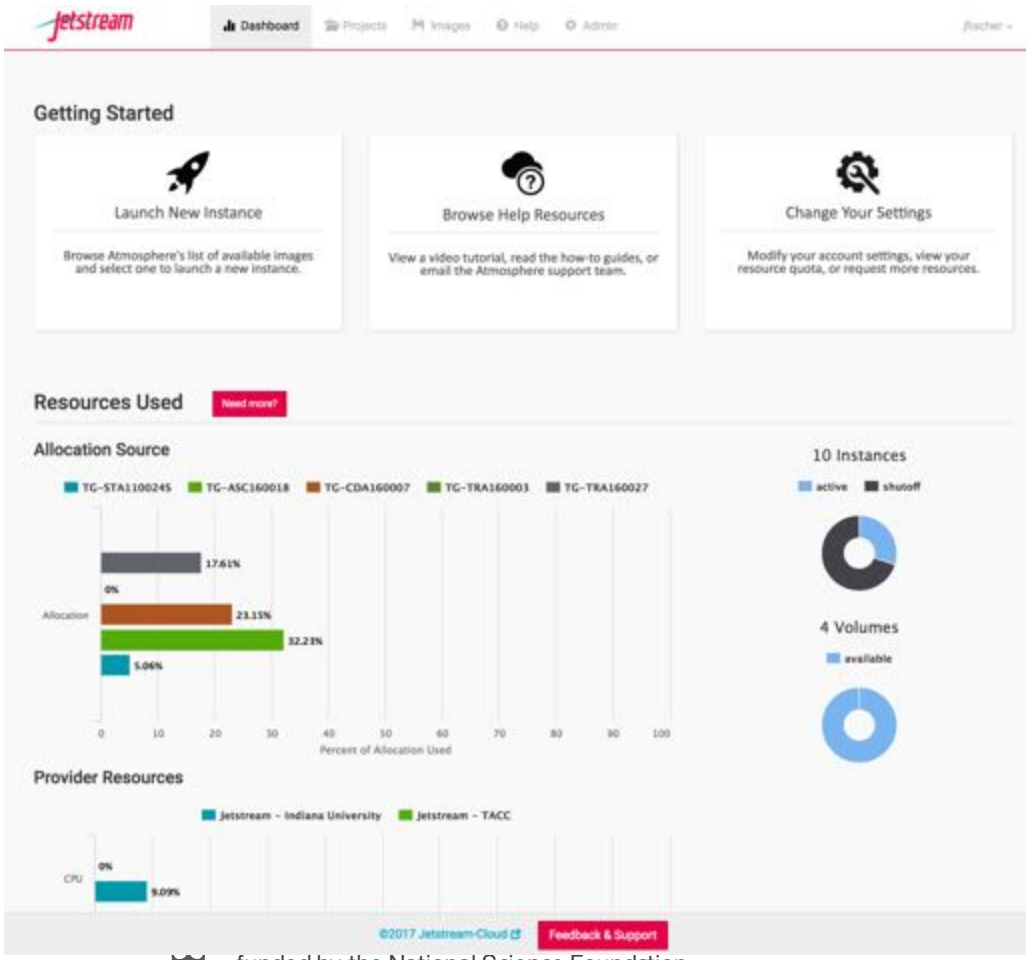
The Jetstream Atmosphere web interface



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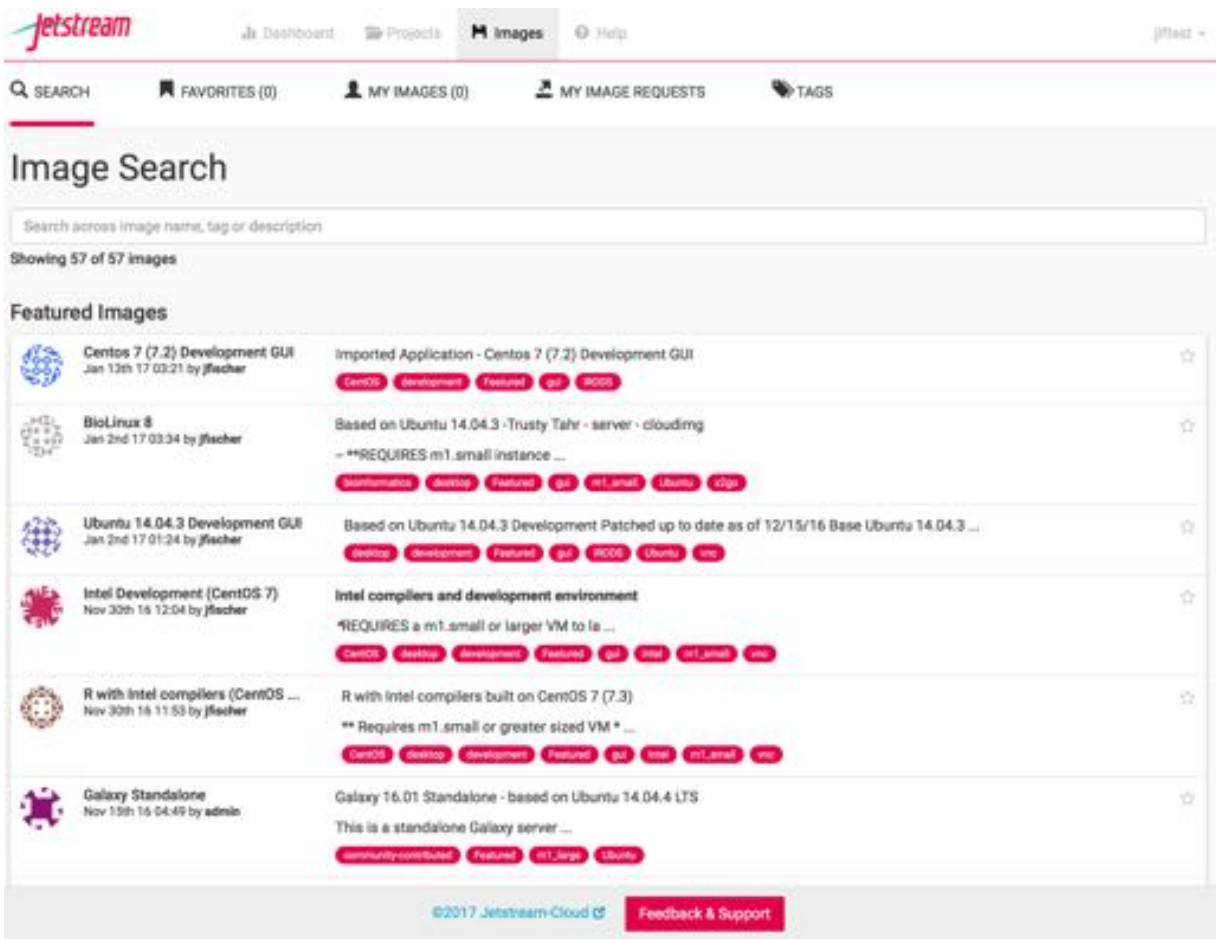
The Jetstream Atmosphere web interface



