Research Cyberinfrastructure Center

| Resources | Update | Utilization |

Philip Papadopoulos ppapadop@uci.edu

Joulien Tatar jtatar@uci.edu

Nadya Williams npw@uci.edu

What do we do?
Infrastructure for Researchers

RCIC builds and maintains real infrastructure for

- ✓ High-performance and high-throughput computing
- ✓ Research data storage and analysis,
- ✓ Scientific software tool integration.

Computing and data infrastructure is operated in a *shared financial model* where campus researchers are given no-cost access to a baseline level of computing and highly-reliable storage.

Faculty can also purchase additional capacity and capability using grant or other funds.

RCIC Faculty Oversight

Executive Committee – Chair Filipp Furche, Professor, Dept. of Chemistry

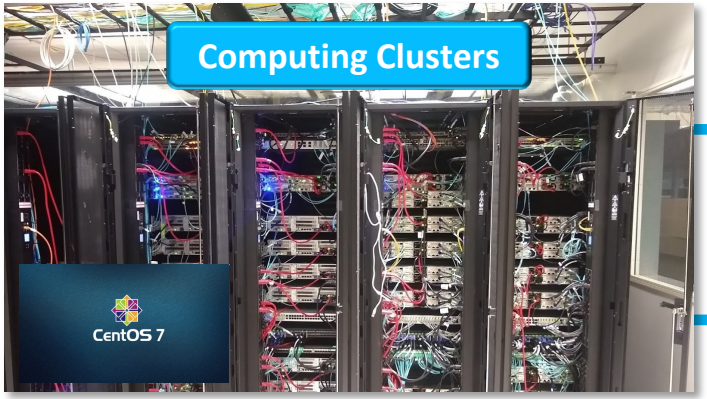
- Help with strategic guidance and direction
- Approval chain for large purchases (> $100K) and high-level policy
- Meet approximately quarterly

Advisory Committee

- About 30 researchers from disciplines across UCI
- Key feedback on what RCIC does right and wrong. They are not shy about expressing their views.

Formation of RCIC was the result of the UCI Cyberinfrastructure Vision 2016

Key Resources @ RCIC



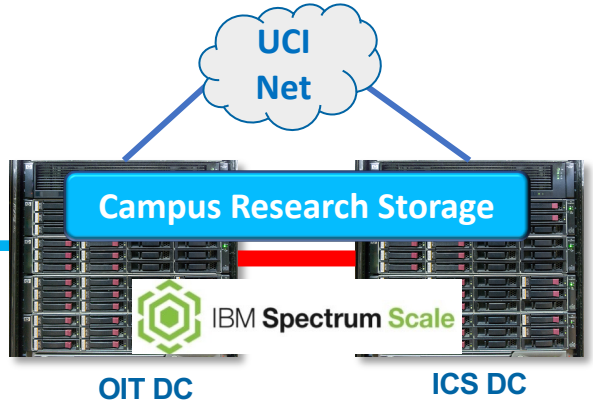
HPC3

- ~6900 Cores/162 Hosts (expanding to ~8500/200)
- 52 Tesla V100 16Gb Nvidia GPUs
- EDR (100Gbps) Infiniband
- 10GbE Ethernet
- Minimum
  - 4GB memory/core
  - AVX2 instruction set (Epyc/Intel CPUs)

Six Parallel File Systems

DFS2, DFS3a, DFS3b, …

- 3.9PB usable storage
- ~6GB/sec bandwidth/System
- Single Copy/No Snapshots



CRSP – Campus Research Storage Pool

- 1 PB usable storage
- Available anywhere on UCI Network
- Dual Copy of All Data
- Snapshots
- Highly available

High-level View of what things cost

No Cost Allocations

Role	HPC3 Core Hours	GPU Hours	Home Area Storage	DFS Storage	CRSP Storage
Faculty	200K hours/year[1]	By Request ~2K hours/year[1]	50GB	1TB in Pub	1 TB
Student	1000 hours	---	50GB	1 TB in Pub	---

Cloud-like Costs

	HPC3 Core Hours	GPU Hours	Home Area Storage	DFS Storage	CRSP Storage
Faculty	$.01/core hour	$0.32/GPU hour	Not expandable	$100/TB/5 years	$60/TB/year
AWS Equivalent	C5n.large $.063	P3.2xlarge $1.95	---	---	S3[2] Standard $242/TB/year

[1] Exact amounts dependent on # requests/available hardware
[2] Comparison difficult - S3 has higher durability, CRSP has no networking fee.

HPC^3 – High Performance Community Computing Cluster

- Short History – And Expansion
- Different Use Cases of HPC3
- How HPC3 is physically connected to UCI
- Queueing and Allocations
- Software Environment
  - What happens when you ask RCIC to install software
  - Organization
  - Insights to usage
- How has HPC3 been used since Jan 1, 2021

Short History of HPC3

Predecessor - HPC

- Catalyzed shared computing at UCI

  Hat-Tip to retired personnel: Joseph Farran , Harry Mangalam, Allen Schiano, Dana Roode, and Garr Updegraff
- Expanded primarily through faculty node purchases (condo computing)
- Reached end of life Dec 2020 – 10500 cores at its peak. Cores 1-9 years in age

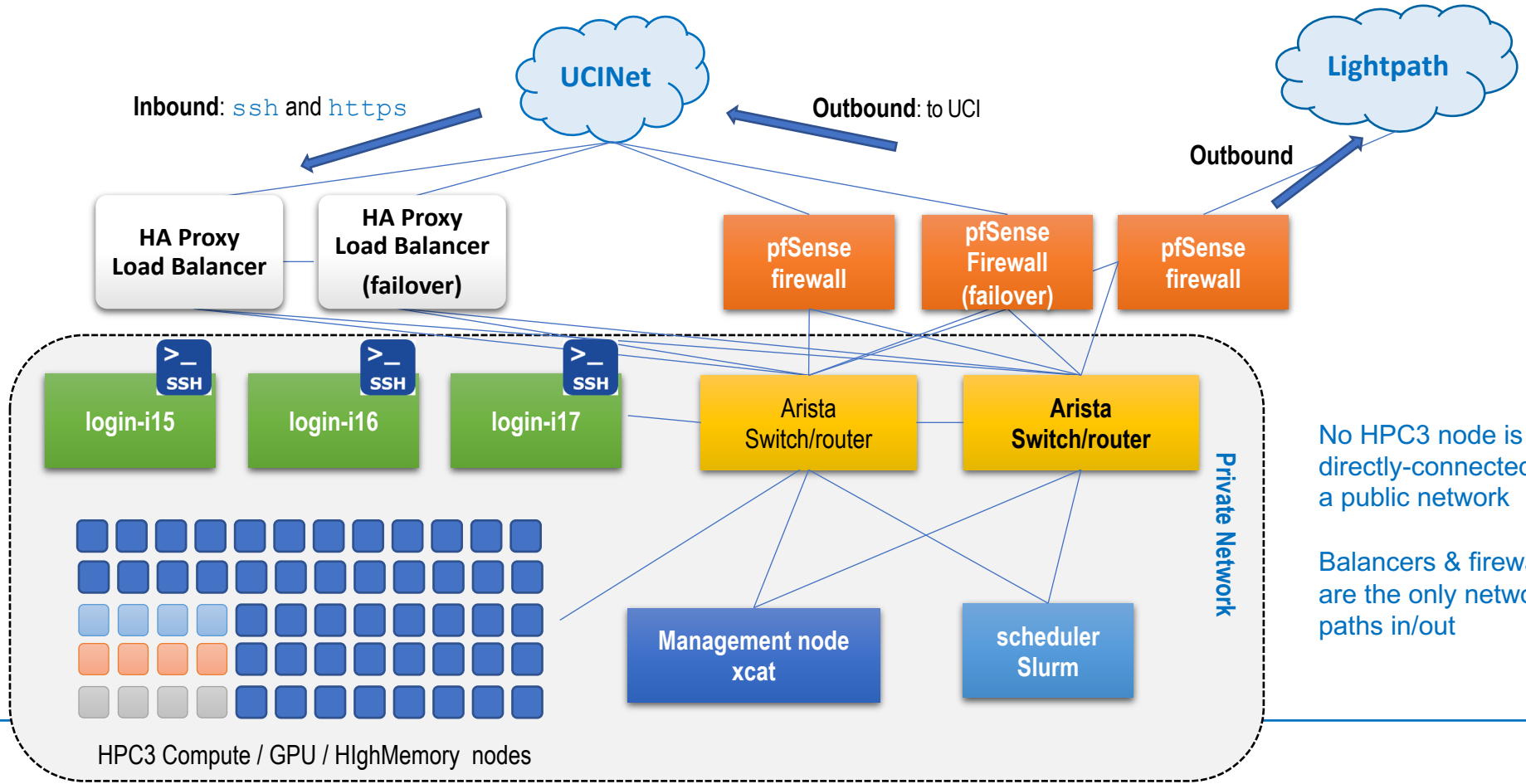
HPC3 catalyzed by NSF Major Research Instrumentation Grant

- PI: Chandramowlishwaran
- Co-PIs: Furche, Roode

Initially constructed from Grant, Faculty Purchase, and Significant UCI investment

- RFP (won by HPE) in Oct 2019. ~100 CPU and GPU nodes (4000 cores total).
- Most nodes arrived after March 2020 during shutdown
- Expanded through faculty/UCI purchase Oct/Dec 2020
- Expanded via compatible HPC nodes moved to HPC3 Jan 2021
- Expanded via UCI/Faculty purchase via April 2021 Competitive Bid (nodes arriving now)

