Biowulf

A High Performance Computing (HPC) Resource for the IRP

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Wolfgang Resch, Support scientist

Accelerate biomedical research at the NIH by providing convenient access to large scale **computational resources** and **scientific software** (and the **know-how** to use them).

Computational resources: The Biowulf system

~100k cores / **~200k CPUs**

~900 TB memory

~50 PB shared high performance storage

5 PB of object storage

~900 GPUs (K80 - A100)

high speed / low latency networks

+12k CPUs

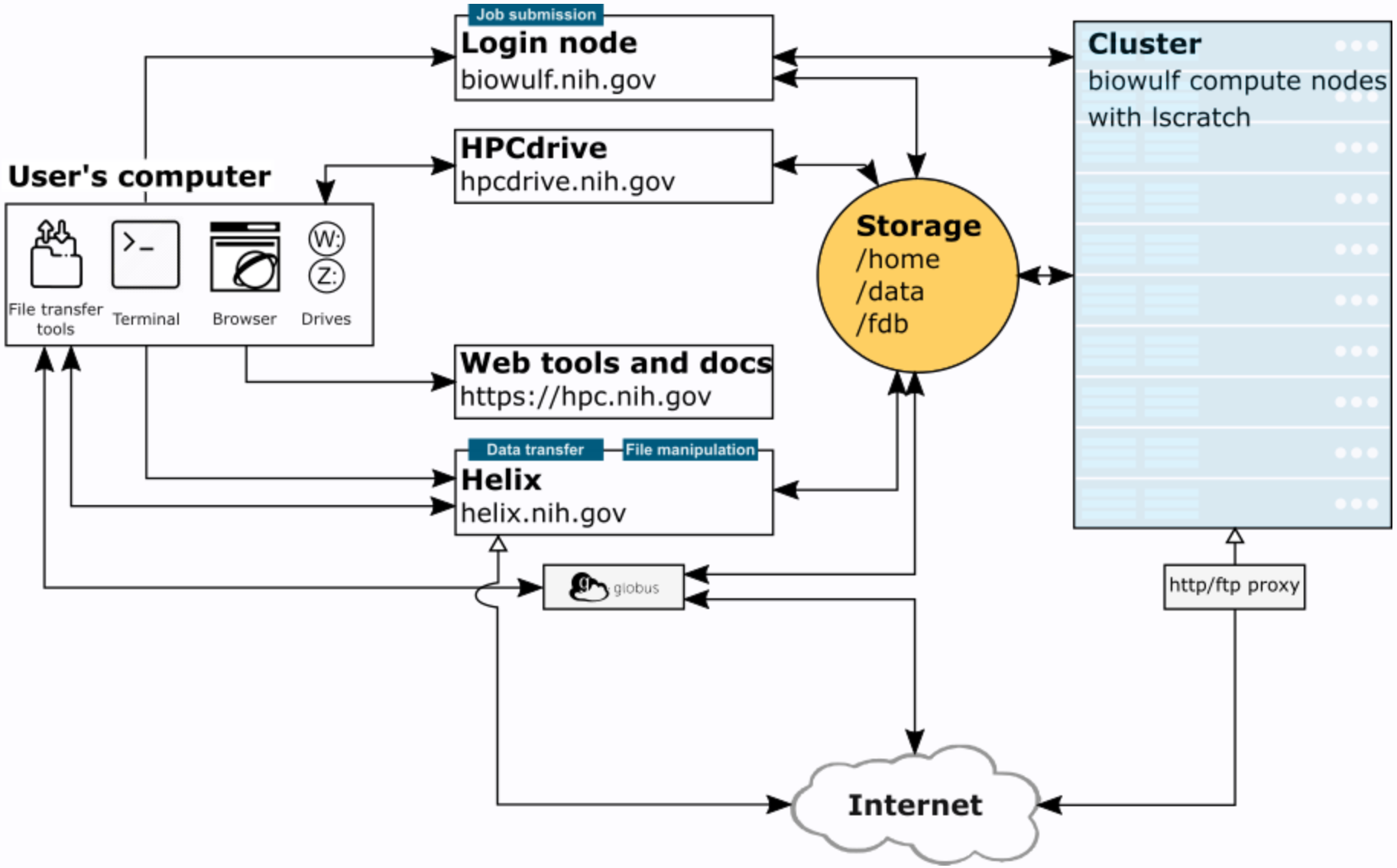
+ 160 A100s

+ 16 3TB largemem nodes

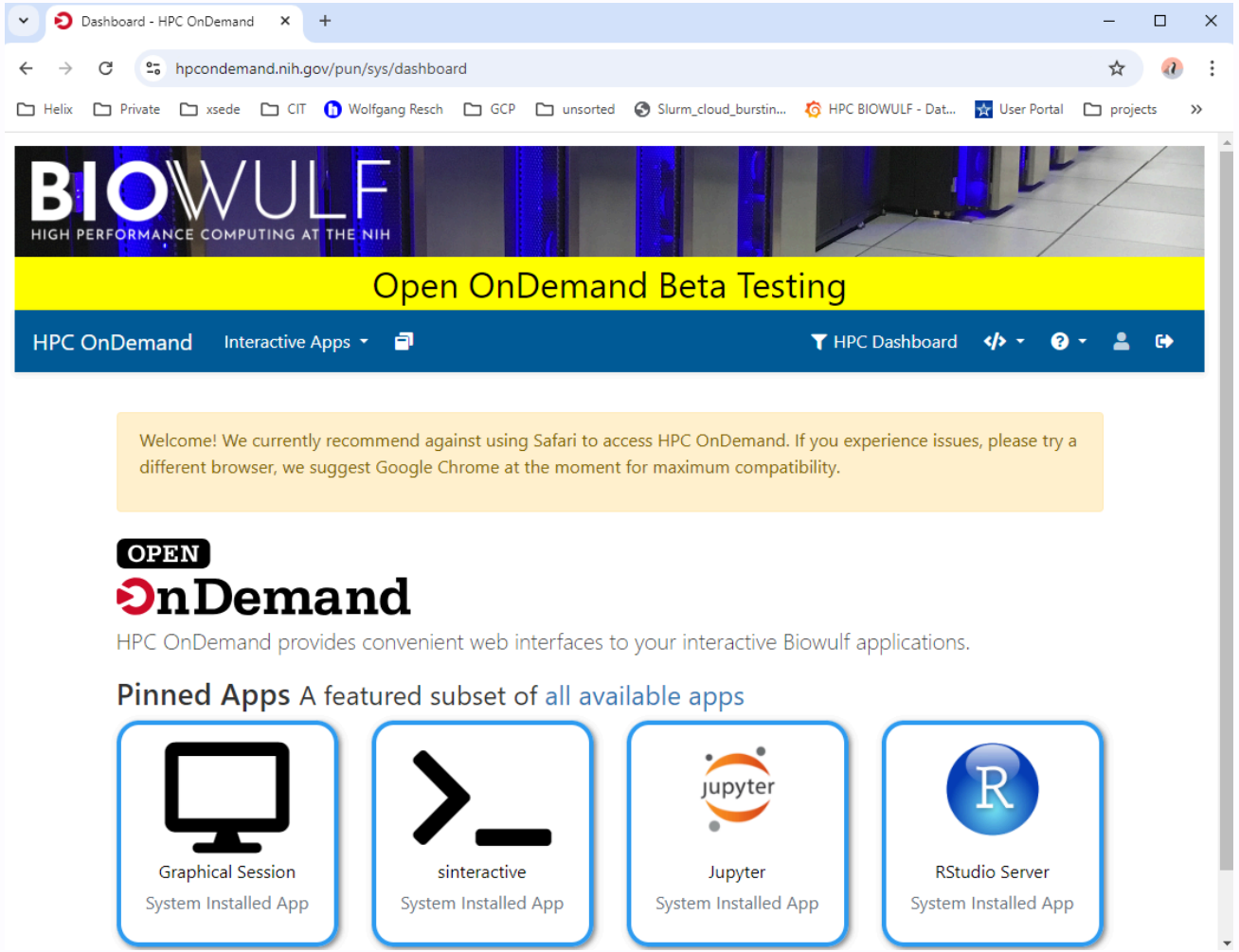
Node classes

- Single node, CPU (56-128 CPUs, 240-500GB)
- Multinode, CPU (56 CPUs, 240GB)
- GPU (K80, P100, V100, A100)
- large memory (1.5-3TB)
- visualization
- buy in nodes

Architecture



Open OnDemand beta testing



https://hpcondemand.nih.gov

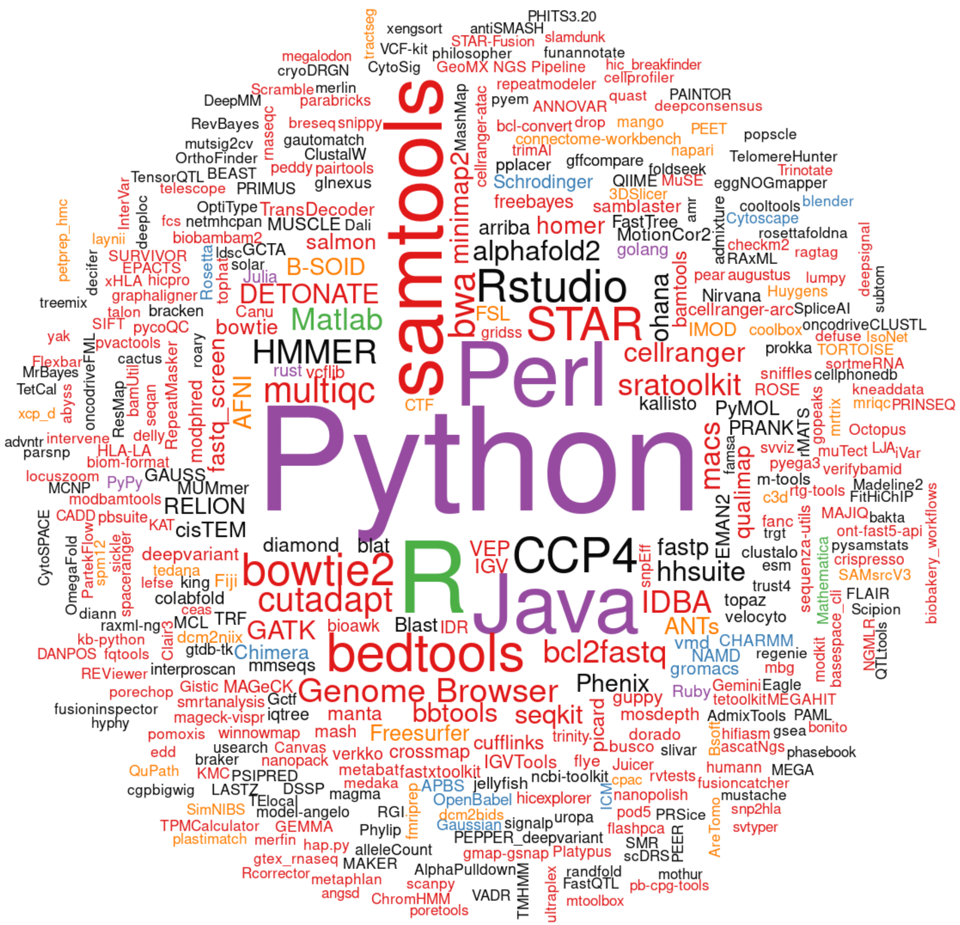
In 2023 **~2400** active users from **~75%** of intramural research groups used **1.1B** CPUh, **4.8M** GPUh and **30PB** of storage

