Using the IU Research Desktop for Interactive Supercomputing

Robert Henschel

Engagement Architect

Research Technologies

UITS

henschel@iu.edu

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My Goal For Today

Raise awareness of the Research Desktop as a way to access IU's HPC systems.

Inspire you to give RED a try the next time you have a computational demanding workflow.

My View of Supercomputing

- I am passionate about enabling broad science with HPC.
- At Indiana University for 17 years, in various roles.
- IU has seen the future of HPC use.

My View of Supercomputing

Posts Replies Media Lists

Andrew Jones (hpcnotes) @hpcnotes.bsky.social · 13d

What happens when people realize that the best High Performance Computing happens when you learn to optimize not so much the performance of the computer, but the performance of the humans using the computer?

#HPC #supercomputing

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Supercomputing at IU

- Have you used RED?
- Have you used IUAnyWare?
- Have you used Quartz or BR200?

- What potential use cases do you have?
- What applications would you run?

Supercomputing at IU

- Create an account:
  - https://access.iu.edu/Accounts/Create
- Join our HPC Users Community Slack:
  - https://iu-hpc-users.slack.com/signup
- Supercomputing for Everyone Series:
  - Sign up on ittraining.iu.edu or events.iu.edu/rssolutions/all

Supercomputing at IU

Personal Workstation

- Easiest to access
- Generally self-managed and completely on-demand
- Limited data storage, computing power, and computing memory (RAM)
- Limited ability to multitask

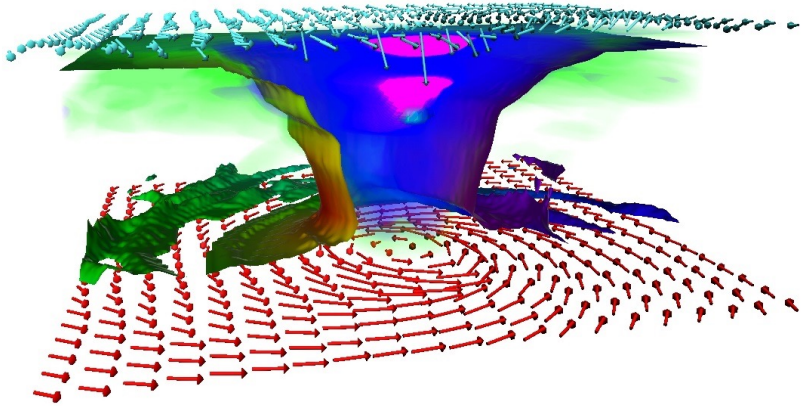
Supercomputing System

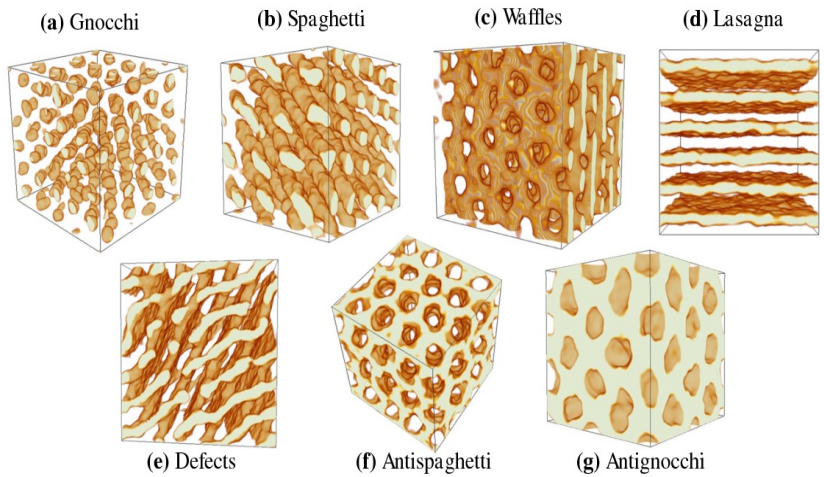
- Users submit jobs (set of commands) to a queue
- Best for Highly Parallel Computations
- Easy to get access to
- Generally free to use, unlimited access

Research Desktop

Supercomputing at IU

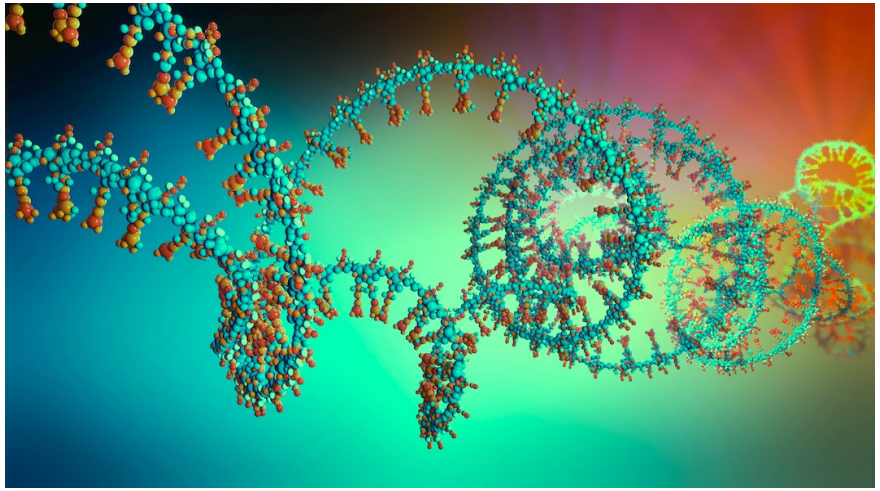
- Quartz / Research Desktop
  - Great for memory-intensive, high-throughput work, and getting started quickly.
  - Open to all Students, Faculty, and Staff
  - 90 compute nodes, each equipped with 128 cores and 512 GB of RAM.
  - GPU partition with 24 nodes and 4 NVIDIA V100s per node.
  - Hopper GPU Partition with 12 nodes with 4 NVIDIA H100. For intensive work that can't fit on the NVIDIA V100s or NVIDIA A100s





Supercomputing at IU

- Big Red 200
  - Compute-intensive, large-scale applications and GPU workflows
  - Open to Graduate Students, Faculty, and Staff
  - HPE Cray EX running SLES15.
  - 640 dual socket AMD Rome nodes (2x 64 core) with 256GB RAM
  - 64-core single socket Rome nodes, 512GB main memory, with 4 NVIDIA A100 40GB GPU cards



Storage at IU

- Slate — Quota based and not purged high-performance file system with 800GB quota allotment, excellent for computing against. Must request to get an account
- Slate-Project — Up to 30TB provided, and more may be provided upon request
- Slate-Scratch — 100TB quota allotment, un-accessed files purged every 30 days.
- Home Directory — 100GB across all accounts, backed up, not for computation.
- SDA — The tape archive. Excellent for long term storage, data replicated between here and Indianapolis.
- Globus — To connect everything!

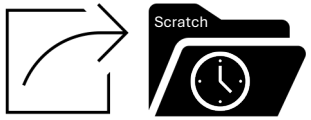
Workflow

Install software to your Home Directory

Store your data on Slate while working on it

Archive your work on the SDA when you're done!

Point your application's temporary directories to Slate-Scratch



Getting Access

- Quartz and Research Desktop: Faculty, staff and students
- Big Red 200: Faculty, staff and graduate students
- Create system and storage accounts at: access.iu.edu/Accounts/Create
  - https://servicenow.iu.edu/kb?id=kb_article_view&sysparm_article=KB0023238
- Submit an RT Project at: projects.rt.iu.edu
  - https://servicenow.iu.edu/kb?id=kb_article_view&sysparm_article=KB0024132
- More info:
  - https://servicenow.iu.edu/kb?id=kb_article_view&sysparm_article=KB0022656

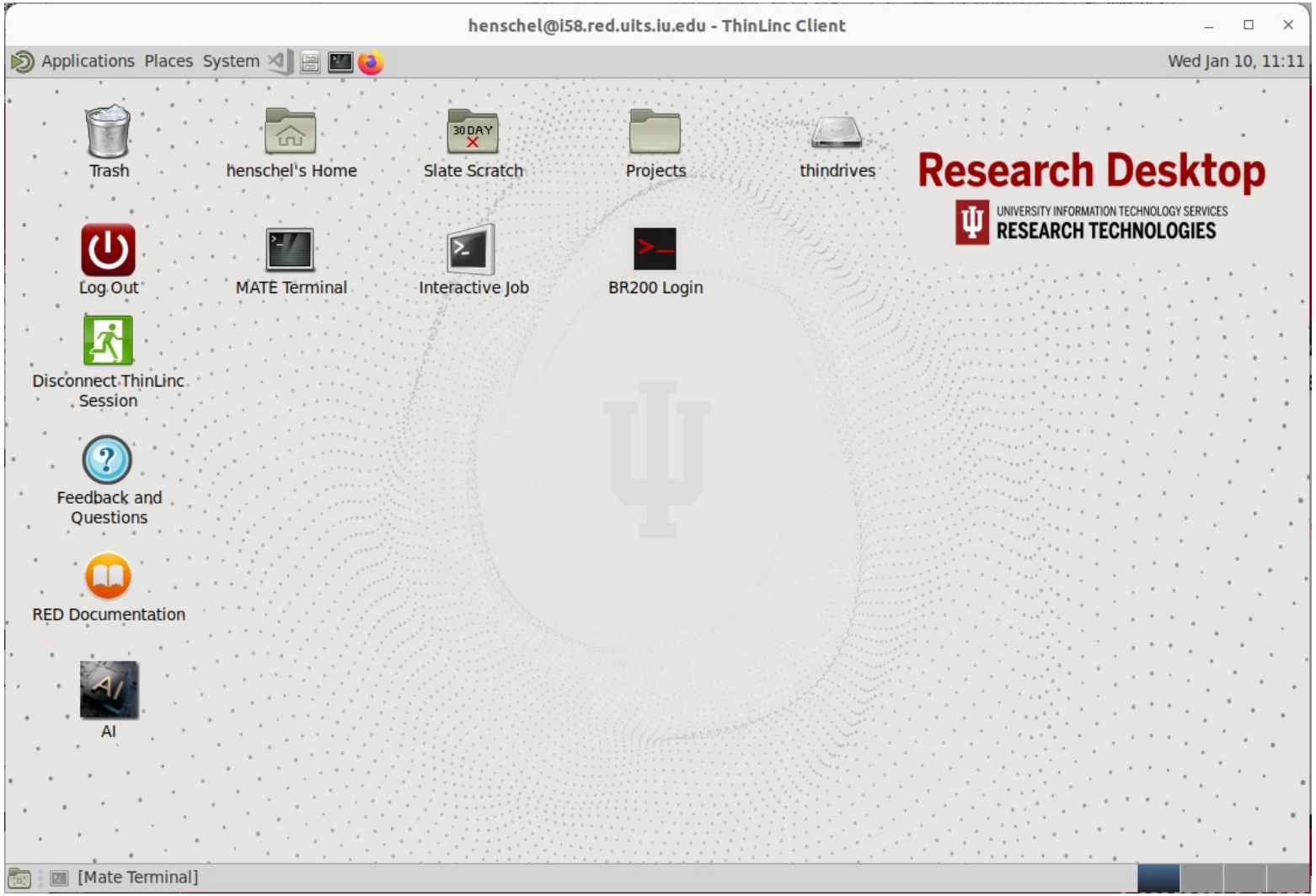
How much does this cost?

