Facilitation Services Updates

Christina Koch

OSG All-Hands Meeting @ Throughput Computing 2023

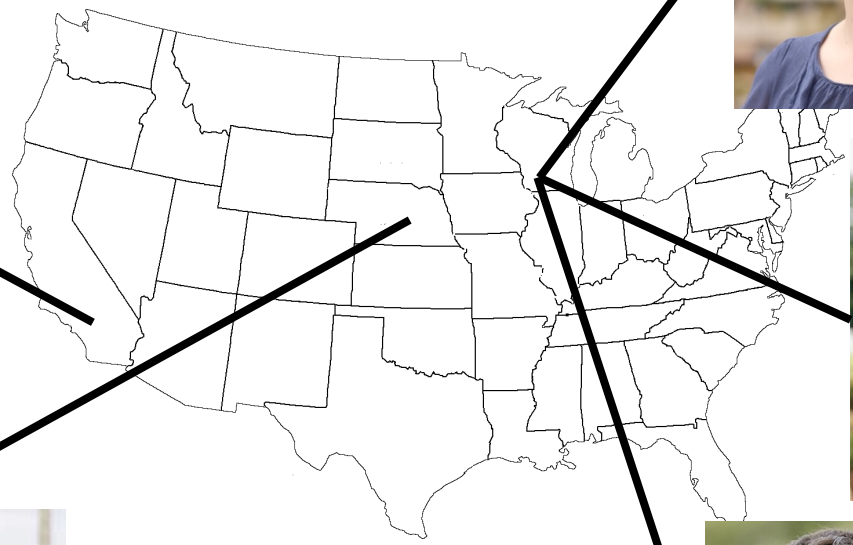
July 10, 2023

PATh PARTNERSHIP to ADVANCE THROUGHPUT COMPUTING

Facilitation Team

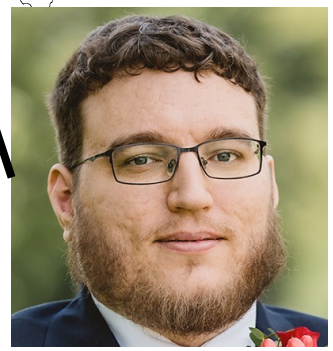
Mats Rynge
OSG/PATh Tenure: 10+ years
Background: Computer Science

Showmic Islam
OSG/PATh Tenure: 2 years
Background: Engineering



Christina Koch
OSG/PATh Tenure: 5 years
Background: Mathematics

Rachel Lombardi
OSG/PATh Tenure: 1.5 years
Background: Biology



Andrew Owen
OSG/PATh Tenure: 6 months
Background: Chemistry

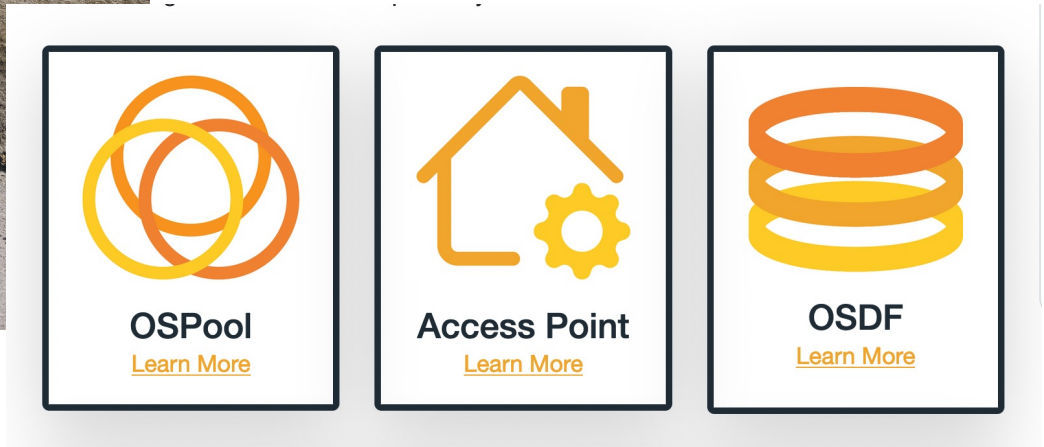
Advancing Science

OSG is a consortium dedicated to the advancement of all open science via the practice of distributed High Throughput Computing (dHTC), and the advancement of its state of the art.

How did the facilitation team advance open science via dHTC?

