Use Cases for High Performance Research Desktops

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UNIVERSITY INFORMATION TECHNOLOGY SERVICES

Contents

- Introduction to HPC Desktops
- Capabilities of an HPC Desktop
- Use Cases
- Future Developments
- Research Desktop at Indiana University

Before I Begin: My Journey in HPC

- Robert Henschel
  - At Indiana University since 2008.
  - Project Director for Research Engagement.
  - Architect of the IU Research Desktop.
  - Working 60% at IU; 40% HPC and Research Computing consulting.
  - Currently consulting for Cendio, maker of ThinLinc.

- I am passionate about broader adoption of HPC and I am pursuing this both at Indiana University and at Cendio.

How this Paper Came to be

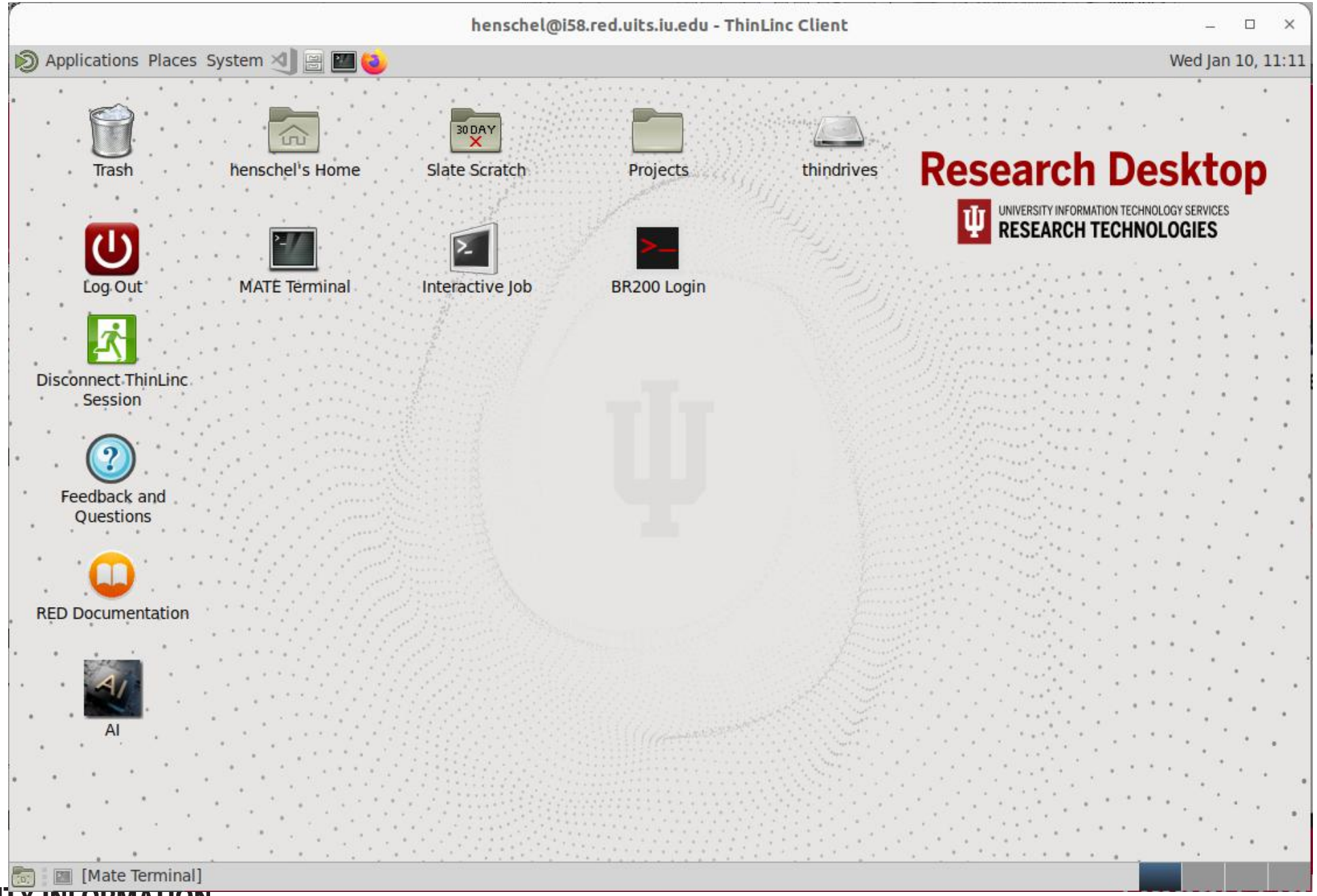
- IU has a long history of open access to HPC resources.
  - 2016: A PetaFLOPS Supercomputer as a Campus Resource: Innovation, Impact, and Models for Locally-Owned High Performance Computing at Colleges and Universities
  - 2019: Research Computing Desktops: Demystifying research computing for non-Linux users
  - 2022: Lightening talk at the Interactive HPC workshop at SC22
- This paper: Collecting a comprehensive list of use cases from multiple institutions.
- This talk:
  - General overview to HPC Desktops
  - Review of IU's Research Desktop of the last 10 years
- Reach out via DM or email to continue the conversation.