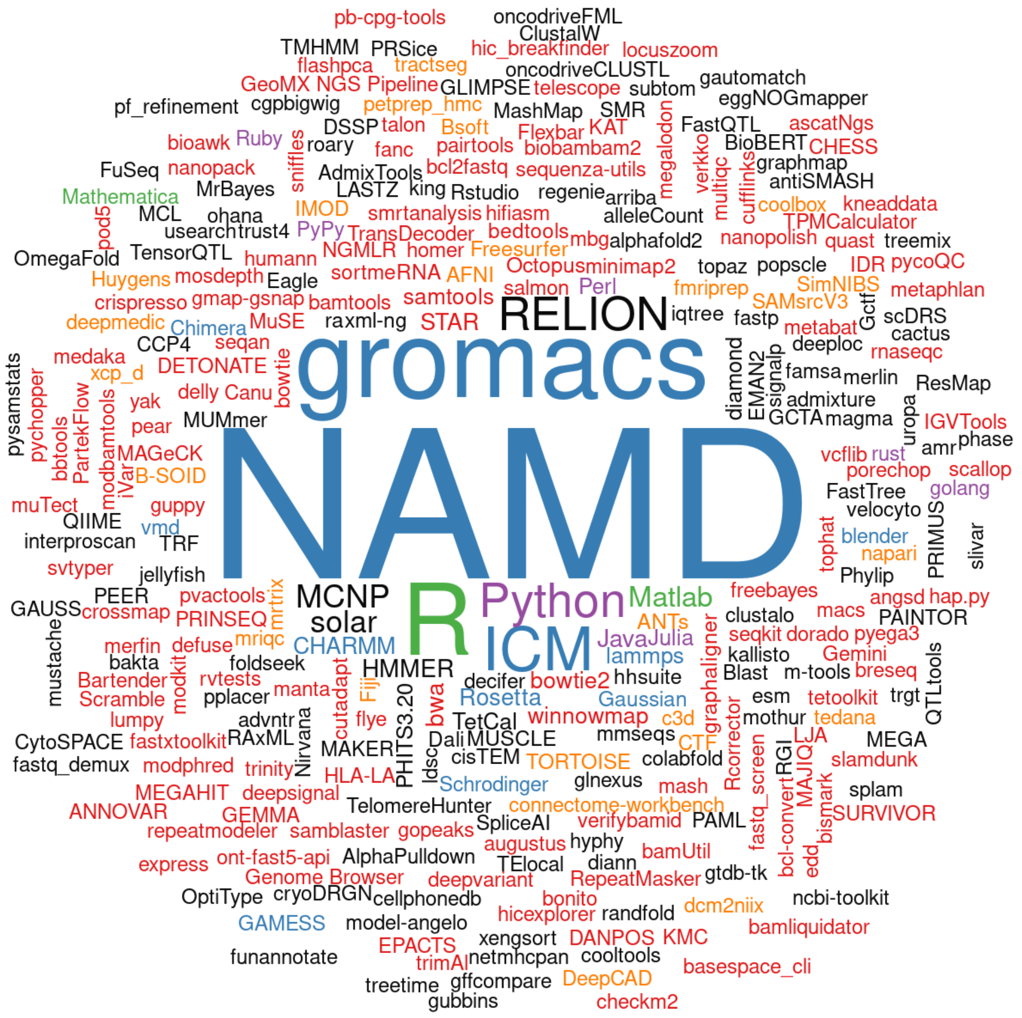
Scientifc Software

Applications

- multiple versions for ~1000 applications available
- Multiple versions of python with ~500 packages each
- Multiple versions of R with about 1600 packages each
- singularity for containerization
- jupyter, rstudio, vscode, desktop sessions