Network Connectivity of HPC3



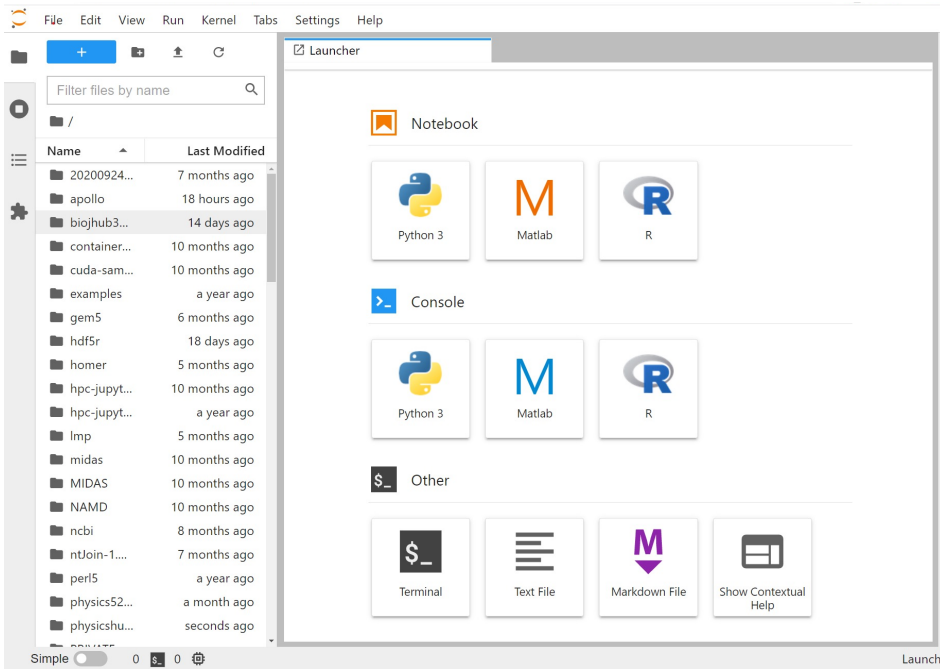
No HPC3 node is directly-connected to a public network

Balancers & firewall are the only network paths in/out

Different Ways People are Using HPC3

1. Most common: command-line, batch queue, job submission
   ssh hpc3.rcic.uci.edu
2. Teaching courses
   Quarter:
   - Grad courses
   - Lower division physics labs

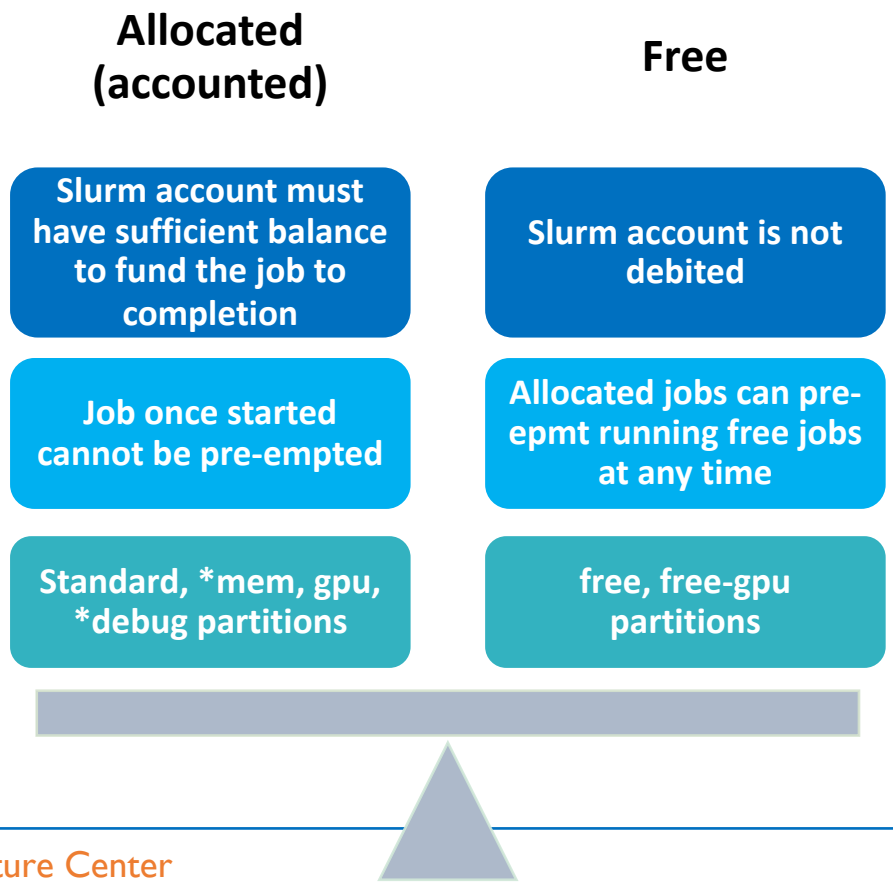
   Short-term:
   - UCI machine learning hackathon
3. Specialized Jupyter Labs
4. Via Singularity Containers



Two Types of Jobs

Q: Why is my job not running and squeue output shows AssocGrpCPUMinutesLimit ?

A: not enough balance in your slurm account



Q: Is there checkpointing?

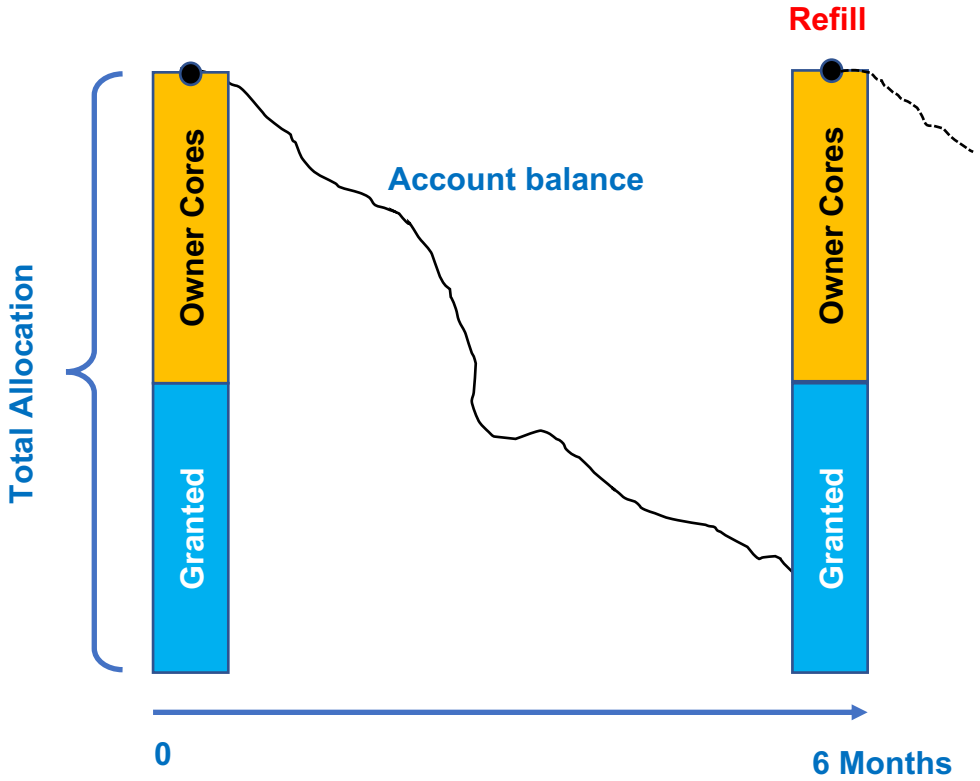
A: **NO checkpointing !** not a viable technology

Allocated Jobs (standard, *mem, GPU queues)

- All allocated jobs use a common "currency" (SU)
- CPU cores cost 1 SU/Hour
  - There is no differentiation on memory used.
- GPUs cost 32 SUs/Hour
- What about owner hardware/queues?
  - Owner queues do NOT exist. Instead
  - Theoretical capacity of owner hardware is converted into SUs
    - 95% * (# cores) * 8760 hours/year – 40 core node ~ 325K SUs/year
    - 95% * (# gpus) * 32 * 8760 hours/year.
  - GPU SUs and CPU SUs are not "convertible". → need a GPU account to charge runs on the GPU queue.

Automated Refill of Allocations for labs

- Account balances are reset every 6 months
- Each Lab is on their own cycle
- Allocations are for "the next 6 months"
- **SUs not utilized in the previous 6 months are lost**
- Purchased cycles can be spent over 18 months.



Policy on allocating UCI-paid cycles

Ideal – every cycle allocated is utilized

Allocation Tiers for CPU Cores (6 months horizon):

- 100K, 75K, 50K, 25K, 12.5K

Your next allocation is based on your previous 6 months of usage

- > 80% of current allocation utilized, go up one tier
- 50% - 80%. Remain in same tier
- 25% - 50%. Go down on tier
- < 25% go down two tiers

Limits

- Philosophy

  Allow users to do what they need to do.