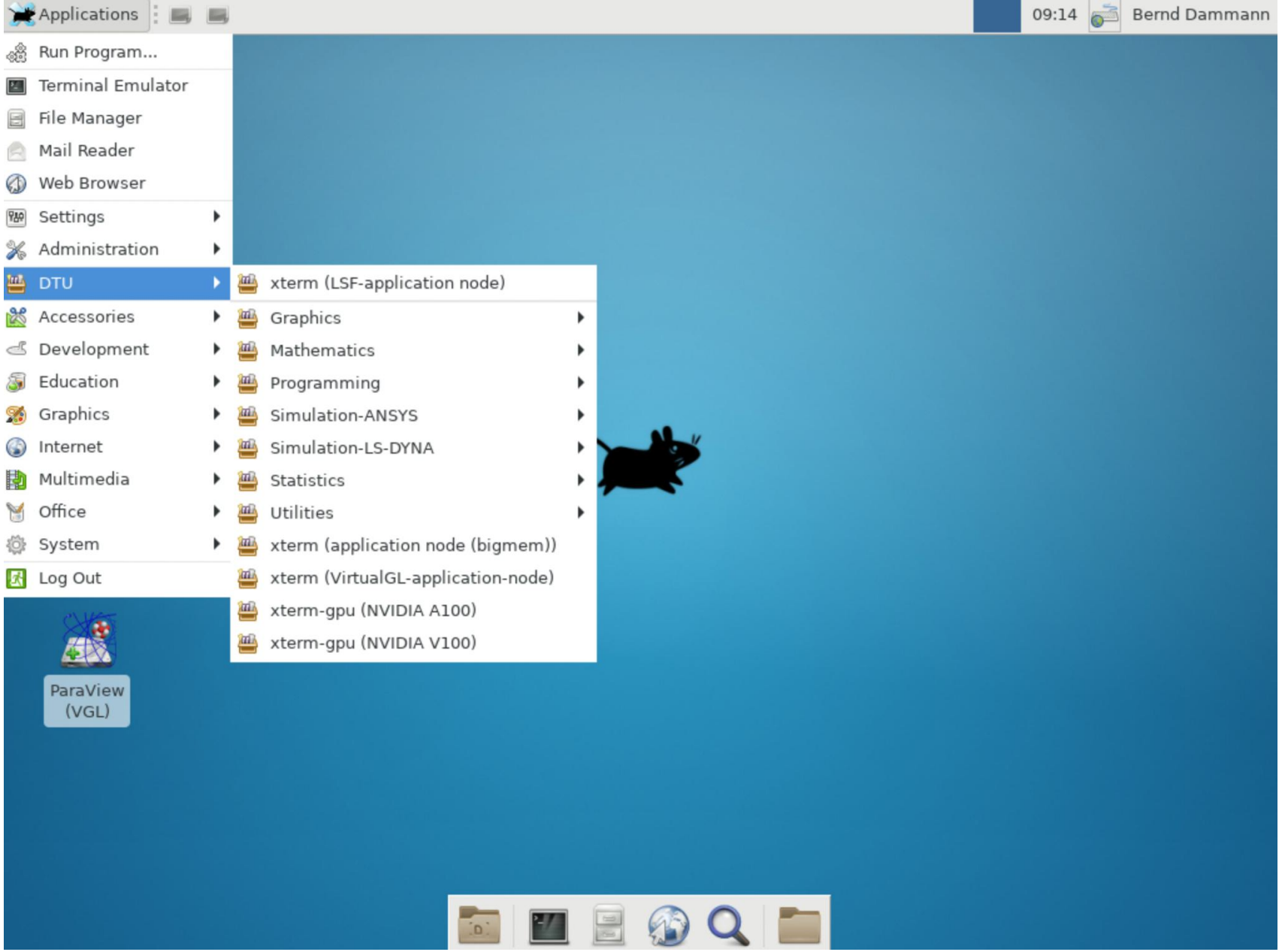
Interactive HPC Workshop at SC22

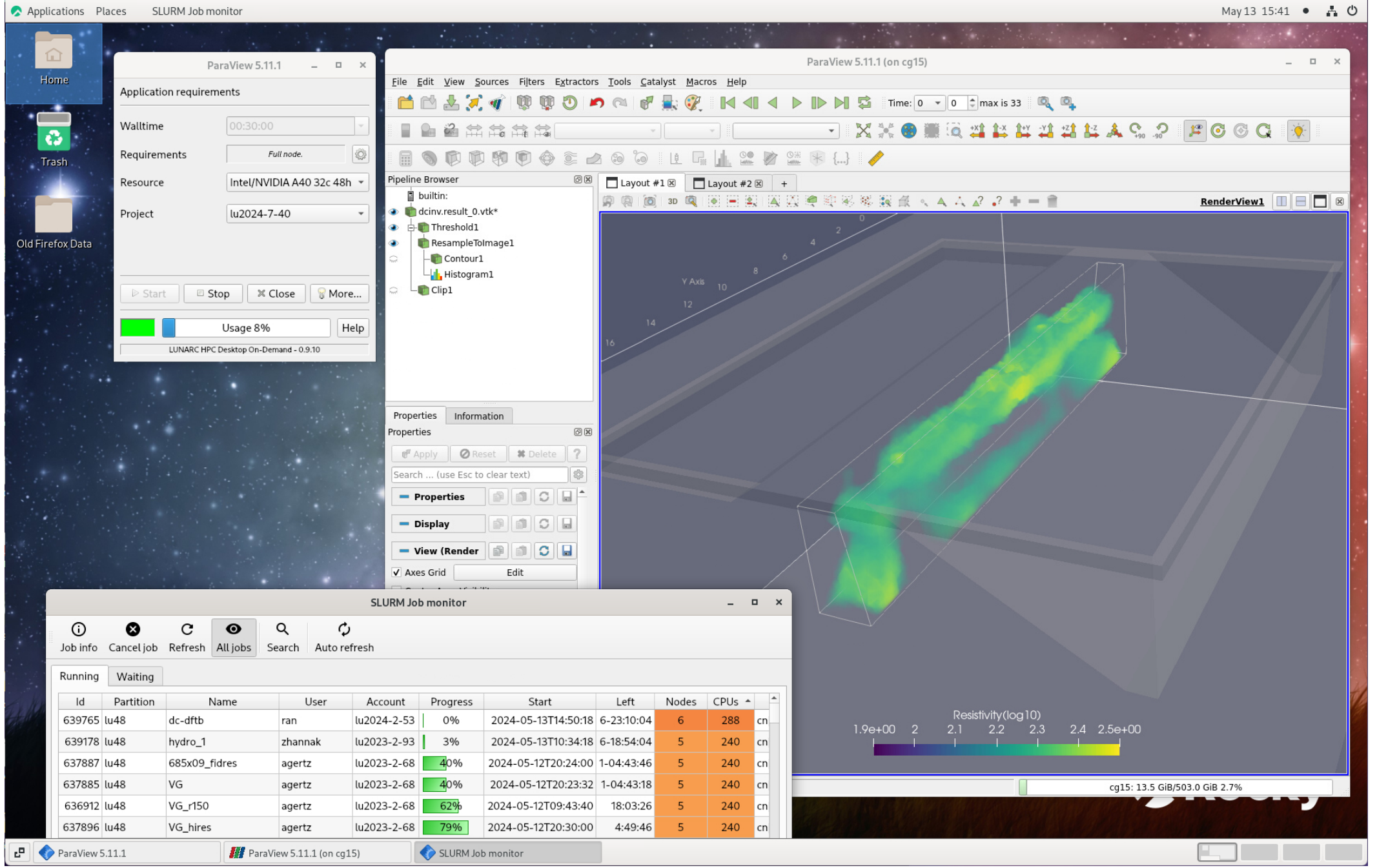
What if you had access to a **high performance desktop from any endpoint device**? What if this desktop allowed you to **launch interactive graphical applications** like MATLAB, Jupyter Notebooks, Ansys and VS Code, as well as **compose scientific workflows** using graphical and command line tools? What 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? Indiana University built such a desktop in 2015 and is evolving it ever since.