Application usage





Know how - training and outreach

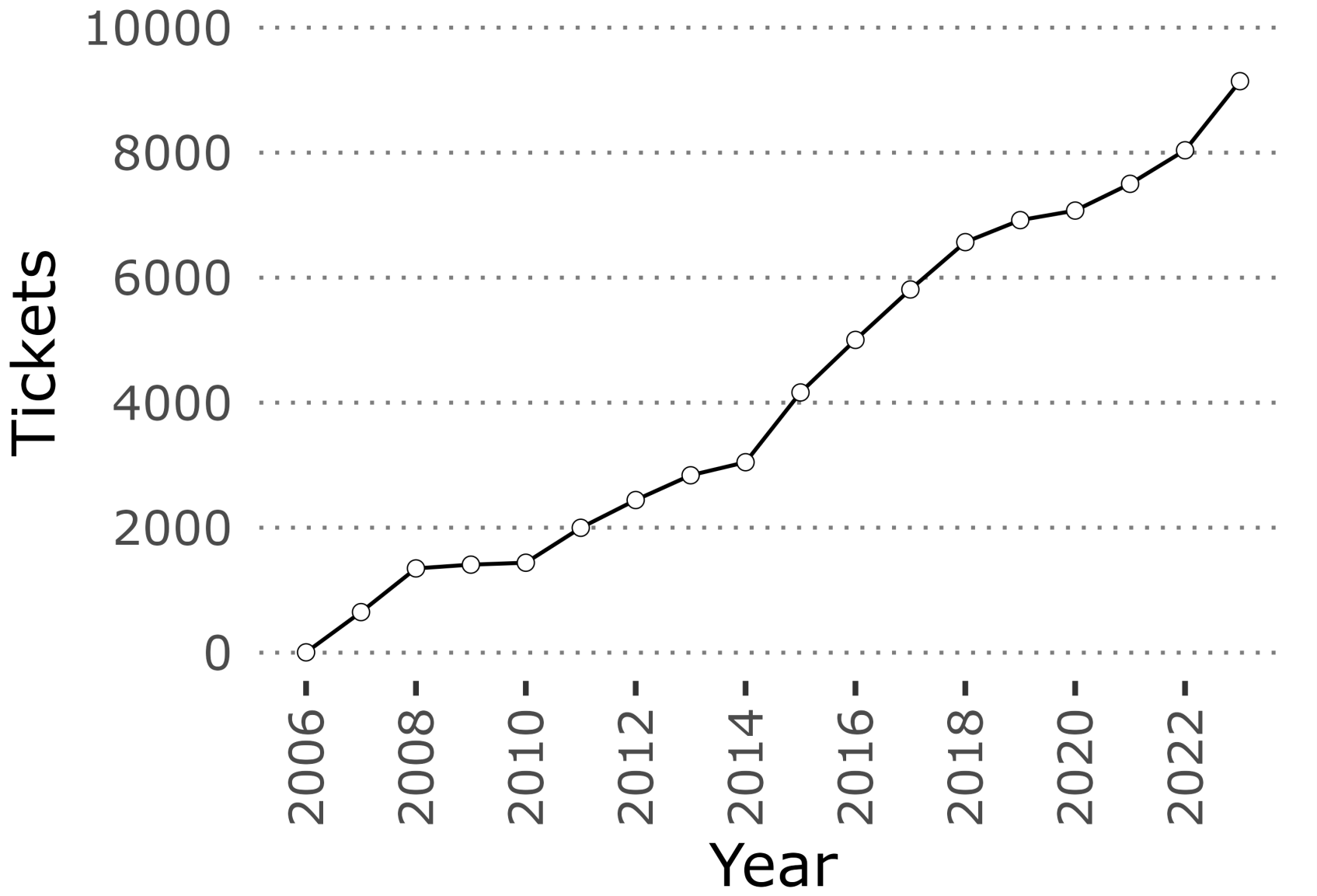
Training

- Online, self-paced clases (intro to biowulf, bash)
- Live/recorded class sessions (e.g. Deep learning by example, R, matlab, snakemake)
- Documentation (https://hpc.nih.gov) and tutorials (e.g. https://hpc.nih.gov/training/gatk_tutorial)
- *Assist in other groups' training*
- Student accounts

Outreach

- Monthly *Zoom-in* consult
- Meeting with individual groups or 1:1
- Cranky email from staff if/when you break something
- Let us know if you'd like somebody to attend lab/branch/group meeting

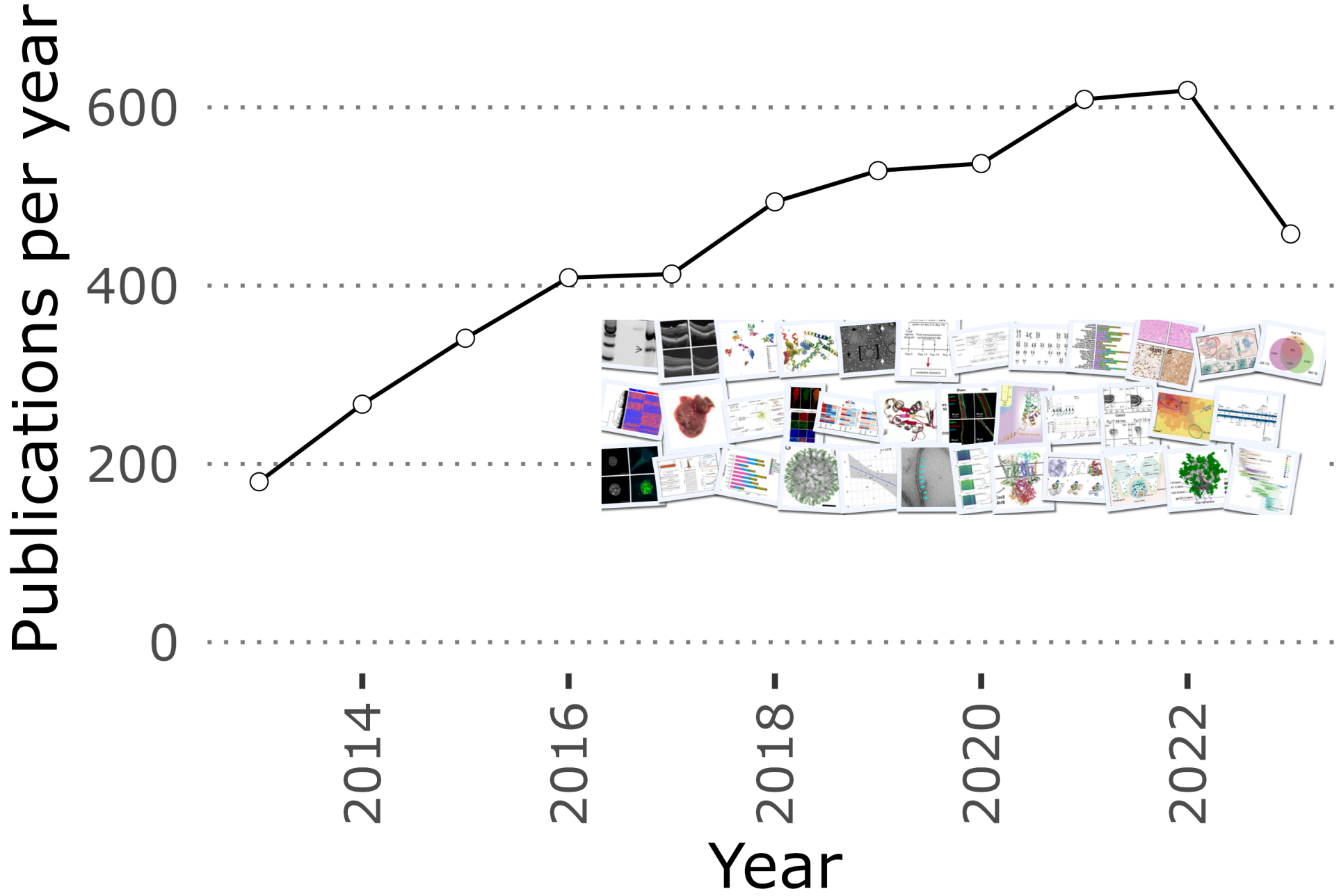
Support - staff@hpc.nih.gov



https://hpc.nih.gov/docs/accounts.html

Flat fee of $40 / user / month

Accelerate research


Publications per year
600
400
200
0
2014
2016
2018
2020
2022
Year

- Acknowledge
- Check the box in NIDB
- Let us know directly

Staff - staff@hpc.nih.gov


Steve Bailey


Tim Miller


David Hoover, Ph.D.