  Generally, only place limits to address: stability, fairness, responsiveness

- Example System-wide limits

  MaxArraySize = 100000

  MaxJobCount = 50000

- When we see a file system "under stress"

  1. Identify user/users
  2. Contact them to find out "what their applications are doing"
  3. Determine if

     limits (like maxjobs or maximum cores) are needed to mitigate

     or

     can a restructuring of jobs address the issue

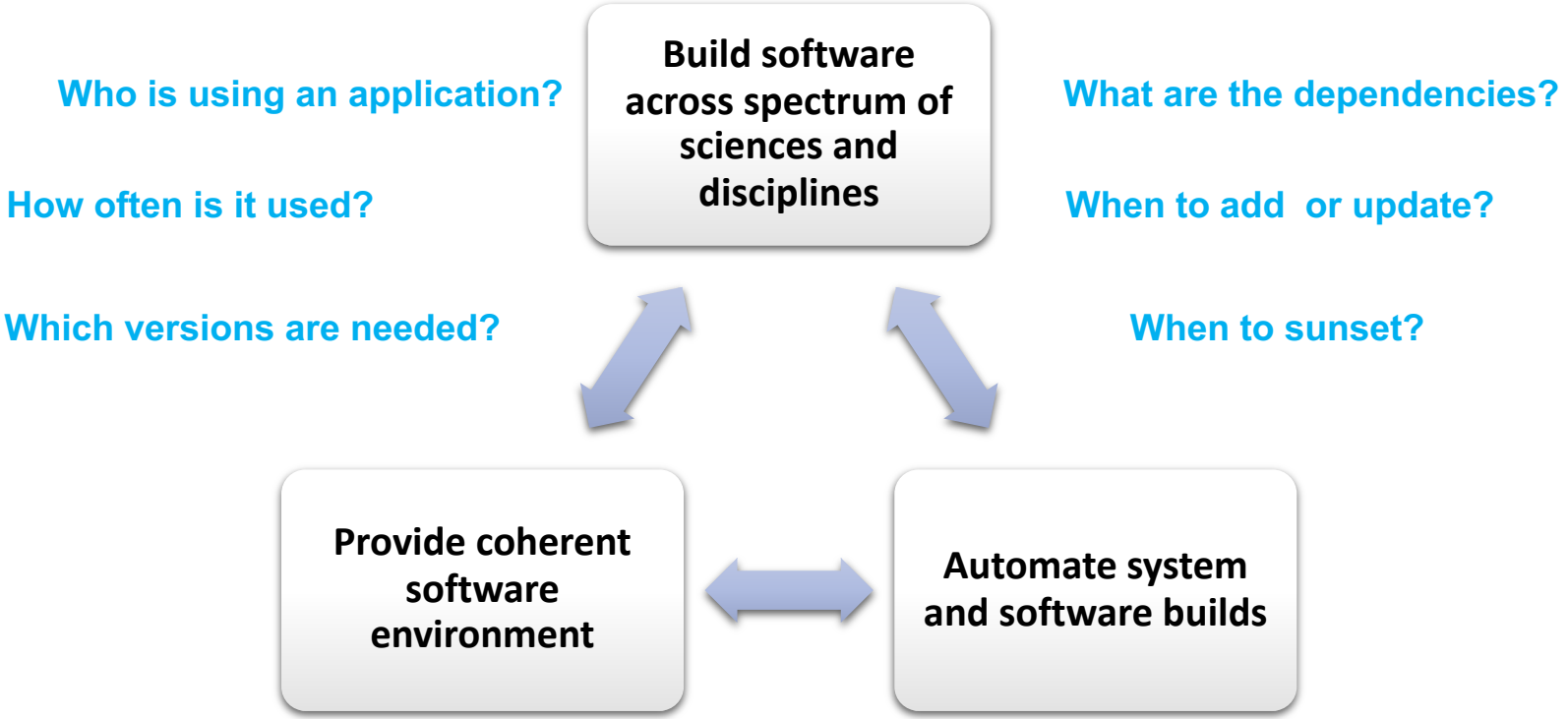
- Example user-specific limit:

```
   Account         User  Partition     Share  MaxJobs       GrpTRES
---------- ---------- ---------- --------- ------- -------------
   uci_lab   panteater                    1     300       cpu=800
```

The most vulnerable part of any cluster is storage

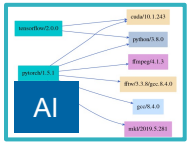
Software environment on HPC3

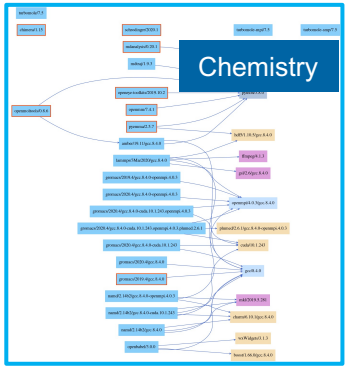
Software Applications

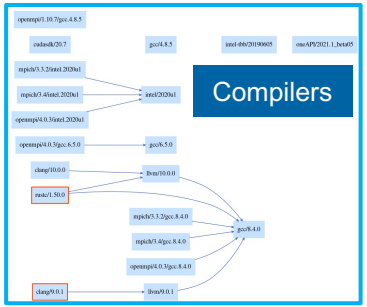


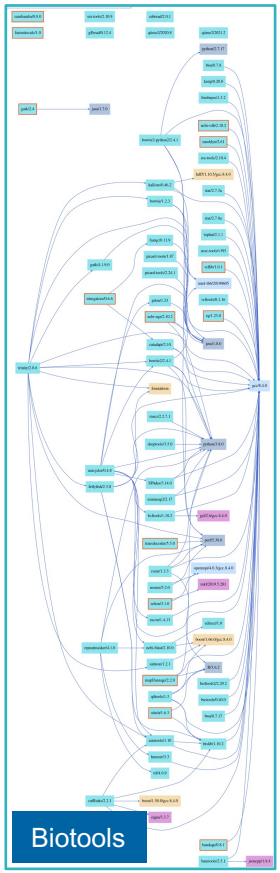
We package most applications in the OS-native format: RPM

