



# ENABLING SCIENTISTS AT SCALE WITH AGAVE

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# TACC AT A GLANCE



## Personnel

160 Full time staff (~70 PhD)

## Facilities

10 MW Data center capacity

New office facility to be completed  
by start of 2016

## Systems and Services

A Billion compute hours per year

5 Billion files, 50 Petabytes of Data,  
Hundreds of Public Datasets

## Capacity & Services

HPC, HTC, Visualization, Large scale  
data storage, Cloud computing  
Consulting, Curation and analysis,  
Code optimization, Portals and  
Gateways, Web service APIs, Training  
and Outreach



# EXTREME SCALE SUPERCOMPUTING



## Stampede

- #7 HPC system in the world for computation 500k CPU core 9.7 PF

## Lonestar 5

- Texas-focused Cray XC40 30,000 Intel Haswell cores 1.25 PF

## Wrangler

- 0.6 PB usable DSSD flash storage w 1 TB/s read rate + 10 PB Lustre

## Maverick

- 132 Fat nodes w dual 10 core Ivy Bridge + NVIDIA Kepler K40 GPGPU

## Chameleon & Jetstream Cloud

- 1400 nodes OpenStack

## Disk and Tape Storage

- 100+ PB storage in HIPAA-aligned data center



## Coming Soon: Hikari

- Green computing system partnership with NEDO and NTT. 10k Haswell cores. HVDC and Solar (partial)
- Support for container ecosystem

# TACC SUPPORTS AN INCREDIBLE AMOUNT & DIVERSITY OF RESEARCH

- Since 2013...
  - Over \*2 Billion\* processor hours delivered to end users
  - 6+ **million** successful jobs
  - About 10,000 students, faculty, and staff use our Stampede directly
  - Over 30,000 more use it indirectly via portals and services
  - Peer-reviewed requests for time (via XSEDE) run ~500% available hours
- **Stampede alone** supports nearly 2,500 funded projects across the United States and abroad

# THE EVOLUTION OF A CYBERINFRASTRUCTURE



Once upon a time, most of us built garage-style clusters...

HPC systems have grown up since then and become much more powerful and sophisticated