OSG Services for Researchers

- Access to computing capacity, data tools, job management
- Facilitation support
- Learn more after the break

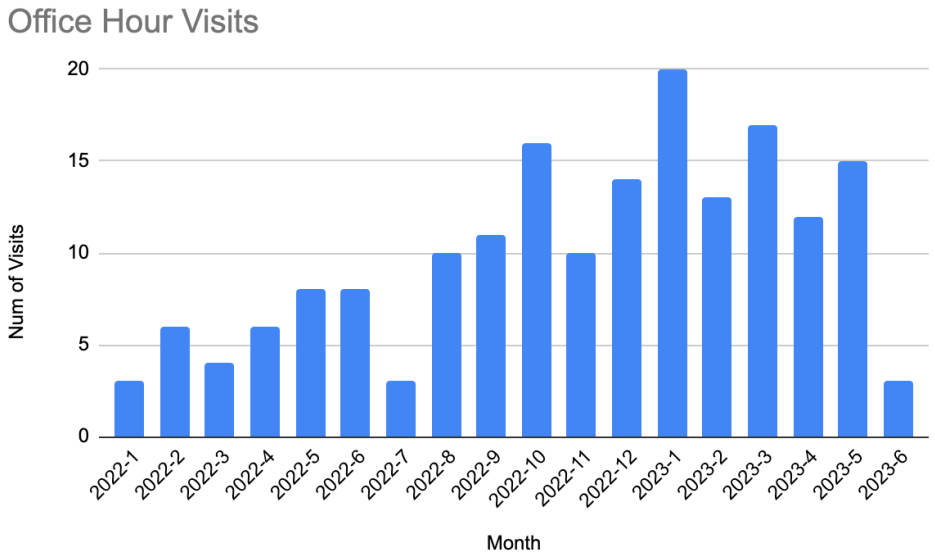


New and continuing support channels

- Have now done over a year of monthly **training** and twice-weekly **office hours**.
- Personalized researcher **orientation**
- Ongoing updates to **documentation**
- **What's Next:** self-serve tutorials

180+
orientations

8
new training topics



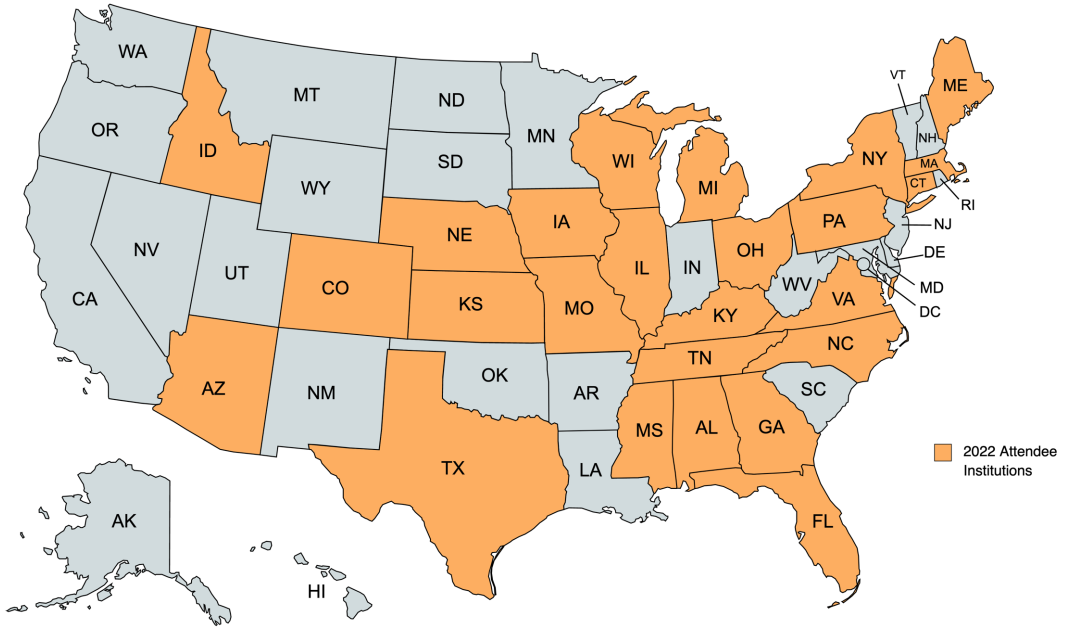
OSG School

- High throughput computing training with hands on-practice
- Community building
- **Emphasis on getting real workflows running**



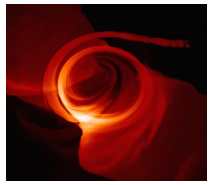

OSG School 2022

In 2022, 58 attendees from 25 states, 3 countries.