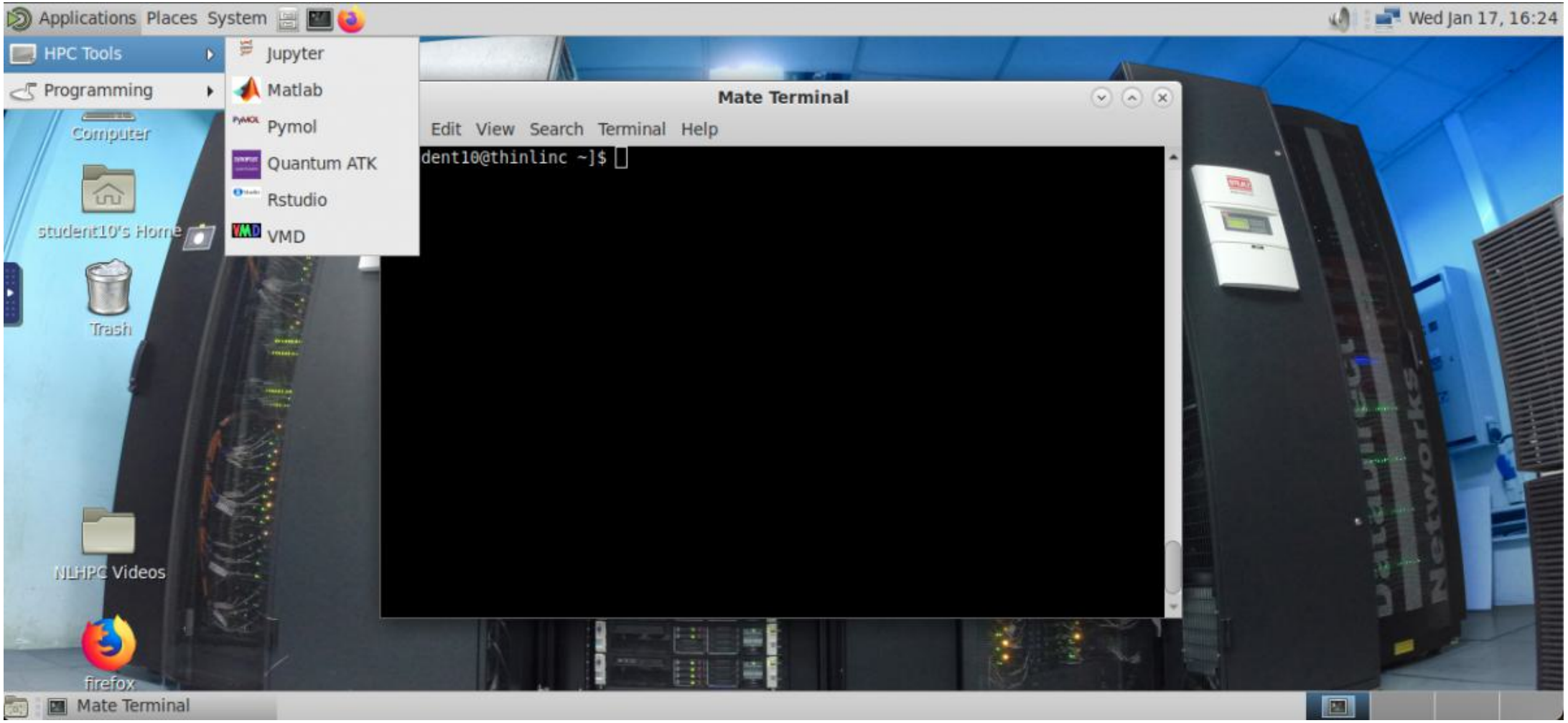
Introduction to HPC Desktops

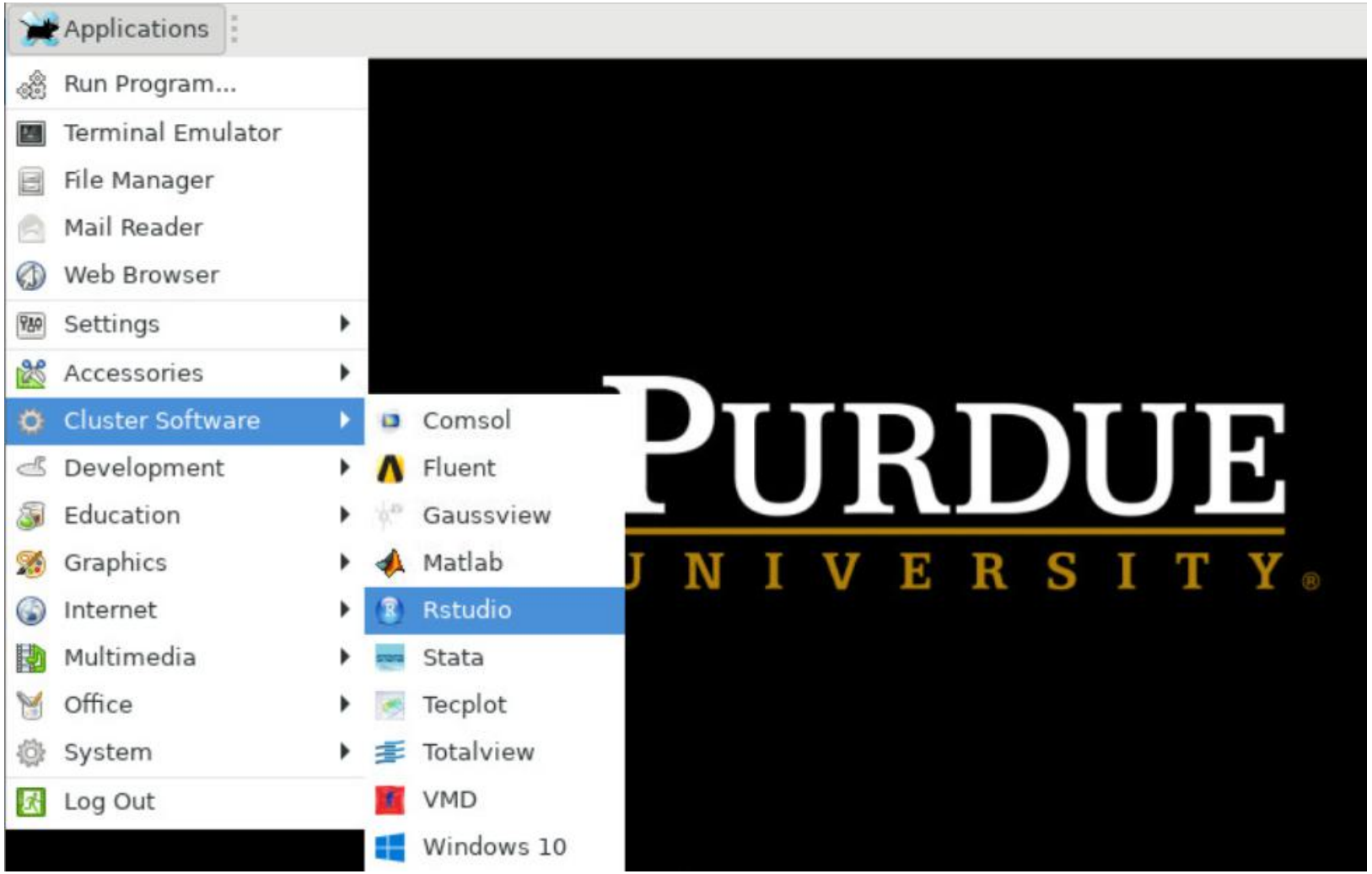
- Use a desktop to make high performance compute and storage systems available to users.
  - Deployed as a gateway to an HPC system and for execution of applications.
  - More than just a visualization resource. Utilize all tools of a desktop environment, and provide graphical tools for HPC access.
- Offer a convenient and persistent environment, that is faster than a users laptop or workstation.
- A customized desktop!
- HPC Desktops have grown in popularity over the last years, but are still a niche.

