



Enabling Research and Education Through the Geddes Composable Platform

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Overview

- Motivation and Goals
- Defining Composability
- Technologies and Components
- Use Cases



Information about the Geddes namesake
This work supported by NSF award #OAC-2018926

Motivation

- The Purdue Community Cluster Program is a reference implementation for campus “condo” HPC, but..
- Researchers increasingly look for more diverse computing resources
 - Cloud style flexibility
 - Persistent services
 - Scalable data analysis tools
 - Web based science gateways and applications
 - **Complementary services to HPC**
- Why not start with the public cloud?
 - Does not leverage existing infrastructure investments on campuses
 - Researchers are their own security teams
 - Can be costly for naïve scientists

A path needs to exist to shift to the public cloud, or national resources like Jetstream for scale and portability!

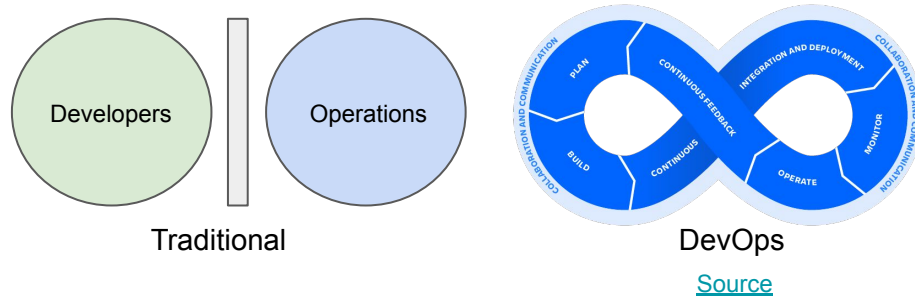
Goals

- Create a campus ecosystem for cloud technologies
 - Many research labs use container and virtualization solutions today
 - Bridge the gap to national resources or public cloud
 - Not just the technology, also knowledge sharing and support
- Empower faculty in the integration of cloud computing technologies
 - For research and instruction
 - Deploy your own services
 - Incorporate version control, automation and continuous integration
 - Create reproducible and shareable science
- Evaluate a sustainable model for campus private clouds

What is a “Composable” platform?

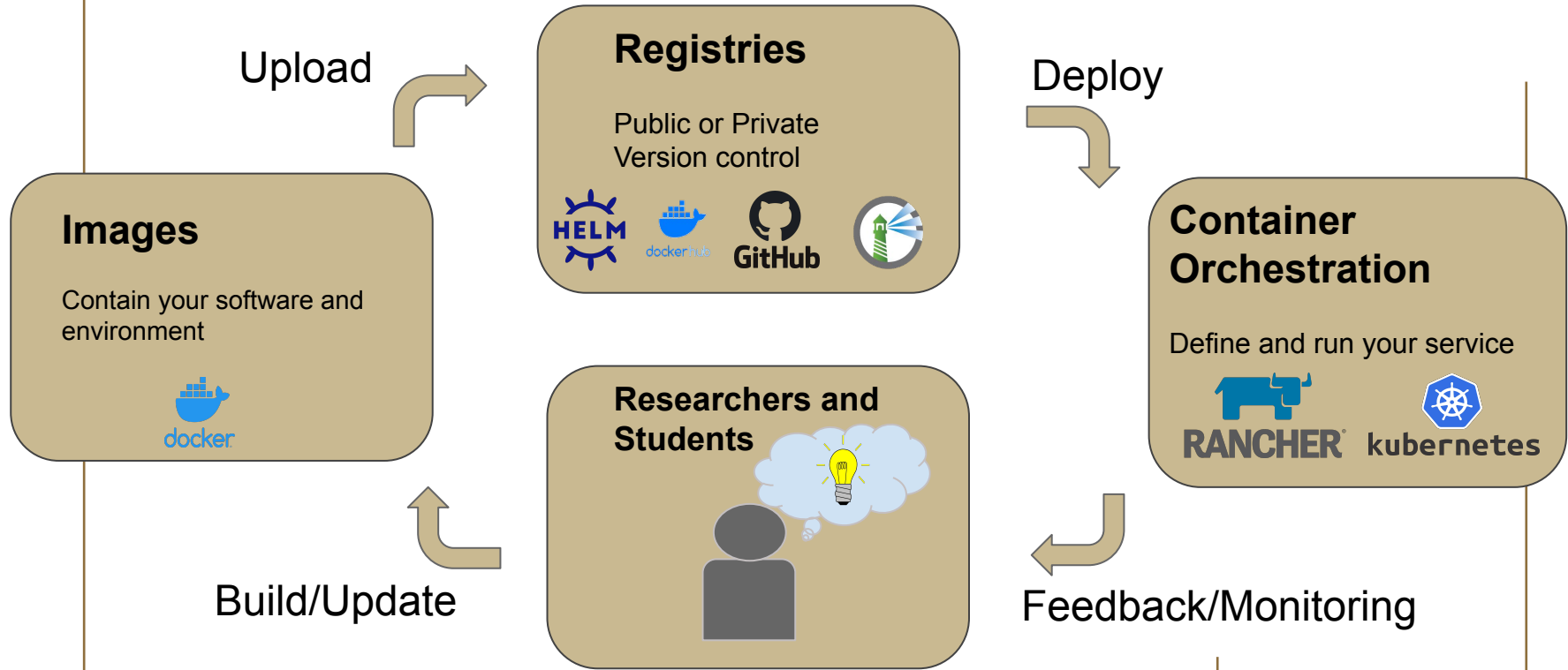
A platform for “SciOps”