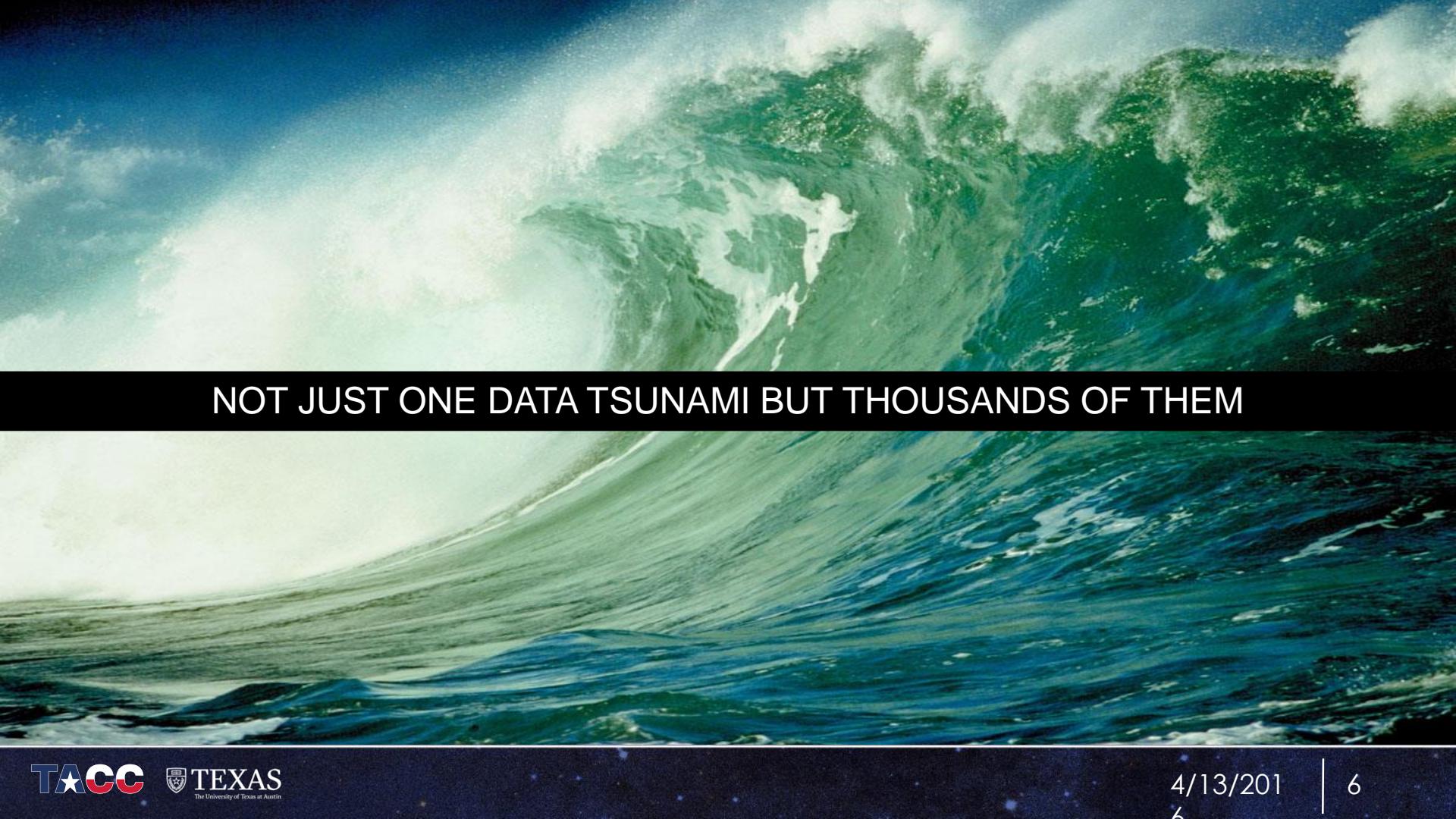


*We built a very successful center based on 3 pillars in our first 7 years*

- *Simulation & HPC*
- *Visualization*
- *People (Consulting & Algorithms)*

*But a curious thing happened while HPC was running its victory lap...*





NOT JUST ONE DATA TSUNAMI BUT THOUSANDS OF THEM

# CAMBRIAN EXPLOSION OF LANGUAGE, TECHNOLOGY, AND HARDWARE

## CATALYSTS

- Triumph of Linux and FOSS
- Rise of collaborative massive scale
- Emergence of Internet-scale technologies
- Rapid innovation to solve IO bound problems
- Repeal of Moore's Law

# WORKFLOWS NOW TECHNICALLY COMPLICATED

## LANGUAGES

- Python 2 & 3
- R
- Julia
- Perl
- Matlab
- Java
- Scala, Clojure, etc
- .NET
- C++
- Swift
- Haskell
- Go
- Javascript

## FRAMEWORKS

- MapReduce: Hadoop, Storm, Pachyderm
- Event & Streaming: Kinesis, Azure Stream Analytics, Camel, Streambase
- Deep/Machine Learning: Watson, Azure BI, Tensorflow
- In-memory parsing: Kognito, Apache Spark
- New data warehouse: Snowflake
- Containers: Docker, Rocket, MESOS, Kubernetes
- Cloud: AWS, GCE, OpenStack, VMWare

## HARDWARE

- Rise of many-core computing means 50-100 threads/node\*
- Xeon / Xeon Phi
- GPU
- OpenPower
- ARM
- Multi-level memory architectures
- Hierarchical storage architectures
- FPGAs

# DIVERSE DISTRIBUTED RESEARCH TEAMS



**Mike**

- Computing novice
- Works remotely at partner site



**Eliza**

- Masters specific analysis skills
- Readily adopts new tech



**Paulo**

- Staff computational expert
- Supports multiple projects



**Nikolaidas Group**

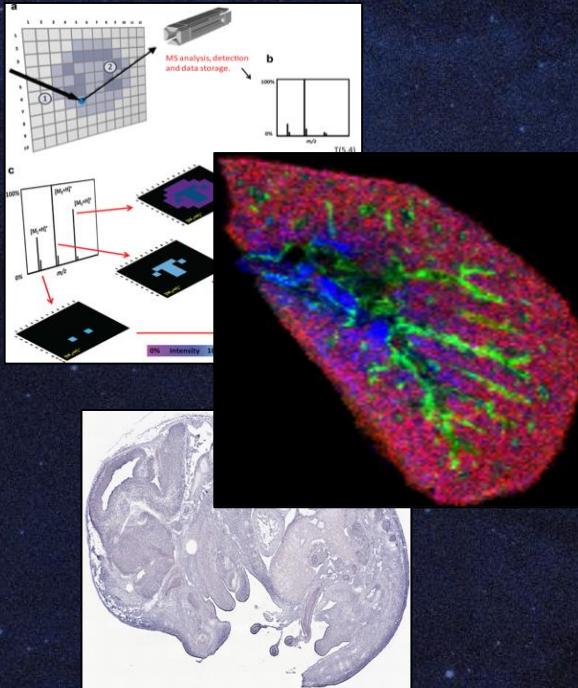
- Mostly experimentalists
- Strict data sharing & access



**Roshan**

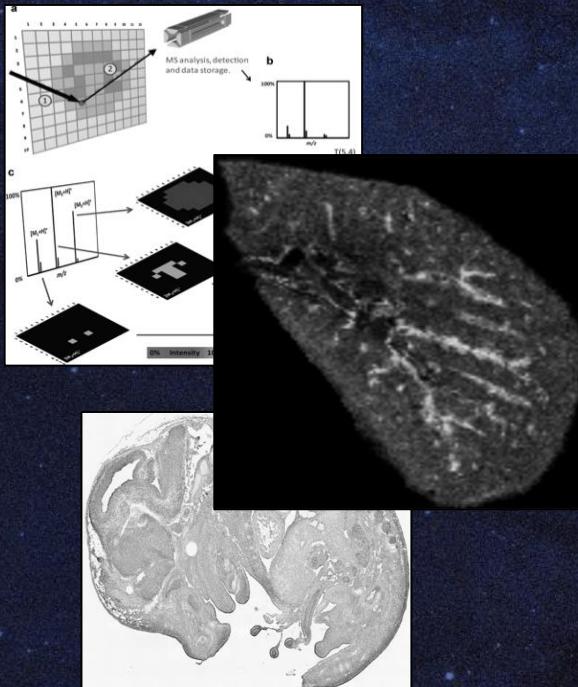
- Computationally experienced
- Focused on interpretation

# THEIR NEEDS (30,000 FT. VIEW)



- ▶ Store, organize, share *primary data*
- ▶ Iteratively perform 1' analyses
- ▶ Store, organize, share *derived data products*
- ▶ Iteratively generate and explore hypotheses
- ▶ Share analytical code with the scientific public
- ▶ Integrate results from new experiments
- ▶ Publish data alongside plots, visualizations and analytical tools