Helen Ashdown


Gennady Denisov, Ph.D.

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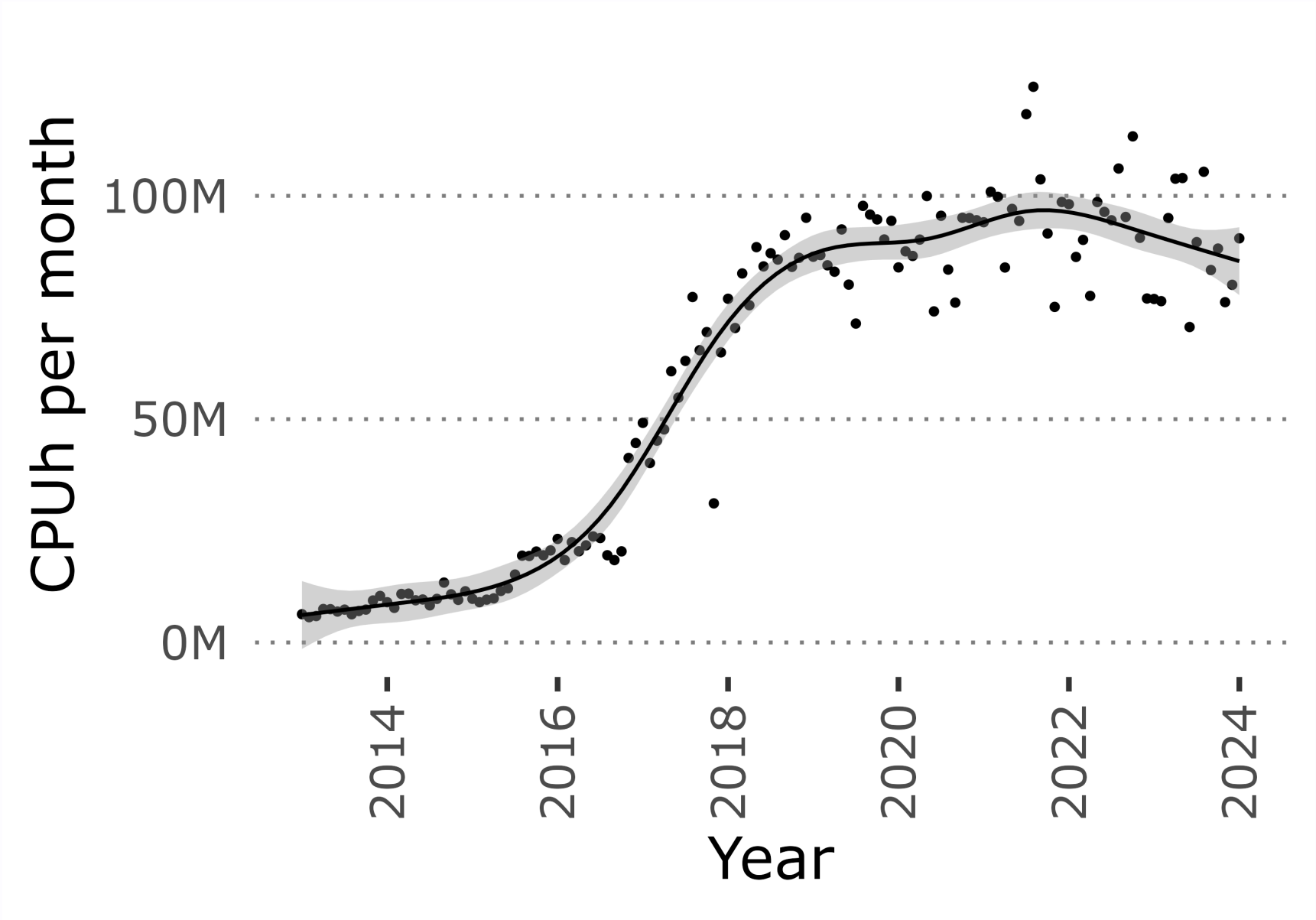
Renbin Yang, Ph.D.

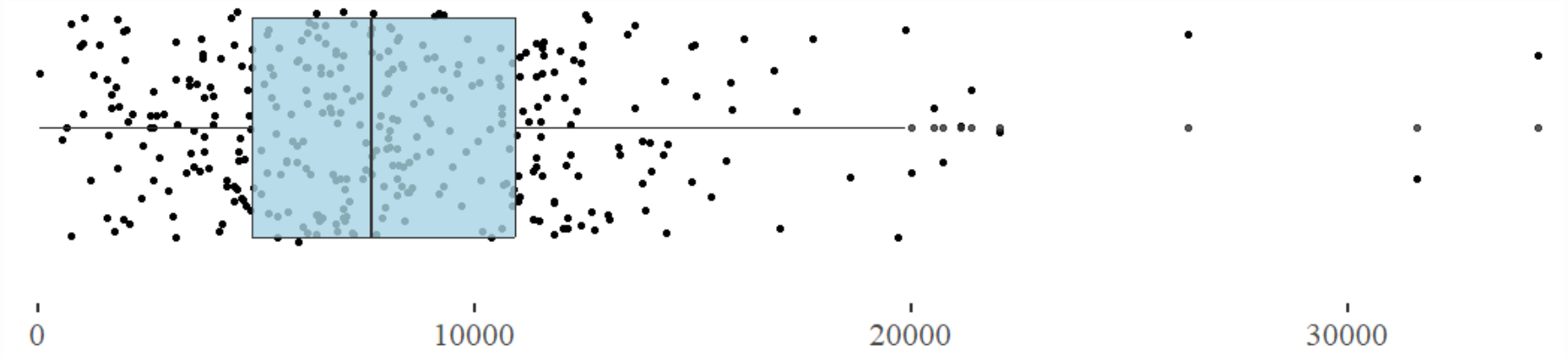

Qi Yu, Ph.D.