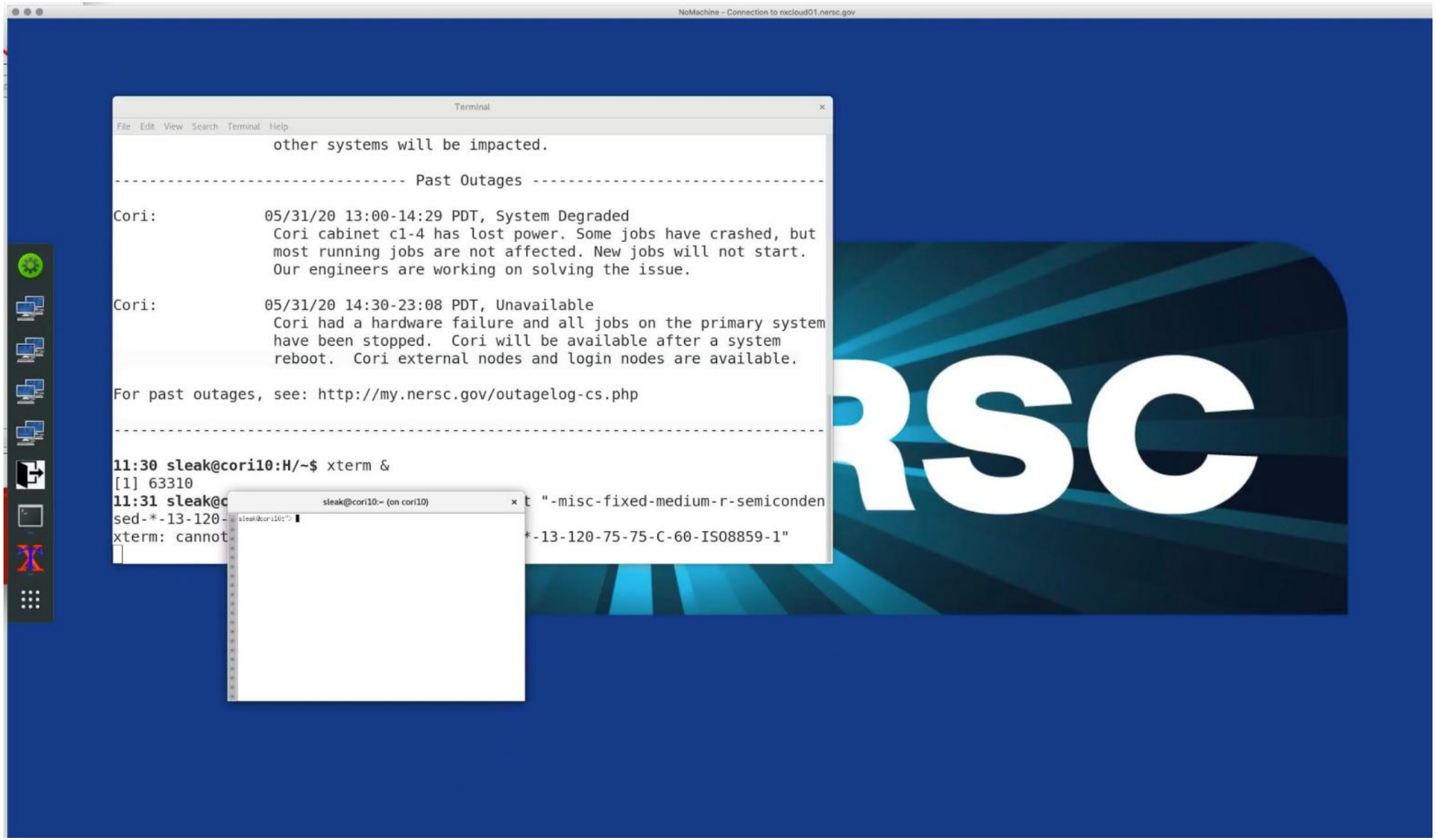

henschel@i58.red.uits.iu.edu - ThinLinc Client
Applications Places System
Wed Jan 10, 11:11
Trash
henschel's Home
Slate Scratch
Projects
thindrives
Research Desktop
UNIVERSITY INFORMATION TECHNOLOGY SERVICES
RESEARCH TECHNOLOGIES
Log Out
MATE Terminal
Interactive Job
BR200 Login
Disconnect ThinLinc Session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


Applications
09:14
Bernd Dammann
Run Program...
Terminal Emulator
File Manager
Mail Reader
Web Browser
Settings
Administration
DTU
Accessories
Development
Education
Graphics
Internet
Multimedia
Office
System
Log Out
xterm (LSF-application node)
Graphics
Mathematics
Programming
Simulation-ANSYS
Simulation-LS-DYNA
Statistics
Utilities
xterm (application node (bigmem))
xterm (VirtualGL-application-node)
xterm-gpu (NVIDIA A100)
xterm-gpu (NVIDIA V100)
ParaView
(VGL)