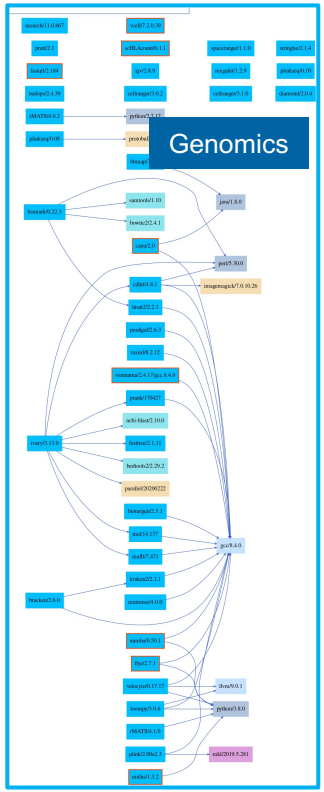
Software Map

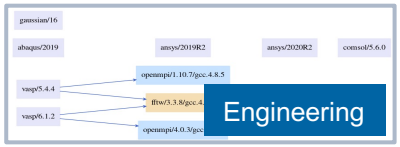


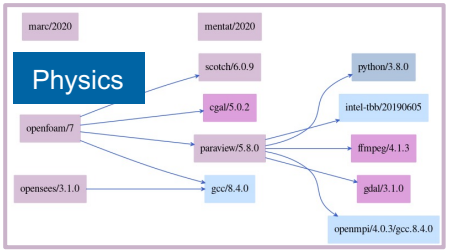


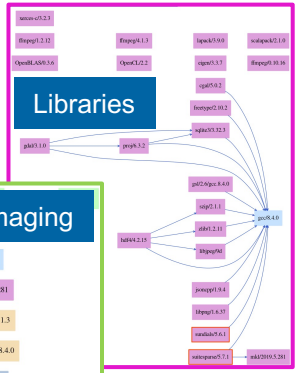


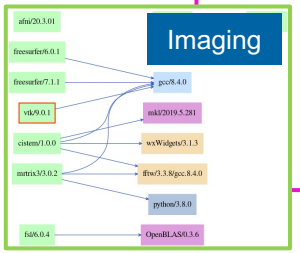


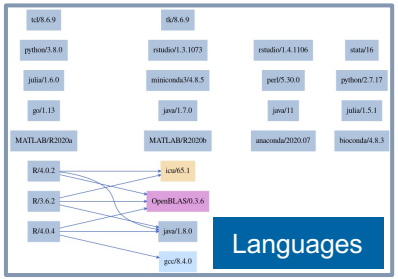


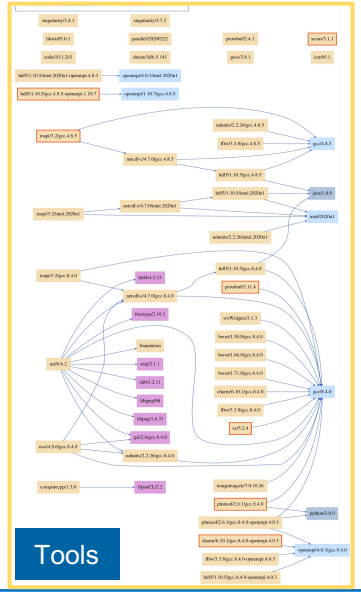




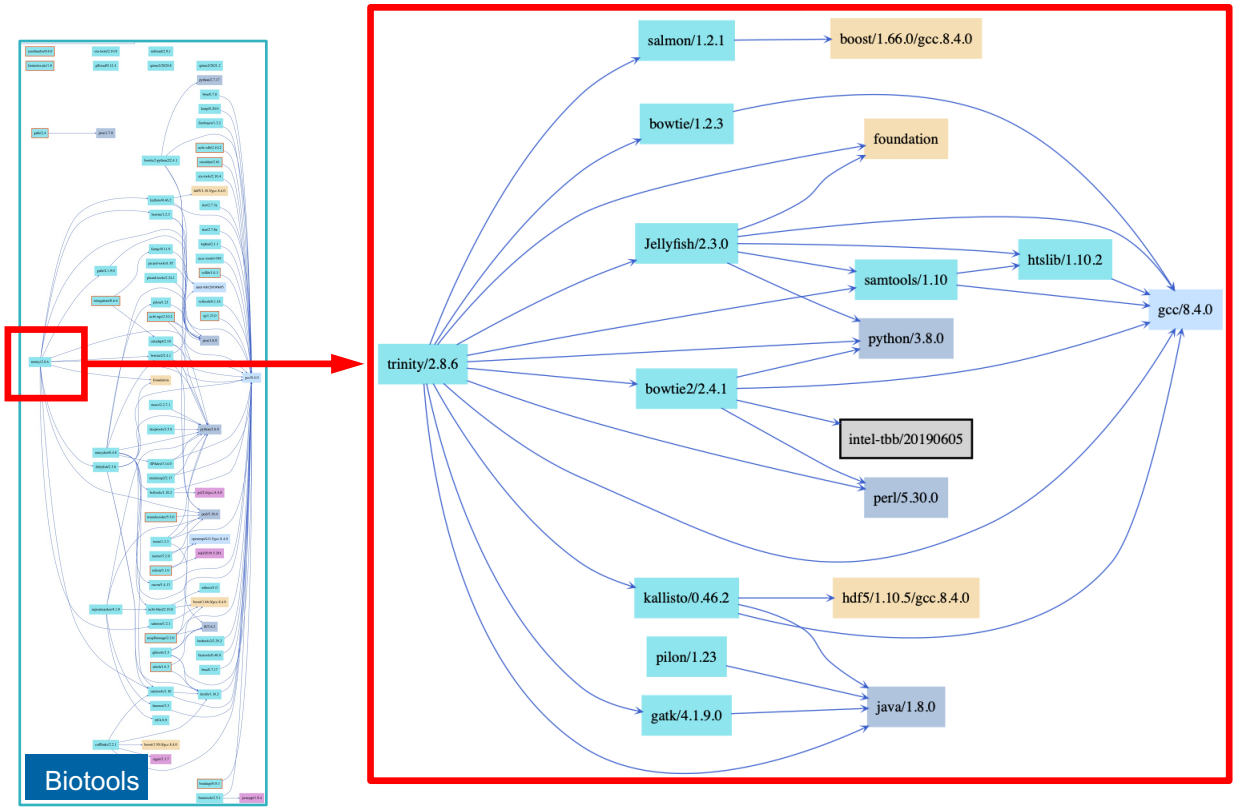








Software Map Detail



- Some apps have very deep dependencies
- Capture dependencies during the build
- Enable auto loading of dependencies
- User needs to load a single module:

module load trinity/2.8.6

Module Dependencies

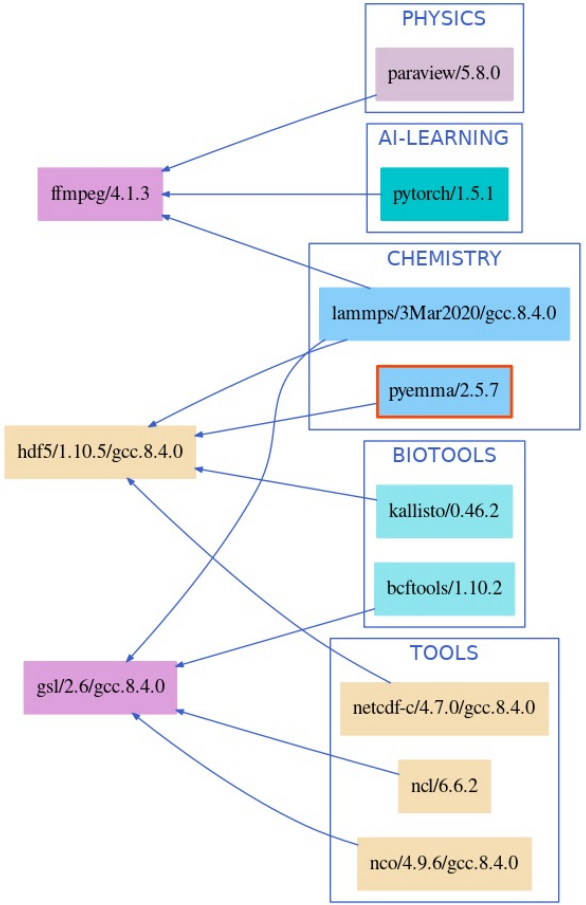
AI-LEARNING:	2
BIOTOOLS:	63
CHEMISTRY:	21
COMPILERS:	20
ENGINEERING:	7
GENOMICS:	40
IMAGING:	9
LANGUAGES:	22
LIBRARIES:	24
PHYSICS:	6
STATISTICS:	1
TOOLS:	42

Most used modules since Jan 1, 2021

python/3.8.0	701,106
gcc/8.4.0	408,170

Updating a single package

Can affect many others, how?
Which ones ?



What we do to install software

Building

Find and download

Build
- create a patch
- prerequisites

Software request

Create package yaml file

Build package RPM (and filter)

Create module yaml file

Build module RPM

Install RPMs

Record build in git

Add source to google drive

Verification

Download from git

Build RPMs and apply fixes

Install RPMs locally

Production

Copy RPMS to HPC3

Update HPC3 nodes using ansible system

Taking advantage of system automation

Goals:

- Automation yaml2rpm
- Reproducibility
- Coherency

Modules Usage (since Jan 1)

Modules:

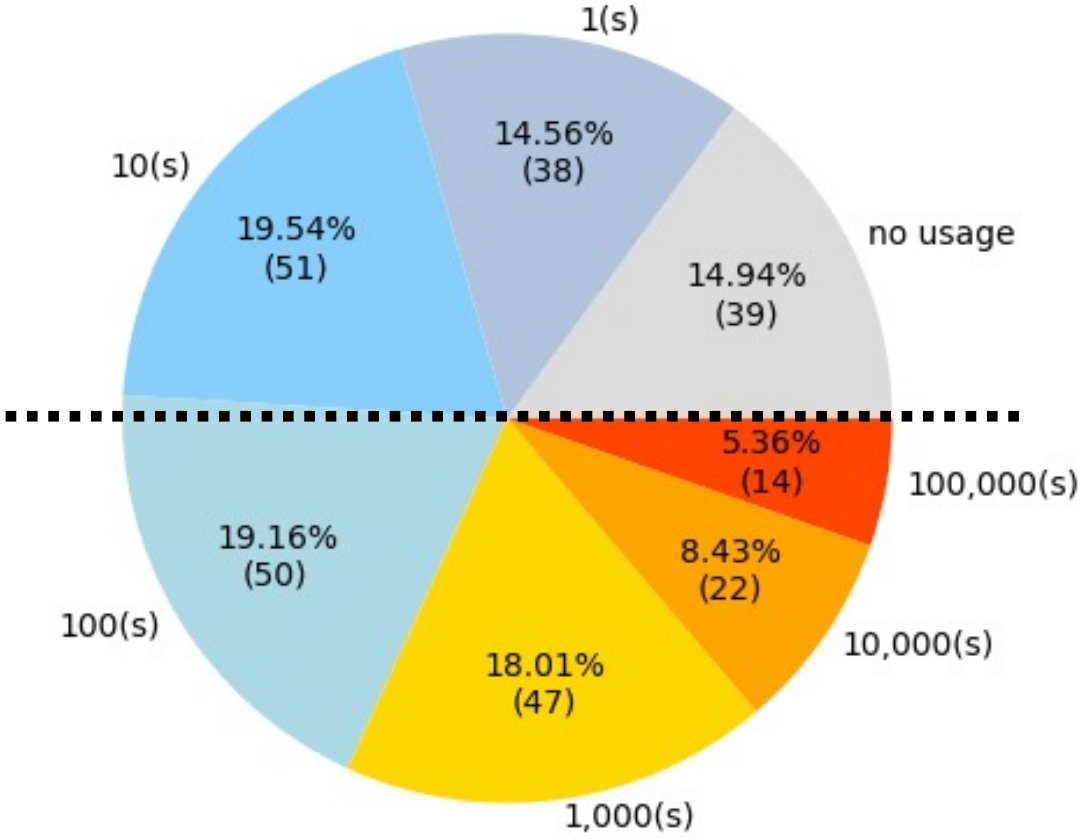
- 261 built
- 39 unused
- 6 user-authored

RPMs:

- ~1700 built and installed

Summary of tracking:

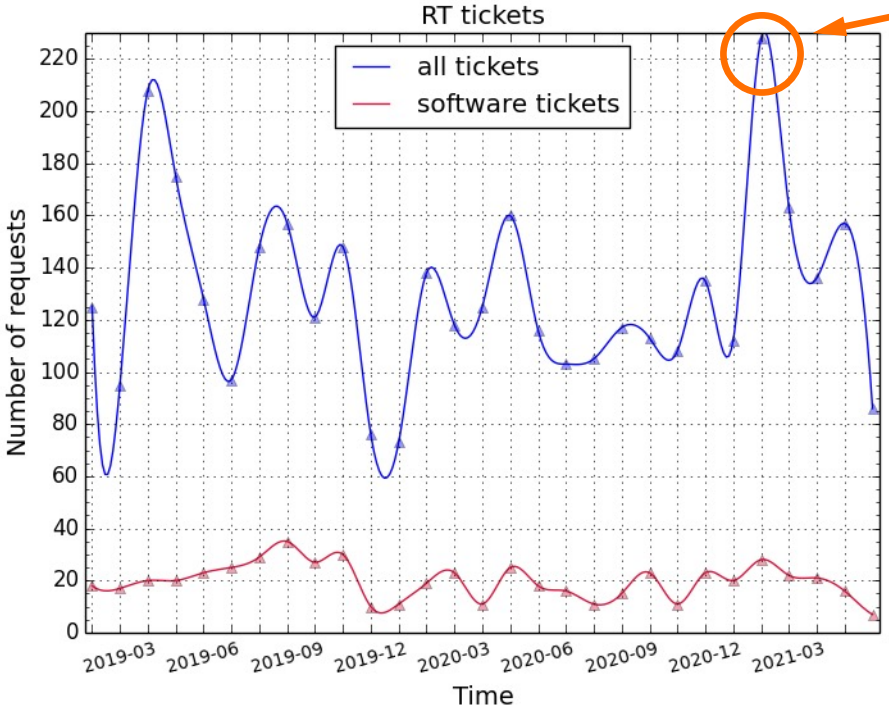
1. All software was requested
2. Fair fraction (~ 49%) is rarely or never (15%) used
3. Helps to answer the question *"When to install, update, or sunset the software"*