- The computing resources and storage are free for normal use
  - (Unless you need huge amounts of dedicated compute time or large data storage)
- Short term support and consulting is also free
  - Involves help with day-to-day issues
  - Installing software
  - Troubleshooting problems, etc
- Long term support and consulting is possible on a paid basis

Contacting Support

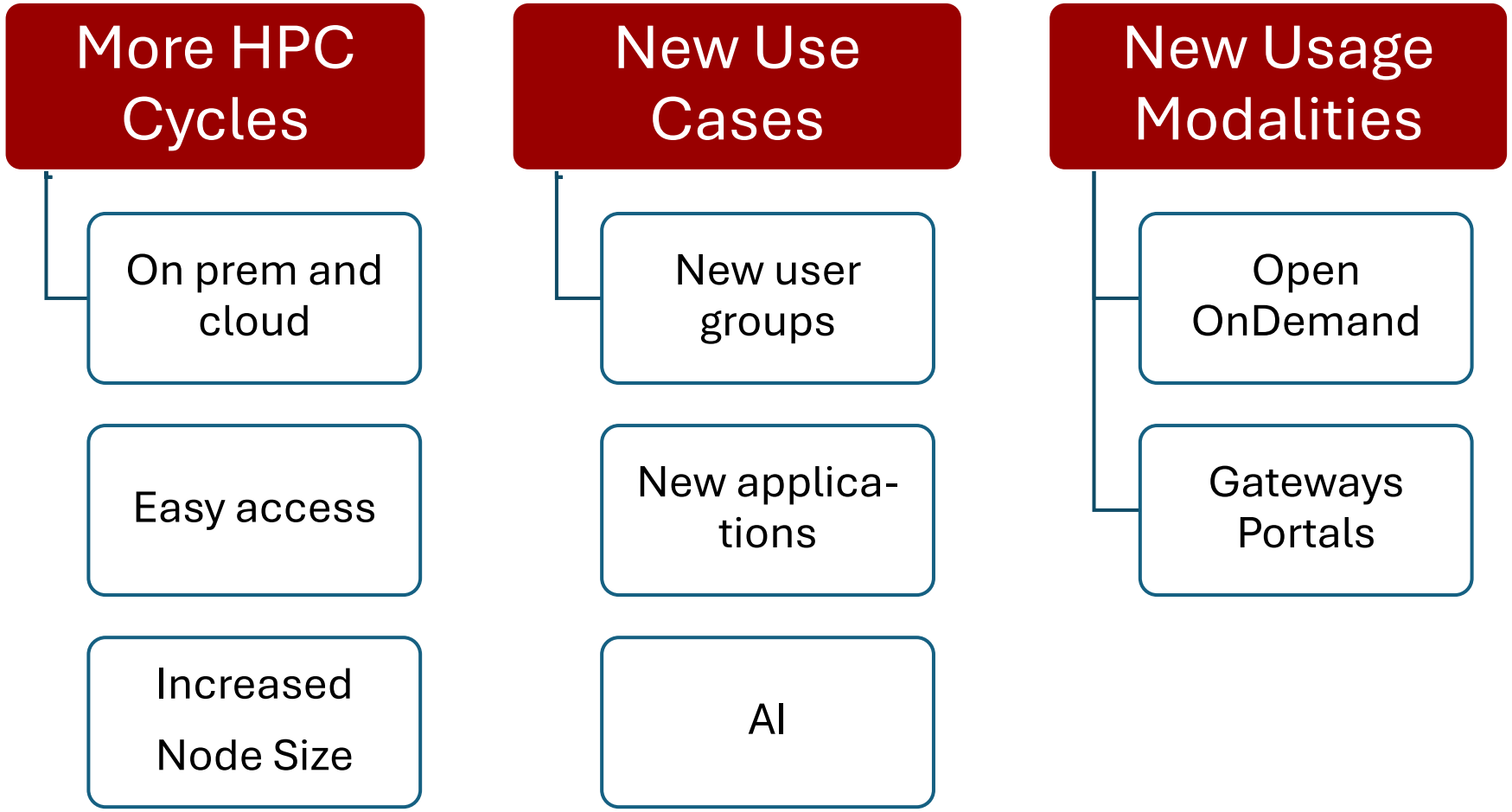
- The KB (kb.iu.edu) is an excellent resource for most of the basics
- Specific addresses for specific issues:
  - HPS (Admins): hps-admin@iu.edu
  - Research Applications: radl@iu.edu
  - HPFS (Slate): hpfs-admin@iu.edu
  - SDA: store-admin@iu.edu
  - RED: red-help@iu.edu

RED Demo

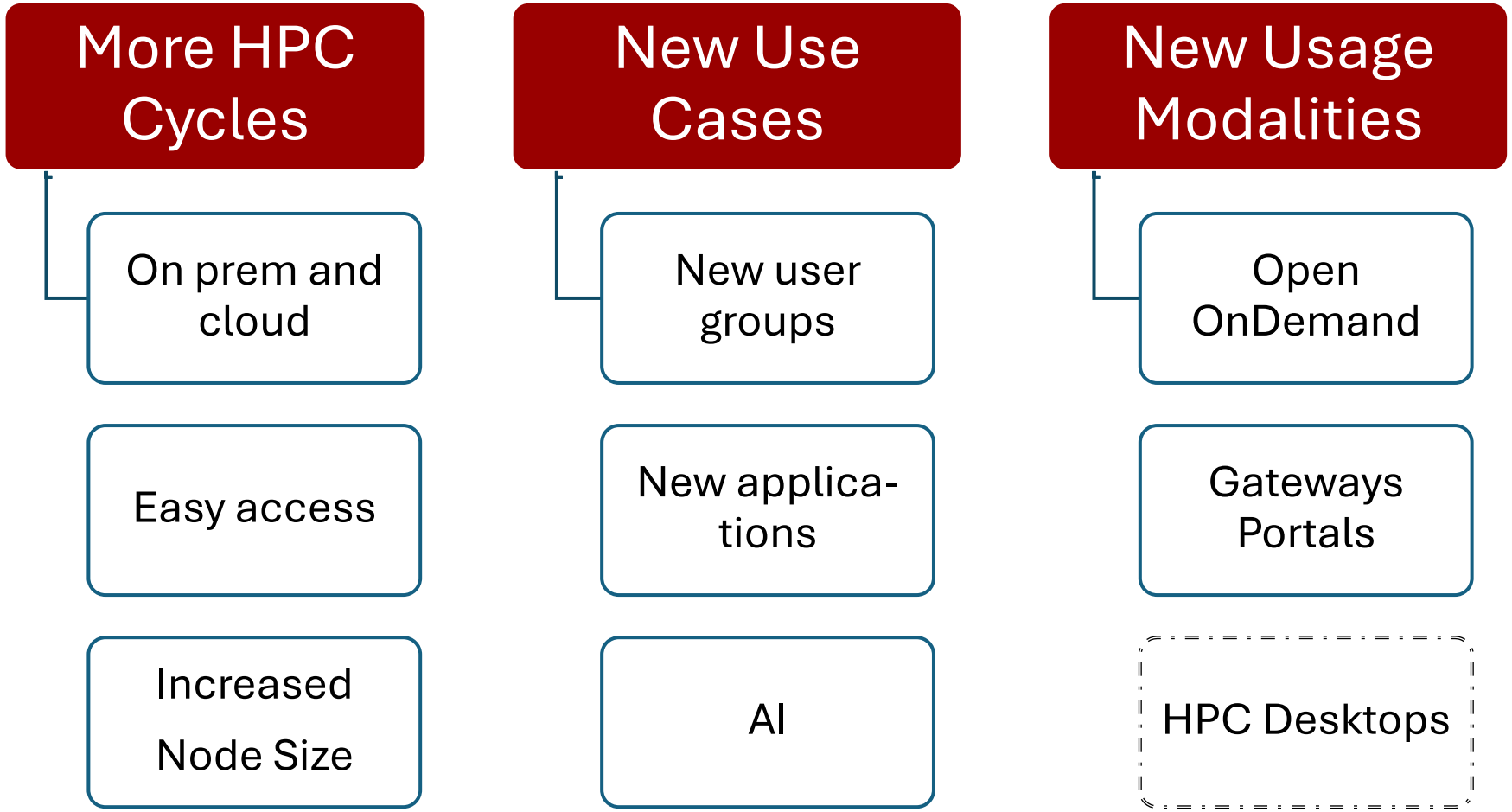

henschel@i58.red.uits.iu.edu - ThinLinc Client
Applications Places System
Wed Jan 10, 11:11
Trash
henschel's Home
Slate Scratch
Projects
thindrives
Research Desktop
UNIVERSITY INFORMATION TECHNOLOGY SERVICES
RESEARCH TECHNOLOGIES
Log Out
MATE Terminal
Interactive Job
BR200 Login
Disconnect ThinLinc Session
Feedback and Questions
RED Documentation
AI
[Mate Terminal]

