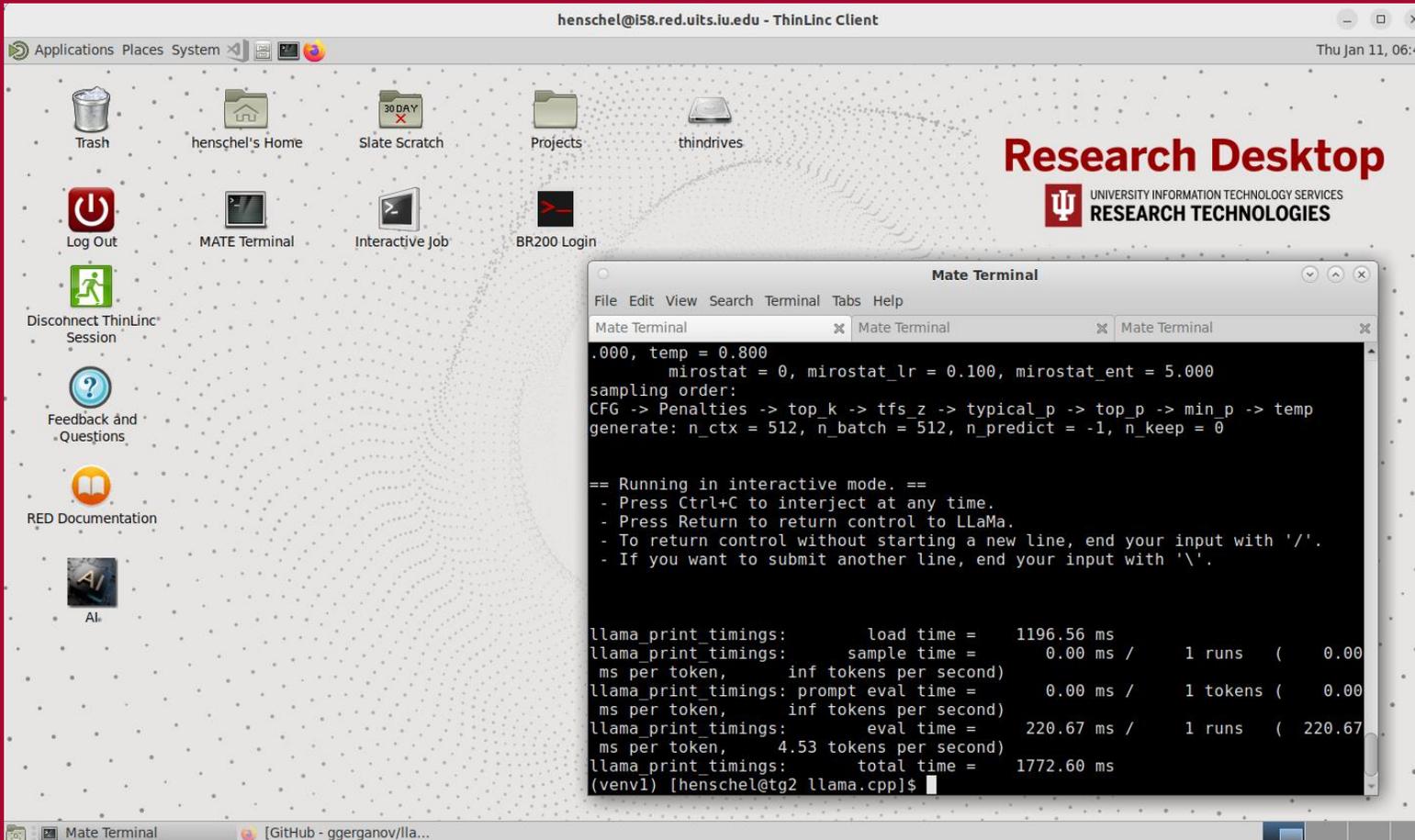


# The Research Desktop



Robert Henschel

Project Director, Research Engagement

Research Technologies

[henschel@iu.edu](mailto:henschel@iu.edu)



UNIVERSITY INFORMATION  
TECHNOLOGY SERVICES

# Thank you!

Sunita and Samantha

## Questions:

- Have you used a Linux desktop?
- How have you used HPC? (researcher, operator, educator,...)

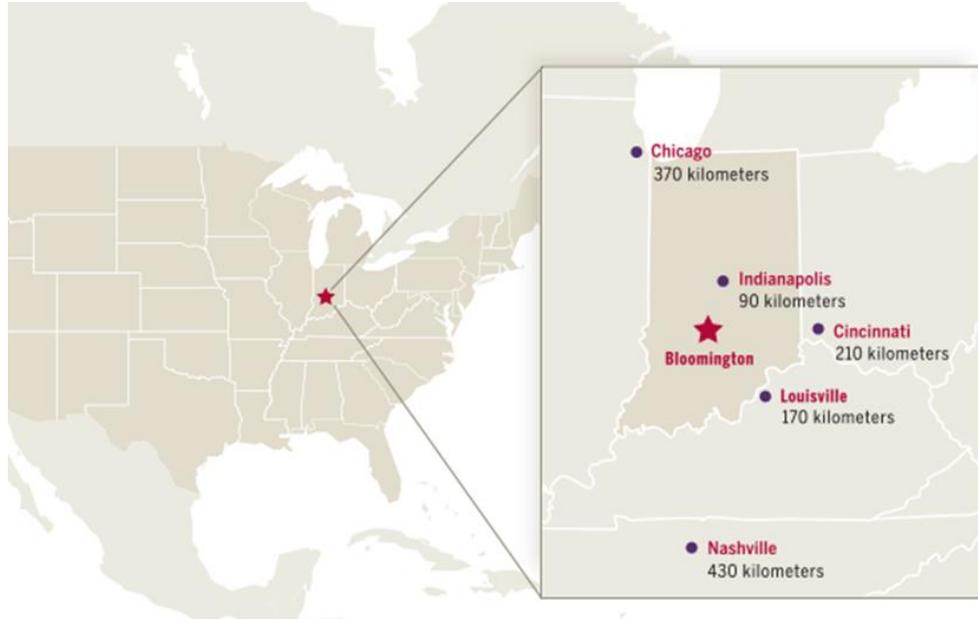
# The next hour...

