



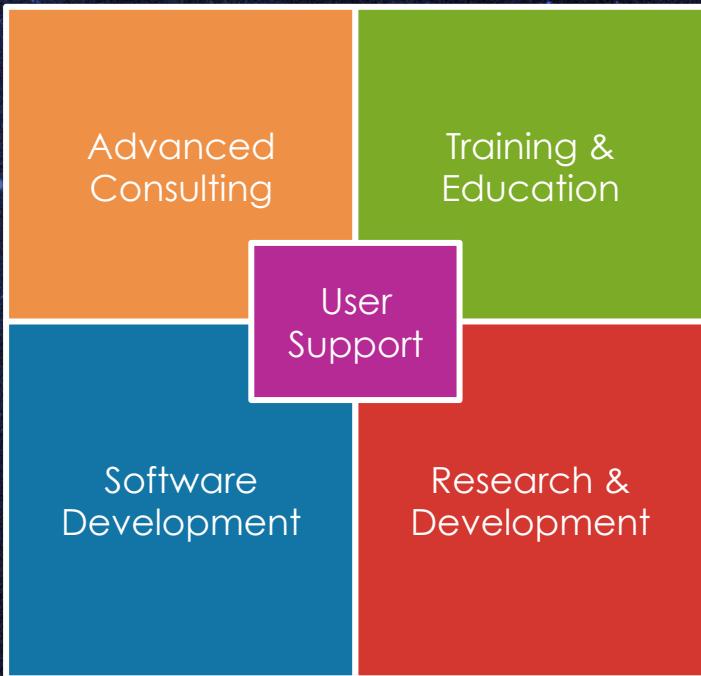
CONTAINERS @ TACC

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Life Sciences Computing, TACC

TACC OVERVIEW

- 160 staff members
 - 70 PhDs, ~25 students
 - 1 in 3 have 10+ years exp
- Over 50 open source software codes
- 30+ active research projects
- Monthly training - Data Science to MPI to UNIX 101
 - 500+ trainees annually
- 300+ K12 students engaged each year



HIGH PERFORMANCE COMPUTING ECOSYSTEM



HIGH PERFORMANCE COMPUTING ECOSYSTEM

Computing System	Specialization
Stampede 2	18PF Intel Skylake and KNL - Capability HPC
Lonestar 5	2PF Intel Haswell - HPC & HTC
Wrangler	600 TB Flash + 10 PB HDD - Data Intensive
Maverick	High-end NVIDIA GPU - ML, Analytics, Visualization
Jetstream & Chameleon	OpenStack clusters - Programmable infrastructure
Rodeo	VMware/OpenStack - Production hosting
Stockyard	20PB Lustre - Compute-optimized filesystem
Corral	15PB GPFS - High-integrity, performant HDD
Ranch	160PB SAMFS - Long-term archival storage

INFRASTRUCTURE AS A SERVICE

Atmosphere

Web Service Training

Instances

Name	Status	Activity	IP Address	Size	Provider
Ubuntu 14.04.3 Development	Active		129.114.17.28	M1.Tiny	Jetstream - TACC
Ubuntu 14.04.3 Development	Active		149.165.156.40	M1.Tiny	Jetstream - Indiana University
Ubuntu 14.04.3 Development	Suspended	N/A	149.165.156.40	M1.Xlarge	Jetstream - Indiana University
CentOS 6 Studio	Active	Networking	129.114.17.140	M1.Medium	Jetstream - TACC

Feedback & Support

[Press Shift-F1 for help]

Host IP or ssh:// URL [localhost]: ssh://vaughn@129.114.104.242:22
Connecting to ssh://vaughn@129.114.104.242:22

The following SSH identities are being used for this connection:
vaughn_default

Last login: Mon Apr 11 07:31:48 2016 from 129.114.104.5

Atmosphere

For assistance, contact help@xsede.org
[vaughn@104-242 ~]\$ uname -a
Linux js-104-242-jetstream-cloud.org 2.6.32-573.22.1.el6.x86_64 #1 SMP Wed Mar 23 03:35:35
[vaughn@104-242 ~]\$ whoami
vaughn
[vaughn@104-242 ~]\$ sudo su -
-bash-4.1# whoami
root
-bash-4.1#