Applications Places SLURM Job monitor
May 13 15:41
Home
Trash
Old Firefox Data
ParaView 5.11.1
Application requirements
Walltime
00:30:00
Requirements
Full node.
Resource
Intel/NVIDIA A40 32c 48h
Project
lu2024-7-40
Start
Stop
Close
More...
Usage 8%
Help
LUNARC HPC Desktop On-Demand - 0.9.10
ParaView 5.11.1 (on cg15)
File Edit View Sources Filters Extractors Tools Catalyst Macros Help
Time: 0 0 max is 33
Pipeline Browser
builtin:
dcinv.result_0.vtk*
Threshold1
ResampleToImage1
Contour1
Histogram1
Clip1
Layout #1
Layout #2
RenderView1
Properties
Information
Apply
Reset
Delete
Search ... (use Esc to clear text)
Properties
Display
View (Render
Axes Grid
Edit
Y Axis
Resistivity(log10)
1.9e+00 2 2.1 2.2 2.3 2.4 2.5e+00
cg15: 13.5 GiB/503.0 GiB 2.7%
SLURM Job monitor
Job info
Cancel job
Refresh
All jobs
Search
Auto refresh
Running
Waiting
Id Partition Name User Account Progress Start Left Nodes CPUs
639765 lu48 dc-dftb ran lu2024-2-53 0% 2024-05-13T14:50:18 6-23:10:04 6 288 cn
639178 lu48 hydro_1 zhannak lu2023-2-93 3% 2024-05-13T10:34:18 6-18:54:04 5 240 cn
637887 lu48 685x09_fidres agertz lu2023-2-68 40% 2024-05-12T20:24:00 1-04:43:46 5 240 cn
637885 lu48 VG agertz lu2023-2-68 40% 2024-05-12T20:23:32 1-04:43:18 5 240 cn
636912 lu48 VG_r150 agertz lu2023-2-68 62% 2024-05-12T09:43:40 18:03:26 5 240 cn
637896 lu48 VG_hires agertz lu2023-2-68 79% 2024-05-12T20:30:00 4:49:46 5 240 cn
ParaView 5.11.1
ParaView 5.11.1 (on cg15)
SLURM Job monitor


Applications
Places
System
Wed Jan 17, 16:24
HPC Tools
Programming
Jupyter
Matlab
Pymol
Quantum ATK
Rstudio
VMD
Computer
student10's Home
Trash
NLHPC Videos
firefox
Mate Terminal
Edit View Search Terminal Help
dent10@thinlinc ~]$
Mate Terminal


Applications
Run Program...
Terminal Emulator
File Manager
Mail Reader
Web Browser
Settings
Accessories
Cluster Software
Development
Education
Graphics
Internet
Multimedia
Office
System
Log Out
Comsol
Fluent
Gaussview
Matlab
Rstudio
Stata
Tecplot
Totalview
VMD
Windows 10
PURDUE
UNIVERSITY


NoMachine - Connection to nxcloud01.nersc.gov
Terminal
File Edit View Search Terminal Help
other systems will be impacted.
---------- Past Outages ----------
Cori: 05/31/20 13:00-14:29 PDT, System Degraded
Cori cabinet c1-4 has lost power. Some jobs have crashed, but
most running jobs are not affected. New jobs will not start.
Our engineers are working on solving the issue.
Cori: 05/31/20 14:30-23:08 PDT, Unavailable
Cori had a hardware failure and all jobs on the primary system
have been stopped. Cori will be available after a system
reboot. Cori external nodes and login nodes are available.
For past outages, see: http://my.nersc.gov/outagelog-cs.php
11:30 sleak@cori10:H/~$ xterm &
[1] 63310
11:31 sleak@c
t "-misc-fixed-medium-r-semiconden
sed-*-13-120-
xterm: cannot
*-13-120-75-75-C-60-ISO8859-1"
sleak@cori10:~ (on cori10)
RSC

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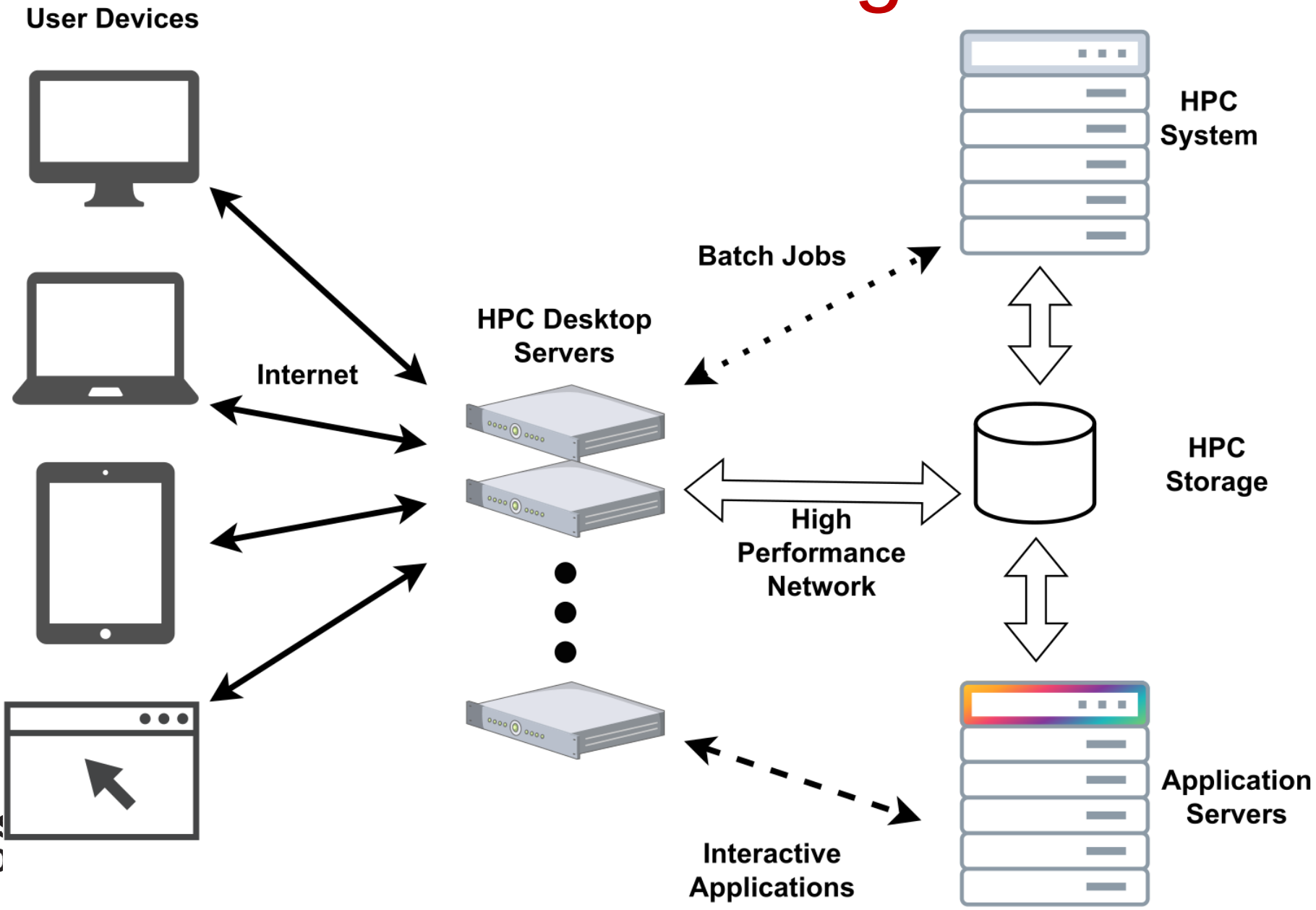
Capabilities of an HPC Desktop

- Guiding principle for the desktop: Convenience over Efficiency
- Desktops provide an environment for light computational and data management work outside of the HPC system.
  - Application servers can support the desktop.
- Leverage the power of HPC infrastructure as much as possible.
  - Network, storage, applications, people, …
- Desktop customizations are key for the user experience.
  - Application menu, desktop icons, storage shortcuts, GFXLauncher
- Policies that enable long running applications and a persistent environment.
- But wait… isn't there Open OnDemand?!