- Introduction
- Motivation for creating a Research Desktop
- Definition and History of the Research Desktop
- Current State and Future Developments
  
- Q&A and Demo

# Introduction

- 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.
- Trying to cover everything that I promised in the abstract of the talk, but always open for questions!

# 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

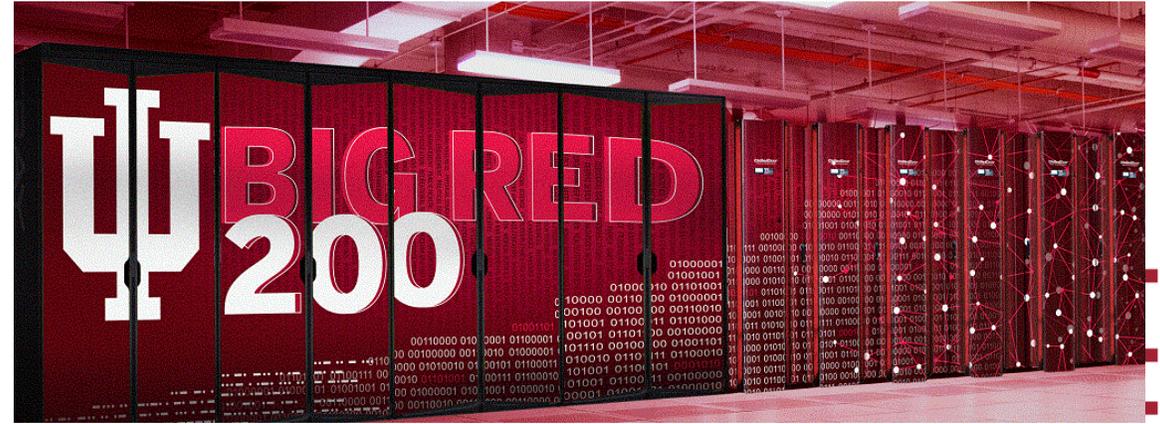
# HPC @ Indiana University

- **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; 34 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)

# The next hour...

- Introduction
- **Motivation for creating a Research Desktop**
- Definition and History of a Research Desktop
- Current State and Future Developments
  
- Q&A and Demo

# History of Supercomputing



# History of Supercomputing



```
henschel@login1:~$ cat /etc/passwd | grep henschel
henschel:x:1000:1000:~:/:bin:/usr/sbin/crontd
henschel@yourhost:~$ ls
backup bin documents downloads images music templates tmp videos
henschel@yourhost:~$ ls -l
total 36
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 backup
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 bin
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 documents
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 downloads
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 images
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 music
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 templates
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 tmp
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 videos
```

```
henschel@login1:~$ cat /etc/passwd | grep henschel
henschel:x:1000:1000:~:/:bin:/usr/sbin/crontd
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backup bin documents downloads images music templates tmp videos
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drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 downloads
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 images
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 music
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 templates
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 tmp
drwxr-xr-x 2 yourname yourname 4096 Apr 30 21:17 videos
```