HPC@NIH in the future

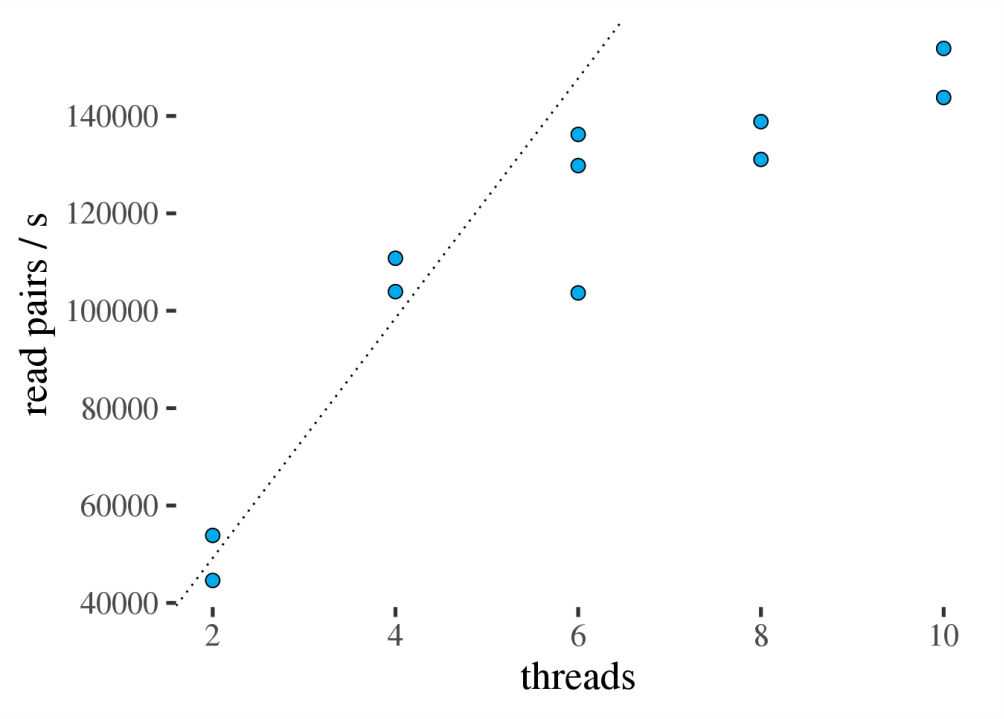

CPUh per month
100M
50M
0M
2014
2016
2018
2020
2022
2024
Year

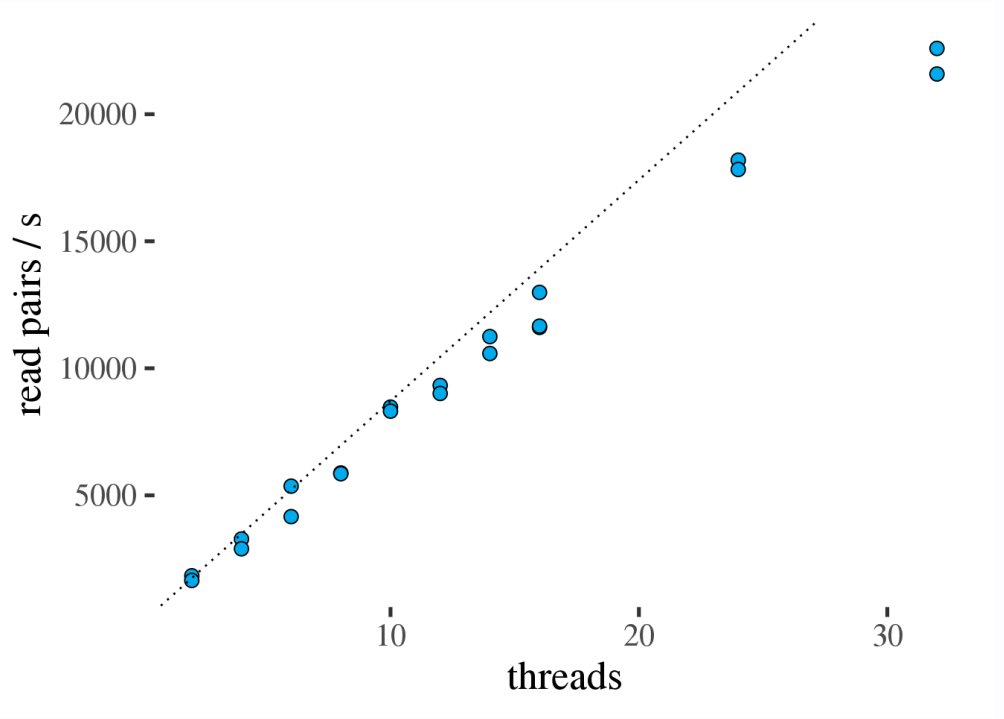
Best practices

Test before running large production jobs



Scaling matters





Left: fastp Right: bwa

Be nice to the **file systems**

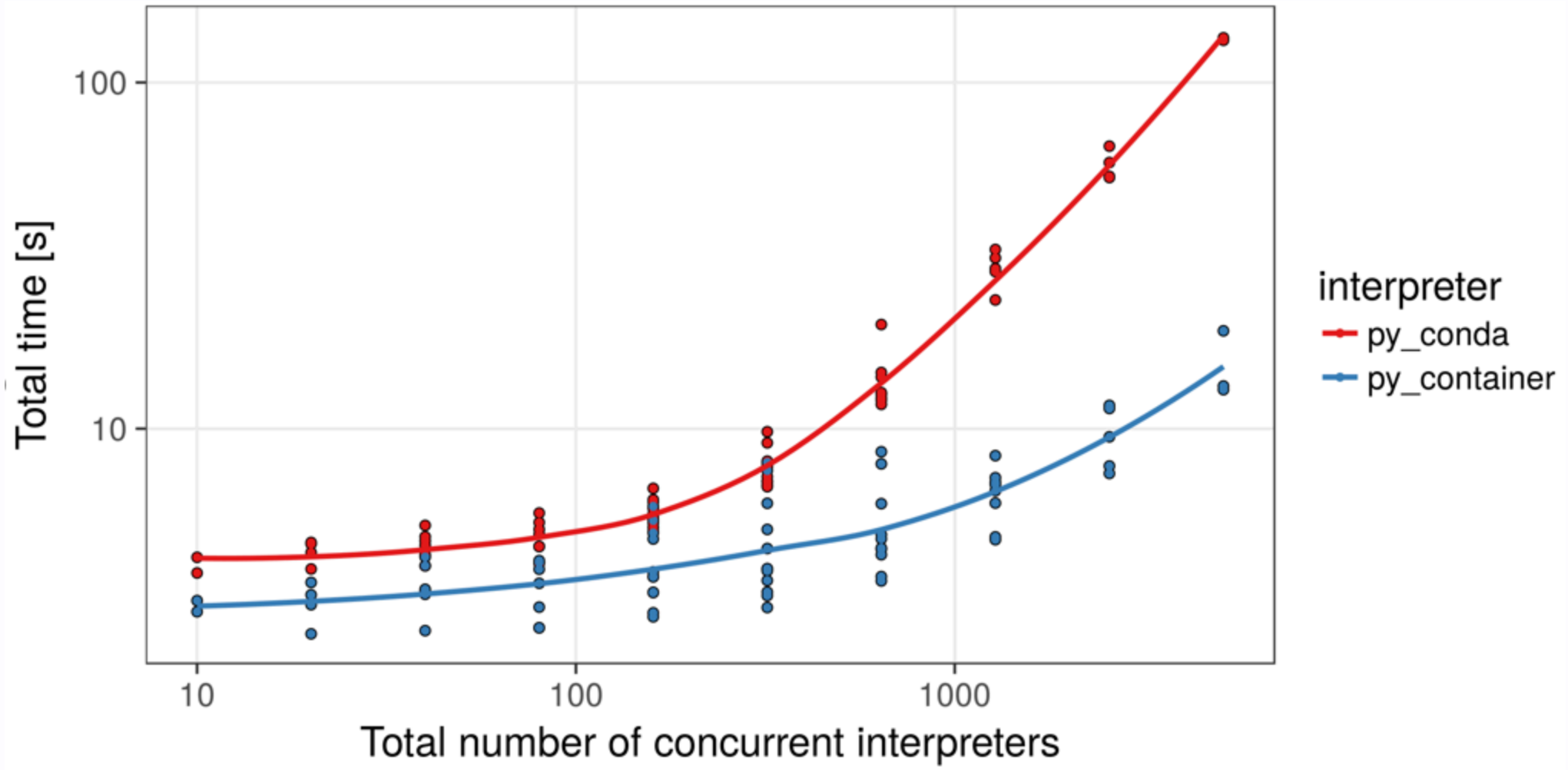
and use `/lscratch`

and pipes

Interpreter startup is

expensive

For example: concurrent python processes