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http://jetstream-cloud.org/

Using Jetstream VMs

- Manipulating Jetstream VMs:
- • Jetstream Atmosphere web interface
- • Direct API access via OpenStack command line or Horizon access
- - API access enables Science Gateways and other always on services or on demand use cases; e.g. elastic compute techniques

- Primary methods of logging into Jetstream VMs to work
- • Interactive user access via web interface with VNC/SSH
- • Direct VNC/SSH to individual instances

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HPC vs Cloud

- Adapting to a different environment:
- No reservations, no queueing
- More interactive use and less/no batch queuing
- What? No parallel filesystem?!?
- Being your own admin – hey, we have root!
- You really can have almost any (linux) software you want**
- Constantly getting new features (https://www.openstack.org/software/project-navigator/)
  - ** Here there be dragons…

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Requesting access to Jetstream

- You can request startup allocations anytime. (Startups are simple!)
- You can request allocations for educational use anytime.
- We are happy to help you prepare a request and create a successful proposal.
- You do not have to have prior use of Jetstream to be successful.

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Allocation types and docs needed for each

- Startup allocation (apply anytime)
- - Current CV for PI and any Co-Pis
- - Brief abstract/description of work
- Education allocation (apply anytime)
- - Current CV for PI and any Co-PIs
- - Syllabus/Class/Workshop description
- - Description of use --> justification of SUs requested
- Research allocation (quarterly allocation window)
- - Current CV for PI and any Co-PIs
- - Main project description (up to 10 pages unless > 15M SUs, then 15 pages)
- - Scaling doc (up to 5 pages)

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Not just the usual suspects…

- Physics, chemistry, and other "usual" HPC suspects are represented, but Jetstream also is home to projects on:
- Financial analysis / Economics
- Political science
- Humanities / Text analysis
- Network analysis
- Computer Science / Machine learning
- Satellite data analysis

Jetstream
http://jetstream-cloud.org/
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Getting help with JetStream

Wiki / Documentation: http://wiki.jetstream-cloud.org

User guides: https://portal.xsede.org/user-guides

XSEDE KB: https://portal.xsede.org/knowledge-base

Email: help@xsede.org

Campus Champions: https://www.xsede.org/campus-champions

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My cloud toolbox

- Ansible for automation
- Docker for execution environment
- Makeflow workqueue for task distribution
  ccl.cse.nd.edu/software/

SPIE Proceedings | Volume 9913 | Data Management and Archives I >

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Proceedings Article

High-contrast imaging in the cloud with klipReduce and Findr

Asher Haug-Baltzell ; Jared R. Males ; Katie M. Morzinski ; Ya-Lin Wu ; Nirav Merchant ; Eric Lyons ; Laird M. Close

[+] Author Affiliations

Proc. SPIE 9913, Software and Cyberinfrastructure for Astronomy IV, 99130F (August 8, 2016); doi:10.1117/12.2234095

Hands On Part

1. Get the training login (paper is going around)
2. Go to: https://use.jetstream-cloud.org
3. Login and browse around choose the image
4. Launch **Ubuntu 14.04.3 Dev w Docker CE**
5. Open web shell and start playing with shell
6. Visit hub.docker.com (store.docker.com)
7. https://github.com/jupyter/docker-stacks/tree/master/datascience-notebook
8. Lets install and run Jupyter notebook and bring something in.
9. docker run -it --rm -p 8888:8888 -v /home/train**70**:/home/jovyan/work jupyter/ datascience-notebook