- Composable infrastructure provides highly customizable, on-demand provisioning of pools of computing resources (cpu/gpu, mem, disk, network)
- DevOps Principles
 - Infrastructure as code
 - Version Control
 - Automation
 - Portability
 - Reproducibility



DevOps principles applied for computational and data intensive science = “SciOps”

SciOps with the Geddes Platform

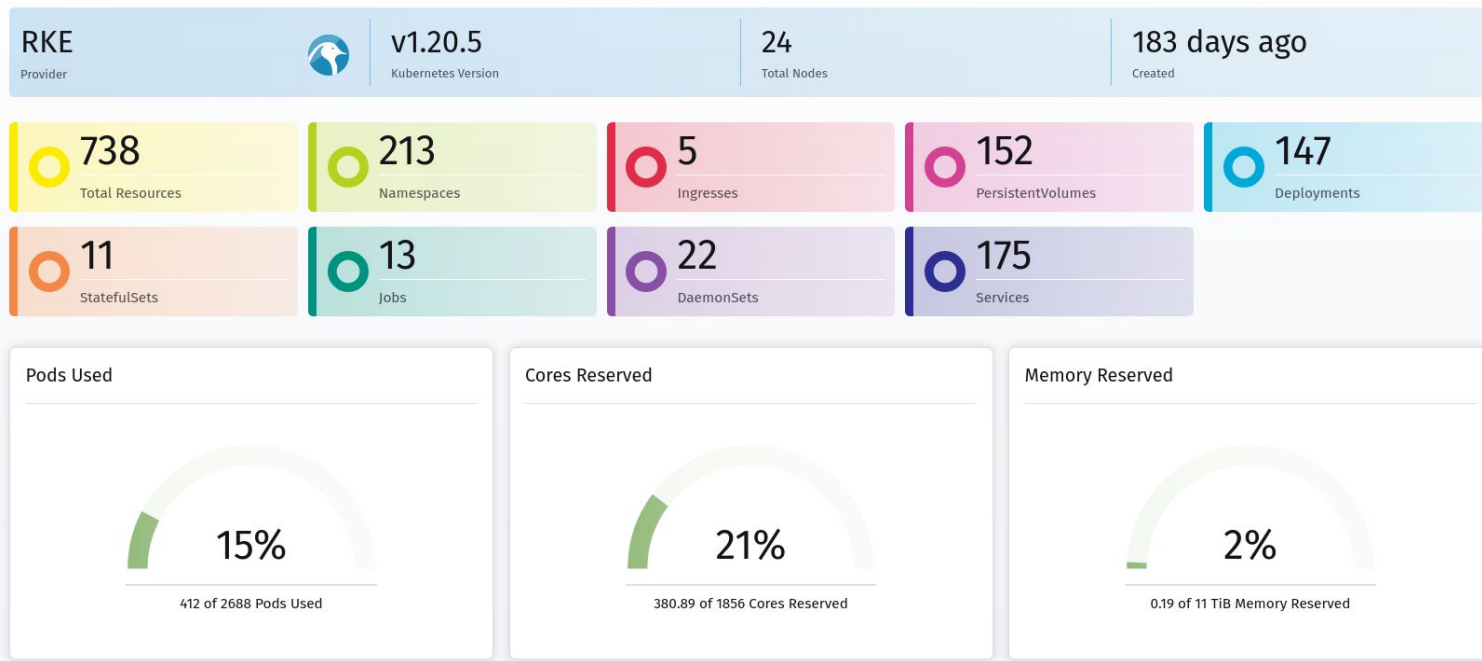


Technical Implementation

- Resources
 - Compute - 3584 cores, AMD EPYC 7662
 - Storage - 384 TB HDD, 672 TB SATA, 192 TB NVMe
 - GPUs - 8 NVIDIA A100 (MIG enabled)
- Stateless server provisioning via xCAT, minimal CentOS 8 + Docker
- Rancher for k8s provisioning, authentication, authorization
- Harbor for private registry
- Kubernetes Configuration
 - CNI - Canal, flannel VXLAN + Calico network policy, Rancher project isolation
 - [metallb](#) - LoadBalancer services for public/private addresses (L2 mode)
 - [k8s_gateway](#) - CoreDNS plugin for Ingress, LoadBalancer DNS records
- Storage
 - Ceph Deployment via [Rook](#) (block, filesystem, object storage)
 - [Longhorn](#) - from Rancher Labs (block storage)
- GPU Management with the NVIDIA [GPU Operator](#)

Usage

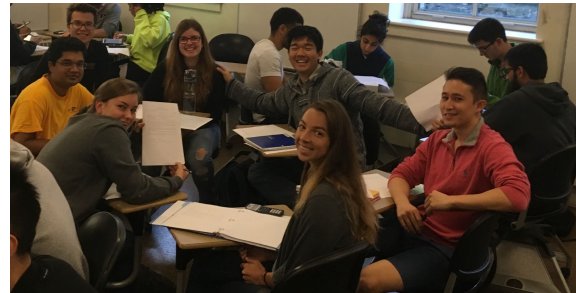
- Geddes has been in an early user access period since May, 2021
 - 60 users across 20 Research Groups
 - 22 Geddes Workshop/Tutorial participants



Use Cases

The Data Mine

- The Data Mine is a living, learning and research-based community
 - Introduces students to data science concepts
 - Enables students to create solutions to real-world problems
 - Serves students from all colleges in the university
 - Open to all students; no background required
 - Open to undergraduate and graduate students
- 20 Learning Communities
- 50 Corporate Partners projects



The Data Mine

- Hosting JupyterHub and notebook deployments, persistent databases used in data science courses
- Utilized for Corporate Partner - student projects
- Integration: Geddes resources taught in online teaching materials, k8s tutorial on DevOps methodologies

Homework 5

HONR 39900

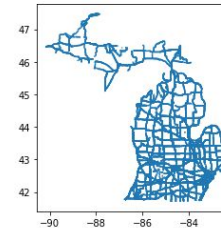
Problem 5

Determining which County in Michigan Has the Highest Mileage of Limited-Access Highways—24 Points

Michigan—particularly the Detroit area—is known for having many highways. Please determine if this is, indeed, true. Given the shapefiles for both the counties (POLYGON) and limited-access highways (LINESTRING) in the state of Michigan, please determine the total mileage of limited-access highways belonging to each county in Michigan.

