

MOUNTAINS  
AND MINDS

# High Performance Computing Advisory Group

Thursday, November 3, 2016



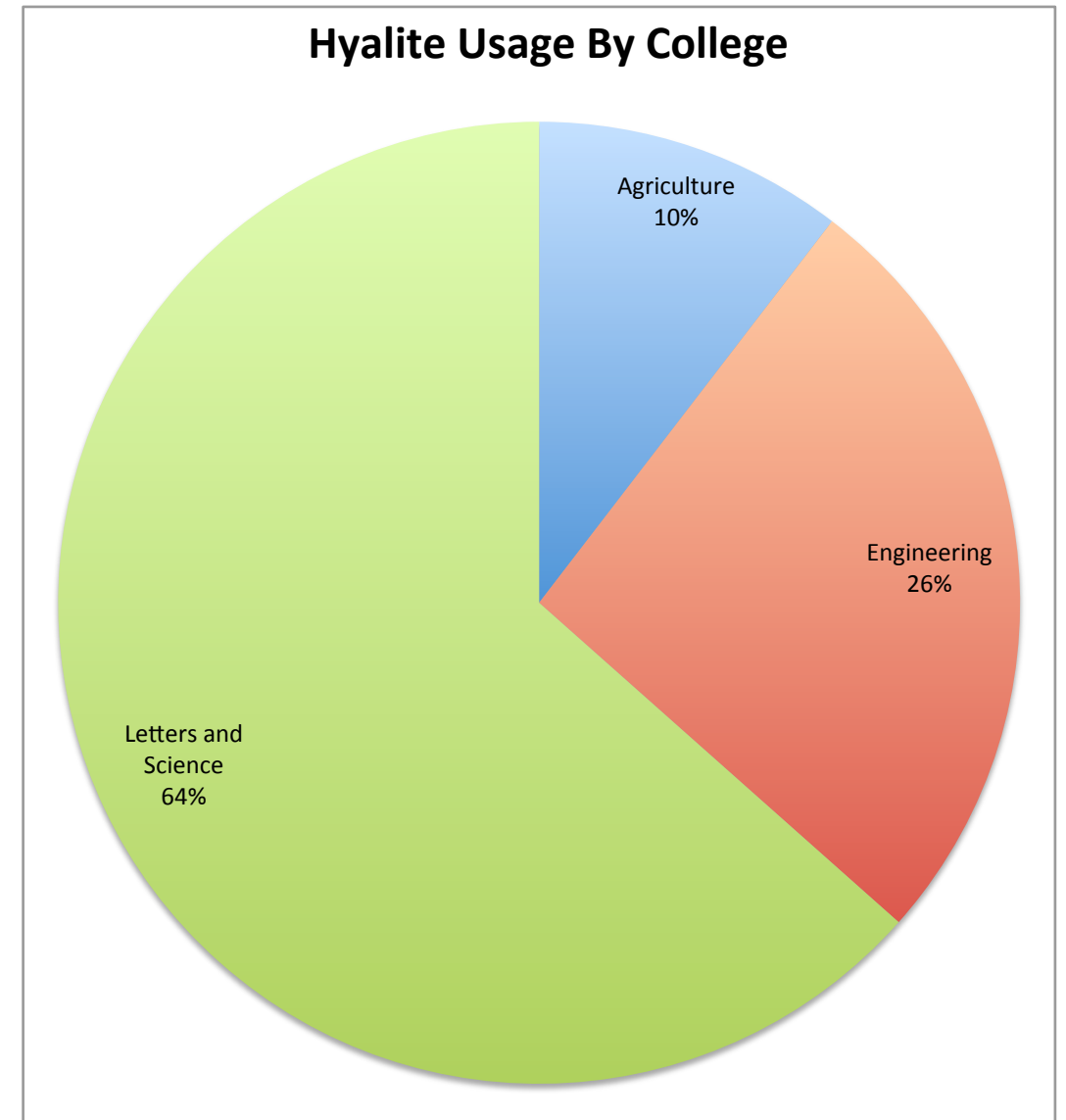
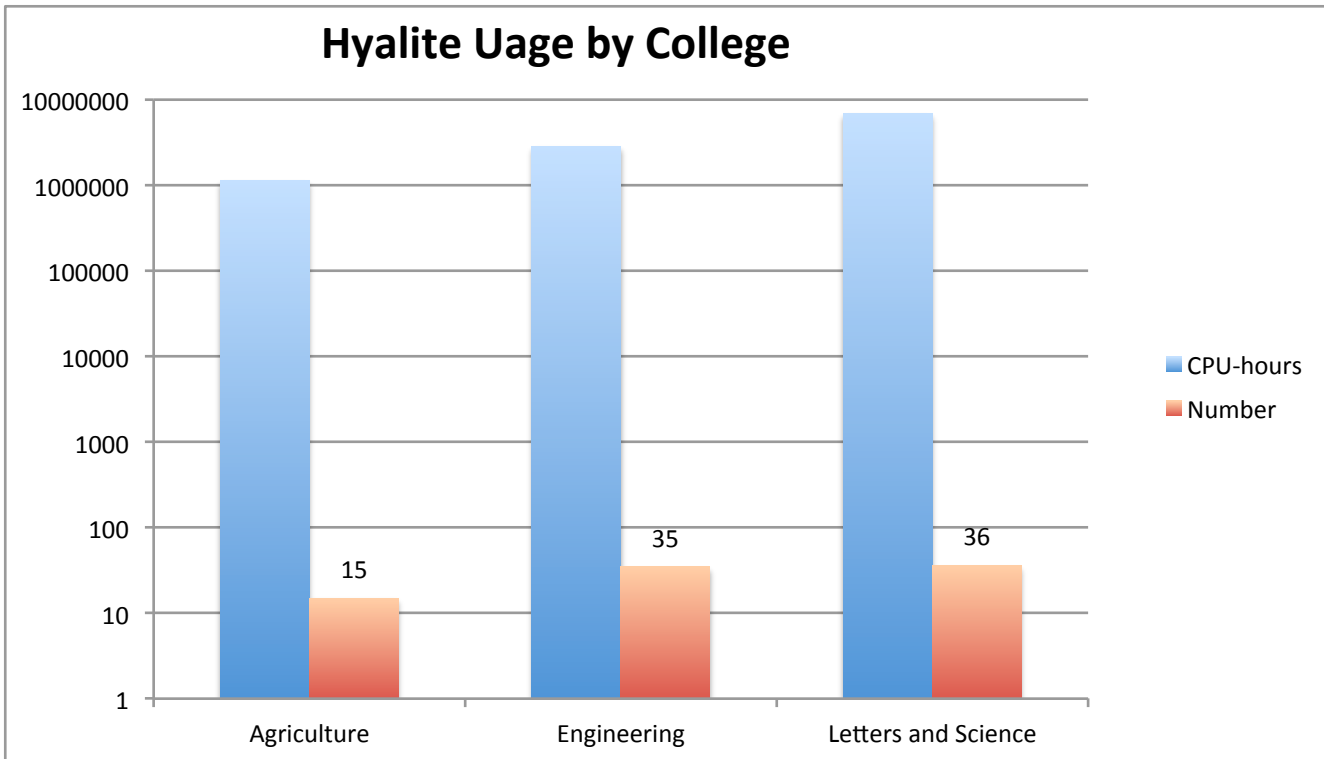