Above: students from NIAID's ACE program who attended the 2022 User School
Left: Institutional locations for 2022 School participants

Reaching Out



PIRE Webinar
September 2022

SGX3 | SGCI
A Center of Excellence and a Software Institute
Serving the Science Gateways Community

Gateways 2022, Panel
September 2022, May 2023

Annual Meeting
May 2023

NIH National Institute of Allergy and Infectious Diseases

NIAID presentation
March 2023

AFRICAN CENTERS OF EXCELLENCE IN BIOINFORMATICS

ACE Global Consortium
September 2022

HPC Symposium
May 2023

PEARC
PEARC CONFERENCE SERIES
Practice and Experience in Advanced Research Computing

Reaching Out

- We want to continue reaching new domains and communities, especially underrepresented groups
- What's Next
  - Identify and target domain science events
  - Highlight existing (or new) domain science examples
  - Consult new advisory board representing minority-serving institutions, tribal colleges, etc.

New Service: the PATh Facility

Q: What happens if your HTC workloads aren't a good fit for the opportunistic structure of the OSPool?

A: Dedicated HTC service: the PATh Facility (learn more this morning)

New Users

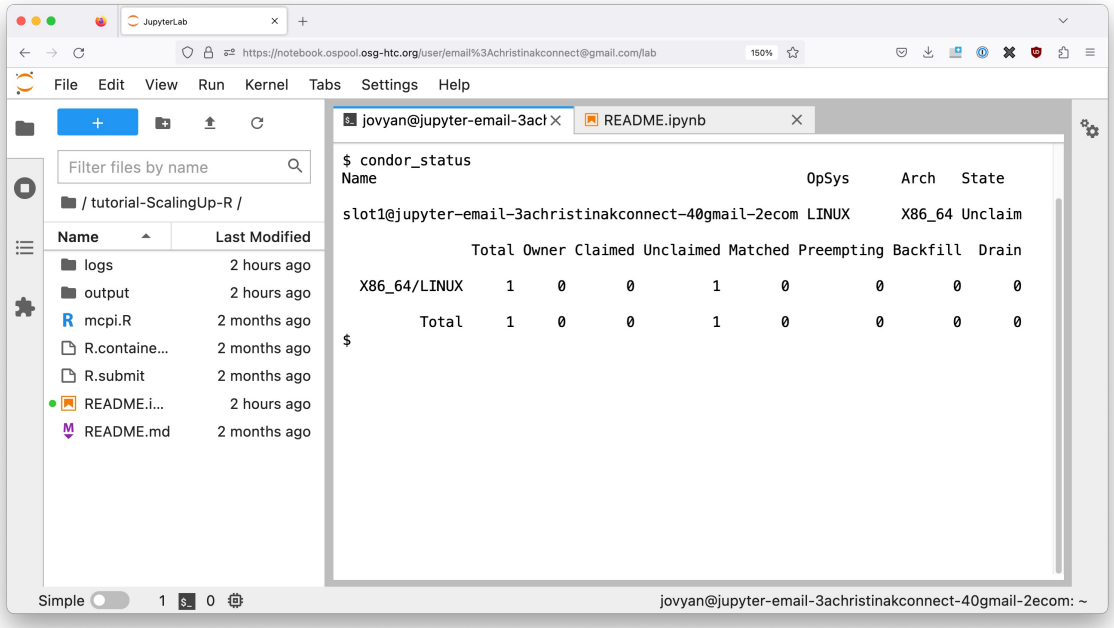
Processes, Templates, Documentation

Office Hours

What's Next:
more users

New Service: OSPool Notebooks

- Jupyter Hub interface to HTC resources
  - Access an HTC resource with just a browser
  - Includes terminal, file browser, notebook capabilities
  - Can be used with or without a full OSPool account
- User interface and training tool
- Talk and demo later this morning!