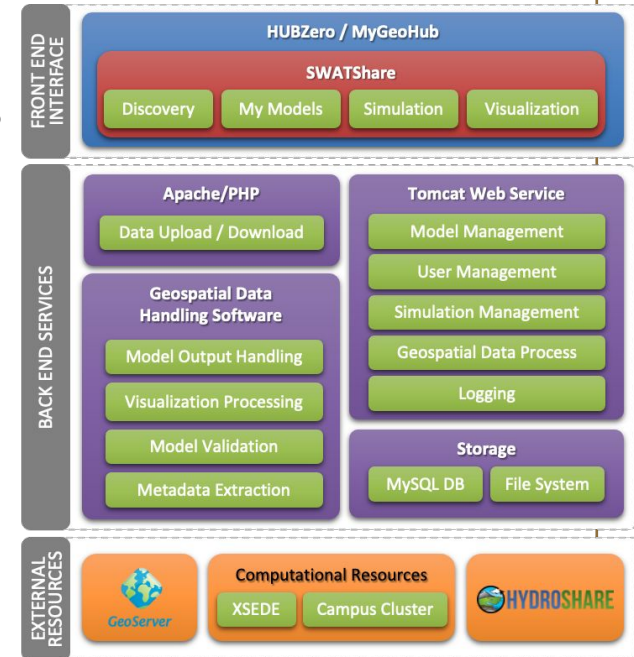
```
In [8]: problem_5.plot()
```

```
Out[8]: <AxesSubplot:>
```



Scientific Solutions Group

- Purdue's Scientific Solutions Group develops innovative CI solutions to advance scientific discovery, education and research reproducibility
- Science Gateways, HUBZero
- SWATShare
 - Publish, share, execute hydrologic models and visualize output via a web browser
 - RHEL6 VM managed by Purdue RC
 - Integrated with XSEDE, Purdue HPC
 - Redesigned with containers on Geddes
- Migrating a “traditional” deployment to a DevOps model allows SSG to maintain software more efficiently



IronHacks

- IronHacks is a Kaggle-like platform for hosting virtual data science hackathons, geared toward educational settings, with hacks focused on societal challenges
- Cloud based platform provides the hackathon environment

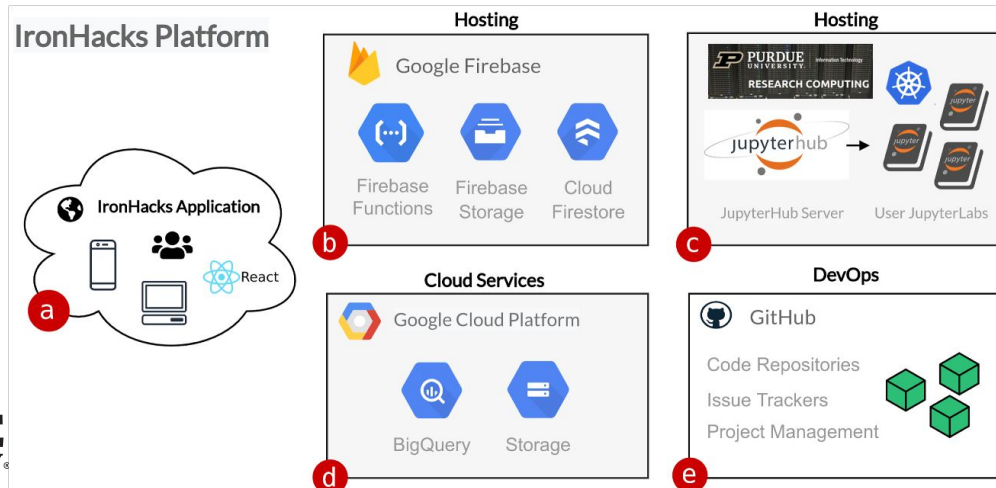
PURDUE
IRONHACKS

Hack for innovation to solve global challenges.



IronHacks

- Data analysis capabilities were provided through a JupyterHub instance deployed in DigitalOcean
- As hackathons become more data intensive, access to GPUs was needed for AI/ML exercises (not available on DO)
- Wanted to tie more closely with Purdue CI, work with local datasets and easily scale notebook deployments to 100s of users
- Migrated JupyterHub from public cloud to Geddes in Fall '21

