



HOLLAND COMPUTING CENTER

hcc.unl.edu

Hongfeng Yu, Director
HCC Kickstart 2022

HCC Provides High-Performance Research Computing Resources for University of Nebraska and Beyond



NU Supercomputing Core

- ~ 100 departments NU system-wide
- ~ 250 research groups
- > 1,700 active users
- > 7 million CPU-hours each month
- ~36,500 cores, 23 PB storage, 100 Gbps to Internet2
- 134 GPUs including 52 NVIDIA V100

Access to HCC machines is **primarily shared and free**

- Usage is accounted per research group (professor)
- This necessitates waiting in queue

Immediate access is available for a priority access fee

Opportunistic access is available to all idle HCC resources

7 system administrators, 5 applications specialists, 2 research personnel, 1 outreach/training specialist, 1 web and database analyst

- 8 PhDs
- Staff members provide expertise for code porting, parallelization, data intensive workflow deployment

HCC Facilities



Schorr Center

- 2200 sq. ft. machine room
- 240 kW
- 12 full-time staff
- 100 Gbps network



Scott Engineering Center (SEC)

Data Center

- 3110 sq. ft. machine room
- Twelve racks of space for HCC
- 95 kW allocated to HCC
- 100 Gbps network



Peter Kiewit Institute (PKI)

- 1800 sq. ft. machine room
- 310 kW
- 4 full-time staff
- 100 Gbps network
- 100 Gbps to Schorr



HCC Facilities



Schorr Center



Red

- US CMS project
- Open Science Grid (**OSG**)
- Over 11 PB storage (CEPH)
- Over 15,000 job slots
- No interactive login accounts



Scott Engineering Center (SEC) Data Center



Silo

- Mirror of Attic
- 3 PB storage



Peter Kiewit Institute (PKI)

Crane

- Analysis and numerical exploration
- > 122 TeraFLOPS
- 10,640 cores
- 1.5 PB (raw) Lustre Storage
- 52 NVIDIA V100 GPUs



Swan

- 8,320 cores
- 5,300 TB Lustre Storage
- 12 nodes each with 2 NVIDIA Tesla T4 GPUs
- 2 high memory nodes



Anvil

- OpenStack Cloud machine
- 1,440 cores
- 532 TB storage (CEPH)



Attic

- 3 PB nearline archive storage fully replicated back to Lincoln in Silo
- Accessible via Globus, rsync, sftp
- 25 Gbps transfer node front end



Common

- Transparent file access between all HCC resources
- 1.9PB storage (BeeGFS)

HCC Ongoing Upgrades

FY22-23



Replacing Common storage



Developing new storage solution NRDStor (Nebraska Research Data Storage)

- Funded by NSF CC* award
- Accessible on HCC's computing clusters
- Mountable by NU researchers on their lab computers and laptops



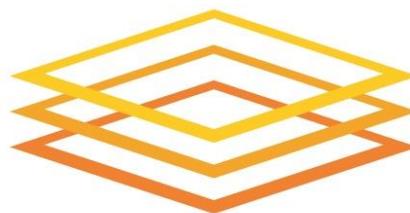
Plan to upgrade Anvil OpenStack cloud resource



- Incorporate faculty researchers' feedback
- Sponsored by UNL Office of Research & Economic Development (ORED), Nebraska Research Initiative (NRI), and National Science Foundation (NSF)

What We Provide

- **Free shared resources** to all NU students, staff and faculty
- Resources maintained by HCC's System Administrators
 - Dedicated computing resources, extended storage and personnel effort available for a fee
- Education
 - hands-on workshops
 - classroom tutorials and course support
 - individual group training
- Consultation
 - research computing facilitation
 - workflow and data management
 - grant preparation
- Extended computing resources offered through partnerships with:



Open Science Grid

High Throughput (Grid) Computing
spanning over 130 institutions nationwide



Petascale HPC Computing, Training and
Collaborative Support Service



HyperScale Kubernetes
GPU Cluster for parallel
machine learning
research

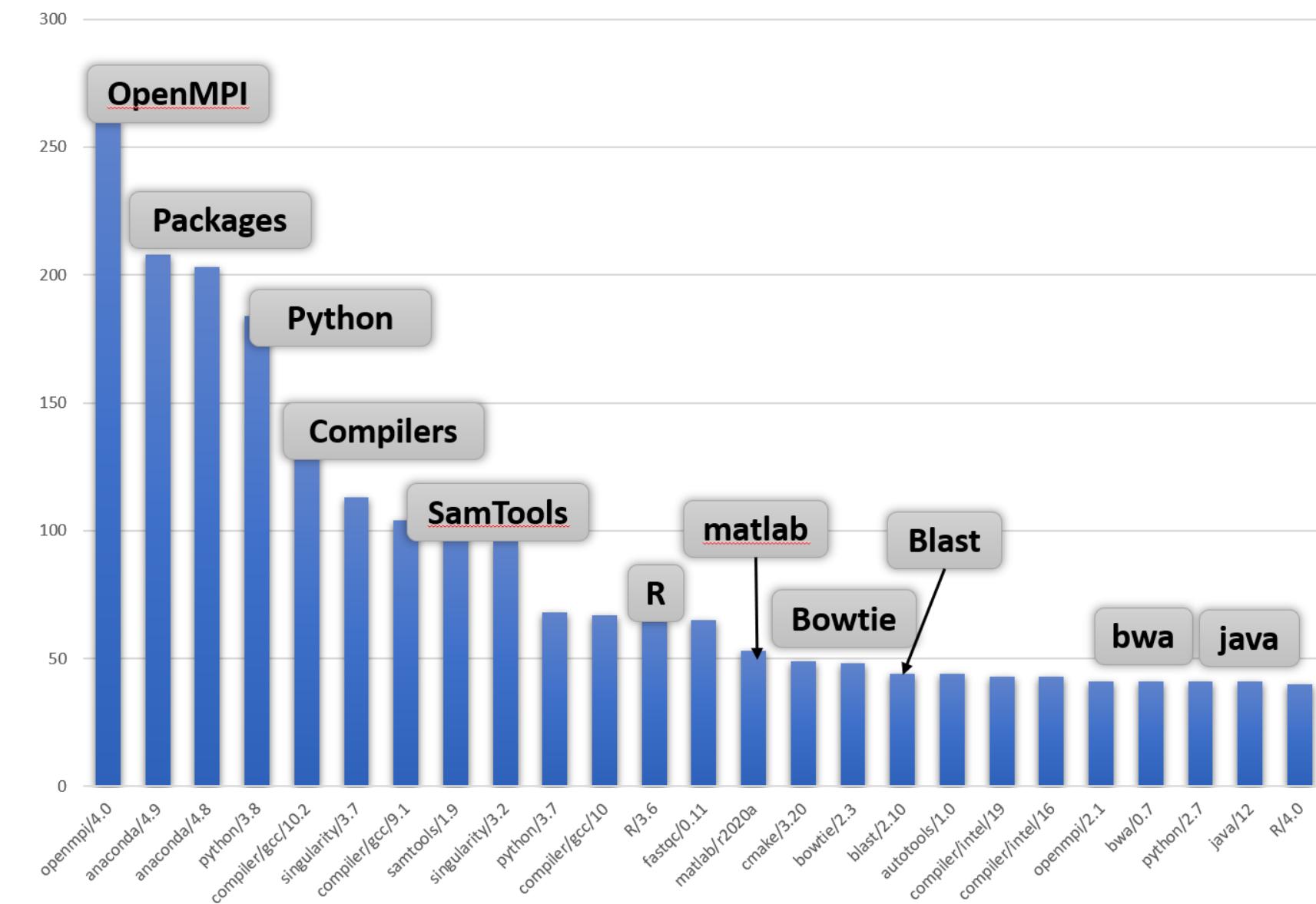


National, All-in-one system
for computing, research and
education resources to
expedite science