The State of Supercomputing

The State of Supercomputing



The State of Supercomputing



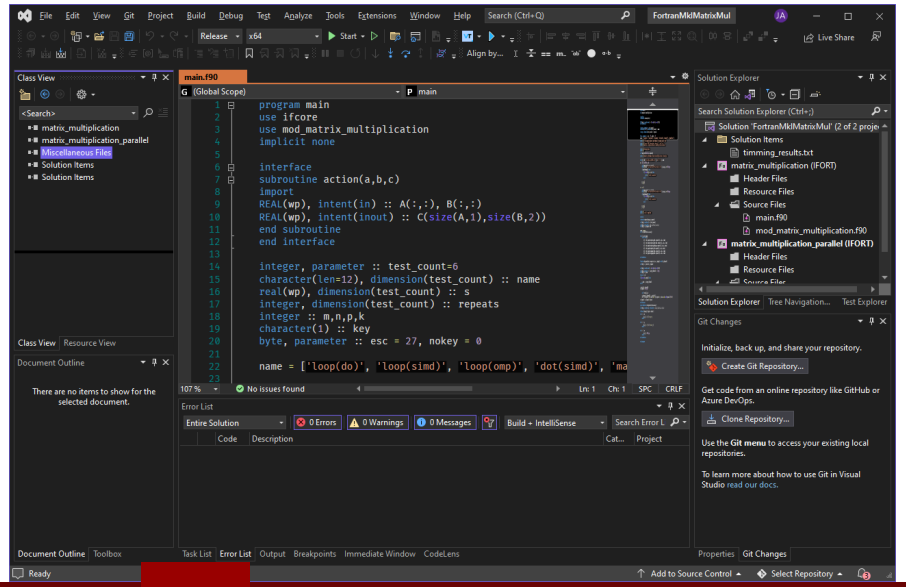
The State of Supercomputing

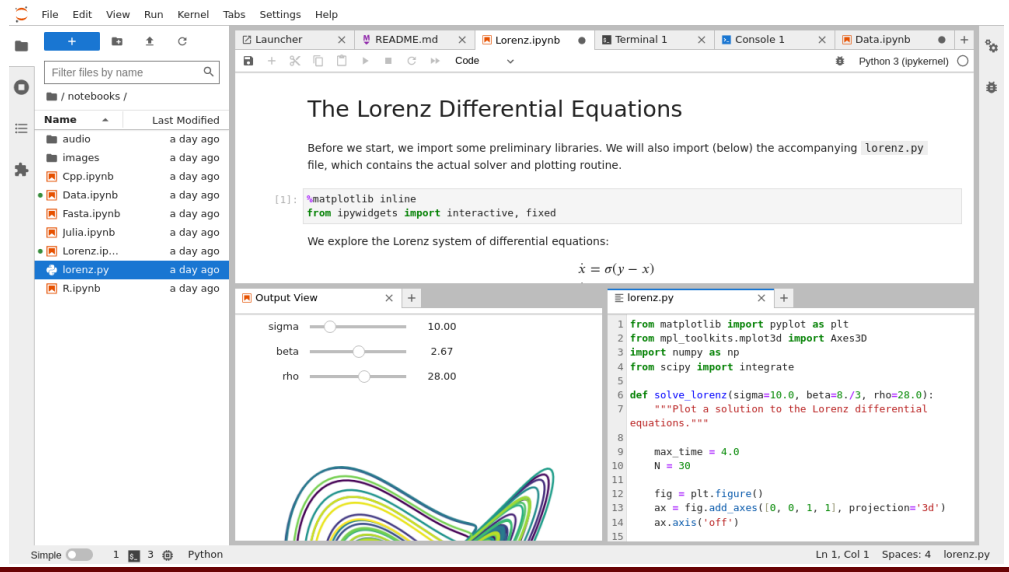
Edit-Compile-Run

REPL / Notebook

File Based

Document Based





The State of Supercomputing

- HPC systems are becoming more widely available.
- Demand is increasing from all fields of science.
- The users are more diverse and so is their skillset.
- The tools they use are more diverse.

- HPC Centers are asked to support it all. (and IU has for the last decade or two)

HPC Users, a Big Picture

Observations about Users

- Users don’t read documentation.
- Users are annoyingly creative.
- Users utilize diverse tools, and tools evolve.
- Users don’t know how computers work.

Thank you Matt Rocklin!

Lessons learnt

- Be familiar, not novel.
- Invite the user to invent.
- Make it visual.
- Tell people about their usage.
- Make it useful on a laptop.

Thank you Matt Rocklin!

Future HPC Users

- We are hopefully heading into a future with more and more HPC user.
- There are developments on all levels to help new users:
  - Better documentation
  - Easier to use applications
  - Container support
  - Custom portals and gateways

- HPC Desktops are another way.

HPC Desktop

What if you had access to a **high performance desktop from any endpoint device**? What if this desktop allowed you to **launch interactive graphical applications** like MATLAB, Jupyter Notebooks, R-Studio and VS Code, as well as **compose scientific workflows**? What if this desktop had **enough performance to run the applications** and also provided **tools to quickly manage and submit jobs** to an HPC system? What if this desktop was **available to you for weeks or months**, allowing you to reconnect whenever you need it?

Lessons learnt

HPC Desktop

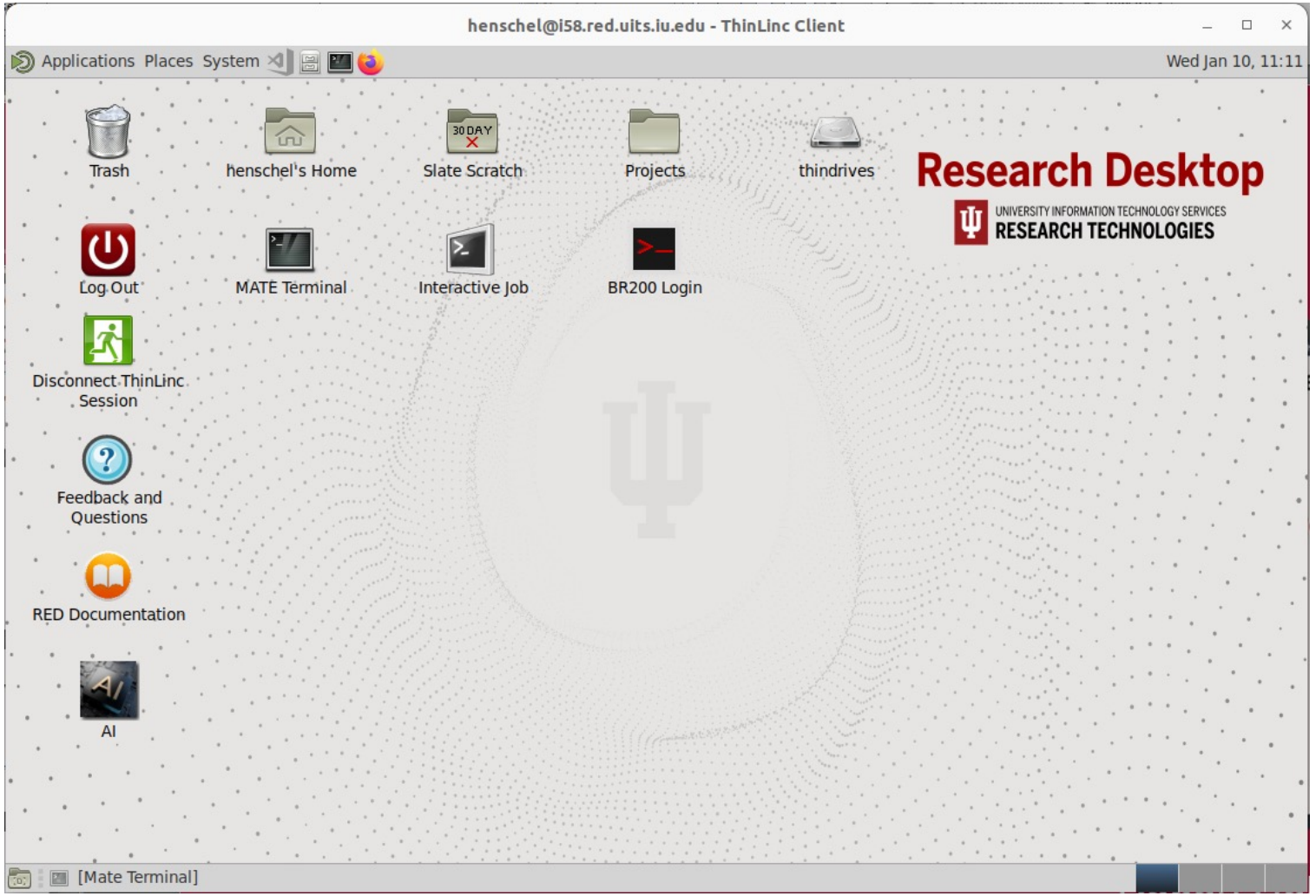
- Be familiar, not novel. 
- Invite the user to invent. 
- Make it visual. 
- Tell people about their usage. 
- Make it useful on a laptop. 