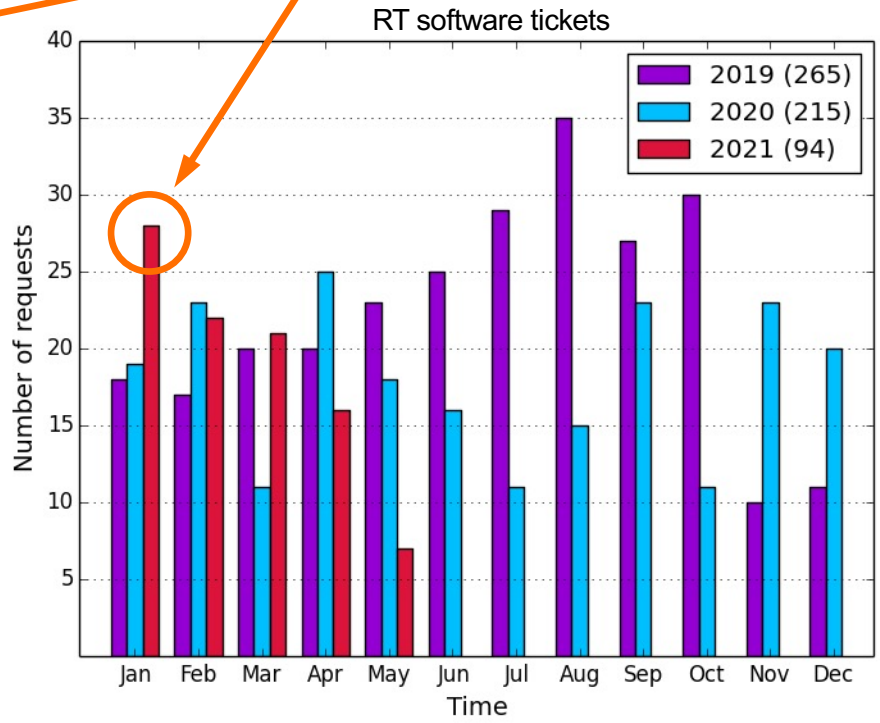


Request Tracker (RT) History

Start: 2019-01-01
End: 2021-05-31

move to HPC3

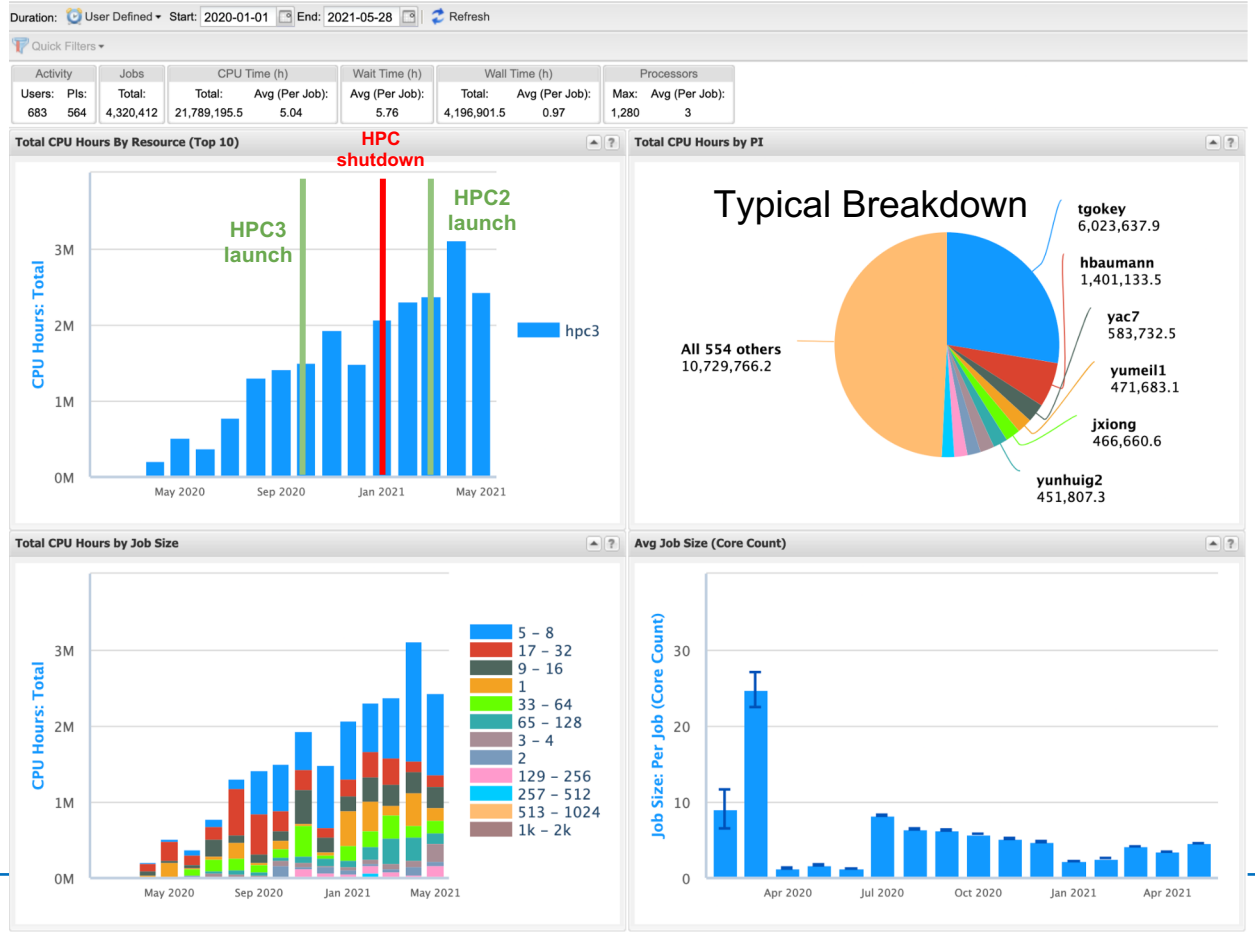




Configuration automation (Ansible) + Applications → fewer issues (and usage has increased)

How has HPC3 been used since Jan 1, 2021

CPU Use Summary: Up Trend



2/1/2020 to 5/28/2021:

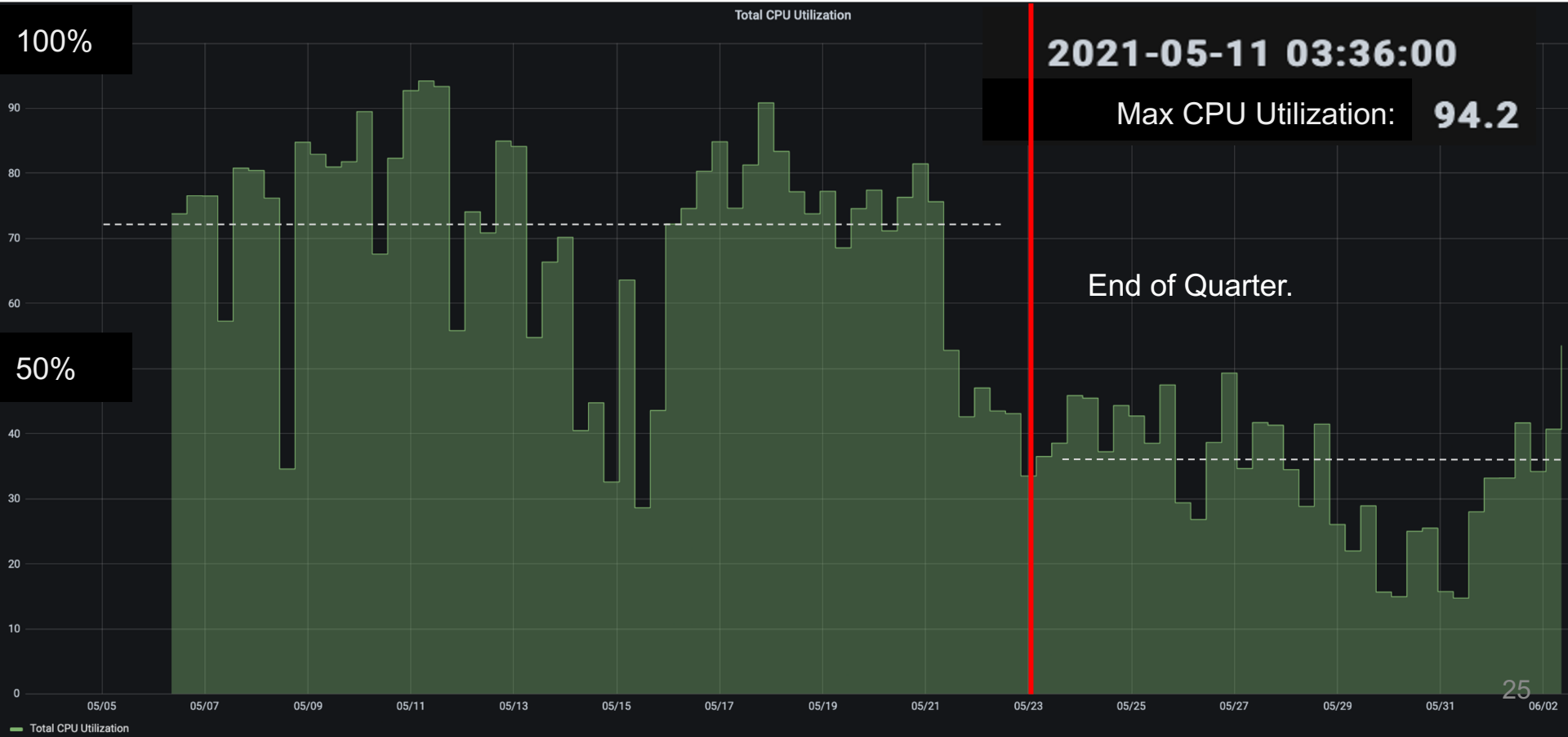
~ 500 active users
~ 1% [power] users

Total core count:
~ 4000 cores 2/2020)
~ 7000 cores 6/2021)
~ 9000 cores 9/2021)
! 16000 cores 1/2025)