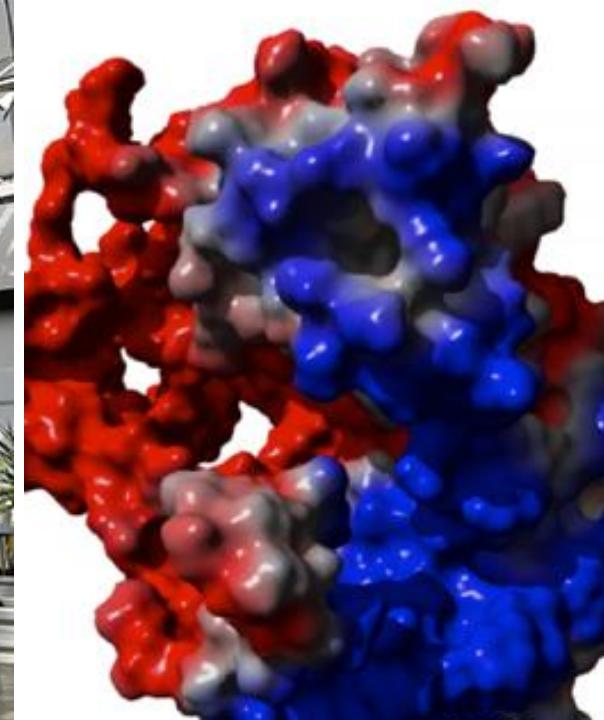
User Diversity at HCC

As of Aug 2022:

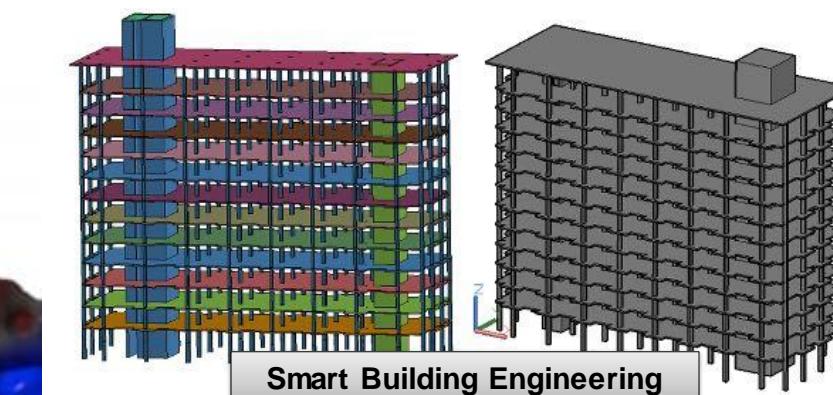
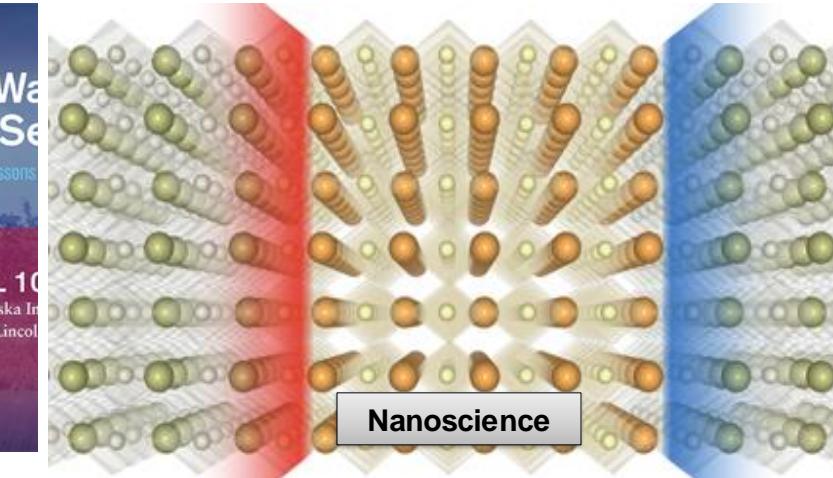
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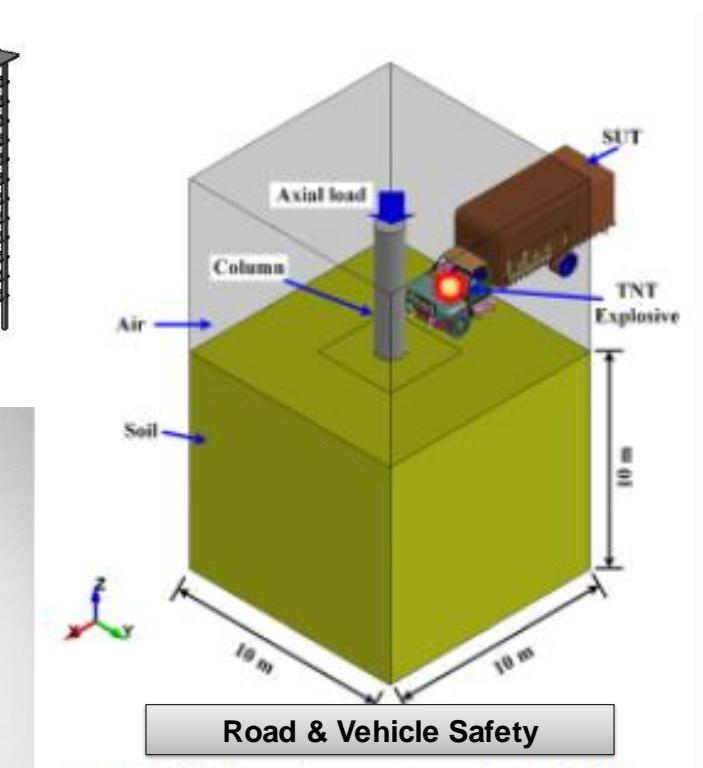
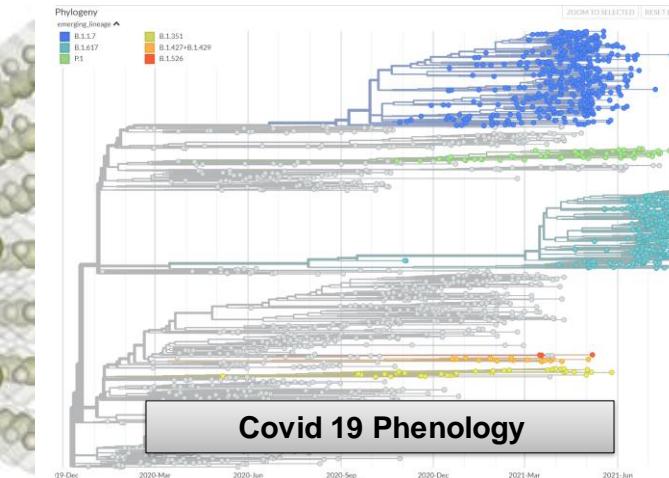
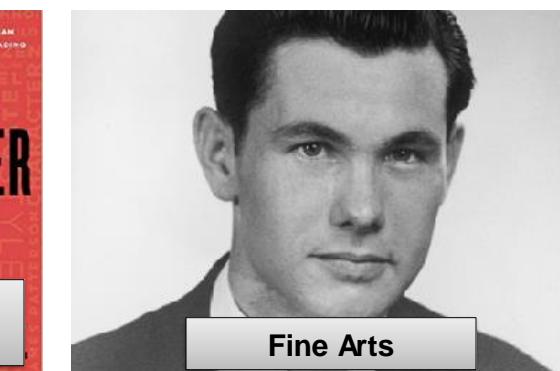
Research at HCC