# THEIR NEEDS (500 FT. VIEW)



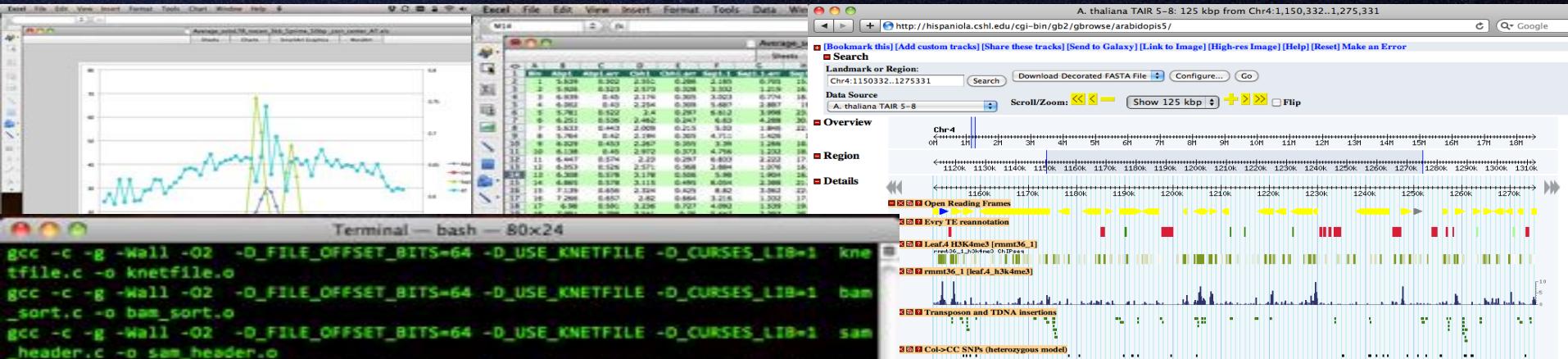
- ▶ Data lifecycle management
  - ▶ Fine-grained permission management
  - ▶ Discoverability
  - ▶ Version control
- ▶ Domesticating promising new analysis codes based on often immature technology
- ▶ Doing reproducible computational science
- ▶ Adopting efficient analytical methods

HOW DO WE HELP RESEARCHERS WITH SUCH  
DIVERSE NEEDS AND BACKGROUNDS?

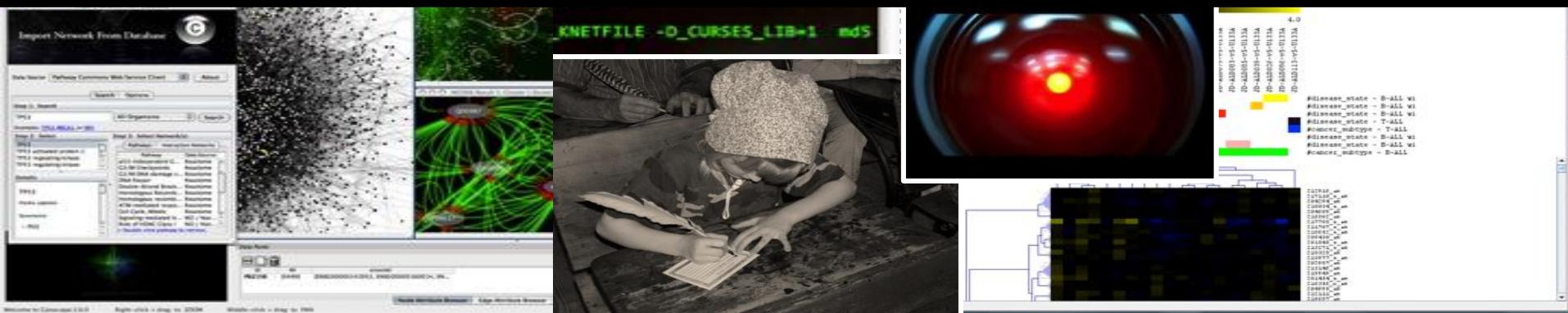


BUILD A MASSIVE STORAGE CLOUD NEXT TO INNOVATIVE, POWERFUL, USABLE COMPUTERS AT THE END OF FAST INTERNET PIPES





MANY DOMAIN SCIENTISTS ARE NOT EXPERTS AT COMPUTING TECHNOLOGY.  
CREATE PURPOSE-BUILT, HIGHLY INTUITIVE INTERFACES



The collage includes:

- DESIGNSAFE CI**: A screenshot of the DESIGNSAFE CI web interface showing a file upload progress bar for "12 Files in...".
- Data on Stampede**: A screenshot of the Stampede data management interface showing a list of files (e.g., alarm, vimento, telem.tcl) with download and delete actions.
- Texas Pandemic Flu Simulator**: A screenshot of the Texas Pandemic Flu Simulator interface.
- API Explorer**: A screenshot of the API Explorer interface for the Agave Community Data service, showing various API endpoints like "apigee\_to\_json" and "apigee\_generator\_alignmentsag".
- stampede.tacc.utexas.edu**: A screenshot of the Stampede system status page showing utilization metrics (CPU, Memory, Network, Disk) and system status.
- VVDJ SERVER**: A screenshot of the VVDJ SERVER interface for managing sequencing projects, showing a list of samples and their details.

## Point-and-click interfaces

- Data management, sharing, and analysis
- Publishing reproducible analysis workflows
- Discovery of new or updated tools and data
- Interactive visualization of results

Backed by world-class computing and data capacity

The screenshot shows a dual-browser setup on a TACC visualization port. The left window is an RStudio session titled 'Console ~/testing/'. It displays the R version 3.0.3 startup message, which includes a 'Warm Puppy' pun. The right window is a Jupyter notebook titled 'pyspark\_genome\_example'. The notebook has a title cell: 'A Genomics Example Using the pyspark Library'. Below it is a text cell explaining the purpose of the example, mentioning k-mers and pathogen detection. A code cell follows, showing Python imports for matplotlib, numpy, scipy, and pyspark, along with the creation of a SparkContext. The bottom of the notebook has a section header 'Pathogens'.