# History of Desktop Computing

```
File Edit Search Layout Mark Tools Font Graphics Help (Press F3 for Help)
IN CONGRESS, JULY 4, 1776
The unanimous Declaration of the thirteen united States of
America

When in the Course of human events it becomes necessary for one
people to dissolve the political bands which have connected them
with another and to assume among the powers of the earth, the
separate and equal station to which the Laws of Nature and of
Nature's God entitle them, a decent respect to the opinions of
mankind requires that they should declare the causes which impel
them to the separation.

We hold these truths to be self-evident, that all men are created
equal, that they are endowed by their Creator with certain
unalienable Rights, that among these are Life, Liberty and the
pursuit of Happiness. - That to secure these rights, Governments
are instituted among Men, deriving their just powers from the
consent of the governed, - That whenever any Form of Government
becomes destructive of these ends, it is the Right of the People
to alter or to abolish it, and to institute new Government,
laying its foundation on such principles and organizing its
powers in such form, as to them shall seem most likely to effect
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```

# History of Desktop Computing

File Edit Search Layout Mark Tools Font Graphics

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powers in such form, as to them shall seem most

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Microsoft Word - README.DOC:2

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### Additional Information About Microsoft Word for OS/2

Since the publication of the *Microsoft Word User's Reference*, additional information has become available. This document contains that information, organized into sections. To see a particular section, use the table below. At the end of many topic titles, you will find a list of page numbers, which refer to pages in the *User's Reference* on which the topic is described.

For a list of	Double-click the box or select box and press Alt+Shift+F9
Important information	<input type="checkbox"/>
Corrections to the <i>User's Reference</i>	<input type="checkbox"/>
Additional printing information	<input type="checkbox"/>

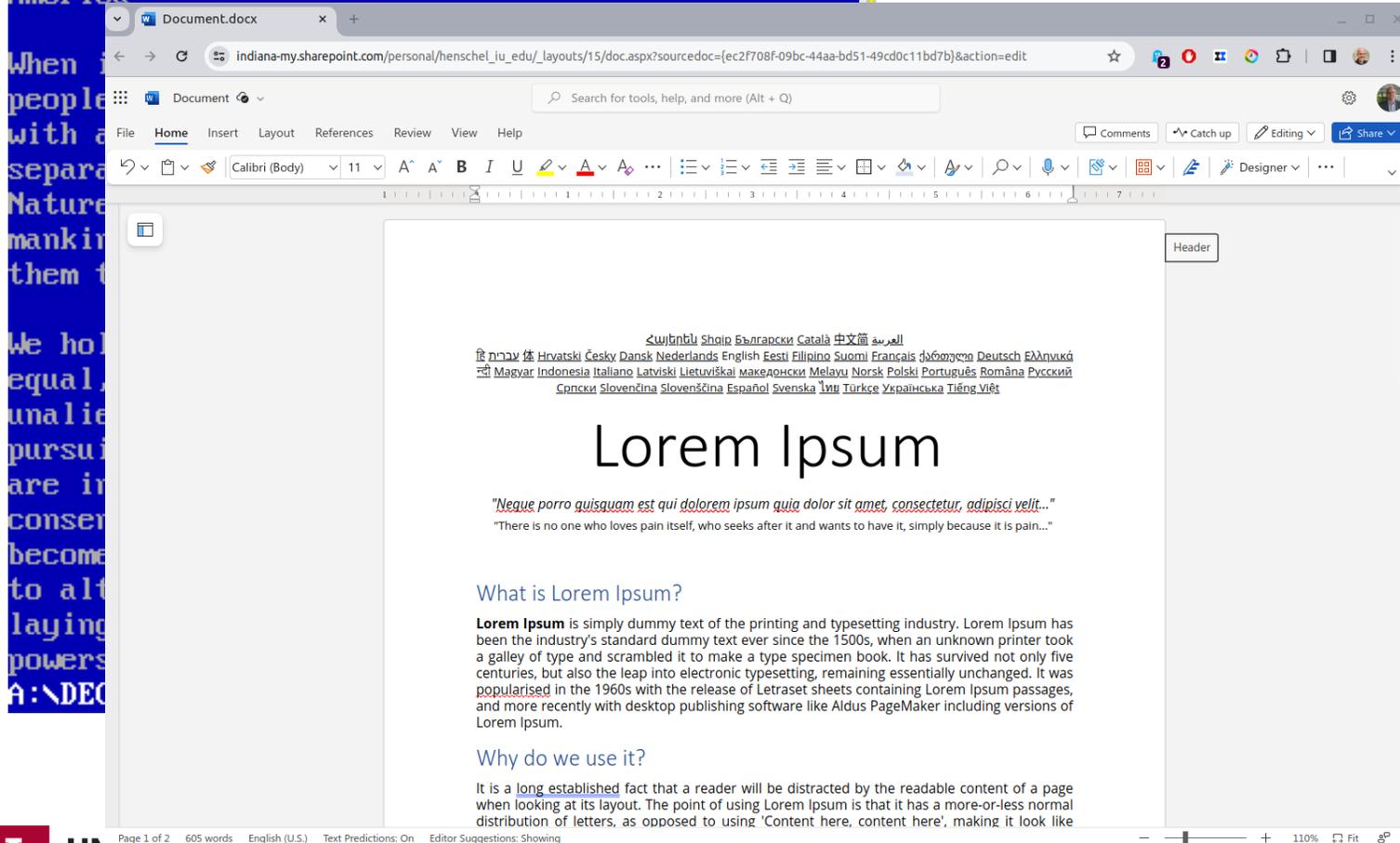
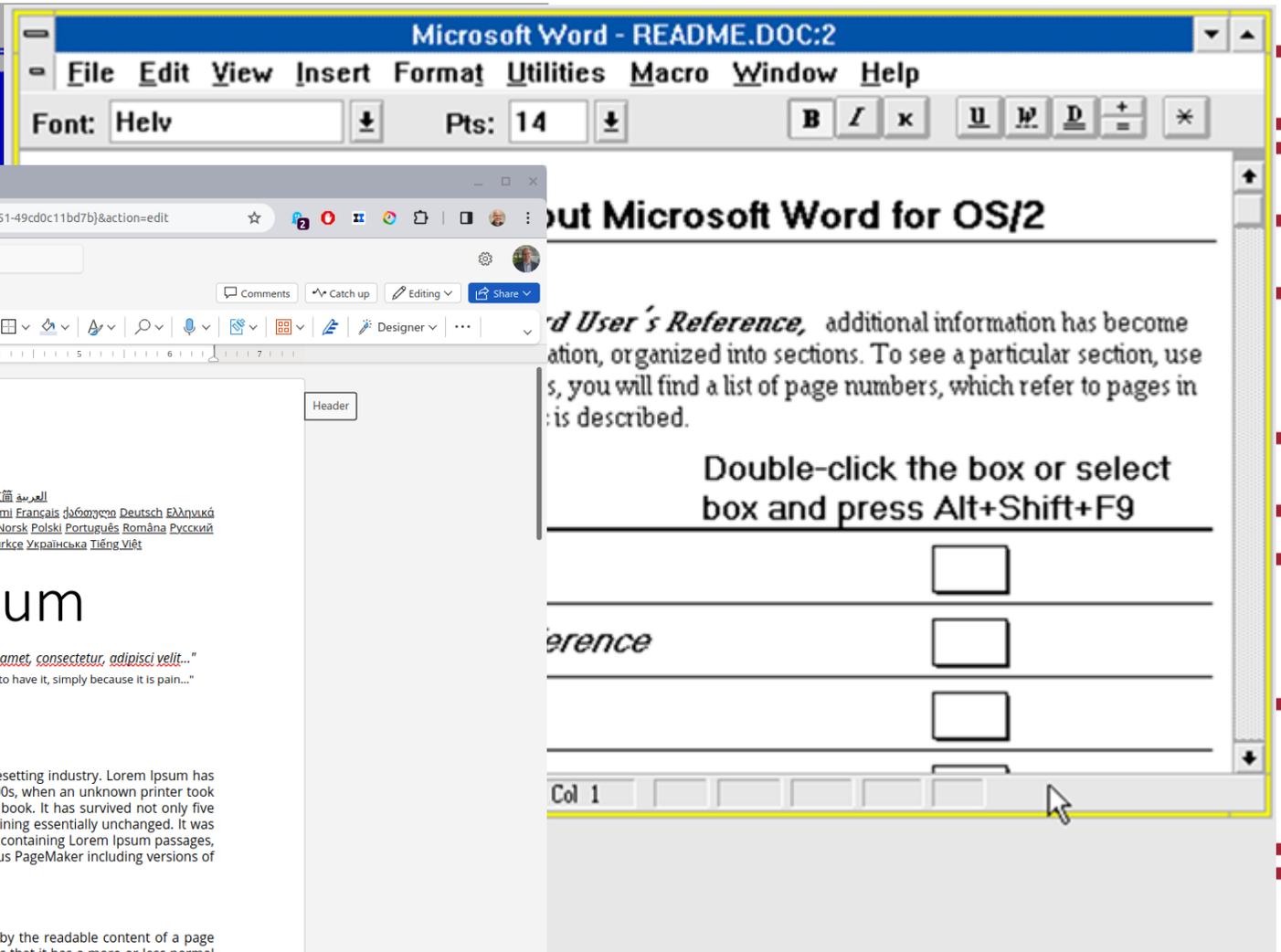
Pg 1 Sec 1 l/ 15 At Ln Col 1

DOS Group - Main

# History of Desktop Computing

File Edit Search Layout Mark Tools Font Graphics

IN CONGRESS, JULY 4, 1776  
The unanimous Declaration of the thirteen united  
America



# Expectations

- Today, new users are coming with a **different skill set than 10 or 20 years ago.**
- What do “new users” really want and what do HPC centers offer?
  - Change in workload for HPC systems.
- IU has an open access policy for all HPC systems, thus needs to support a very diverse user base. IU experiences this problem sooner than others, and at a higher magnitude.