High Throughput Computational Drug Screening



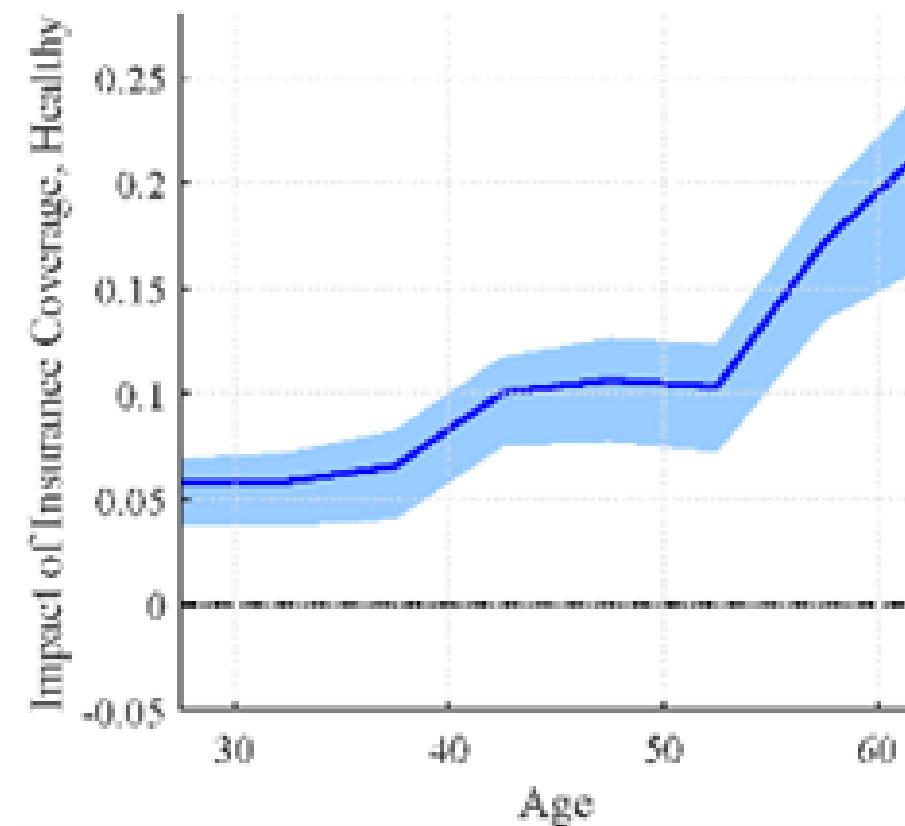
Digital Humanities



Research at HCC

Examples: Computational Method for Designing Optimal Health Insurance

Prof. Zhigang Feng



Develop quantitative theoretical models to study how private sectors (including households and businesses) response to government's policies (e.g., tax policy and health care policy)

- Use the computing facility at HCC to analyze large-scale national data
- Simulate the economic behaviors of millions of American households and businesses with diverse social-economic characteristics
- Lead to novel finding on social welfare, income inequality and health disparity

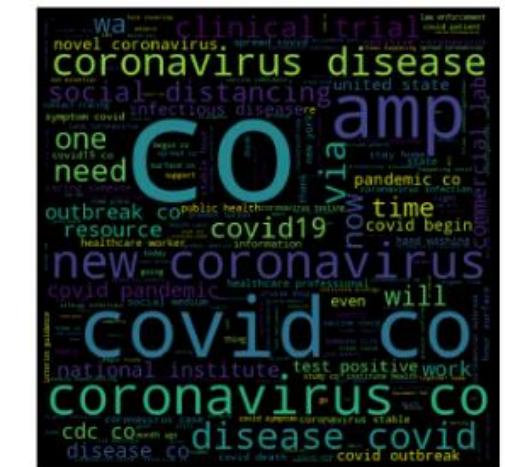
Research at HCC

Examples: Machine Learning Enhanced Social Media Analysis

Prof. Mohammad Hasan

Explore the frontier of machine learning and deep learning by leveraging HCC resources, in particular GPUs

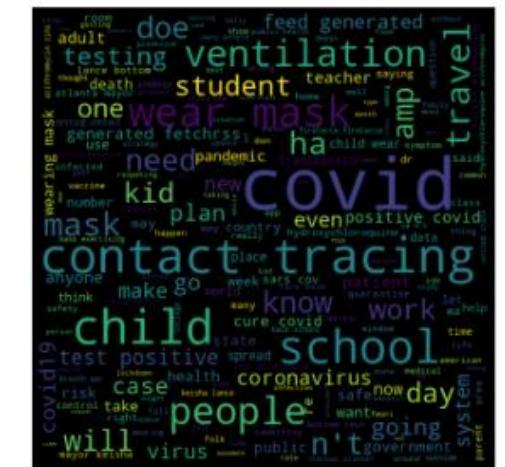
- Develop a machine learning-based generalizable framework for automatically detecting COVID-19 misinformation on social media
 - Design a multi-dimensional study to investigate the efficacy of deep learning based natural language processing