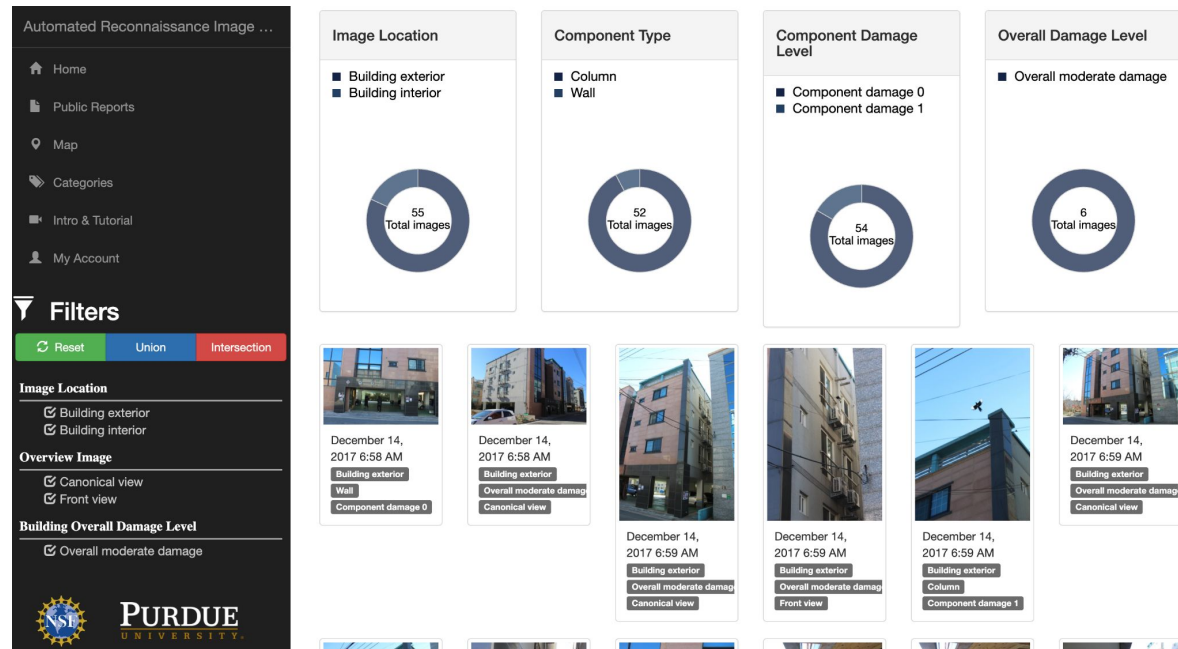


Inference as a Service

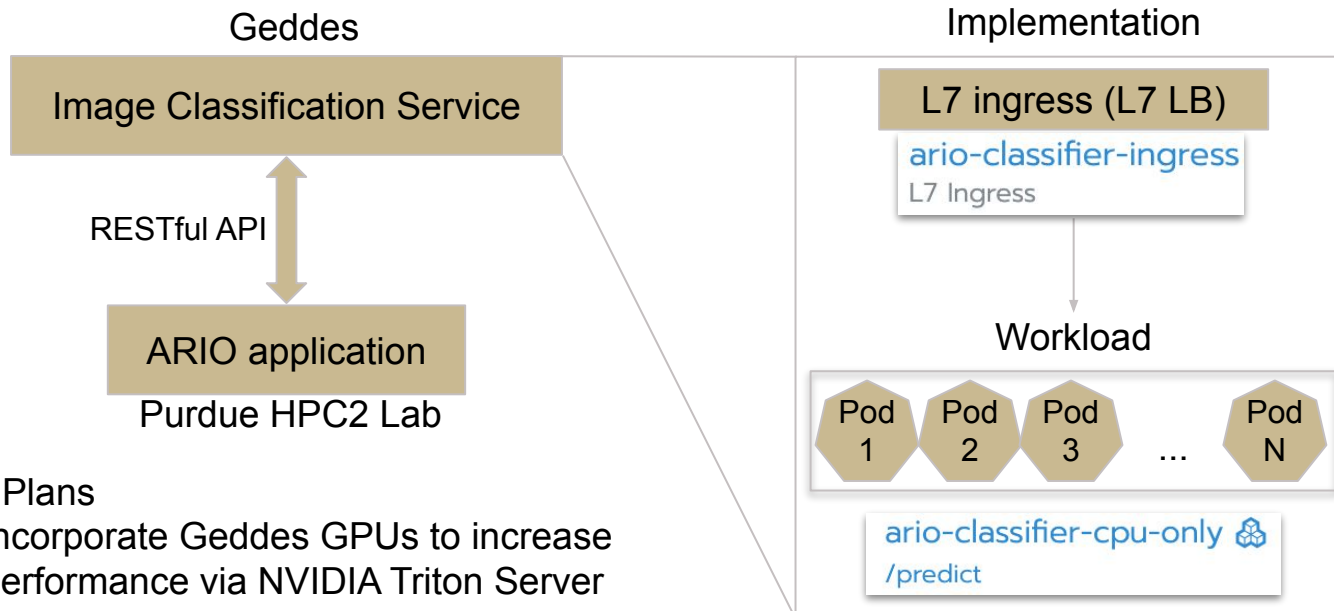
Automated Reconnaissance Image Organizer