# Leveraging HPC for Research Computing

- **Competing with cloud providers** PR is hard. Their sales pitch is very convincing and should not be underestimated!
- HPC centers have to **balance convenience and efficiency**.
- Can HPC centers provide what new users really want? Can HPC centers create something that is truly compelling, both from a performance point of view and a convenience point of view... and that also offers a path to efficient HPC usage?

# Summary: Motivation

- Attract more users and new users.
  - Broaden the reach of HPC systems.
  - Lower the barrier of entry.
- Offer a service that users truly want to use.
- Stay relevant in the era of cloud computing.
- Graduate Research Desktop users to HPC users and train the next generation of HPC users.

# The next hour...

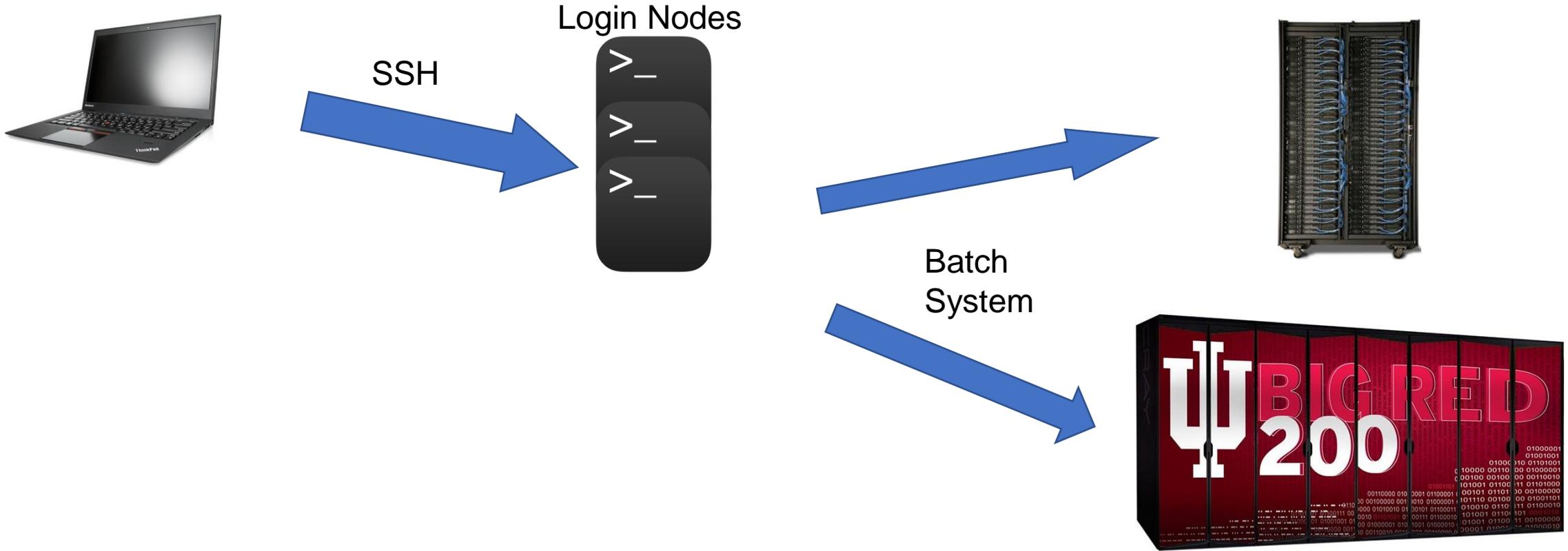
- Introduction
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# Challenge: Research Desktop

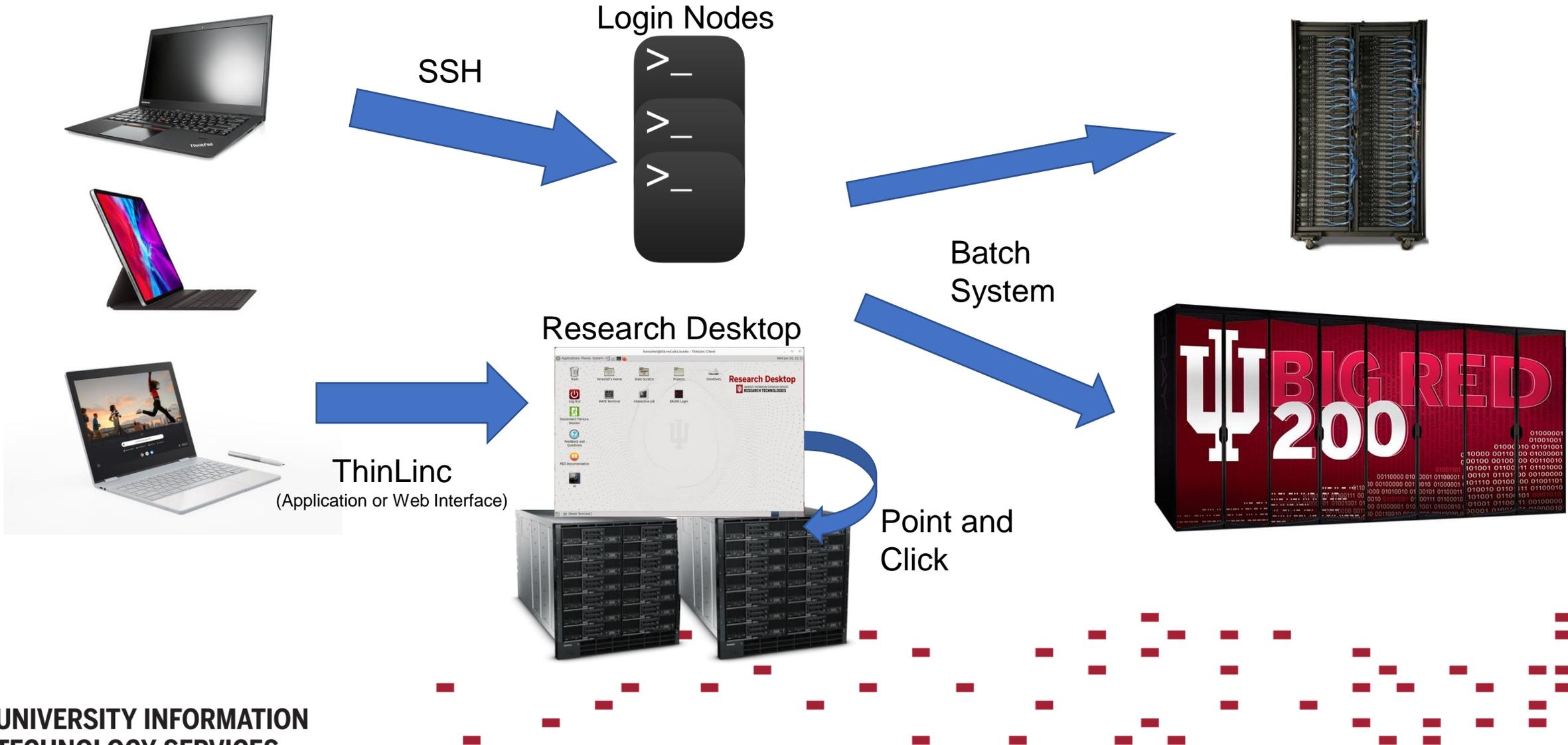
What if you had access to a **high performance desktop from any endpoint device**? What if this desktop allowed you to **launch interactive graphical applications** like MATLAB, Jupyter Notebooks, Ansys and VS Code, as well as **compose scientific workflows** using graphical and command line tools? What 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 2017 and is evolving it ever since.

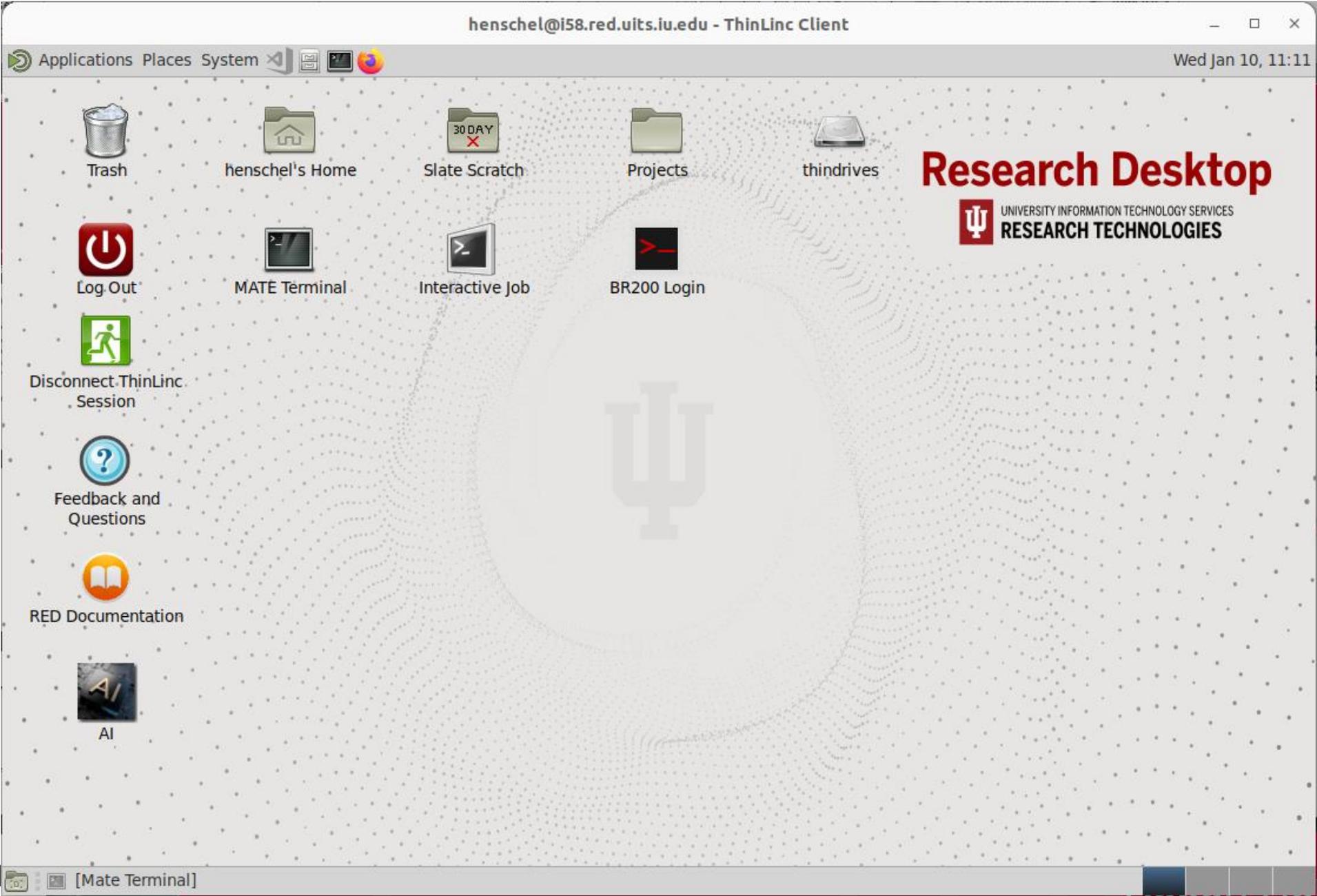