# Hyalite Usage: Overall Summary

<b>Total Jobs Submitted</b>	<b>258,448</b>
<b>Total CPU Hours</b>	<b>11,576,145.48</b>
<b>Total Active Users</b>	<b>107</b>
<b>Avg Wait Time</b>	<b>8.78 hours</b>
<b>Avg Wall Time</b>	<b>2.54 hours</b>
<b>Total Wall Time</b>	<b>656,111 hours</b>
<b>Avg CPU Count</b>	<b>19</b>



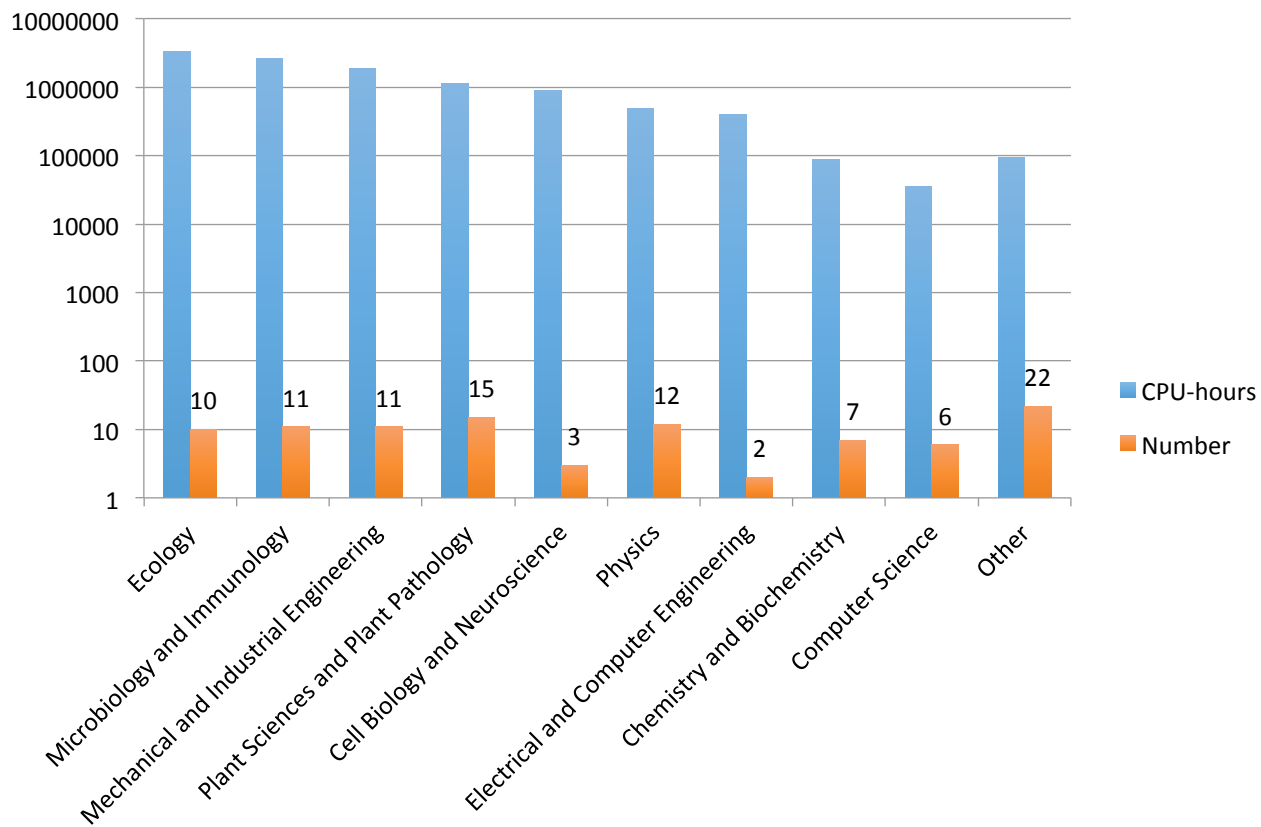
# Hyalite Usage: by College



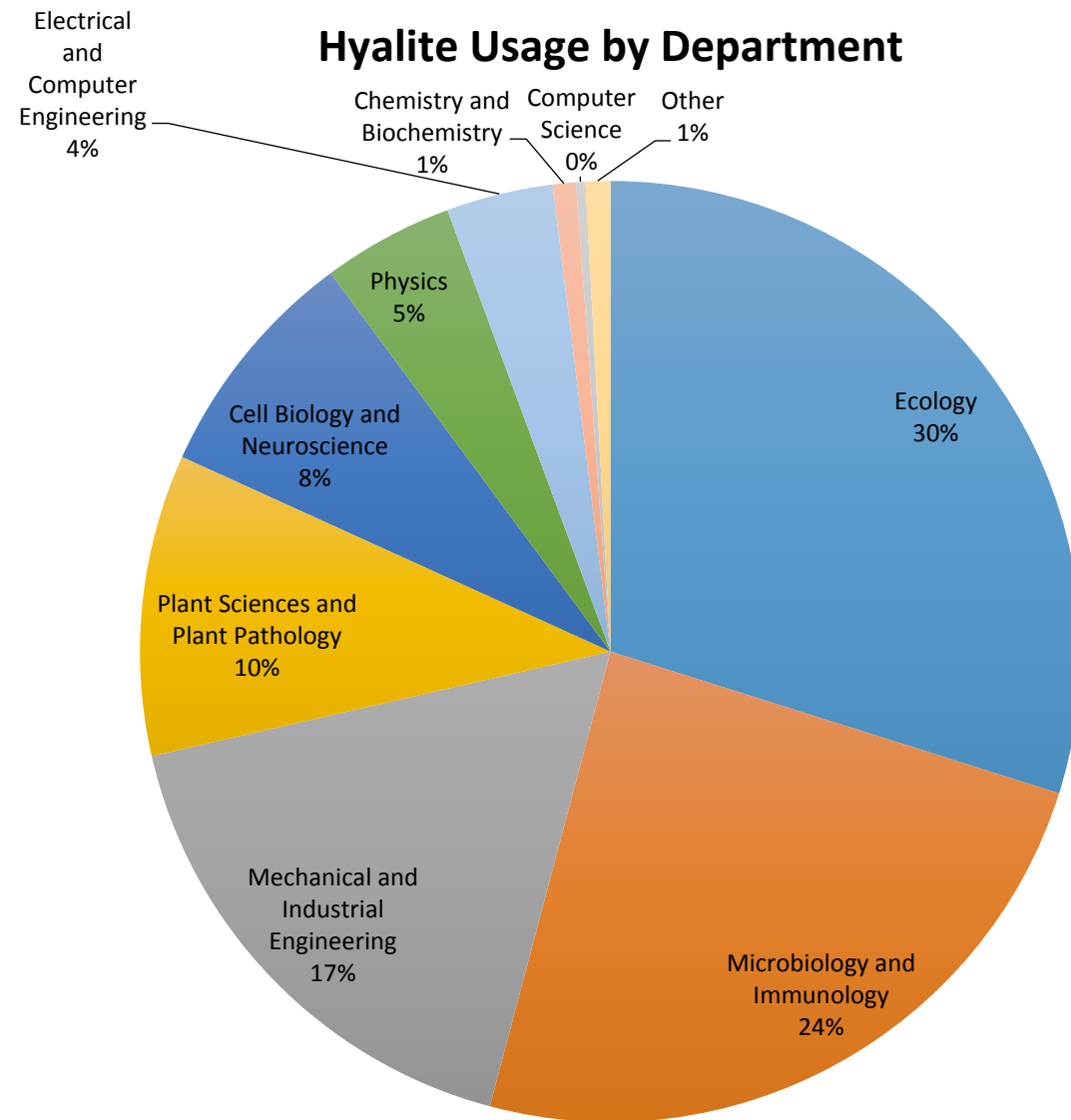


# Hyalite Usage: by Department

### Hyalite