- ARIO provides a multi-label image classification service for reconnaissance teams documenting damage after natural disasters
- Geddes provides large scale inference as a service for the system

Image classification
results from ARIO



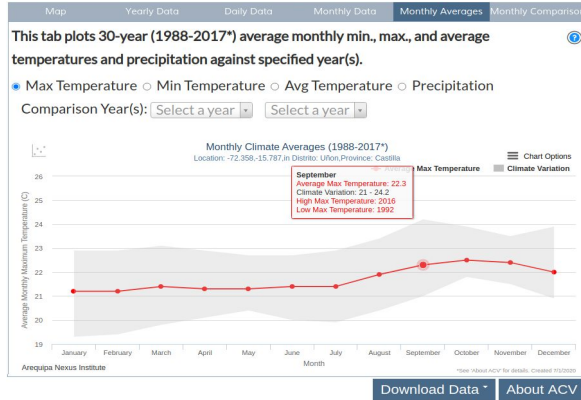
ARIO Implementation



Future Plans

- Incorporate Geddes GPUs to increase performance via NVIDIA Triton Server
- Migration of ARIO application to Geddes

Personal Science Gateways

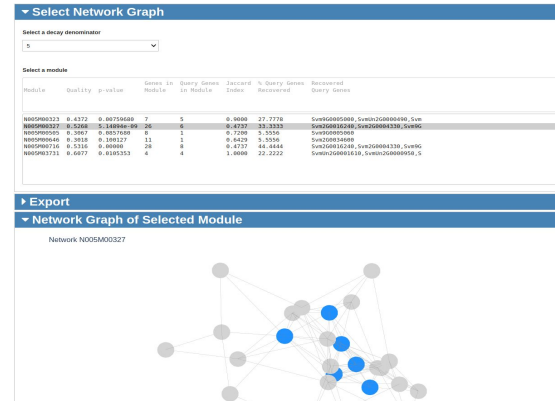


Arequipa Climate View
("ACV"): Temperature and precipitation data over 30 years in the Arequipa region of Peru

voilà



CoExplorer - Wisecaver Lab
("CoEx"): Expression of specific genes in setaria viridis (a type of grass)



Closing Thoughts

- Operations
 - Deploying things in Kubernetes is easy, but troubleshooting can be hard
 - k8s is rapidly evolving, sort by date on search results
 - Github issues are often the best place to find information
 - Things can easily go “poof”... etcd snapshots are your friend
 - Finding the right balance between flexibility and security can be difficult
- User support
 - Train user support staff early
 - Tutorials and workshops
 - Users will leave random things deployed and won't clean up PVCs
 - Documentation, documentation, documentation
- Evaluation of Geddes cost model vs. public cloud is in the works
- The same composable capabilities are available on the **Anvil XSEDE Resource**



THANK YOU

Early users

- The Data Mine - Prof. Mark Daniel Ward, Justin Gould, Kevin Amstutz
- IronHacks - Prof. Sabine Brunswicker, Manthan Keimm
- ARIO - Prof. Tom Hacker, Zhiwei Chu
- SSG - I Luk Kim, Lan Zhao, Rajesh Kalyanam
- Science Gateways - Prof. Jennifer Wisecaver, Prof. Diane Wang
- And many others...

Geddes Team

- Alex Younts, Brian Werts, Sam Weekly, Chuck Schwarz
- PI Preston Smith, Co-PIs Thomas Hacker, Norbert Neumeister, Jennifer Wisecaver

NSF

- CC* Award #OAC-2018926