# Architecture (HPC)



# Architecture (HPC + RED)





# History

- 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.

# History (cont'd)

- Desktop servers increased from 10 to 34.
- Concurrently active users increased from 100 to 530.
- Upgrade from RHEL 6 to 7 to 8 (GNOME 2.28 to MATE).
- Substantial customization:
  - Heavily customized desktop
  - rclone for cloud storage (Google Drive, Box, DropBox, OneDrive,...)
  - Zenity for graphical dialogs
  - Dynamic cgroups CPU limits
  - Usage statistics scripts
- Enabling web interface and 2-factor authentication.

# 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 (background, menus, icons)
- Tools
  - Request/Help form
  - Batch system GUI
  - Interactive job icon/tool
  - rclone for cloud storage
- Usage statistics scripts

# Summary: Definition and History

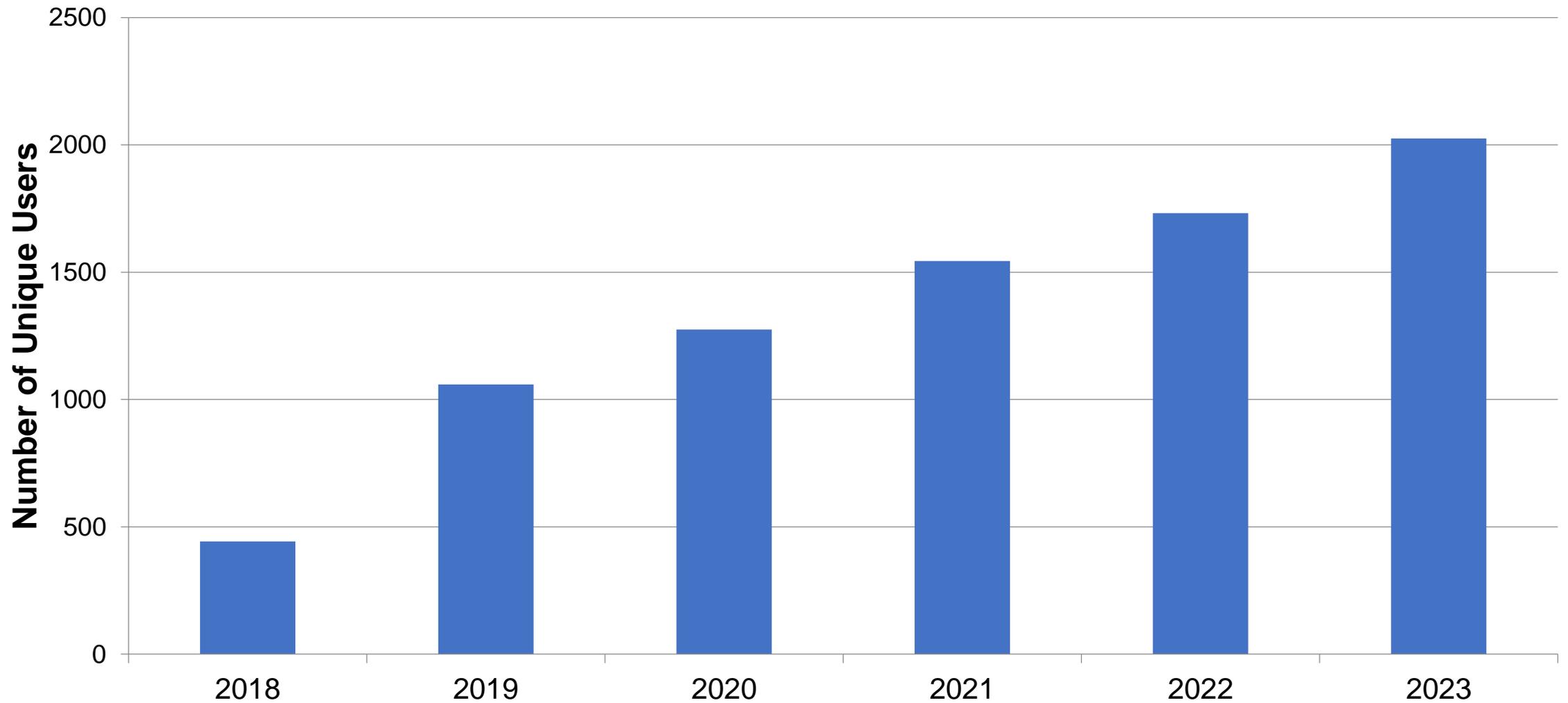
- The Research Desktop is “a place where you want to do all your computational research”.
  - Convenient enough that you want to use it every day.
  - Performant enough that it can handle most demanding workflows.
- Growing service at IU - default way how to access IU HPC systems.
- Always trying new things, new customizations, new opportunities, new use cases.



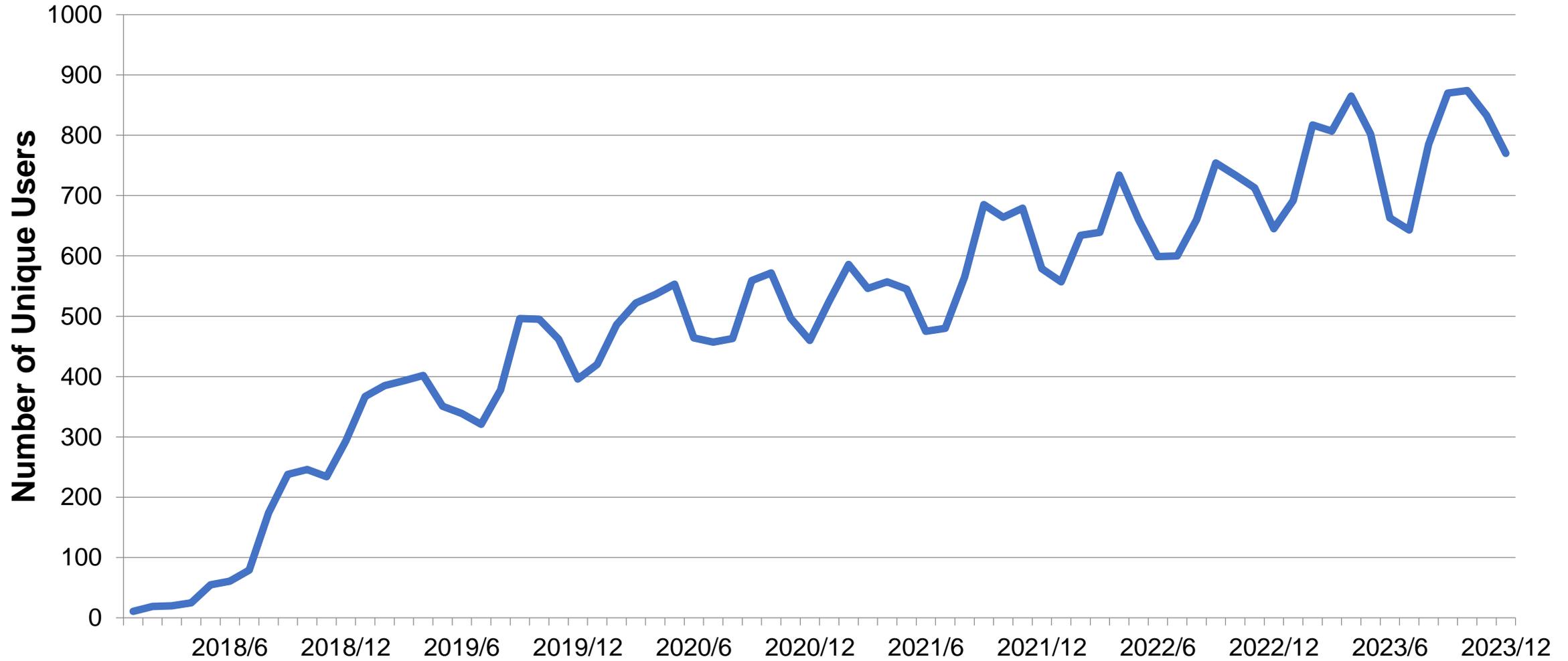
# The next hour...

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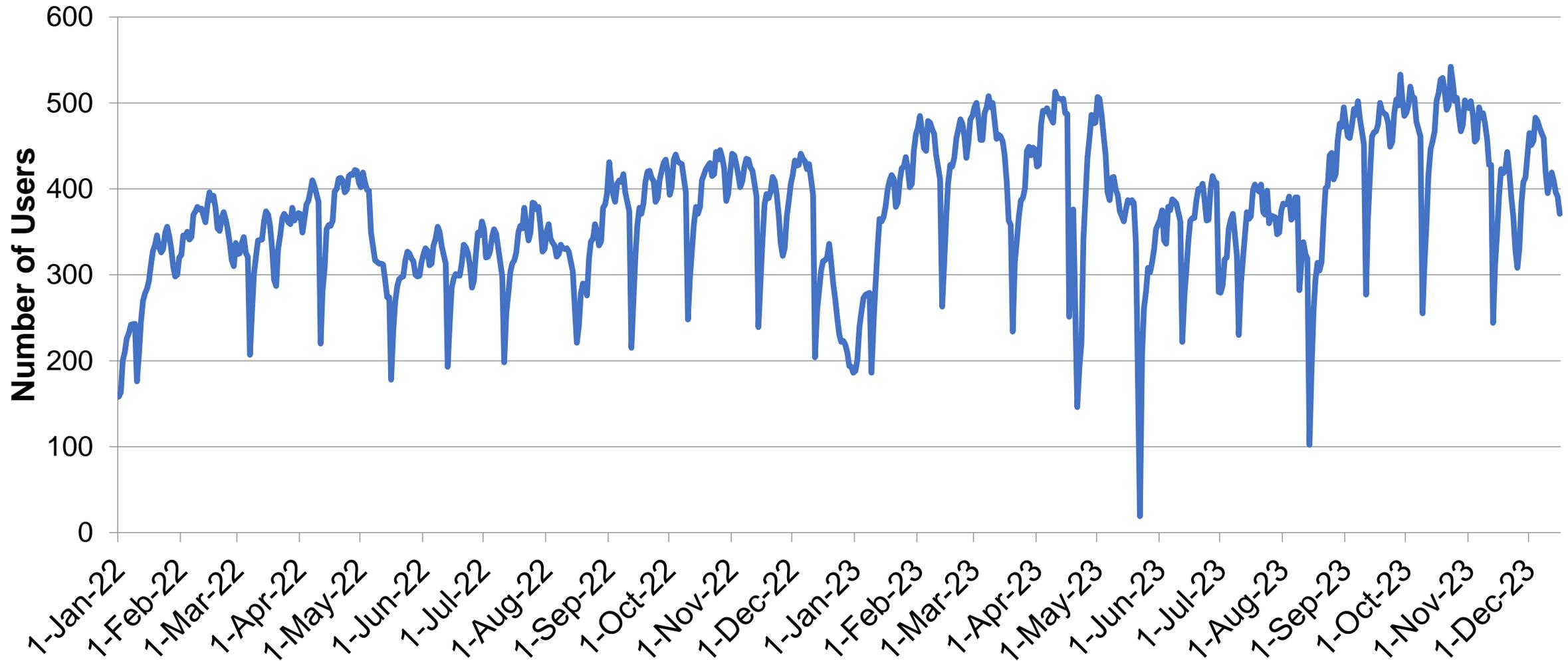