Hardware Configuration



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Use Cases

- Based on 10 years of operation at IU, LU and DTU.

Use Cases: File Manager

- File managers are a game changer for new users
  - Nobody gets the concept of “run a command to do something with 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
- The pitfall of “trash” and “.snap”

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
- GfxLauncher to simplify “job submission”, “Interactive Job” icon
- “ml-browse” tool for module selection
- Graphical development tools, IDEs, debuggers, performance tools
- Preview of job results

Use Cases: Teaching and Learning

- Intro to HPC classes
- 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, ABAQUS CAE,…
- Visualization software

Use Cases: Secure Enclaves

- Graphical secure enclaves
- ePHI / HIPAA, FISMA, NIST 800-171/53

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Let’s Dream – The Future

- What if we exposed robust compute and storage infrastructure using old and new desktop metaphors.
  - User interface design students took on the Research Desktop…
  - Chat bot integrated into the shell.
  - “OS/2 Warp 4 WarpGuide”
- Test out modern Linux desktop environments
  - Modern GNOME makes heavy use of extensions for every desktop function, why not expose some HPC functions that way?
- “Recently run jobs” in the file manager
- “Run In Batch” context menu entry
- “Archive” functionality with metadata collection
- Browse HPC help from the desktop

Build an HPC Desktop Community

- Everything you have heard about is open source and available.
  - But is it findable?
- How about an “All Things HPC Desktop” repository.
  - Share technical recipes
  - Also share statistics scripts and use cases, to make it easier for an institution to get started and justify the investment of time and money.

https://github.com/RobertHenschel/ResearchDesktop

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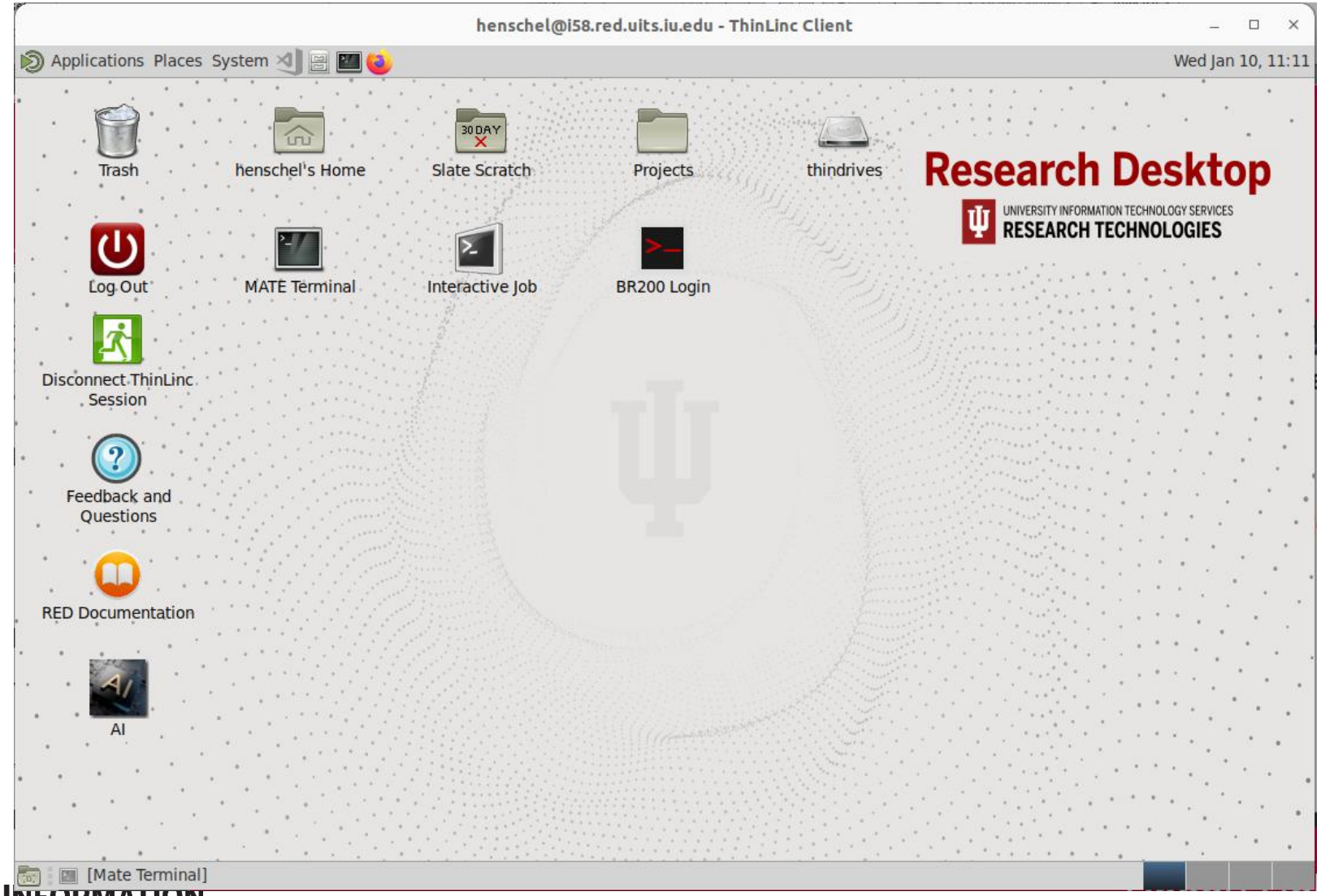
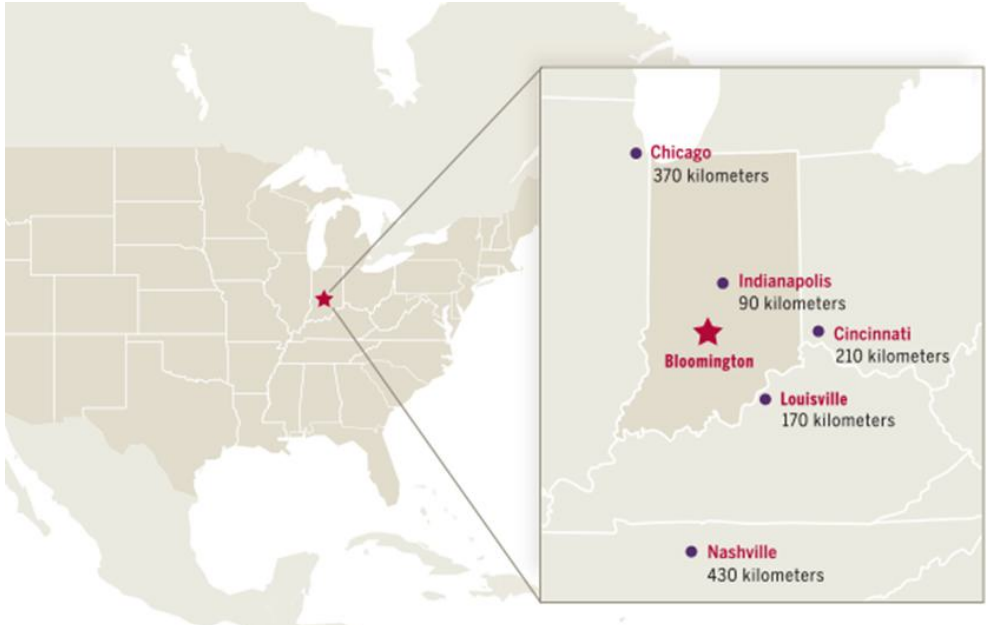
IU Research Desktop