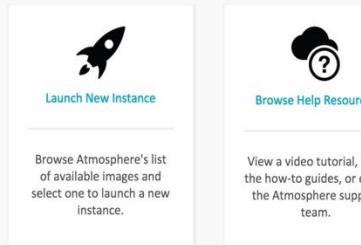
```
In [1]: import string, os
import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import Image, display, Math, Latex, SVG, HTML
import numpy as np
from scipy.cluster.hierarchy import linkage,dendrogram
from scipy.spatial.distance import pdist
# from urllib2 import urlopen
from urllib.request import urlopen
import pyspark
sc = pyspark.SparkContext('local[*]')
```

## Hosted SaaS

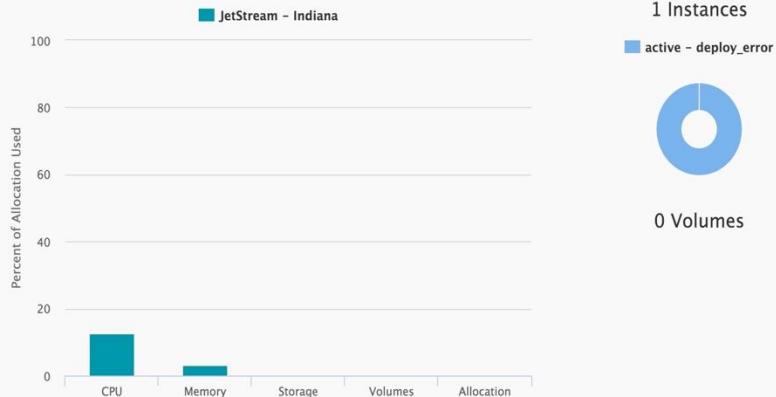
- JupyterHub notebooks
- Rstudio
- Web-based VNC

Also, backed by world-class computing and data capacity

## Getting Started



## Resources in Use Need more?



## Instance History (5 instances launched)



Updated a few seconds ago

Feedback & Support

<https://use.jetstream-cloud.org/application/images/>

## Community Activity

- edwintest3 created an image Nov 16, 2015 02:31 am MAKER-P 2.28 with CCTools 5
- edwintest3 created an image Nov 16, 2015 02:31 am TSW Workshop Williams 1.2
- atmodadmin created an image Oct 23, 2015 12:06 am Trusty Tahr (x64)
- atmodadmin created an image Oct 23, 2015 12:06 am cirros-0.3.4-x86\_64
- atmodadmin created an image Oct 23, 2015 12:06 am CentOS-7-x86\_64-GenericCloud-20150628\_01
- atmodadmin created an image Oct 23, 2015 12:06 am CentOS-6-x86\_64-GenericCloud-1508
- atmodadmin created an image Oct 23, 2015 12:06 am CentOS-7-x86\_64-GenericCloud-1508