# RED - Yearly Unique Users



# RED - Monthly Unique Users



# Red – Daily Active Users



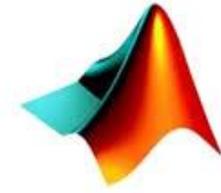
# Use Cases

- Mathematical and statistical applications like SPSS, SAS, STATA, MATLAB
- Graphical tools, IDEs, etc.
- Visualization applications
- GUIs of HPC performance analysis applications such as Vampir, Allinea MAP, TotalView
- Client/Server applications like COMSOL Multiphysics, Schroedinger, Ansys
- Replacement for screen / nohup
- Teaching (Easy access to compilers and editors for classes)
- HPC training
- Secure Data Enclave (FISMA and HIPAA)
- Long running data movement jobs
- Support collaboration across institutions
- User Support



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MAP

R Studio®

 MATLAB®

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PERFORMANCE  
REPORTS

R

jupyter

Wolfram  
Mathematica®  


sas

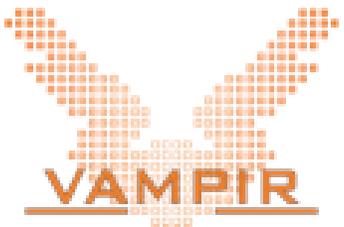
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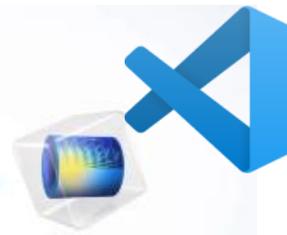
 TOTALVIEW  
TECHNOLOGIES

python™

VMD  
Remote

SPSS®

 VAMPIR

COMSOL  
MULTIPHYSICS®  


 Schrödinger

# Research Desktop vs. HPC vs. OOD

Category	Research Desktop	HPC	OOD
Run text mode applications	Run in terminal	Write batch script, submit to batch system	Batch job via Web UI
Run Graphical applications	Pick application from menu	X11 Forwarding SSH connection + X11 Forwarding batch jobs + X-Server on client	App in Web UI
Up/Download files	File browser / ThinDrives	SCP, SFTP	Web UI for upload/download