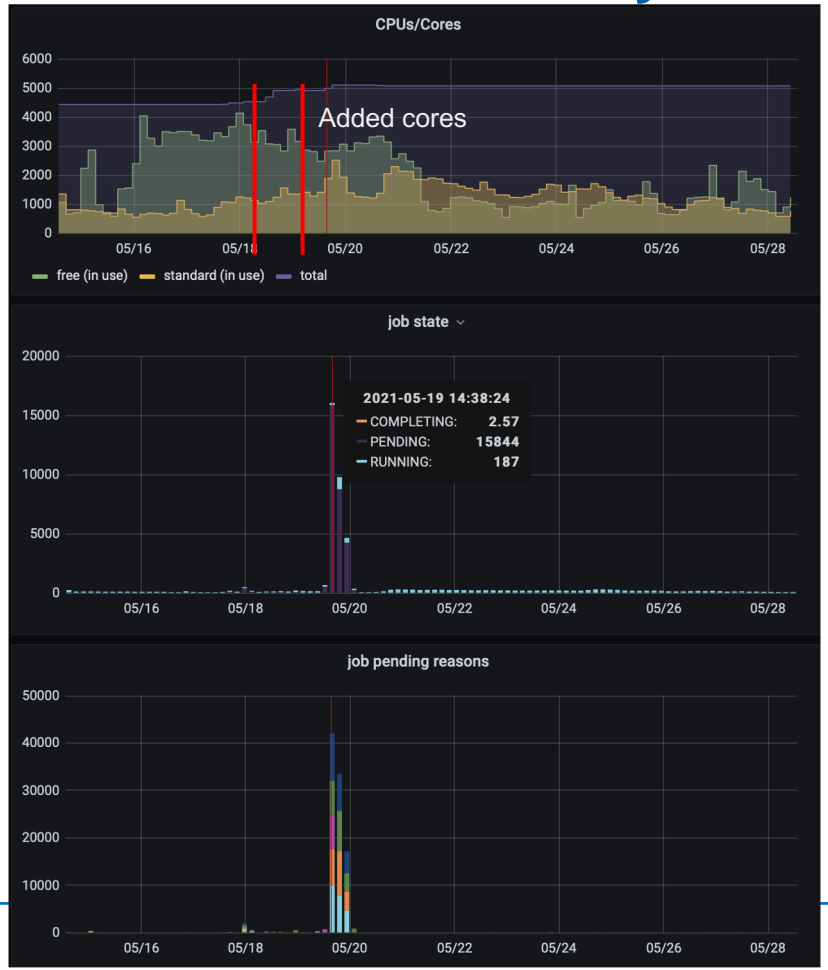
~ 22M CPU hours delivered
~ 5 cores per job on average
- 1280 cores largest jobs

70% average CPU utilization

HPC3 CPU Utilization



Standard Partition Jobs Summary



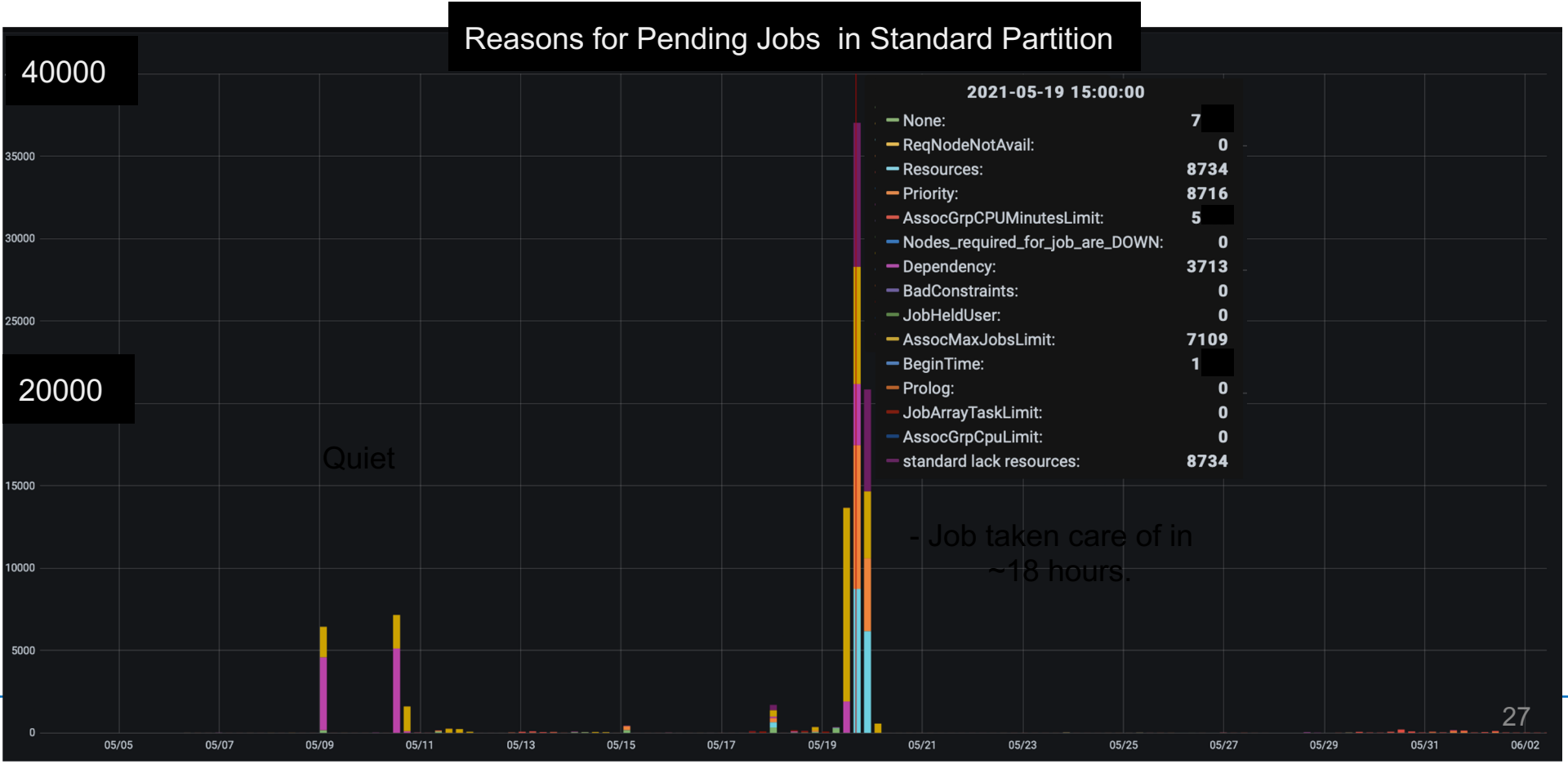
- Partition (queue) has ~5500 cores.
- Standard partition dominates by day
  - Free partition by night and weekend
- ~ 40% of jobs go through standard partition
  - Users not spending their allocations

Waiting for a job a Standard job to run is rare:

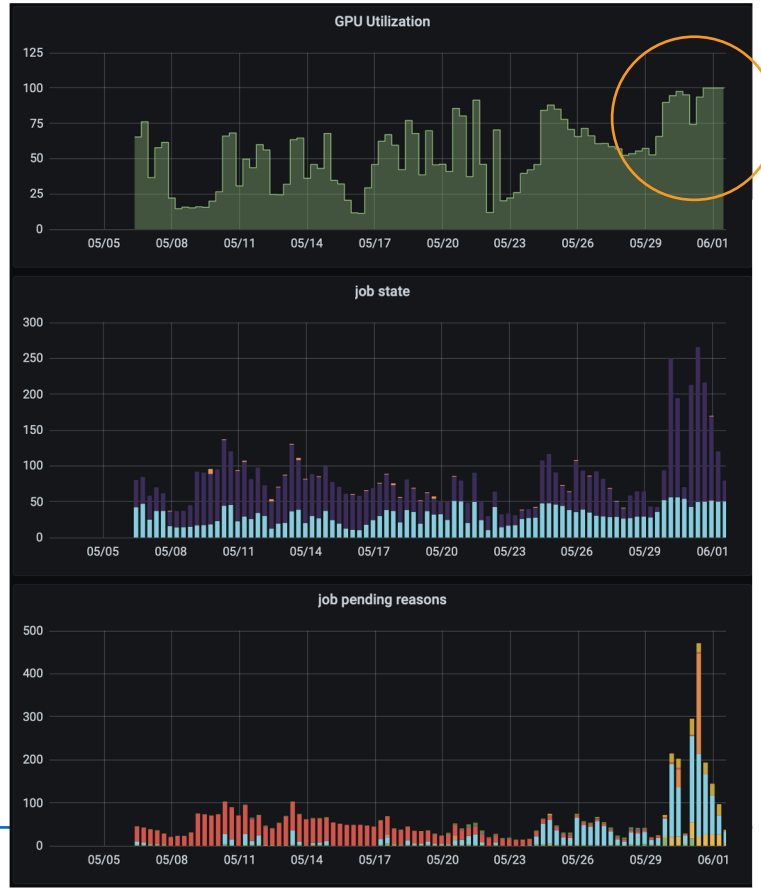
Example: Standard Pending Jobs on 5/19/21 ~ 14:35pm
~ 16,000 cores requested

Reason for pending job? See next slide...