Usage by Department



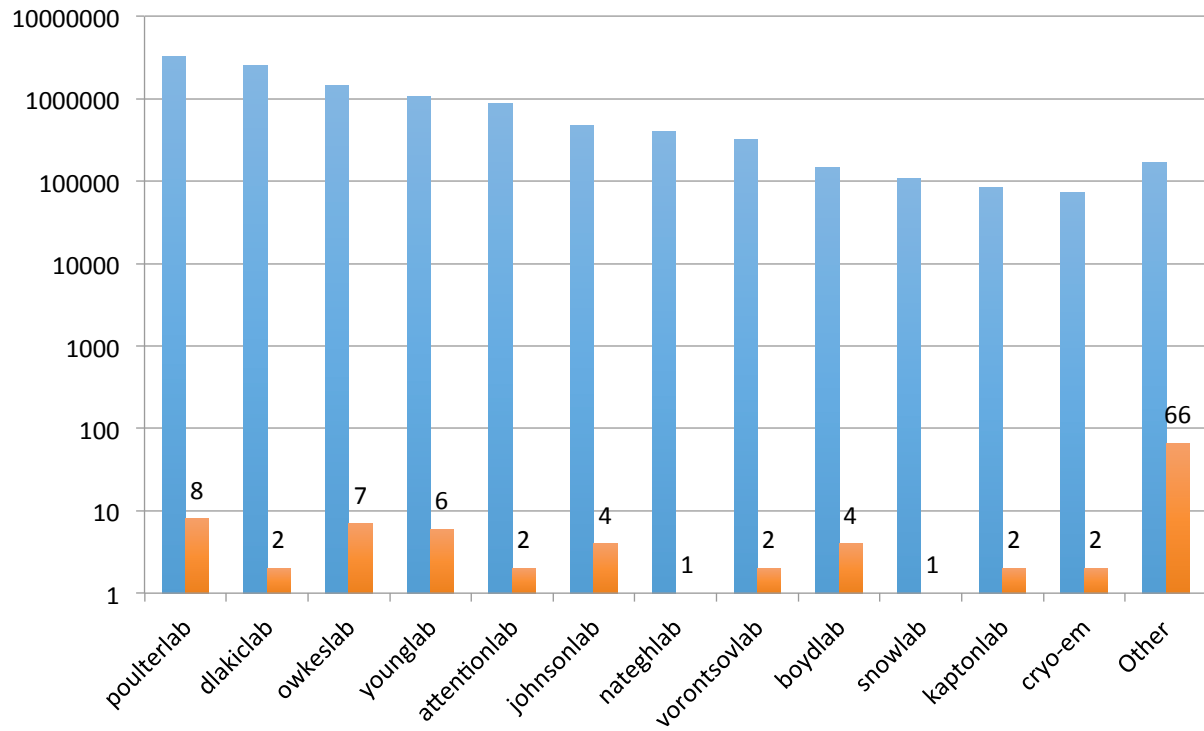
### Hyalite Usage by Department



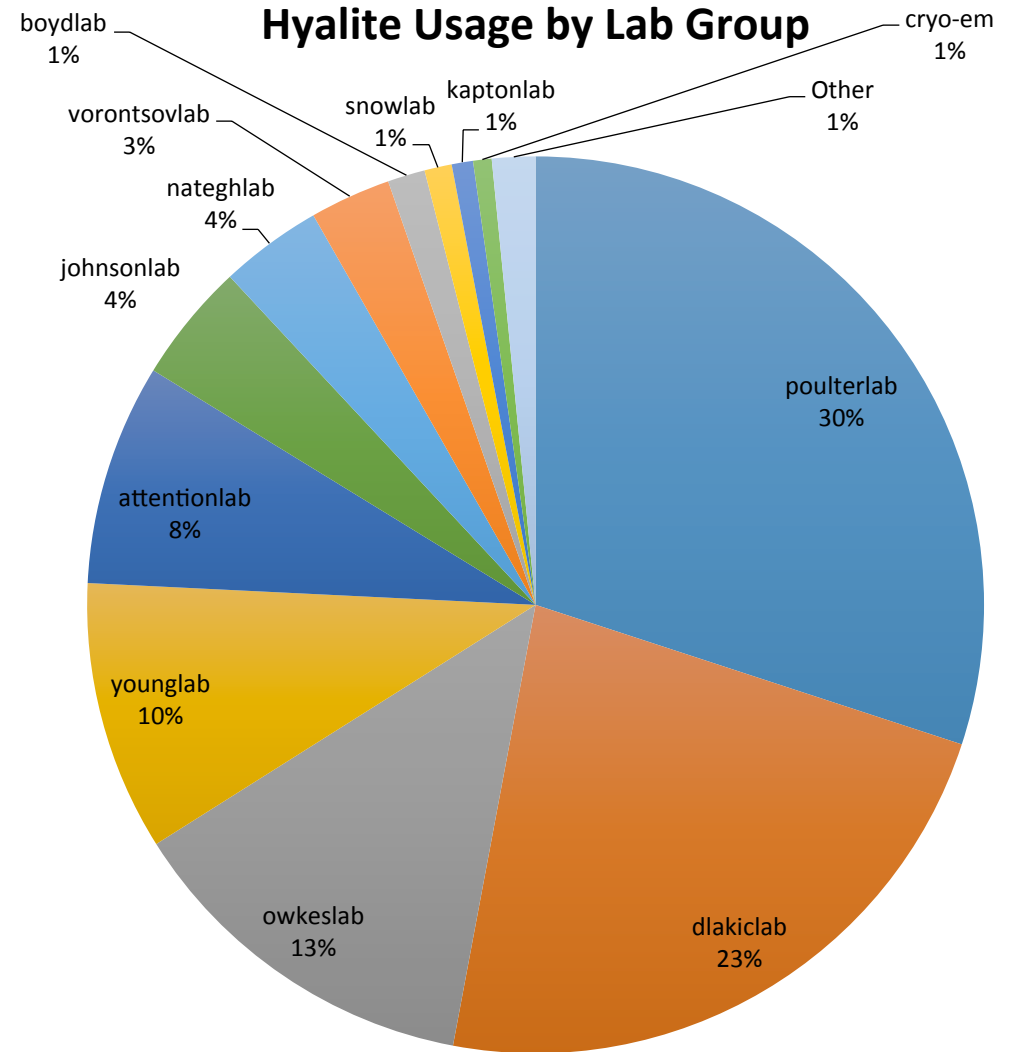


# Hyalite Usage: by Lab Group

## Hyalite Usage by Lab Group

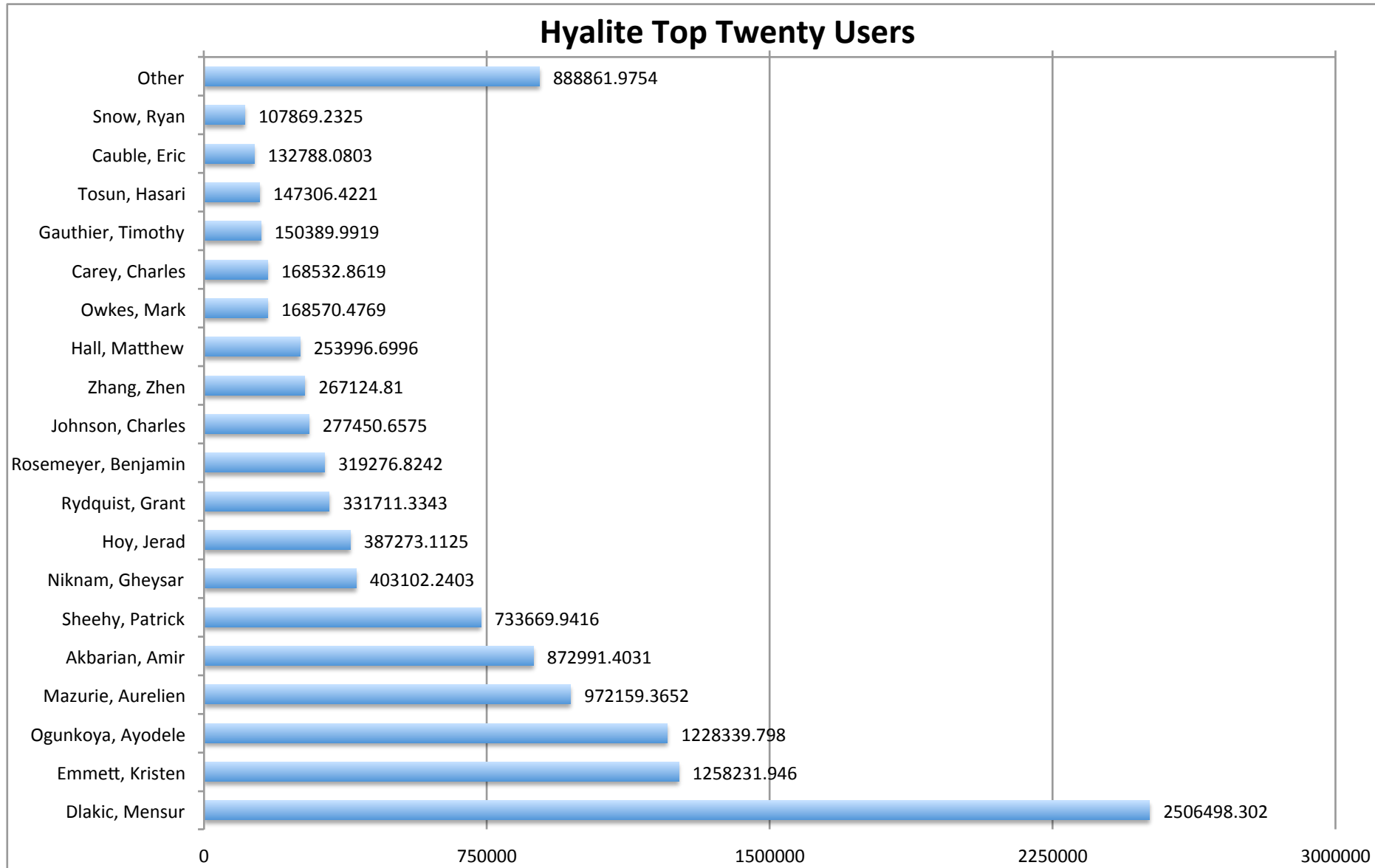