https://notebook.ospool.osg-htc.org

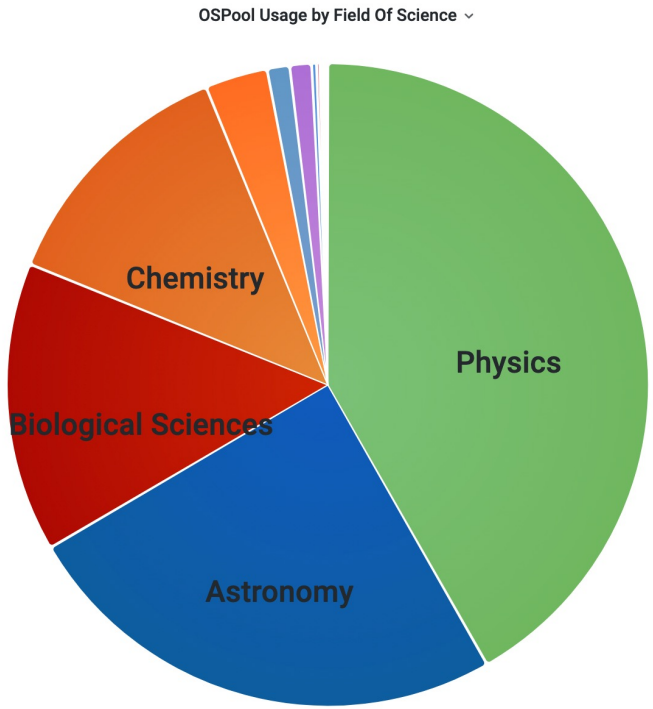
Research Highlights

Active Users

303

Total Jobs

91.5 Mil

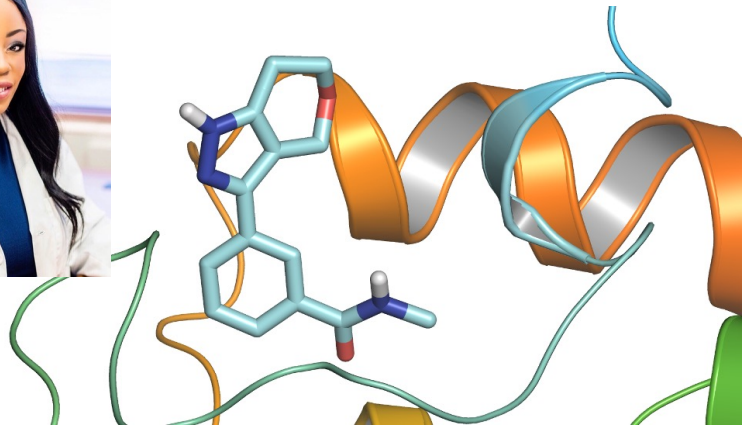


Browse projects: https://osg-htc.org/projects

Research Highlights: Talks Today

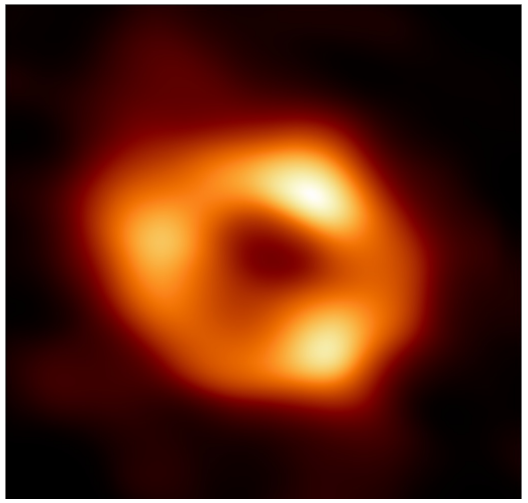
Rousselene Larson

Building a library of molecular compounds and proteins



Chi-Kwan Chan

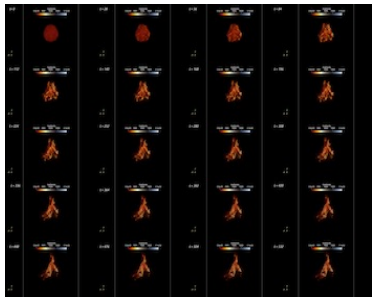
Black hole imaging with the Event Horizon Telescope project

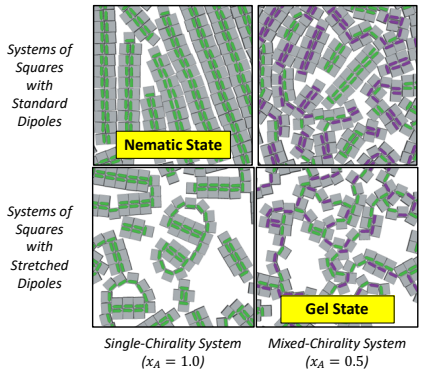


Research Highlights: PATh Stories

OSG User School Researchers Present Inspirational Lightning Talks

https://path-cc.io/news/2022-12-19-Lightning-Talks/





Merging fine arts and “hard science”,
Using AI for healthcare
Searching for properties of the Higgs boson
Mapping invasive species
Analyzing traffic camera video
Developing colloidal particles
Predicting forest productivity
...and more...