Standard Jobs Wait Time: Minimal



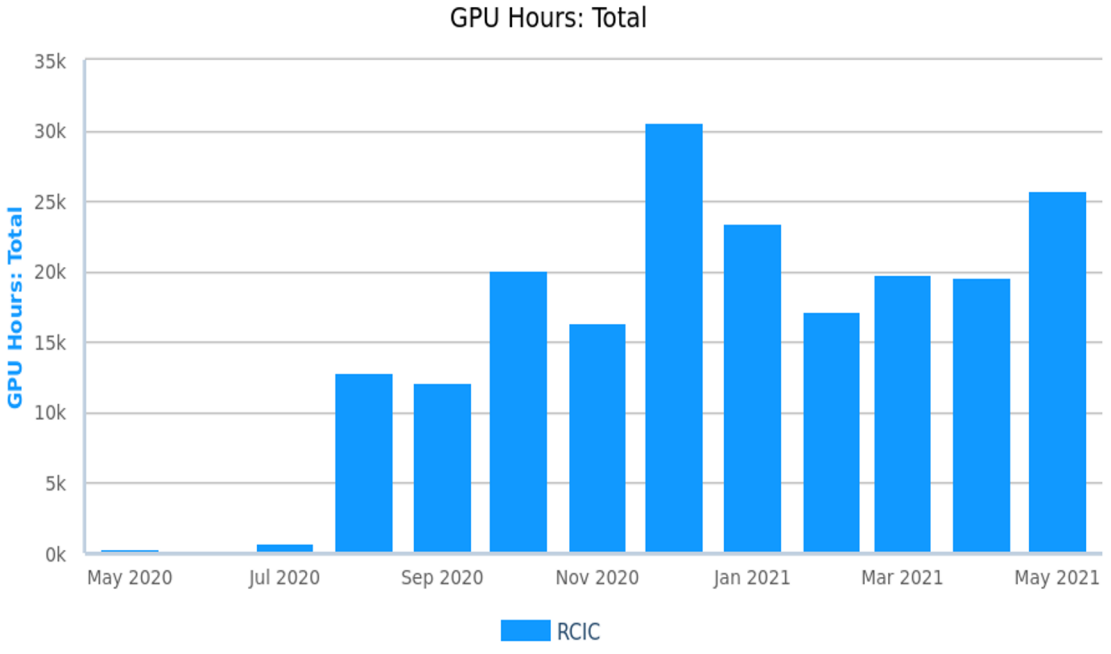
GPUs Summary



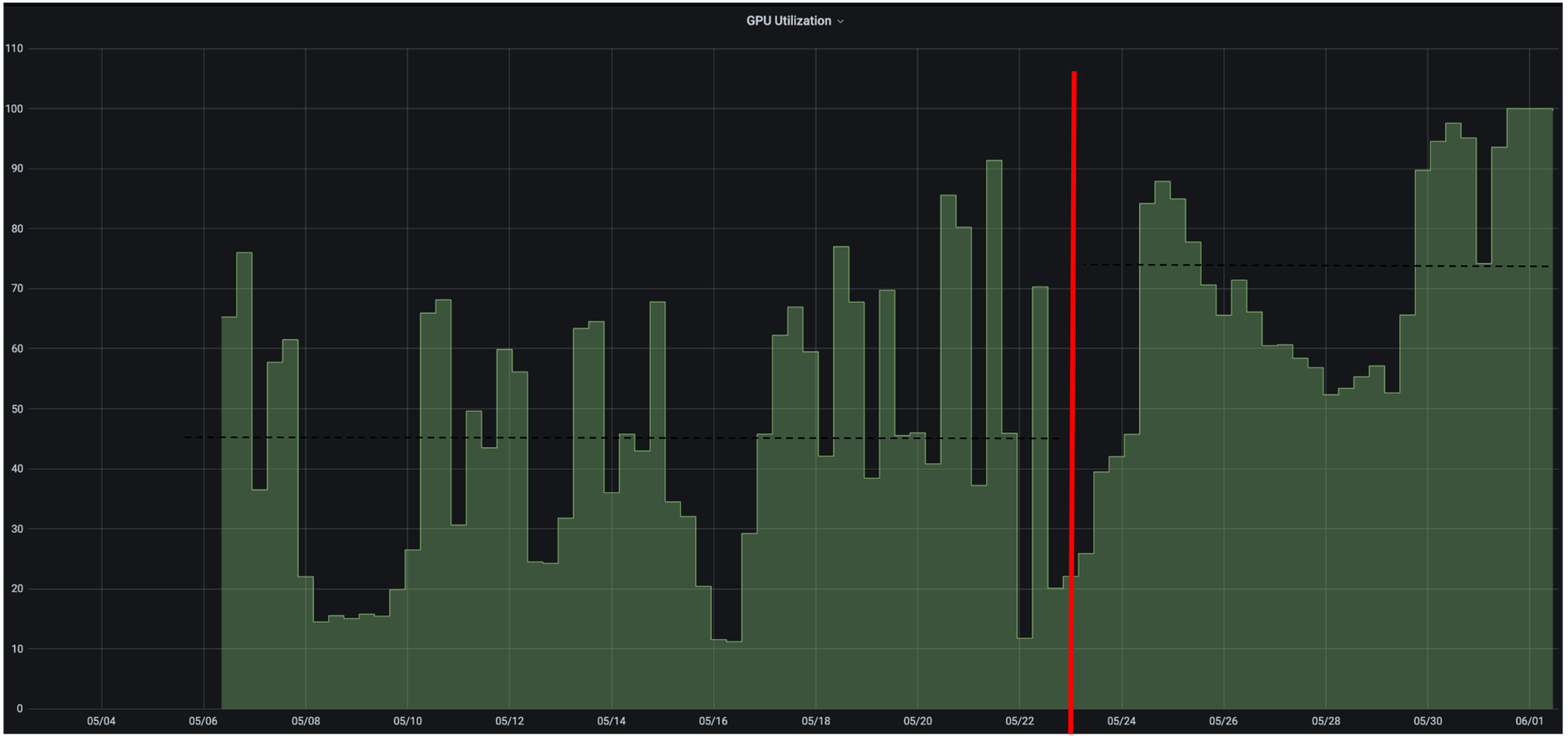
~ 14 nodes = 56 GPUs (V100)
~ 170,000 total gpu hours
~20k/month
~ 65% avg gpu utilization

- Increasing as people learn how to use them
- There is a longer wait for GPUs than CPUs