Edit text documents	Any Linux editor	VI/EMACS/NANO	Build in editor
Look at images, PDFs	Double click in file browser	X11 Forwarding	App in Web UI
Run multiple applications	Just launch them on the desktop	Separate batch jobs	Separate tabs in the browser
Long running application	Launch, disconnect/reconnect	Batch job, tail output file	Batch job, observe output file



# The Future - Building a Community

- Explore new concepts of how to integrate an HPC system into a modern desktop environment. (GNOME 3 and extensions, gfxLauncher, VirtualGL)
- Interactive and Urgent HPC workshop/BoF at SC and ISC.
- IEEE CiSE special issue paper:
  - Interactive And Urgent HPC: Challenges And Opportunities
  - <https://arxiv.org/pdf/2401.14550.pdf>



# Summary: Today and Tomorrow

- Growing service at IU - default way how to access IU HPC systems.
- New use cases every year.
- Explore new Desktop environments and abstractions for HPC.
- International movement for more “interactive HPC”.
  - Community building
  - Maybe UD should join the community?

# The next hour...

- Introduction
- Motivation for creating a Research Desktop
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- Current State and Future Developments
  
- **Q&A and Demo**

# Q&A and Demo

- Connect
- Applications in menu, VS Code
- How to import data using ThinDrives
- Disconnect / Reconnect with web app
- Modules
- Connect to BigRed 200
- Interactive Job