The Case for HPC Desktops

HPC Desktop – History

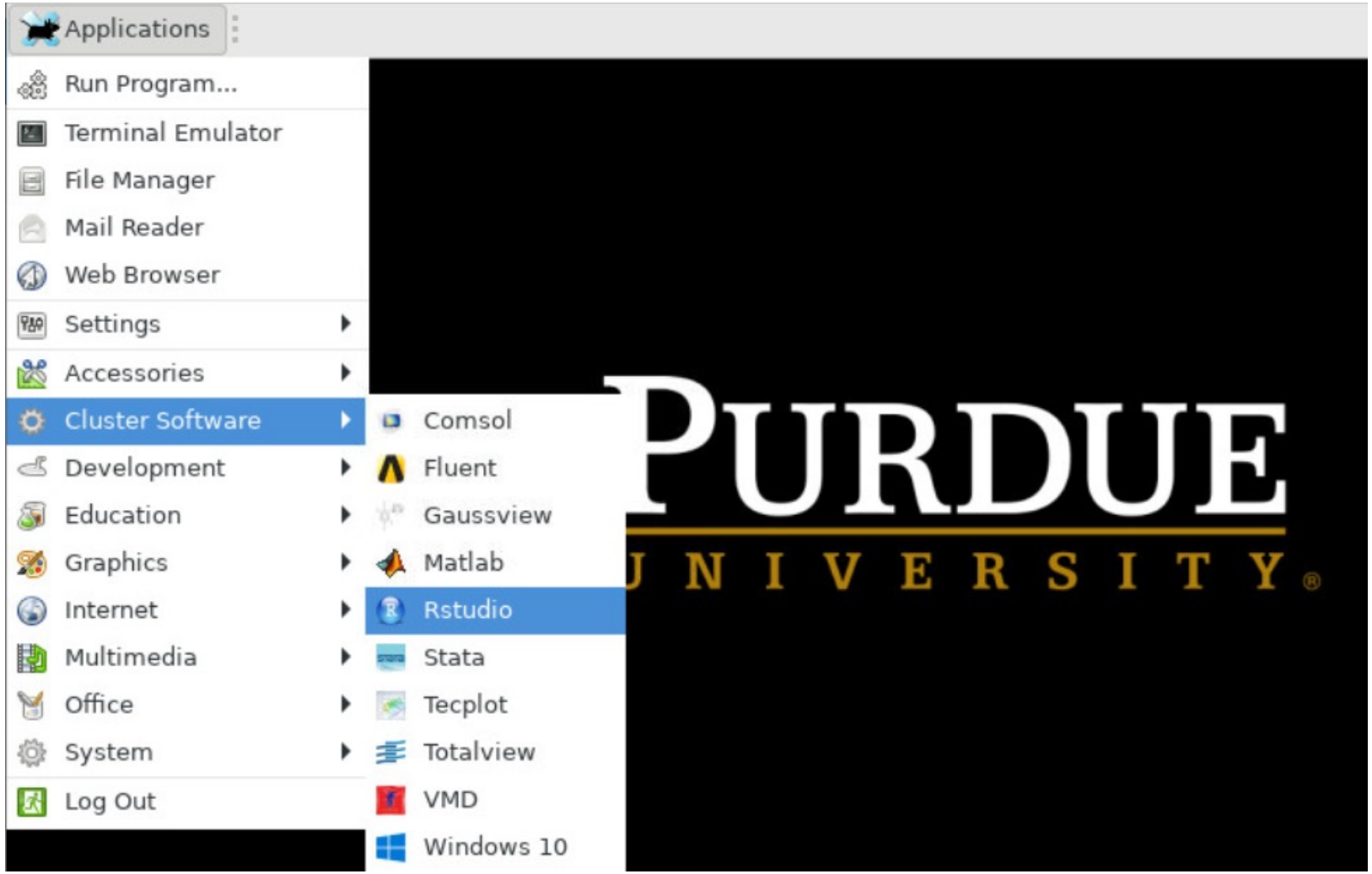
- Indiana University has a long history of open access to HPC
  - 2016: A PetaFLOPS Supercomputer as a Campus Resource: Innovation, Impact, and Models for Locally-Owned High Performance Computing at Colleges and Universities
  - 2019: Research Computing Desktops: Demystifying research computing for non-Linux users
  - 2022: Lightning talk at the Interactive HPC workshop at SC
  - 2024: Use Cases for HPC Desktops, at the Interactive HPC workshop at ISC
- Interactive and Urgent HPC: Challenges and Opportunities
  - https://arxiv.org/abs/2401.14550