Indiana University



Fall 2022	Number
Research Campuses	2
Regional Campuses	7
Undergraduate	71,000
Graduate + Doctoral	19,000
Total Students	90,000
Staff	11,000
Faculty	9,000
Grand Total	110,000

Overall

- Founded in 1820
- Annual operating budget - $4B
- Grant Awards of $772M in 2023

Centralized IT - UITS

- 650+ professional staff
  - 100 Research Technologies
- 500+ part time staff

HPC @ Indiana University

- **Quartz** – HPE/Cray system; 92 dual CPU nodes; 36 4-way V100 GPU nodes
- **Big Red 200** – CRAY Shasta system; 640 dual CPU nodes; 64 4-way A100 nodes
- **Research Desktop** – Dell servers; 30 dual CPU servers

- **Jetstream 2** – NSF's second production cloud environment, main system at IU and small regional clouds in 4 regions. 8 petaflops of VM capacity (CPU + GPU)

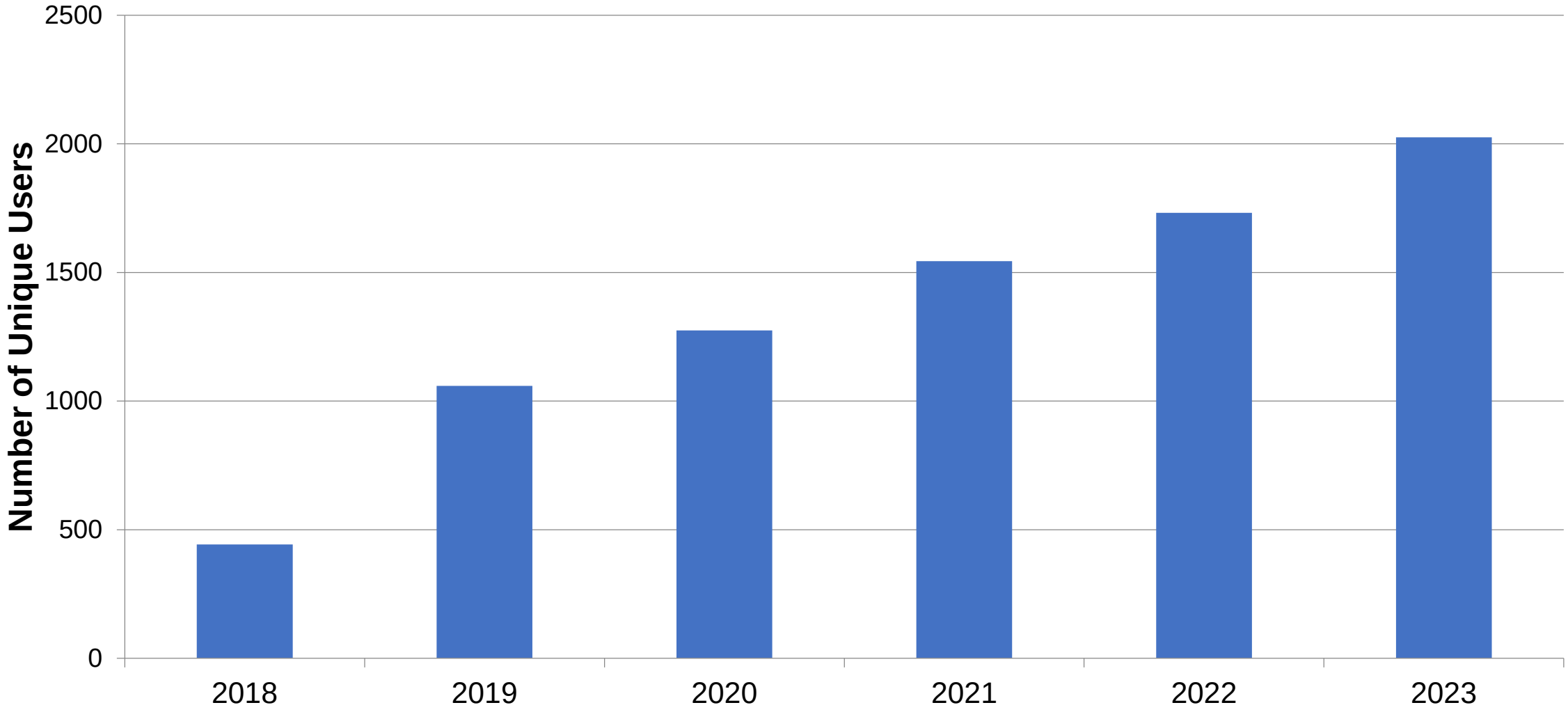
History

- Research into desktops started in 2013.
- Launched as “Karst Desktop” in 2015.
- Closed Beta for 6 months, open beta for 2 years.
- General Available since July 2017.
- Renamed to Research Desktop in August 2018.
- Expanded into OpenStack managed VMs in 2021.
- Migration to new hardware and VMs in 2023.