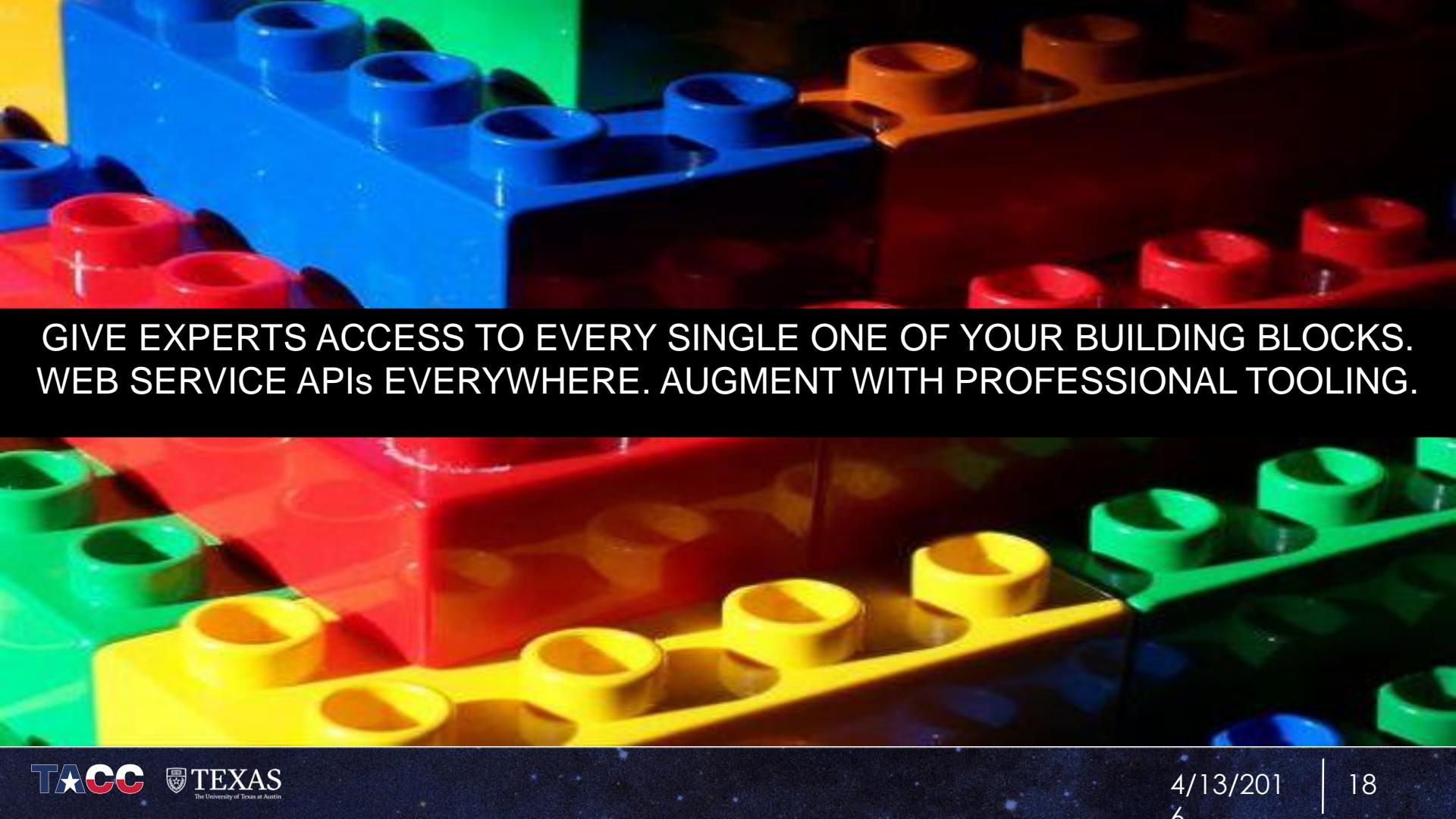
## Easy to use Cloud Computing

- Atmosphere (Cyverse)
- Jetstream (IU,UA,TACC)
- Chameleon (UC,TACC )

Cloud consoles are aimed at sysadmins and unintuitive.

We're changing that with improved UX and support

- APIs are still available
- No cost to end user



GIVE EXPERTS ACCESS TO EVERY SINGLE ONE OF YOUR BUILDING BLOCKS.  
WEB SERVICE APIs EVERYWHERE. AUGMENT WITH PROFESSIONAL TOOLING.

# MIKE: LEARNING COMPUTATIONAL SKILLS



**Mike generates mass-spec data from his samples, which are used to decide on future experiments**

- ▶ Eliza and Paulo have published analytical scripts for his data as 'apps' into a project web portal
- ▶ Paulo has wired up the lab's equipment to send data directly to remote storage
- ▶ Mike can perform basic analysis and reporting on his data from the web interface
- ▶ Roshan can see Mike's results in the project portal and discuss them with him.
- ▶ Mike collaborates with Eliza to improve the results of their analytical scripts

# ELIZA: AUGMENTING HER RESEARCH CAPABILITY



**Eliza collects and analyzes *in situ* hybridization imagery as a major part of her inquiry**

- ▶ She uses code developed by Paulo and others to perform feature detection
- ▶ She helps Paulo develop code for Mike to use in his proteomics work
- ▶ She has developed scripted workflows that run locally on her laptop to complete her analyses
- ▶ She writes her own code in Python and R for aggregate analysis and shares it via the Docker Hub and the project portal
- ▶ She presents her data viz via interactive Rshiny apps that she deploys to the project portal

# PAULO: CONCENTRATING ON COMPUTATIONAL RESEARCH



**Paulo likes to solve hard computational problems but is also responsible for lab research infrastructure**

- ▶ He has automated data movement from instruments to remote storage, including duplication to AWS Glacier. Roshan gets the bill ☺
- ▶ He builds and maintains the project web portal. He didn't have much experience with such technology when the project started
- ▶ Paulo has used Spark to developed new software for feature extraction from *in situ* hybridization images – he can automatically deploy it to the portal, powered by TACC Wrangler, as part of his build process
- ▶ He is working on a paper describing his software and is getting valuable feedback from other folks he has shared it with via the project portal and public source repositories

# ROSHAN: FOCUSING ON THE BIG PICTURE



- ▶ Roshan has deep experience in gene expression analysis - Paulo has populated the project portal with many of the tools she needs to accomplish her goals
- ▶ She collaborates with Mike and Eliza on interpreting their experimental results
- ▶ Because Eliza has included a custom notification in her scripting workflow, Roshan knows when new image analyses have been completed and can schedule time to look at them
- ▶ She can work with Paulo to enable the project web portal to make use of her newly-awarded XSEDE computing and storage allocation
- ▶ She routinely shares results with experimentalist colleagues and reviewers via a simple Dropbox-like interface

The logo for the Agave Platform. It features the word "Agave" in a large, white, sans-serif font. The letter "A" is stylized with a fan-like graphic of white lines extending from its left side. Below "Agave", the word "Platform" is written in a smaller, white, sans-serif font.

# Agave

Platform

AGAVE IS A MULTI-TENANT PAAS  
DELIVERING SCIENCE-AS-A-SERVICE SOLUTIONS  
IN HYBRID CLOUD ENVIRONMENTS

Think of it like



salesforce

for Science

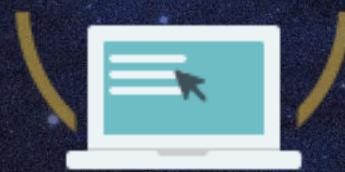
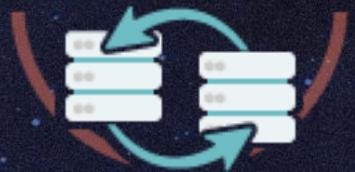
# WHAT DOES IT DO?