HPC Desktops – Examples



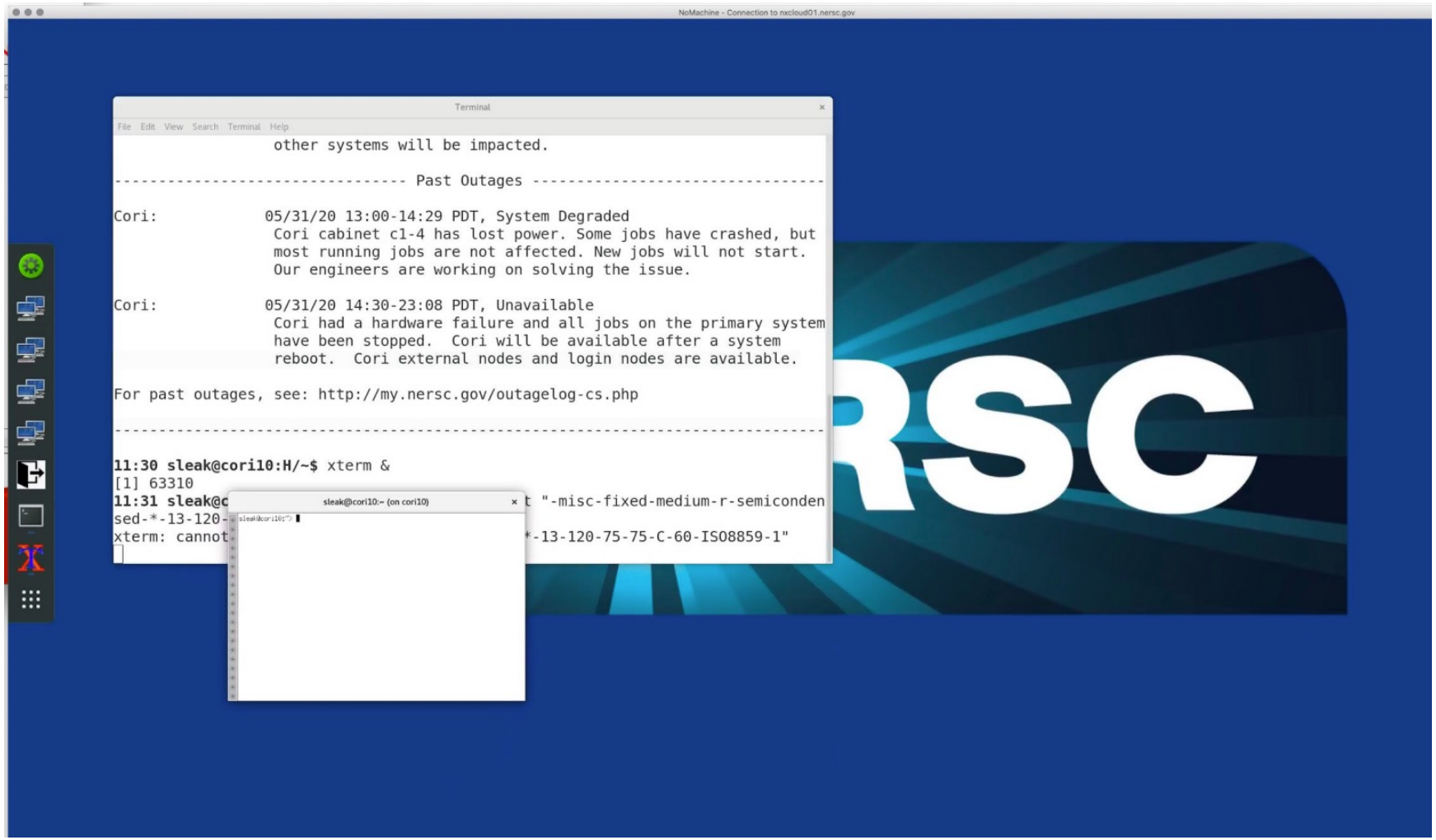
Indiana University

HPC Desktops – Examples



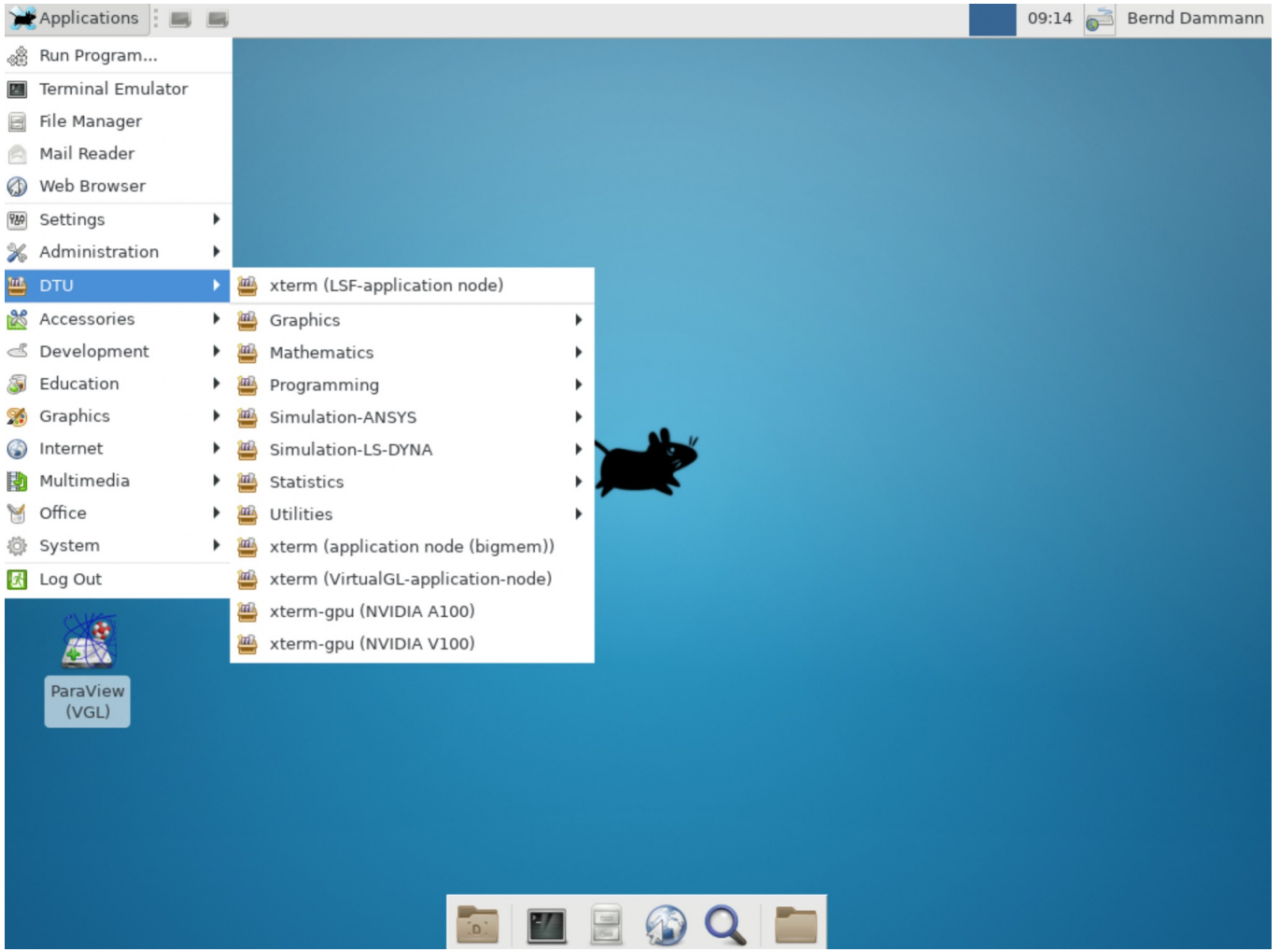
Purdue University

HPC Desktops – Examples



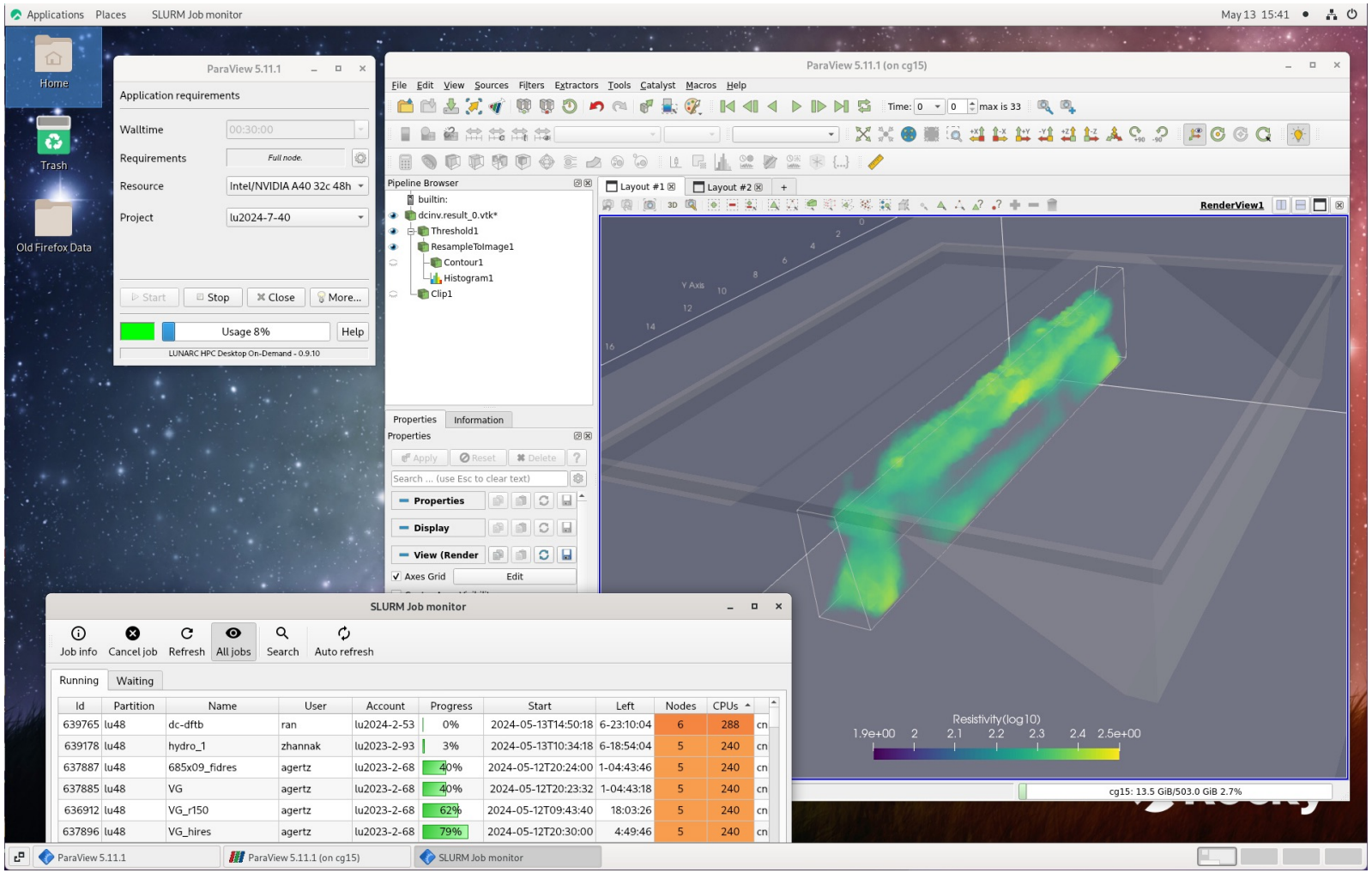
NERSC

HPC Desktops – Examples



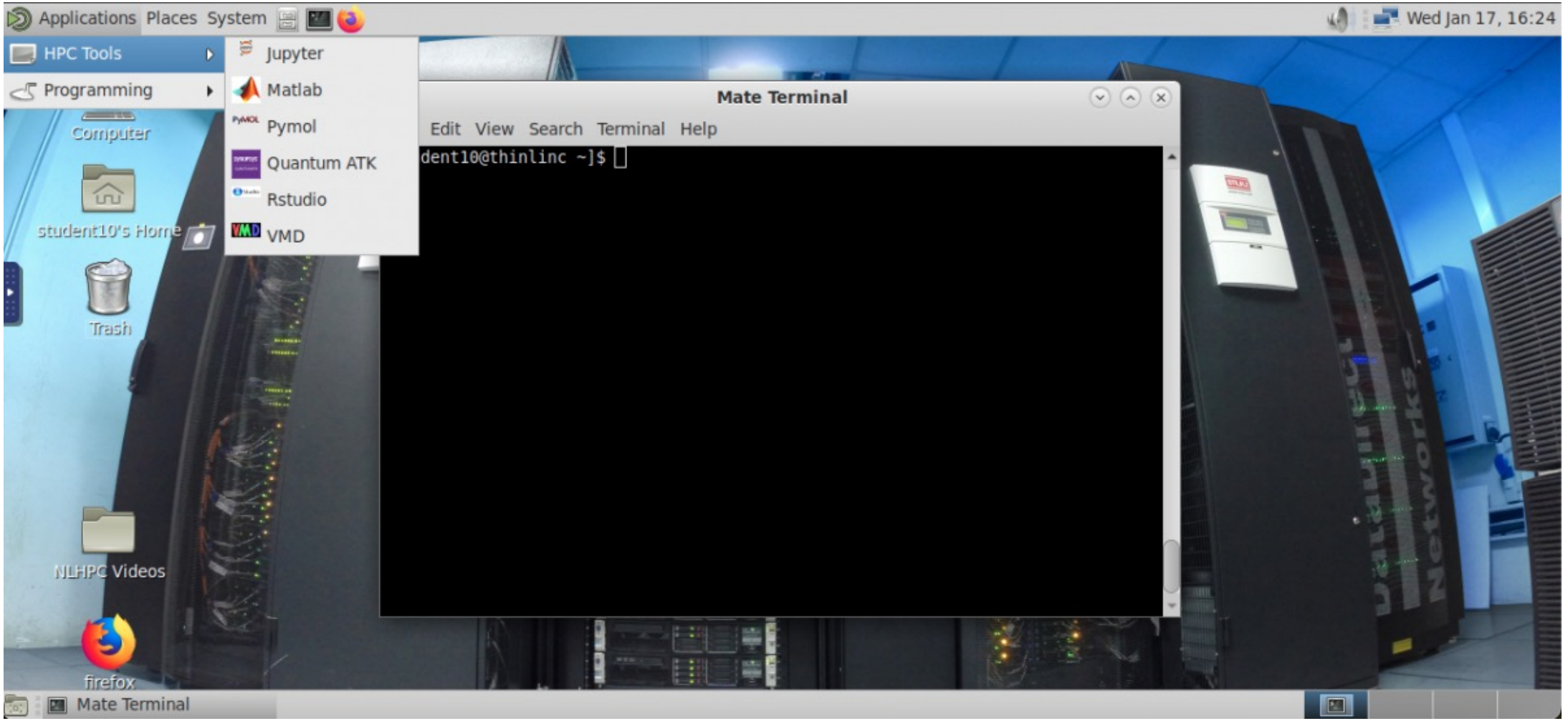
Denmark Technical University

HPC Desktops – Examples



Lund University

HPC Desktops – Examples



HPC Desktop – Use Cases

- Use Cases for High Performance Research Desktops
  - Combined report from Indiana University, Lund University Sweden and Denmark Technical University
  - https://arxiv.org/abs/2404.03298

HPC Desktop – Use Cases

- File Manager
- Non HPC Computations
- HPC Jobs Workflow
- Client Server Applications made easy
- Teaching, Classes
- Secure Enclaves

Use Cases: File Manager

- File managers are a game changer for new users
  - Nobody gets the concept of “run a command to copy a file”
- Create and extract archives
- Graphical “du”, why am I over quota?
- Moving files between storage systems, move to tape.
- Bookmarks in the file browser
- “Connect to Server” functionality

Use Cases: Non-HPC Computation

- Long running graphical and interactive applications like MATLAB, Jupyter Notebooks, RStudio,…
- Statistics applications like SAS, STATA, SPSS,…
- Visualization software like VMS, Paraview,…
- Software and scripts that run for a long time, but with minimal CPU and memory demands
- Leverage centrally licensed software

Use Cases: HPC Jobs Workflows

- A graphical editor for SLURM scripts
- “ThinDrives” functionality to transfer small files
- Download software and datasets right to the HPC filesystem
- Facilitate long running data movement operations
- Simplify “job submission”, “Interactive Job” icon
- Graphical tools, IDEs, debuggers, performance tools
- Preview of job results

Use Cases: Teaching and Learning

- Intro to HPC training
- Use HPC system in classes
- Equal access, powerful desktops for everyone, anywhere.