## Hyalite Usage by Lab Group





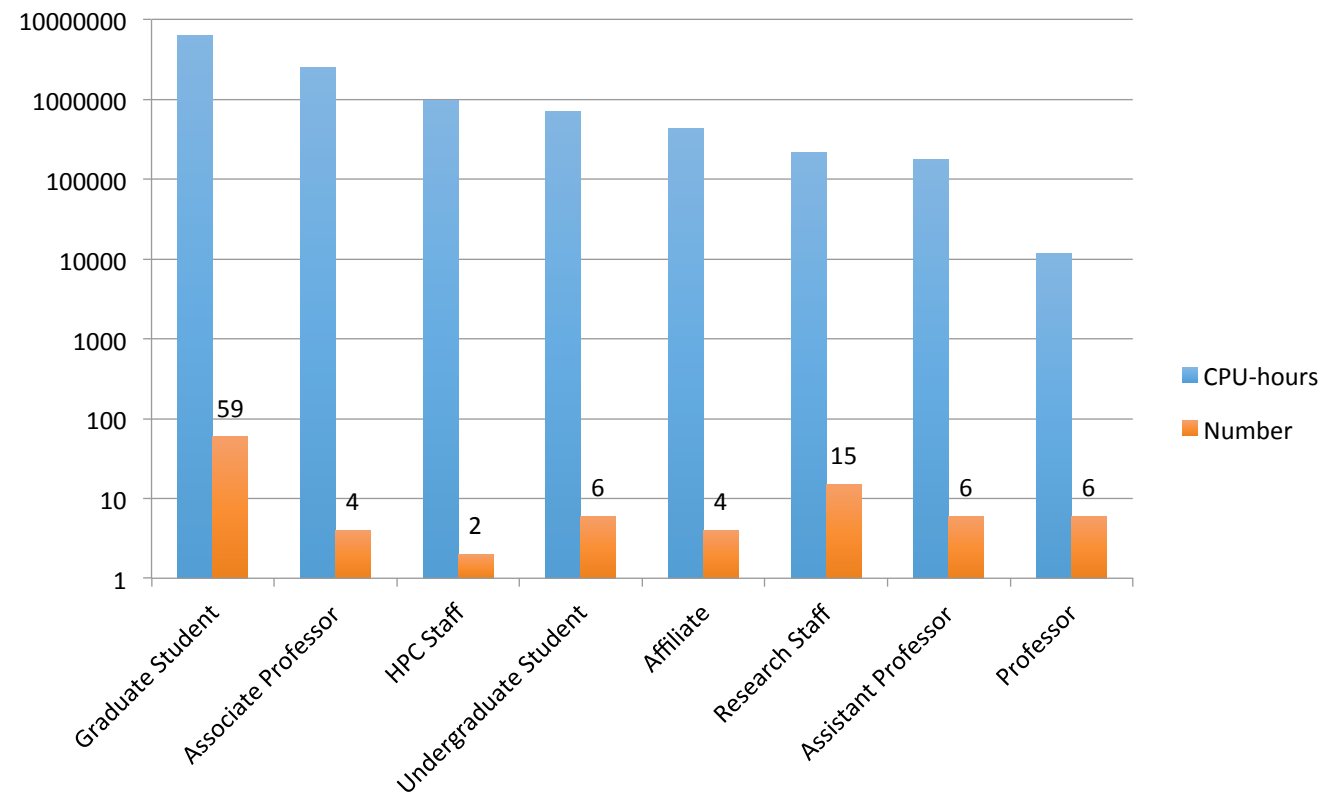
# Hyalite Usage: Top Twenty Users



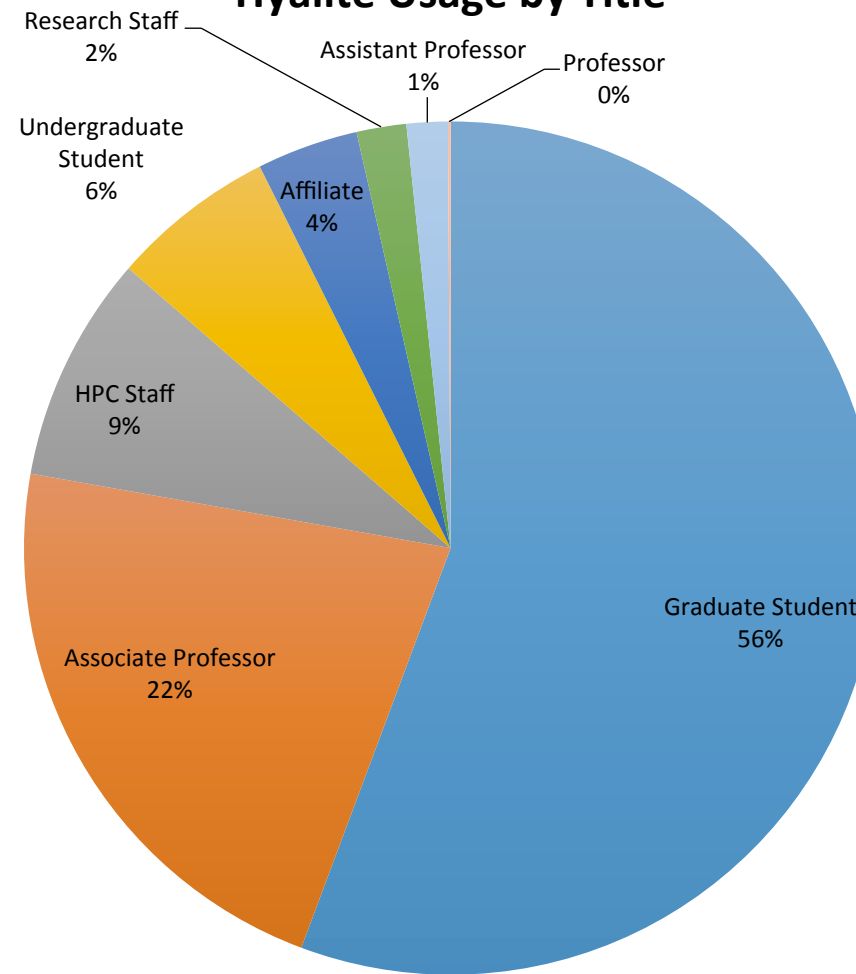


# Hyalite Usage: by Title

### Hyalite Usage by Title

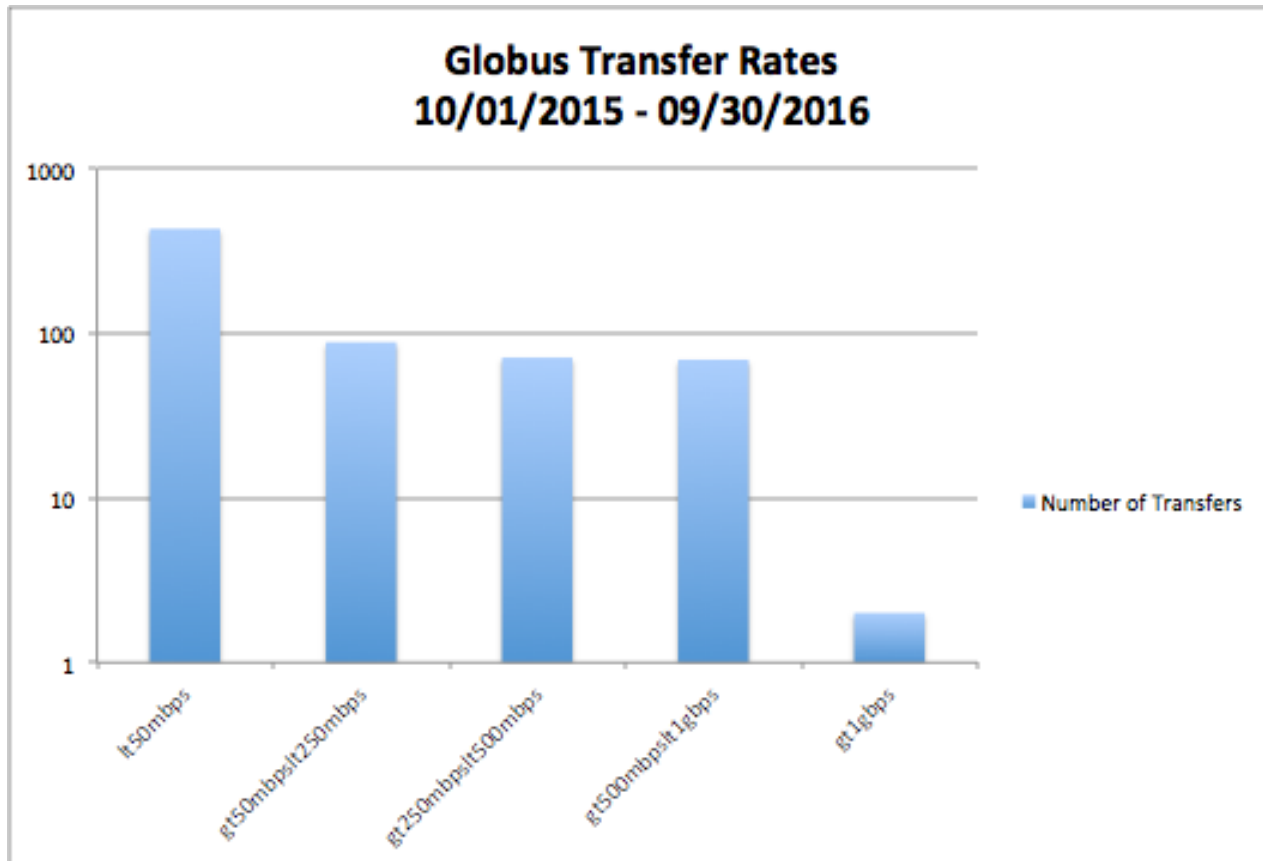


### Hyalite Usage by Title





# GLOBUS: Usage last 12 months



Total Transfers	660
Total Data Transferred(TB)	132.25
Total Files Transferred	30,287,479.00
Total Transfer Time (days)	350.55
Unique Users	54
Unique Sources	62
Unique Destinations	44
Max Transfer Rate (Mbps)	1,469.02
Mean Transfer Rate (Mbps)	133.26

- Globus Plus Account
  - Montana State University – Globus Plus
  - Users may request access
  - Allows GCP <=> GCP transfers