MANAGE  
DATA

RUN  
CODE

COLLABORATE  
ANYWHERE

CONNECT  
ANYTHING



# MANAGE DATA

- Single, consistent interface to access distributed data
- Managed, tenacious data movement
- Opinion-free metadata management
- Full provenance and searchable audit trail.
- Events, alerts, and notifications
- Horizontal scaling

# RUN CODE

- Bring your own code and/or leverage our catalog
- Run your apps as interactive, batch, or event driven processes
- Full lifecycle management
- Full provenance and searchable audit trail
- Reproducibility as a feature
- Publish entire experimental runs

# COLLABORATE MEANINGFULLY

- Secure by default, share as desired
- Deep link to any resource in the API
- Generate disposable links to securely share with others
- Events, webhooks, and web sockets to integrate circa 2016
- Web standards come standard

# CONNECT ANYTHING

- Support for protocols powering the IoT and your PC
- Push and pull information publication
- Sync, async, and event driven interactions
- Hacker friendly

# WHAT'S UNDER THE HOOD





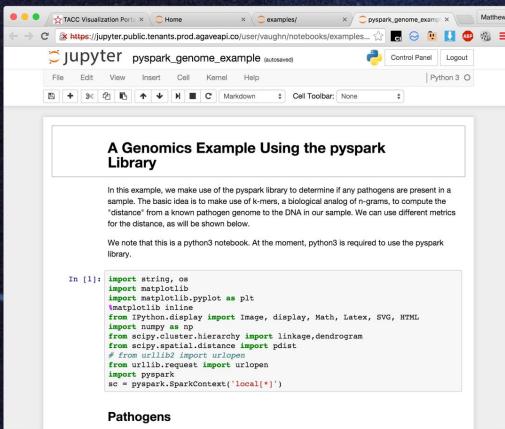
# Agave

To Go

# AGAVE TOGO

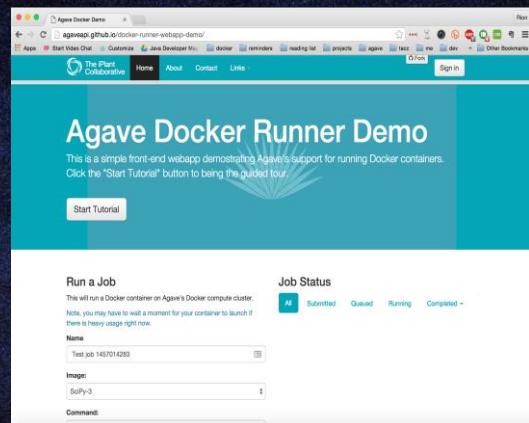
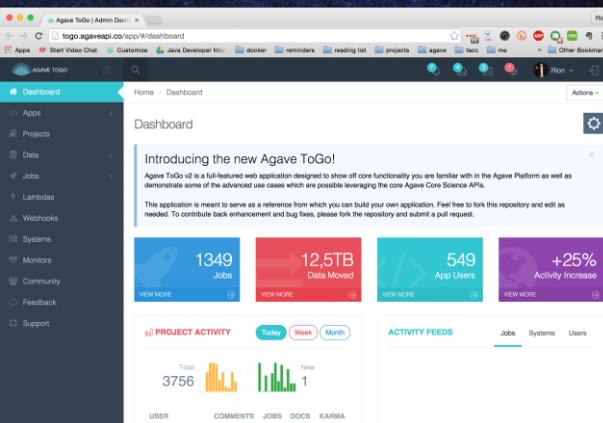
- Client SDK: Python, JavaScript, Java, PHP, *Perl*, *R*
- Command Line Interface
- Plugins: AngularJS, Wordpress, Drupal, Tomcat
- Web applications (ToGo)
- Integrated environments (Jupyter Hub)
- Workflow management (End of Day)

# AGAVE TOGO



```
In [1]: import string
import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline
from IPython.display import Image, display, Math, Latex, SVG, HTML
import numpy as np
from scipy.cluster.hierarchy import linkage,dendrogram
from scipy.spatial.distance import pdist
from collections import defaultdict
from urllib.request import urlopen
import pyspark
sc = pyspark.SparkContext('local[*]')

Pathogens
```