=> Need more GPUs

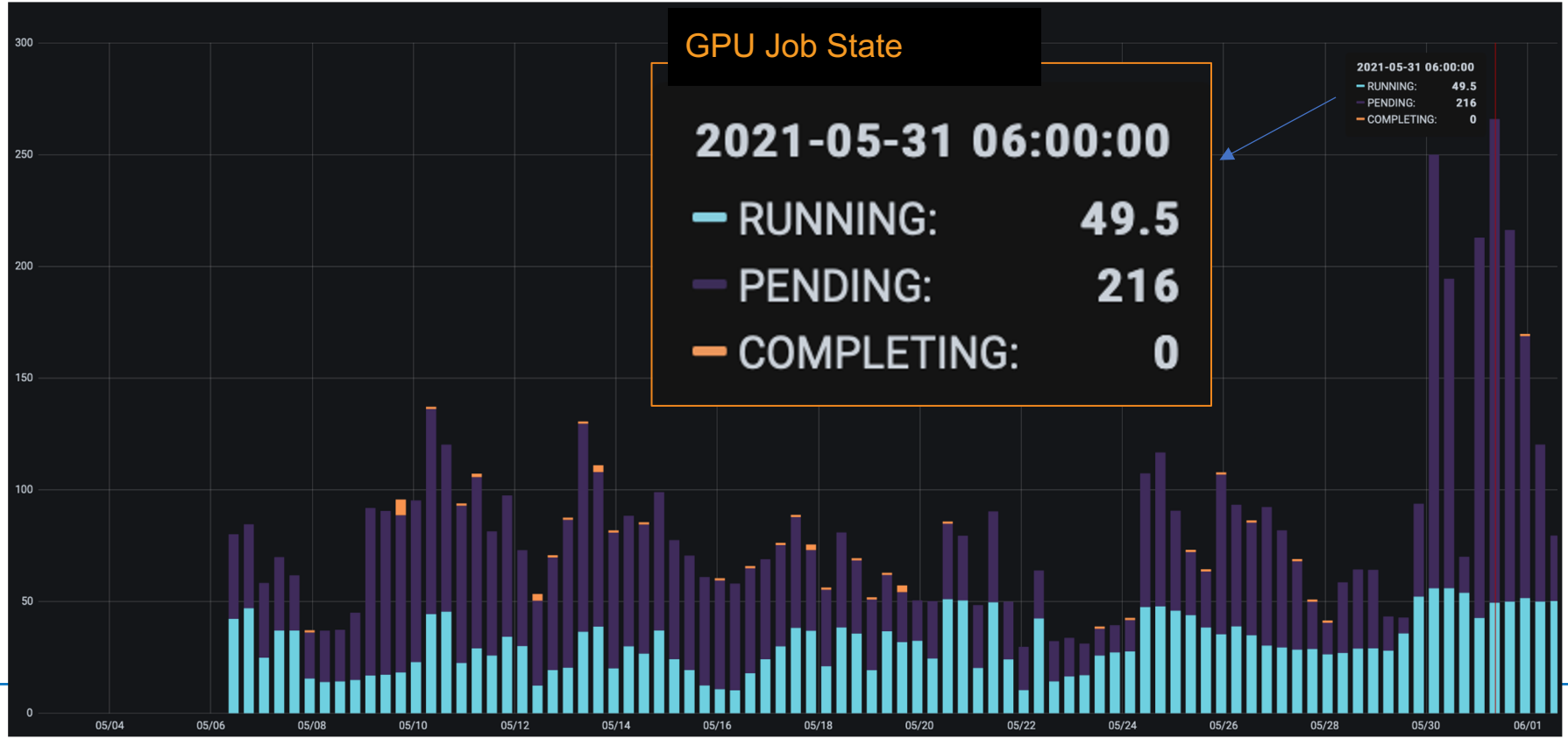


GPU Partition Utilization - Detail

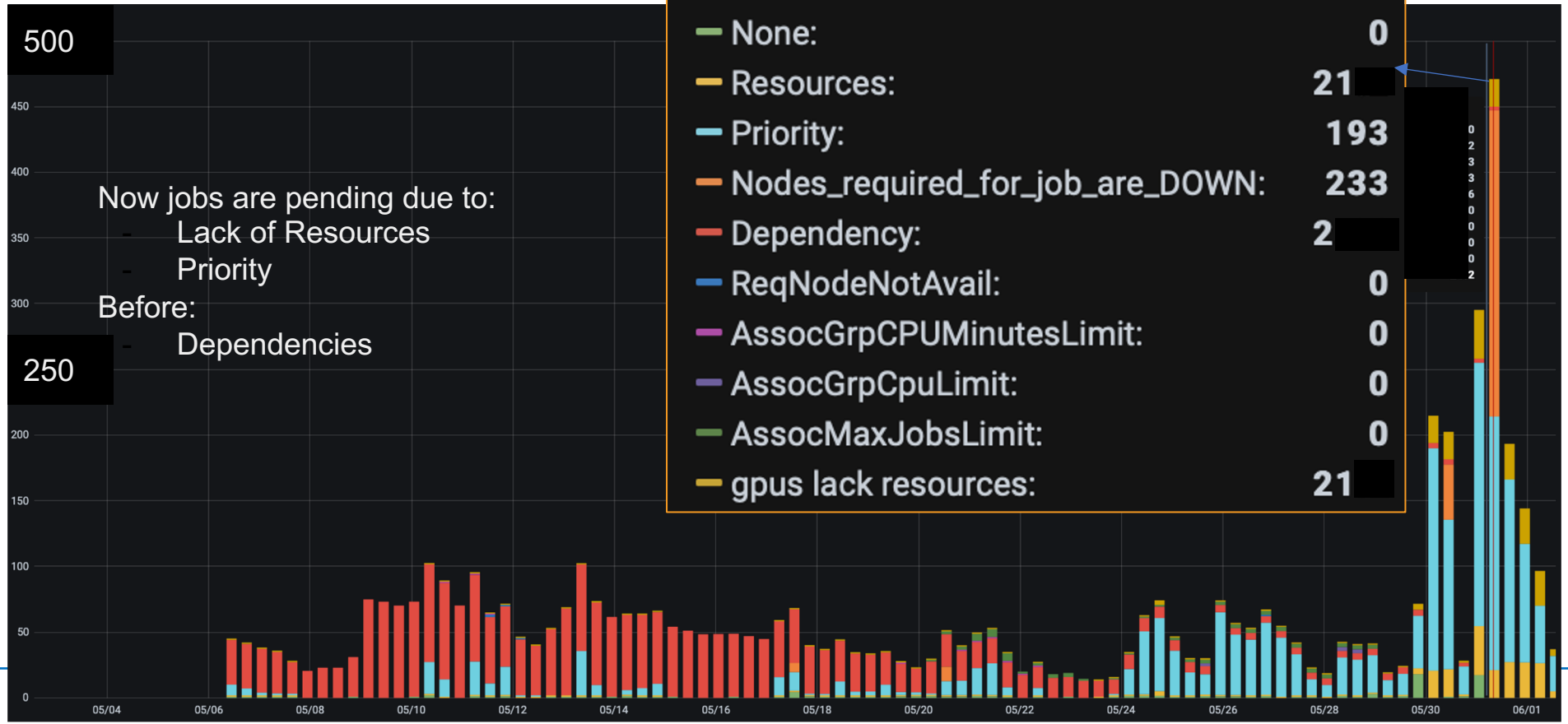


GPU Partition Job State

Different from Standard Partition: there are Always Pending Jobs



Reasons for Pending Jobs in GPU Partition



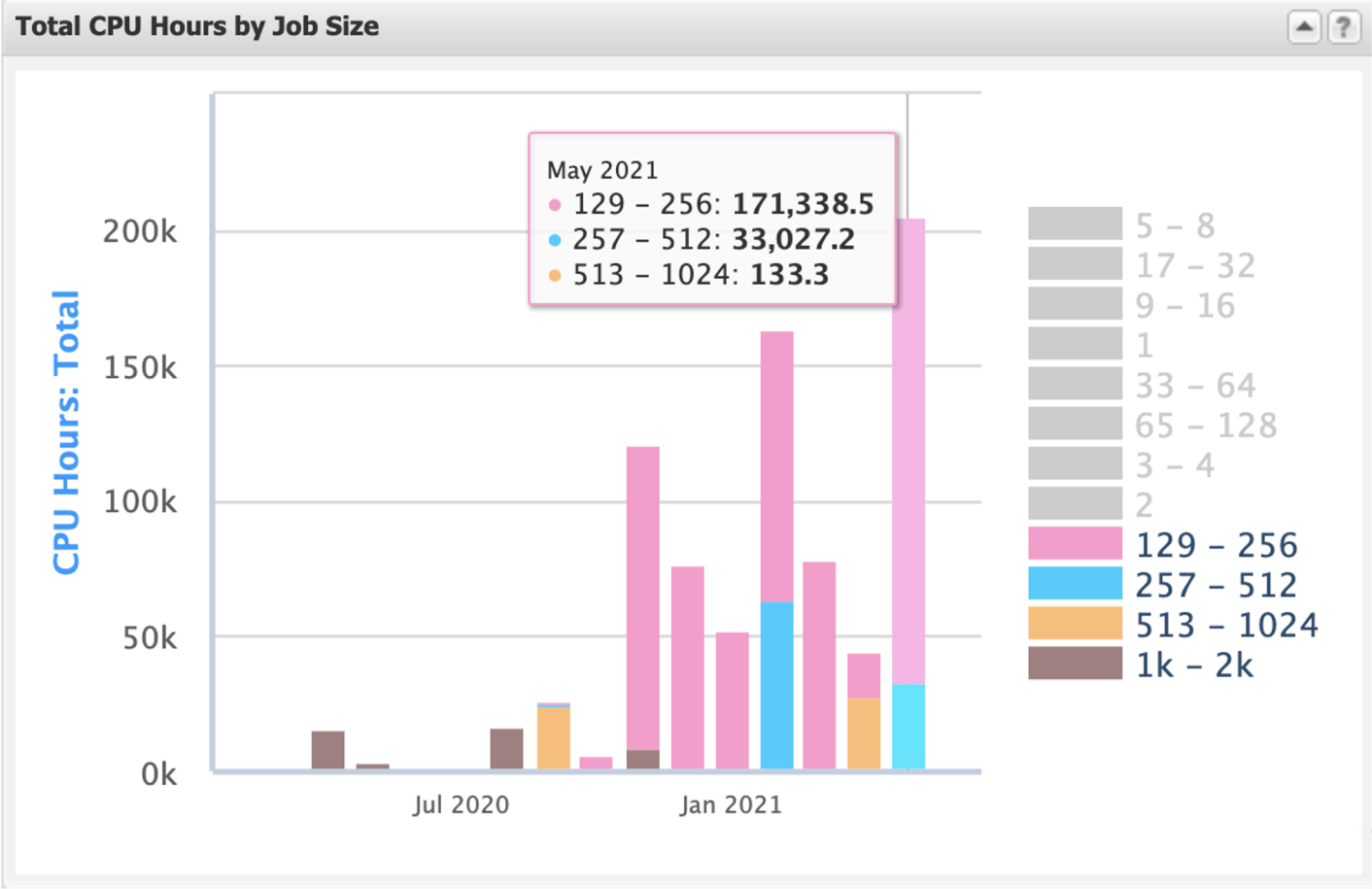
Now jobs are pending due to:

- Lack of Resources
- Priority

Before:

- Dependencies

Large Multi-node Jobs: No special provisions needed to run



10^3 range in core requests

- Avg. Job size: 5 cores
- Max Job size: 1280 cores

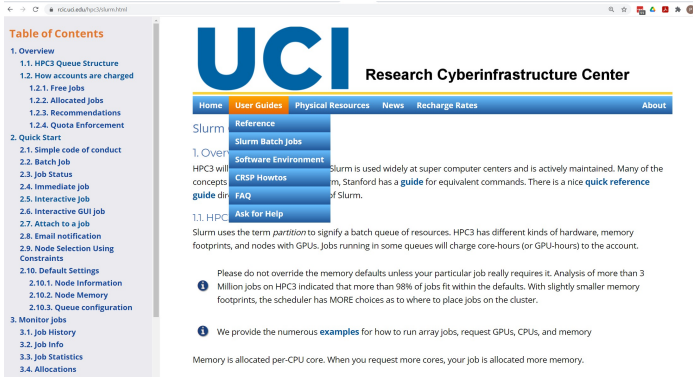
Large Jobs [129, 1280] cores

- Use ~3% of CPU time
- Reasonable wait time

Talking to RCIC and to Each Other

- **How do I ask for help/talk to RCIC?**
  - Send email to hpc-support@uci.edu

    This automatically creates a help ticket
  - Read that fine website: https://rcic.uci.edu



- **What about talking to RCIC and the other users at UCI?**
  - Join the new! Google group

    https://groups.google.com/a/uci.edu/g/rcic-users
  - Chat with us on Slack: https://rcicos.slack.com/

Resources

- Github repositories for the software builds
  https://github.com/RCIC-UCI-Public
- RCIC website https://rcic.uci.edu