# Hyalite Software Usage

- Software is a hard problem
  - Even if we were to track the executables running, there is no guarantee that the user hasn't renamed the executable
  - Loaded modules aren't necessarily what are being run
    - User may load same 10 modules for everything, or may load modules then not run anything from those modules.
- Matlab Usage
  - Faculty/Staff/Lab usage: 148 licenses activated
  - Student usage: 574 licenses activated
  - Hyalite Cluster Usage
    - Uses a single concurrent license
    - Working on current usage stats





# HPC Class Overview: CHMY591

Course: **Computational Chemistry - CHMY591**

Instructor: **Robert Szilagyi**

Number of Students: **5**

## PREPARATION

- Prior to the course starting, we did a training with Robert going over the cluster and how it works. It was a fairly standard cluster training, with a bit more information about class-specific topics.
- Robert prepared custom scripts that built and ran sbatch job files to make things easier for the students.

## COURSE PROGRESS

- Start with an introduction to the software, get the students running the software on their own computers using the GUI to tweak the settings.
  - Get them to use scripts or a text editor to manage the settings.
  - Mac students used Parallels in order for everyone to be in Windows.
- Do the HPC Training,
  - Add a group for the class, add the users to the cluster and group
  - The training started with an overview of the cluster (and HPC in general) and a tour of the cluster hardware
  - The training took ~1 hour longer than usual (2.5 hours instead of 1.5 hours)

- Have the students use exported files from the work they did on their own computers as the initial input files on the HPC cluster
  - Use custom scripts that builds the sbatch files for job submission
  - Use WinSCP “command submission” feature to trigger the job so that the student doesn’t need to learn the command line.
    - Maybe better than MobaXterm?
  - Students run on the test (express) queue

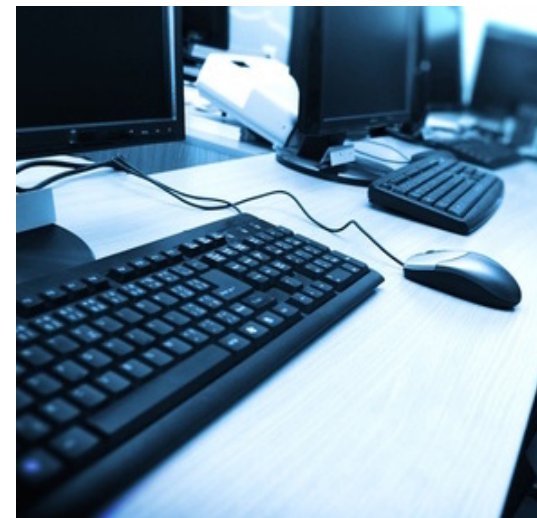
## NEXT STEPS

- Prep a custom queue for the class to run preemptively (still working on this)
  - Students will use the express and default queue in the meantime.



# CHMY591 Jobs

- Jobs will mostly be Gaussian
  - 8 cpu, 16GB RAM
  - 72 hour job runtimes max
- Set up a custom class queue for runtime limit
  - Limit to 4 machines
- Impact on the total cluster usage will be minimal





- Paper published by Ryan Snow (Physics), citing Hyalite:
  - H. Bhatkar, R.J. Snow, E. Arenholz, Y.U. Idzerda, Elemental moment variation of bcc FeMn<sub>1-x</sub> on MgO(001), Journal of Magnetism and Magnetic Materials, Volume 423, 1 February 2017, Pages 46-50, ISSN 0304-8853, <http://dx.doi.org/10.1016/j.jmmm.2016.09.060>.
- Cited Hyalite as:
  - Calculations were performed on the Hyalite Research Cluster at Montana State University.
- Working on a better boilerplate citation for Hyalite



# NSF CyberTraining Solicitation

The overarching goal of this program is to prepare, nurture and grow the national scientific workforce for creating, utilizing, and supporting advanced cyberinfrastructure (CI) that enables cutting-edge science and engineering and contributes to the Nation's overall economic competitiveness and security. This solicitation calls for developing innovative, scalable training programs to address the emerging needs and unresolved bottlenecks in scientific and engineering workforce development of targeted, multidisciplinary communities, at the postsecondary level and beyond, leading to transformative changes in the state of workforce preparedness for advanced CI in the short and long terms. In the short term, the projects shall result in innovative, scalable, informal training models and pilot activities, complementing and leveraging the state of art in curricular offerings, material, and best practices in academia and elsewhere. In the long term, the projects should contribute to the larger goals of an educational ecosystem enabling "Computational and Data Science for All," with an understanding of computation as the third pillar and data-driven science as the fourth pillar of the scientific discovery process.

Prospective PIs are strongly encouraged to contact the Cognizant Program Officers (POs) in CISE/ACI and in the participating directorate/division(s) relevant to the proposal at least a month in advance of the submission deadline to ascertain whether the focus and budget of the proposed activities are appropriate for this solicitation, and include the names of POs consulted in their Project Summary.

**Deadline: January 25, 2017**

**Standard grant: \$4.5M, 10-15 awards**

**NSF 17-507, <https://www.nsf.gov/pubs/2017/nsf17507/nsf17507.pdf>**