Use Cases: Client Server Applications

- Use client server applications without tunneling through a login node
  - An HPC Desktop can easily connect to compute nodes
- Comsol Multiphysics, Schrödinger, MATLAB parallel server, Jupyter Notebooks, Ansys Workbench, …
- Visualization software

Use Cases: “Secure Enclaves”

- Graphical secure enclaves
- ePHI / HIPAA, FISMA, NIST 800-171/53
- Optum, Market Scan datasets

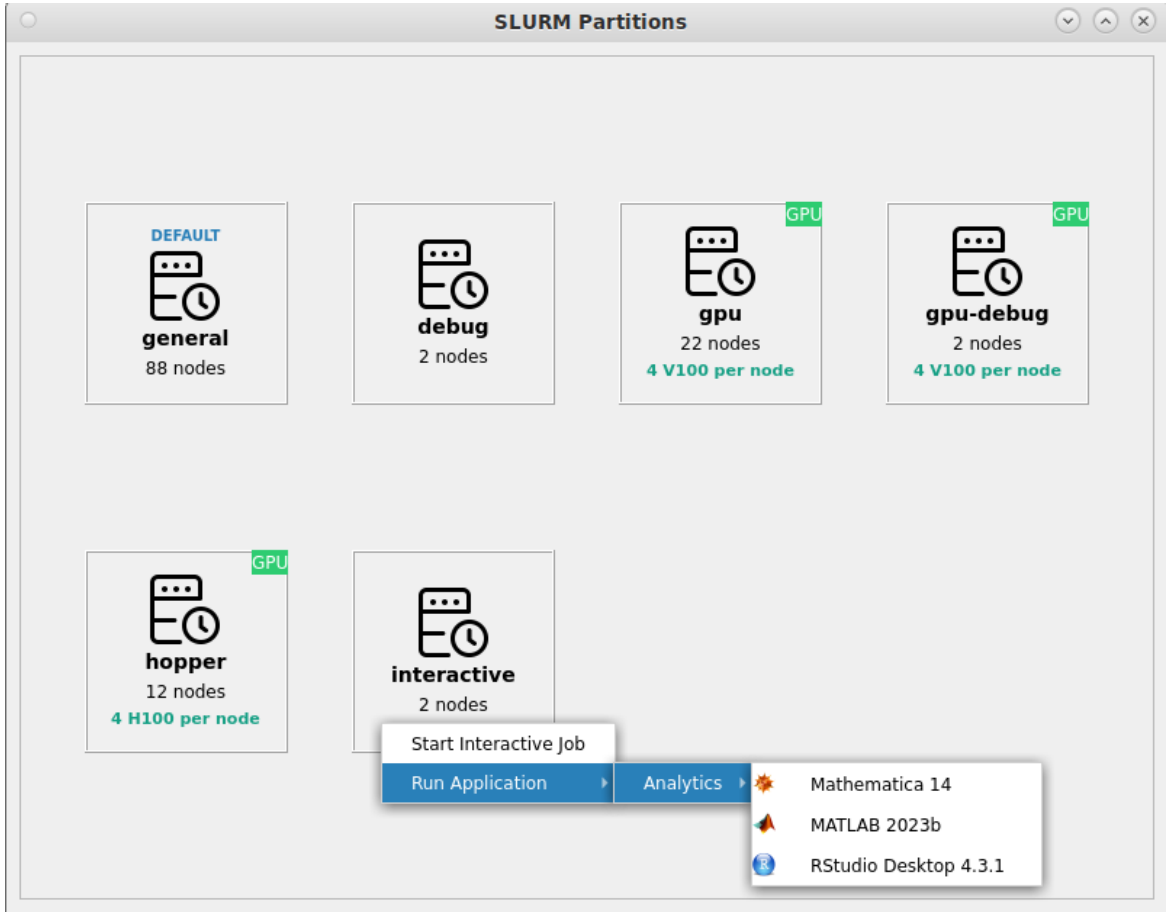
HPC Desktop – Big Picture

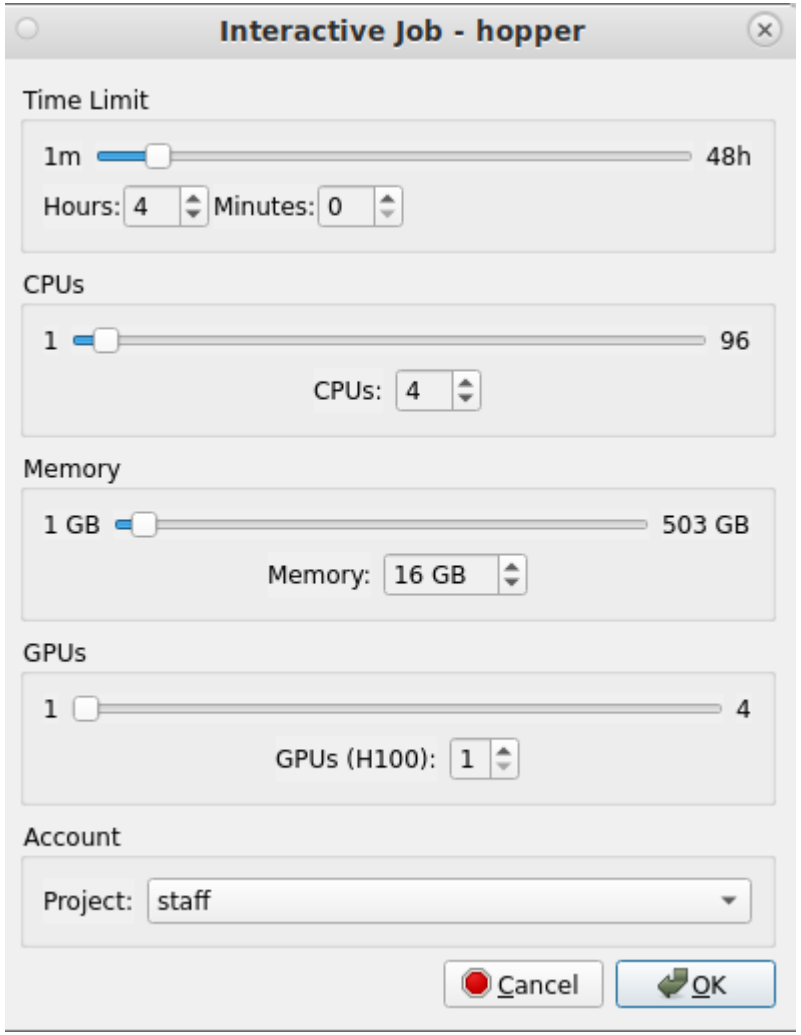
- Disconnect and reconnect. (Similar to laptops)
- Help overcome the initial barrier and people will learn!

- Leveraging HPC investments to attract more users, serve a broader range of scientists.
- Onboard the next generation of HPC users.

- It should be the goal of HPC Centers to attract more users.
- An HPC Desktop is one way to do it.

The Future – App Delivery Platform





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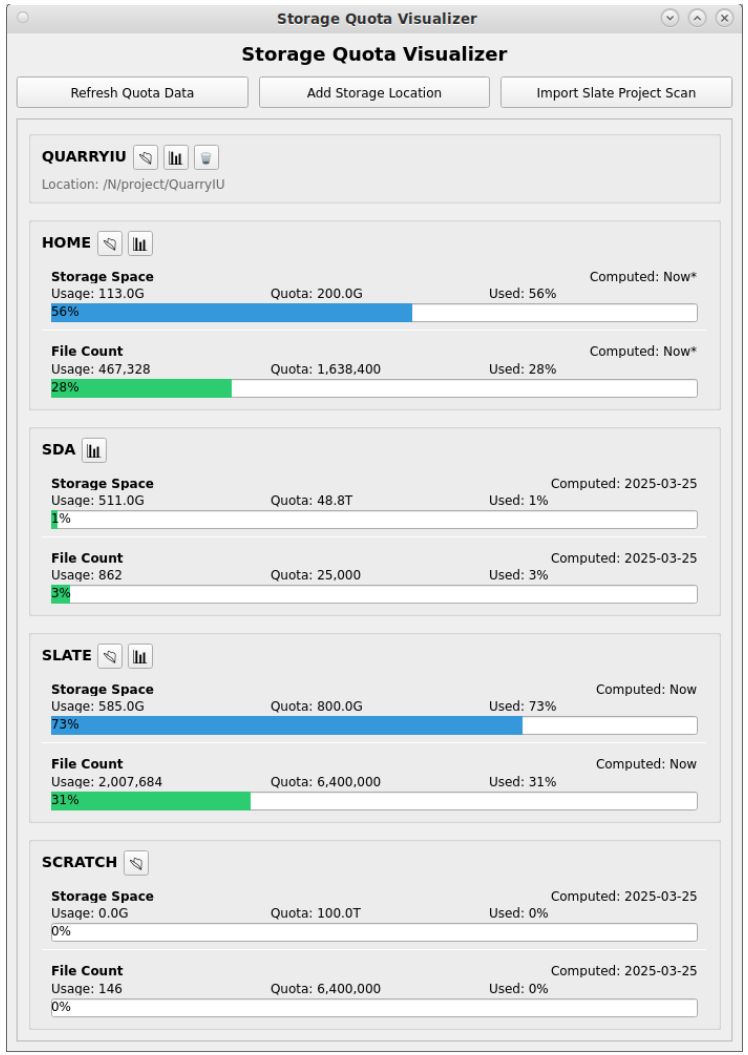