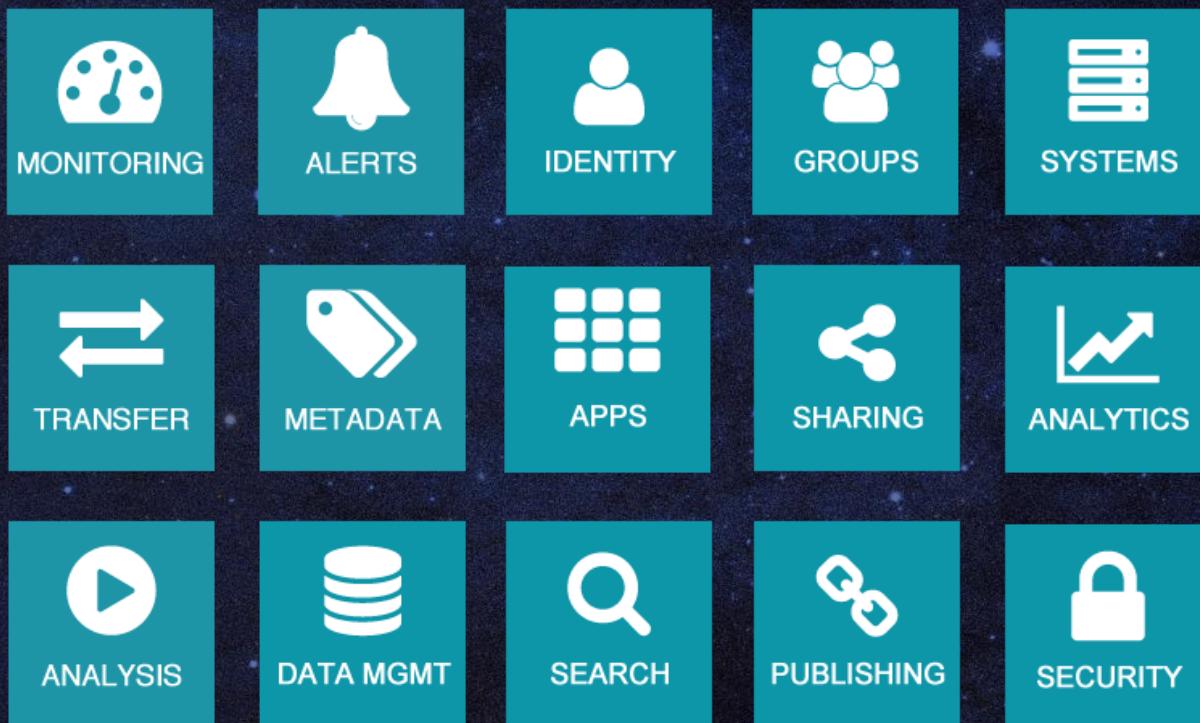




# Agave

Science API

# AGAVE SCIENCE APIS

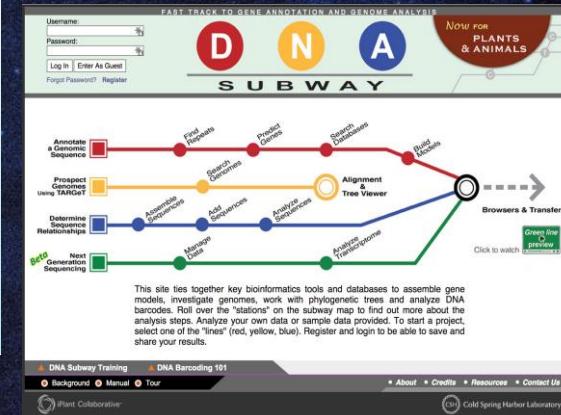


# BUILD AND RUN

- App publishing and discovery services allow you to define, share, and recreate your experiments or use one of the thousands of apps already available in the public app catalog.
- Job execution services to run code in a reproducible, recorded way through interactive, batch, or event driven interfaces.
- Bring Your Own storage and compute systems to allow you to use your own systems, wherever they be to store data and run HPC, HTC, Cloud, and container apps.
- Manage and move your data from anywhere to anywhere using any of the dozen protocols supported out of the box.

# WHO'S USING THIS STUFF?

The screenshot shows the iPlant Discovery Environment's search interface. A sidebar on the left lists categories like Apps, Workspace, Public Apps, and Experimental. The main area displays a search result for 'bam' files, showing 43 items. Each item includes a thumbnail, name, integrated by (e.g., Roger Barthelemy), rating, and a preview link. Below the search results is a 'Details' section with a file browser.



The BioExtract Server interface includes a header with a feedback link and user status. It has tabs for Query, Extracts, Tools, Workflows, Groups, and Help. The main area has sections for Available Data Sources (listing All, Miscellaneous, Nucleotide Sequences, Protein Sequences, Viridiplantae, and Viridiplantae Protein) and a Query Form. The Query Form includes fields for Search Field (All Text) and Search Term(s). A note at the bottom provides details about the service's purpose and funding.