Research Highlights: Biological Sciences

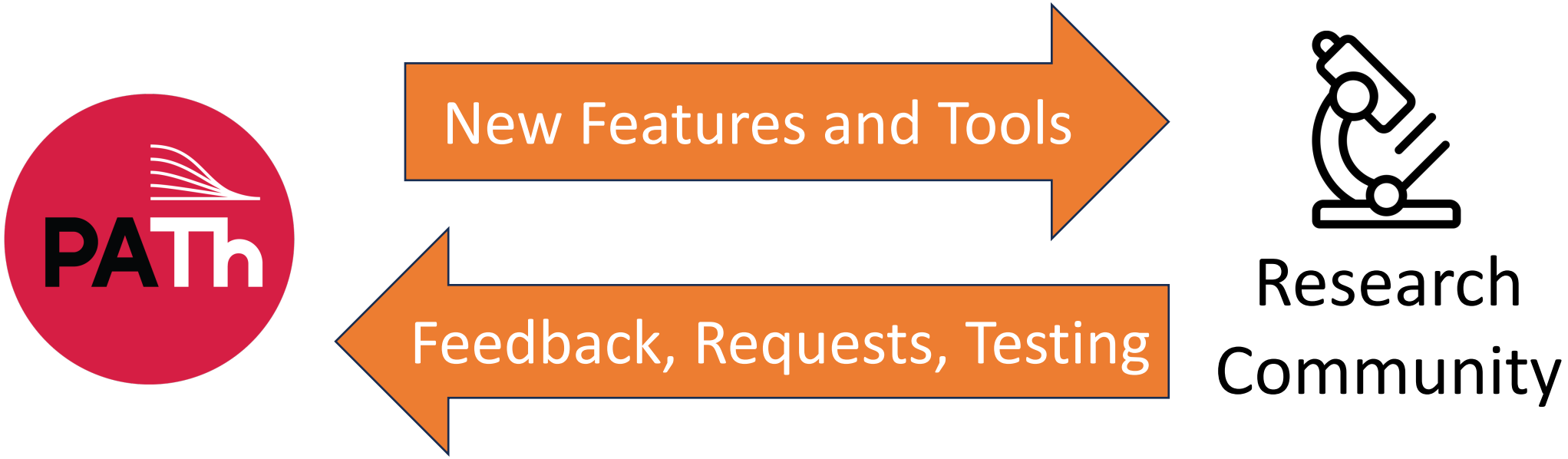
- Eric Wright (University of Pittsburgh)
  - Large scale biomedical informatics on microbial genome sequence data.
- Summer Thyme (University of Alabama – Birmingham)
  - Drug Discovery: development of a conformer library containing a set of over 30 billion conformers from over 2 billion unique ligands
- Oana Carja (Carnegie Mellon University)
  - Evolutionary simulation tracking gene frequencies under a variety of environmental conditions.

Advancing dHTC State of the Art

OSG is a consortium dedicated to the advancement of all of open science via the practice of distributed High Throughput Computing (dHTC), and the advancement of its state of the art.

How did the facilitation team advance the state of the art for dHTC?

Translational Computer Science



User-Driven Changes

- Request for data privacy and sharing on the OSDF
  - Now support authenticated access for individuals
  - Next up: supporting authenticated access for groups
- Using additional resources from an OSPool Access Point
  - Development of “annex” tool to “bring your own capacity”
- **What’s Next**: Tools for users to monitor and learn about their jobs
  - Identifying use cases
  - Developing template commands and dashboards

Advancing Teamwork

OSG is a ~~consortium~~ team dedicated to the advancement of all of open science via the practice of distributed High Throughput Computing (dHTC), and the advancement of its state of the art.

- Building up our “people and process” capacity along with our technical capacity
  - Team lead transition, new facilitation hire
  - Dedicated user documentation work time
  - Strengthening coordination between OSG Services teams
  - Adding support for campuses

Acknowledgements

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