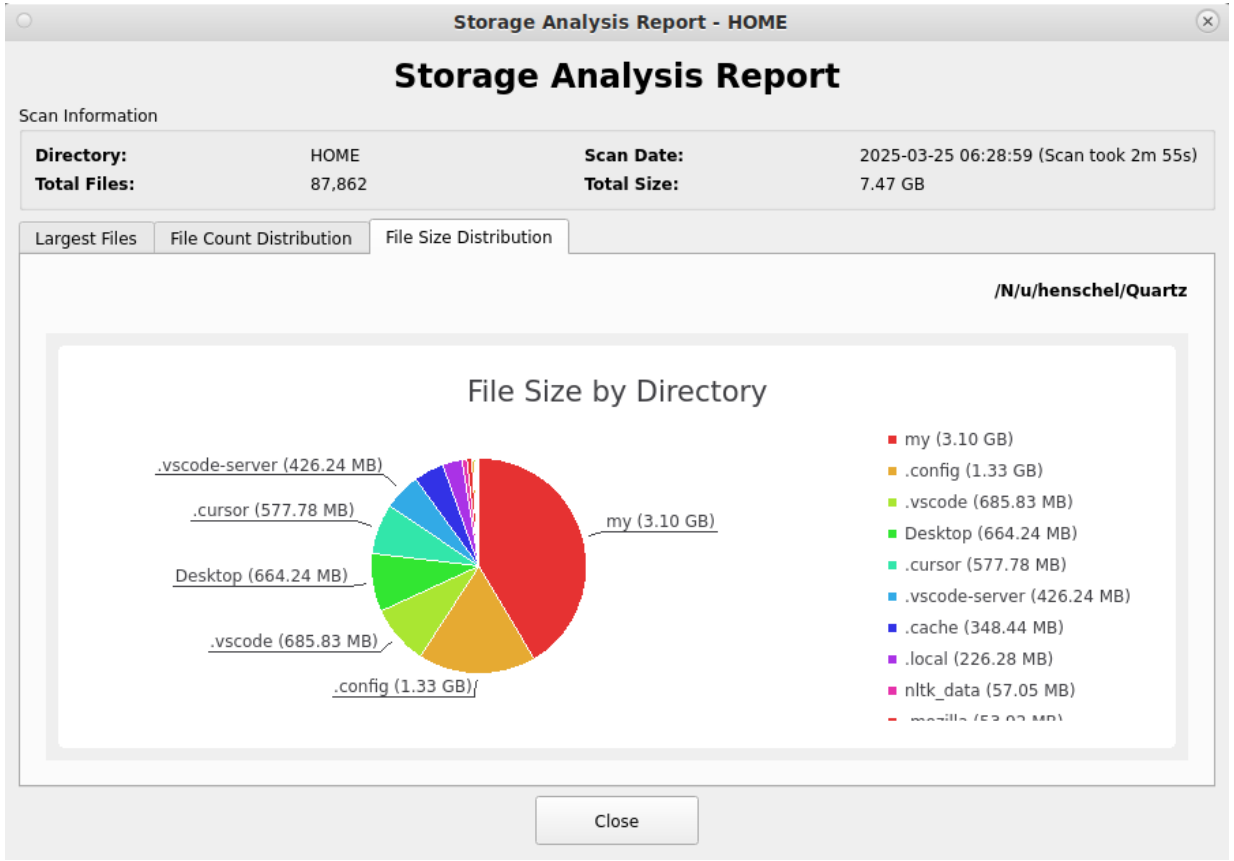

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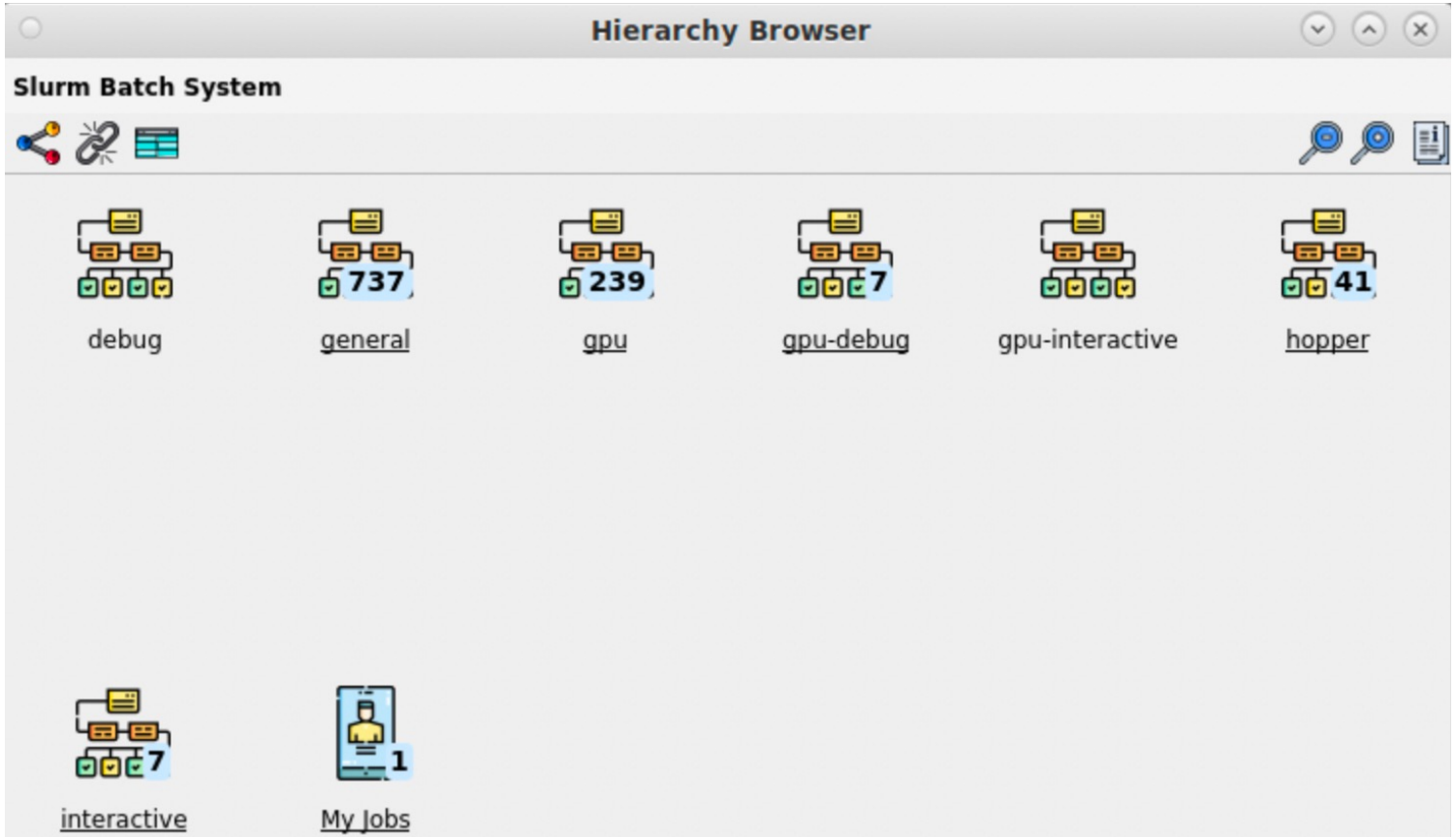