<http://iplantcollaborative.org>

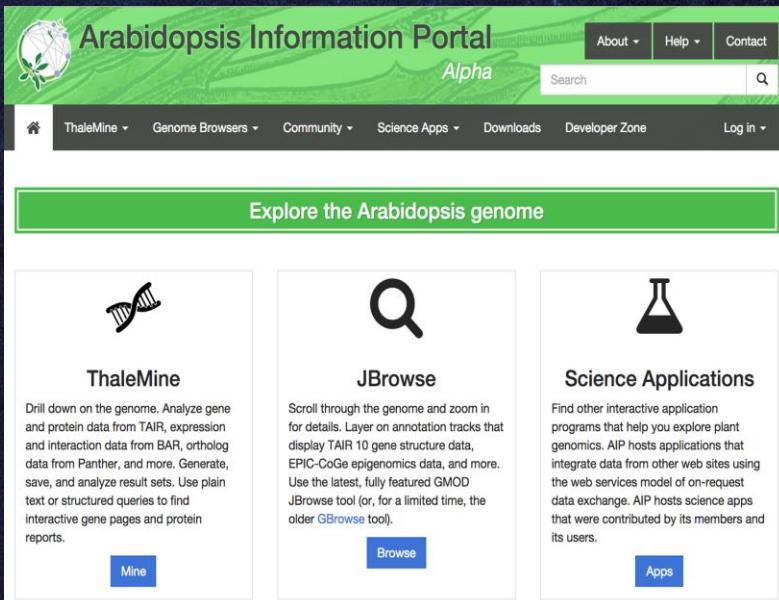
<http://dnasubway.org>

<https://www.bioextract.org>

# SHARE AND CARE

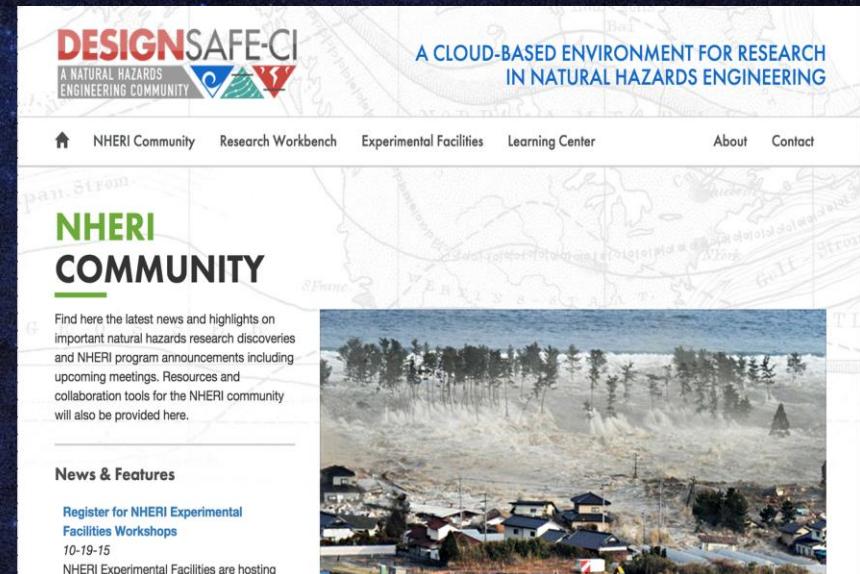
- Fine-grained access control for secure, documented, collaboration with another user, group, or third-party service.
- Publish/subscribe notifications, infrastructure monitoring
- Scalable metadata management and with bulk interfaces
- Scheduled, reliable data movement
- Deep provenance, analytics, and reporting support
- Collaboration and publication support
- Pre-authenticated disposable URLs

# WHO'S USING THIS STUFF?



The screenshot shows the homepage of the Arabidopsis Information Portal (AIP). At the top, there's a green header bar with the title "Arabidopsis Information Portal" and a sub-header "Alpha". Below the header is a navigation bar with links for "About", "Help", "Contact", "Search", and "Log in". The main content area has a green banner at the top with the text "Explore the Arabidopsis genome". Below this, there are three main sections: "ThaleMine" (with a DNA helix icon), "JBrowse" (with a magnifying glass icon), and "Science Applications" (with a flask icon). Each section contains a brief description and a blue "Mine", "Browse", or "Apps" button.

<http://araport.org>



The screenshot shows the homepage of DESIGN-SAFE-CI, a natural hazards engineering community. The top features a logo with the text "DESIGN-SAFE-CI" and "A NATURAL HAZARDS ENGINEERING COMMUNITY". To the right, it says "A CLOUD-BASED ENVIRONMENT FOR RESEARCH IN NATURAL HAZARDS ENGINEERING". Below the logo is a navigation bar with links for "Home", "NHERI Community", "Research Workbench", "Experimental Facilities", "Learning Center", "About", and "Contact". The main content area has a large image of a coastal area affected by a disaster. Overlaid on the image is the text "NHERI COMMUNITY". Below this, there's a section for "News & Features" with a link to "Register for NHERI Experimental Facilities Workshops 10-19-15".

<https://www.designsafe-ci.org>

# FOCUS ON THE “WHAT IF...”

- ▶ Large Synoptic Survey Telescope
- ▶ 15 TB/night of data
- ▶ 1PFLOP/sec compute
- ▶ Built on top of a mountain
- ▶ Has great cell reception...super fast 4G

Built next to this 7-11



# AGAVE SCIENCE APIs

- Event-driven workflows supporting your own custom events
- Real-time & async data transformation
- Streaming data & “always on” data sources
- Support for JSON, pagination, caching, CORS, search, and webhooks on all APIs

# AGAVE SCIENCE APIS

- Real-time & async data transformation
- Support for JSON, pagination, caching, CORS, search, and webhooks on all APIs
- Federation authentication
- On-premise deployments
- Elastic scalability

# WHO'S USING THIS STUFF?



The iReceptor website features a green logo with a stylized Y-shaped antibody structure. The main navigation menu includes links for ABOUT, NEWS, ARCHITECTURE, and CONTACT. Below the menu, a section titled "What is iReceptor?" provides a brief overview of the project's goal: "iReceptor is a distributed data management system and scientific gateway for mining 'Next Generation' sequence data from immune responses. The goal of the project is to: *improve the design of vaccines and therapeutic antibodies by integrating Canadian and international data repositories of antibody and T-cell receptor gene sequences.*" A sidebar on the right lists "LATEST NEWS" items such as "CANARIE Workshop Oct 20-21, 2014 10/20/2014 - 06:59", "Antibody & T-Cell Receptor Data Integration Planning Meeting 09/10/2014 - 15:07", "iReceptor CANARIE announcement 06/23/2014 - 11:31", and "iReceptor is live!!! 06/22/2014 - 04:44".

<https://ireceptorgw.irmacs.sfu.ca/>



The VDJ Server website has a "WELCOME!" banner at the top. It features a circular graphic with various scientific icons like microscopes, test tubes, and DNA helixes. Below the banner are four main functional sections: "UPLOAD" (with an upward arrow icon), "ANALYZE" (with a magnifying glass icon), "PUBLISH" (with a document icon), and "SHARE" (with a person icon). Each section contains a brief description of its purpose.

<https://vdjserver.org>



# Agave

Platform

# AGAVE PLATFORM

- On-premise and hybrid deployments
- Federated identity and access management
- API Management
- Single sign-on
- White label tooling and documentation
- Developer portal and documentation
- Training materials and engagement programs
- Application catalog development

# WHAT KICKING THE TIRES LOOKS LIKE

## MONTHLY USAGE

30 compute sites

100 clients

1,000 apps

6,000 simulations

1,000,000 transfers

2,000,000 GB data moved

## AVG. MONTHLY GROWTH

45 new systems

30 new clients

50 new apps

2000 docs shared

100,000 new transfers

150,000 GB data moved

### WORLDWIDE PLATFORM USAGE





## WE'RE HIRING

Platform development, DevOps, Life Science, Data Science,  
Machine Learning, Web and Mobile, Cloud, HPC, Sysadmin  
[jobs@tacc.utexas.edu](mailto:jobs@tacc.utexas.edu)

## FOLLOW US

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[www.tacc.utexas.edu](http://www.tacc.utexas.edu)