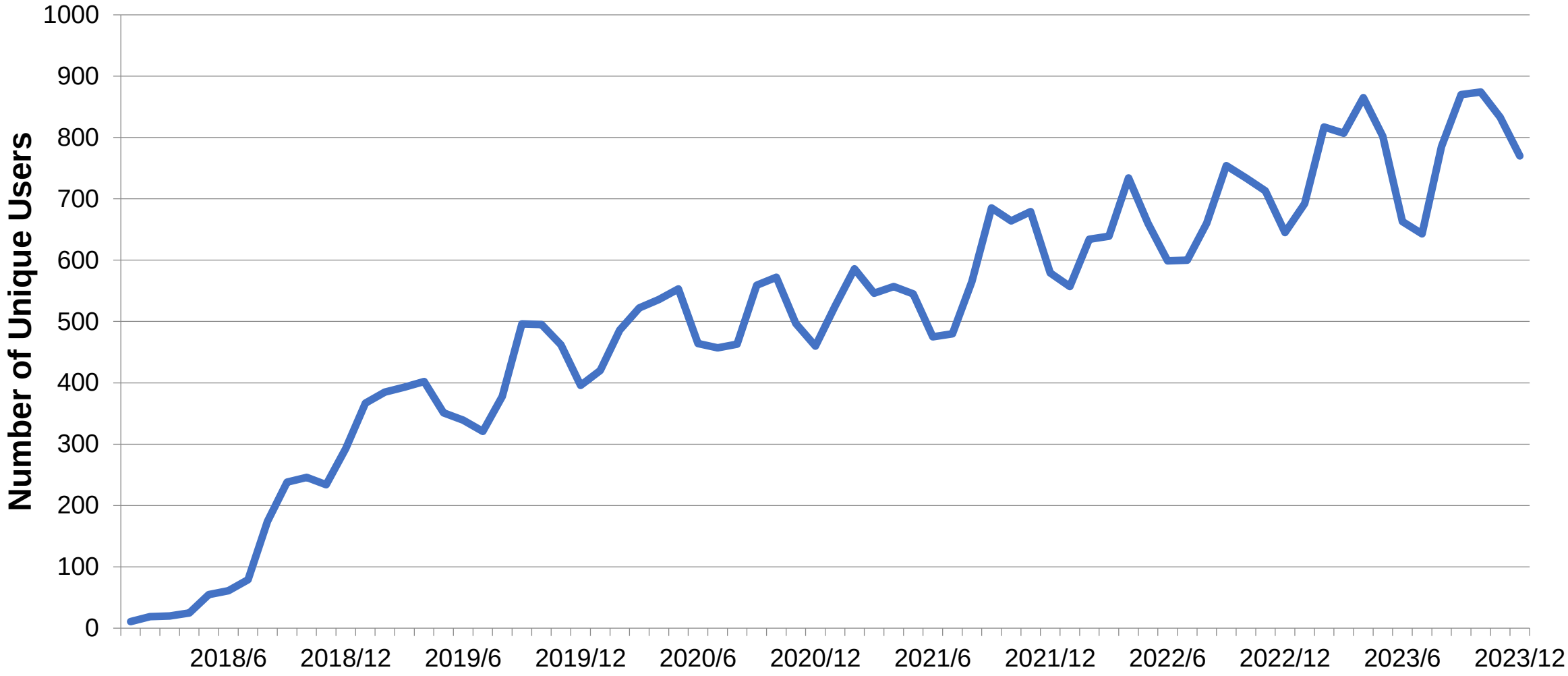
Policies and Customizations

- 100 GB of RAM per user session.
- Soft limit of 8 cores per user.
- Long runtime of disconnected sessions. (7 days)
- Only full desktops, only one desktop environment, only one session per user.
- An interactive systems needs more care and feeding than a batch system.
- Custom desktop (wallpaper, menus, icons)
- Tools
  - Request/Help form
  - Batch system GUI
  - Interactive job icon/tool
  - rclone for cloud storage
- Usage statistics scripts

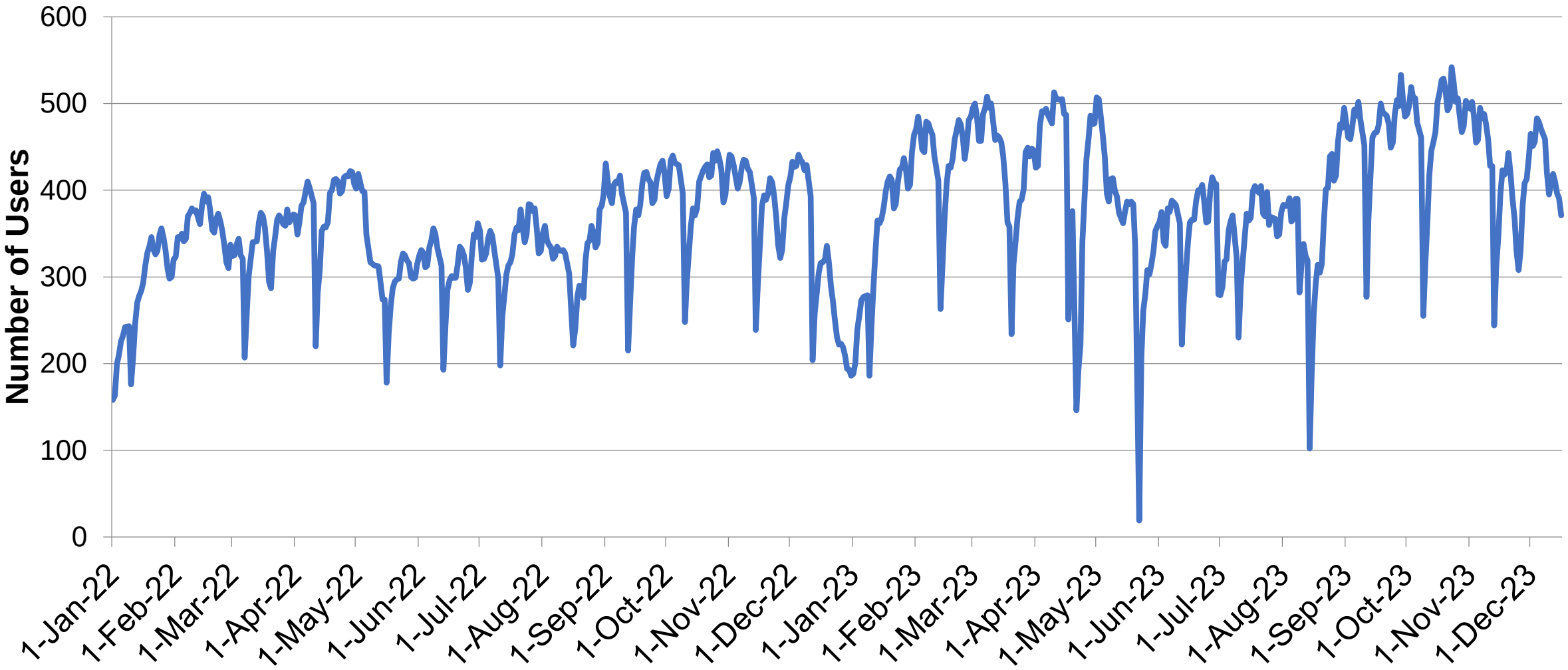
RED - Yearly Unique Users



RED - Monthly Unique Users



Red – Daily Active Users



Thank you!