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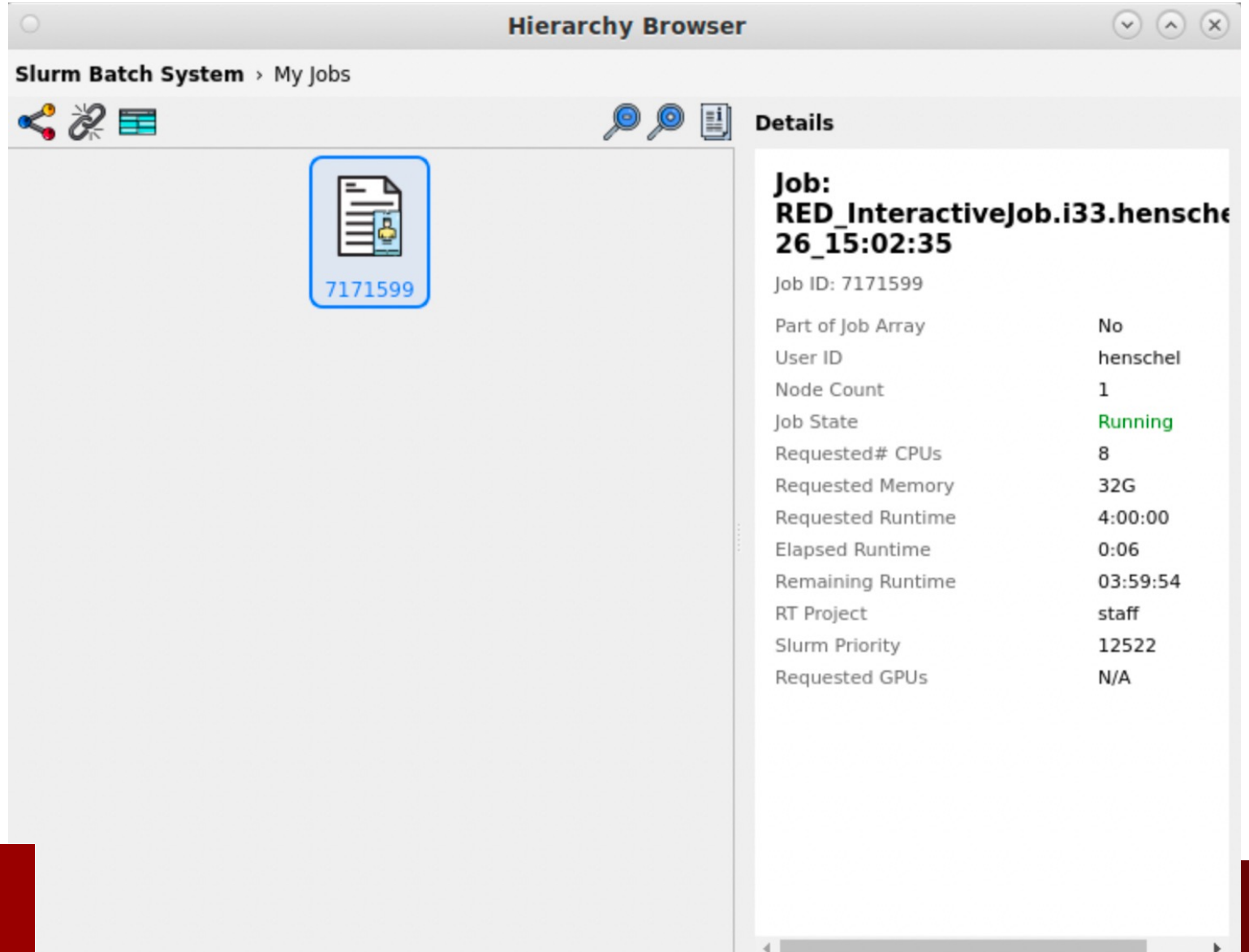

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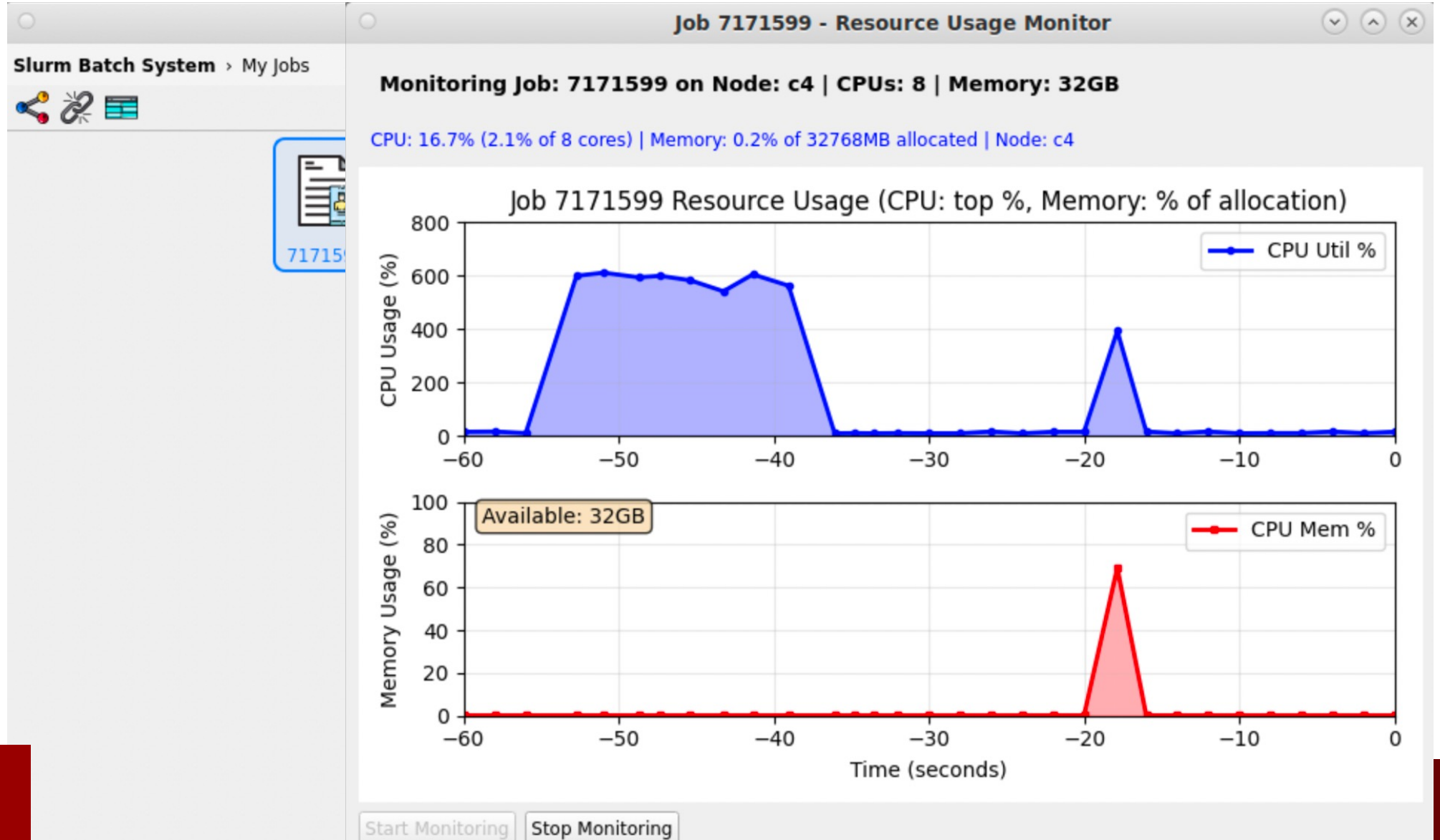

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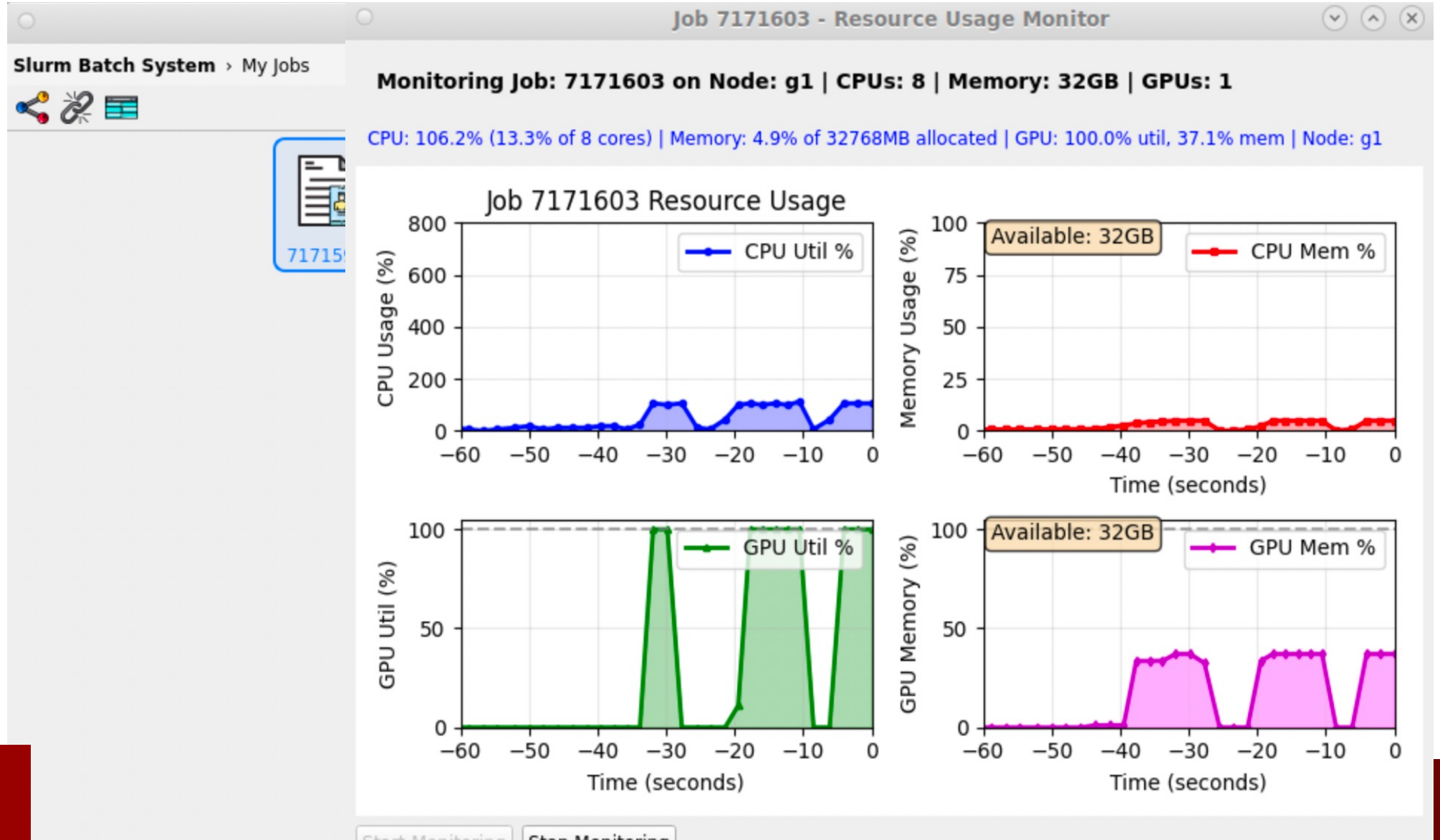

The Future – App Delivery Platform

Demo!

Summary

- IU Research Desktop has been available since 2015.
- RED is the easiest way to get started with HPC at IU.
- Let’s grow the next generation of HPC users.

Thank you!