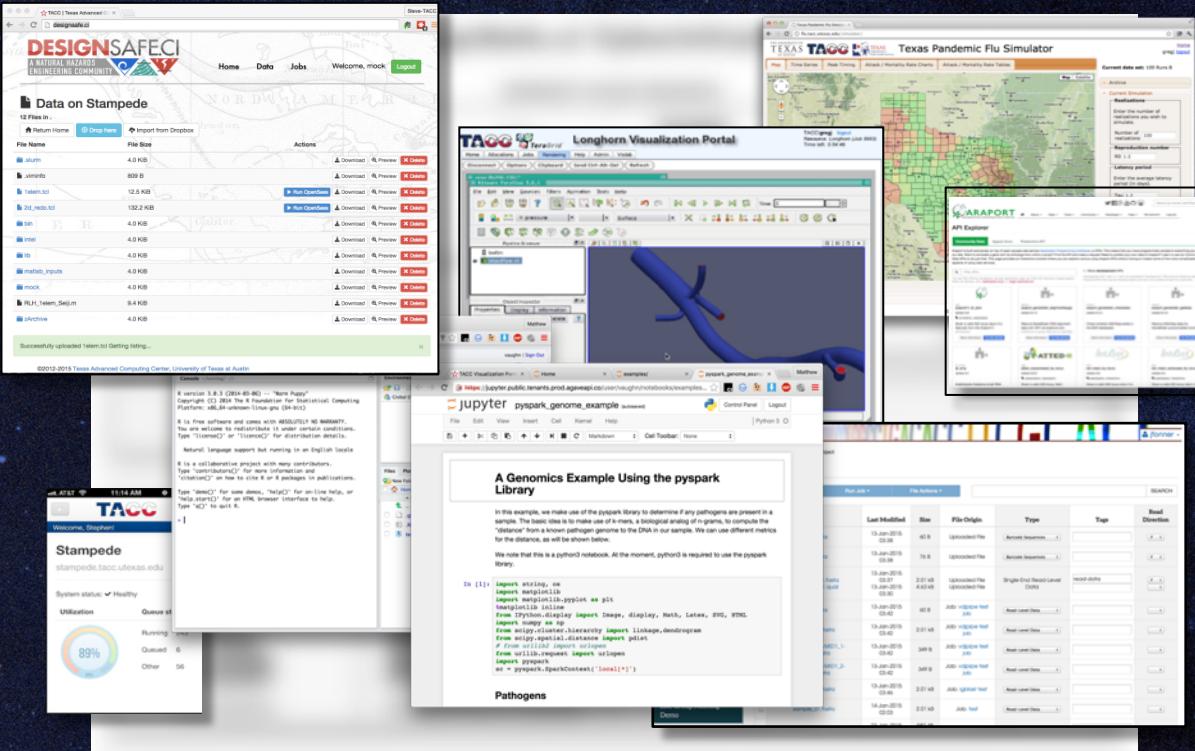
elasticcluster start slurm-js-iu

"Launch a 3-node SLURM cluster with Gluster storage"

IaaS enables support for

- ▶ Containers
- ▶ Container orchestration engines (k8s, Swarm)
- ▶ Configuration management tools like Ansible, Vagrant, Chef, Puppet
- ▶ Custom infrastructure solutions like ElastiCluster

SOFTWARE AS A SERVICE



- DesignSafe Discovery Workspace
- Araport API Explorer
- VDJserver
- JupyterHub
- Rstudio
- TACC Vis Portal

PLATFORM AS A SERVICE

The screenshot shows the "Live Documentation" page for The Agave Platform. The top navigation bar includes links for HOME, ABOUT, DOCUMENTATION, STATUS, and SUPPORT. Below the navigation, there's a section for the iPlant Agave API, which includes links for Terms of service and Contact the developer, and a clients section for managing API keys.

The main content area features a grid of 15 icons representing different platform services:

- MONITORING
- ALERTS
- IDENTITY
- GROUPS
- SYSTEMS
- TRANSFER
- METADATA
- APPS
- SHARING
- ANALYTICS
- ANALYSIS
- DATA MGMT
- SEARCH
- PUBLISHING
- SECURITY

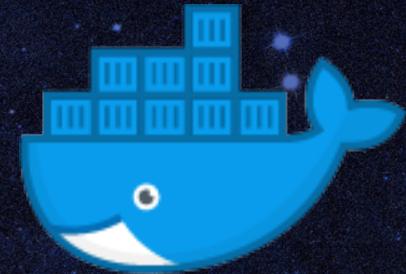
Below the icons, there's a section for Available Platforms with icons for Windows, Mac, Linux, and several application logos (Apache, MySQL, PostgreSQL, etc.).

A terminal window on the right side shows a bash session with command-line output related to system and application management.

- ▶ Agave API
- ▶ Abaco
- ▶ OpenStack API
- ▶ TAS API
- ▶ XSEDE API

DOCKER @ TACC

- ▶ Early adopters in containerizing web services
- ▶ Agave (for example)
 - ▶ Ansible + Docker + Jenkins
 - ▶ 12+ tenants in 3+ clouds
- ▶ DesignSafe JupyterHub is a multi-host Docker setup
- ▶ Available to Jetstream users
- ▶ No path forward for use on HPC systems
 - ▶ Kernel requirements
 - ▶ Security issues



SINGULARITY @ TACC

- ▶ Runtime available on all TACC HPC systems
 - ▶ Modest kernel requirements
 - ▶ Fully user-space execution (no known escalation risk)
- ▶ ~2,400 Singularity containers centrally hosted on TACC's "Stockyard" file system (more on this next)
- ▶ Started with request from Russ Poldrack ~12 months ago
- ▶ First singularity-powered module a few weeks ago
 - ▶ currently using aliases to make it act like a native command



WHY CONTAINERS ON HPC?

► PROS

- support apps with lots of dependencies
- improve reproducibility for NIH's FAIR data initiative
- reduce burden to build bespoke RPMs for every software package
- Facilitate user-extensible software environment

► CONS

- limited to single node
- learning curve for non-technical (and technical) users
- large size of some containers

TOWARD AN APP CATALOGUE

BIOCONDA[®]



 **QUAY**

BioConda
bioconda.github.io

BioContainers
biocontainers.pro

Singularity Hub
singularity-hub.org



ONGOING / FUTURE EFFORTS

- ▶ Connect BioConda's CI to TACC (Björn Grüning)
- ▶ Connect TACC to Singularity Hub (Vanessa Sochat)
- ▶ Support container building as a service (Jacquelyn Turcinovic)
- ▶ Use traditional LMOD modules as Singularity "wrappers"
 - ▶ How far can this be automated?
- ▶ Expose multi-format app catalogue execution through APIs
 - ▶ Hard to generically get past CLI expression
- ▶ Workflow support (e.g. Common Workflow Language)

OTHER THOUGHTS

- ▶ Are there downsides to such a user-friendly user-extensible software catalogue?
- ▶ Where to store metadata / standard interfaces / docs?
 - ▶ BioContainers – only standard executable goes in the container
 - ▶ BioBoxes – containers provide standard interfaces to all software
- ▶ Anyone had successes with MPI enabled containers?
- ▶ Specialized hardware support (very different between container formats)



QUESTIONS?