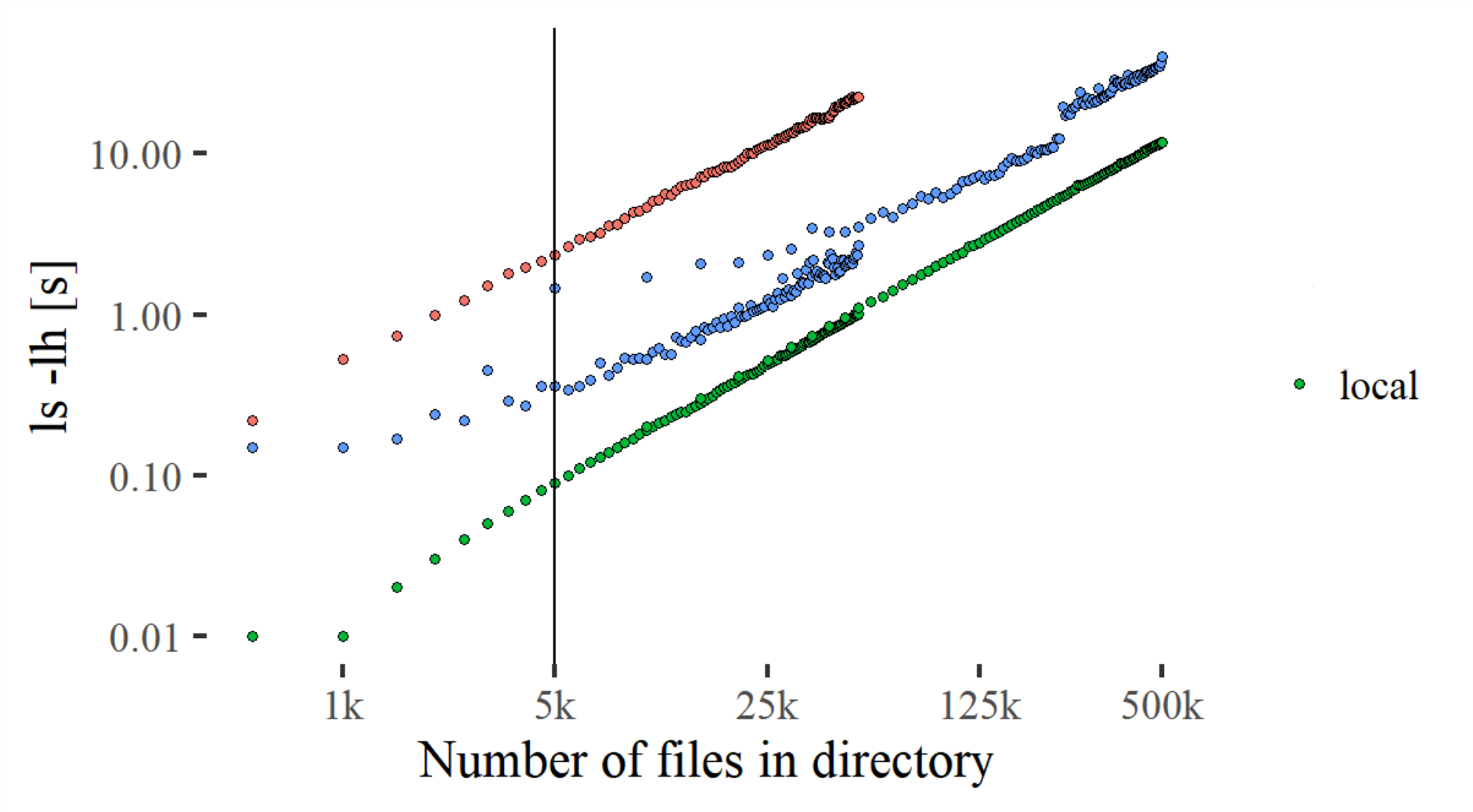


https://github.com/wresch/python_import_problem

Make sure you have **space** in /data for your jobs' output

Keep **< 5000 files** in a directory

listing files in large directories



and listing files is the least of the problems

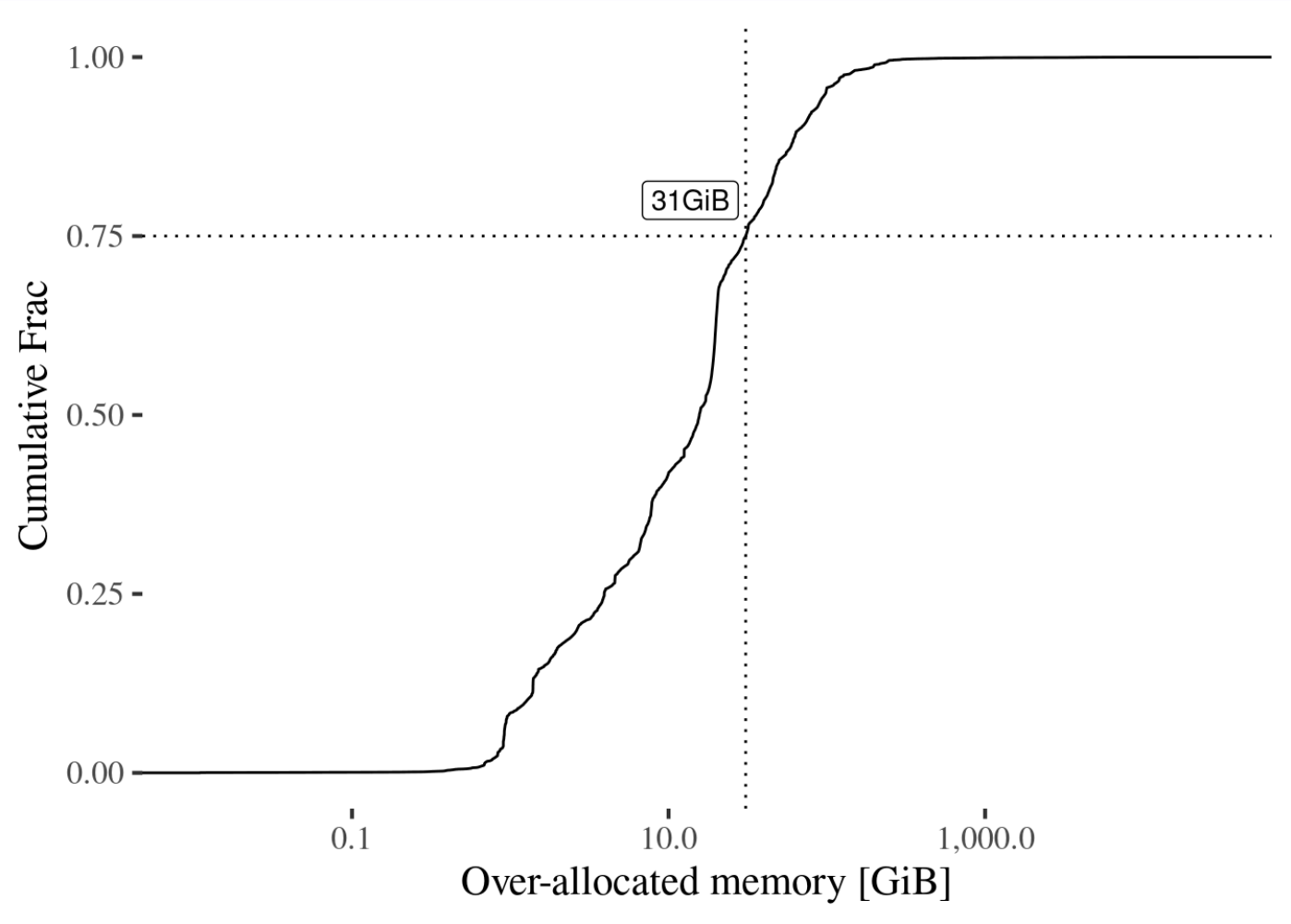
Biowulf storage is not for **archiving**(*)

(*) except the object store, kind of

Backup your data

Have **good resource estimates** for your jobs

Completed jobs in 2023



Don't **abuse** newwall

Use **job arrays / swarms**

when you can

Try to run jobs with

walltime > 15 min

Keep startup files **simple**

(no conda please)

Please **read your email**

Be **detailed** and **specific**
when you file an issue (and
use text
instead of screenshots)

Please **acknowledge biowulf** in your publications

Talk to us

`staff@hpc.nih.gov`