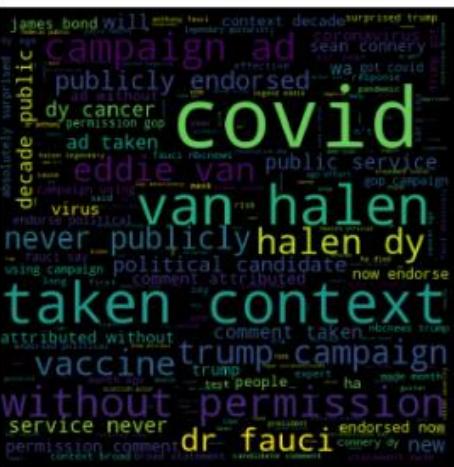
(a) Ma



(b) July



(c) September



(d) November

Evolution in high-frequency words visualized in Tweets Word Cloud.

Research at HCC

Examples: Science Gateway for Designing and Optimizing RNA Nanostructures

Profs. Joseph Yesselman and Derek Weitzel

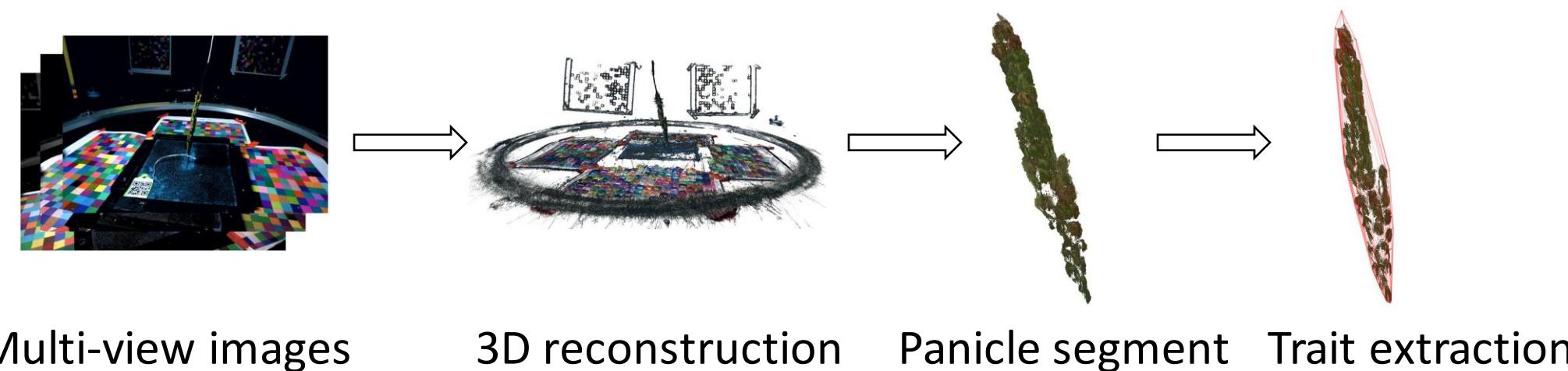
Develop a comprehensive science gateway for the design and optimization of RNA nanostructures powered by RNAMake

- Consist of discrete applications in RNA design that can run on high-performance computing centers through HCC
- Provide the community with easy access to RNAMake through a web-based user interface rather than command line, as well as taking care of the computing and data management of large scale processing with RNAMake
- Undergraduate students of the School of Computing contribute to the development via senior design project

Research at HCC

Examples: Advanced Image Analysis for High-Throughput Phenotyping of Plants
Profs. Harkamal Walia and Hongfeng Yu

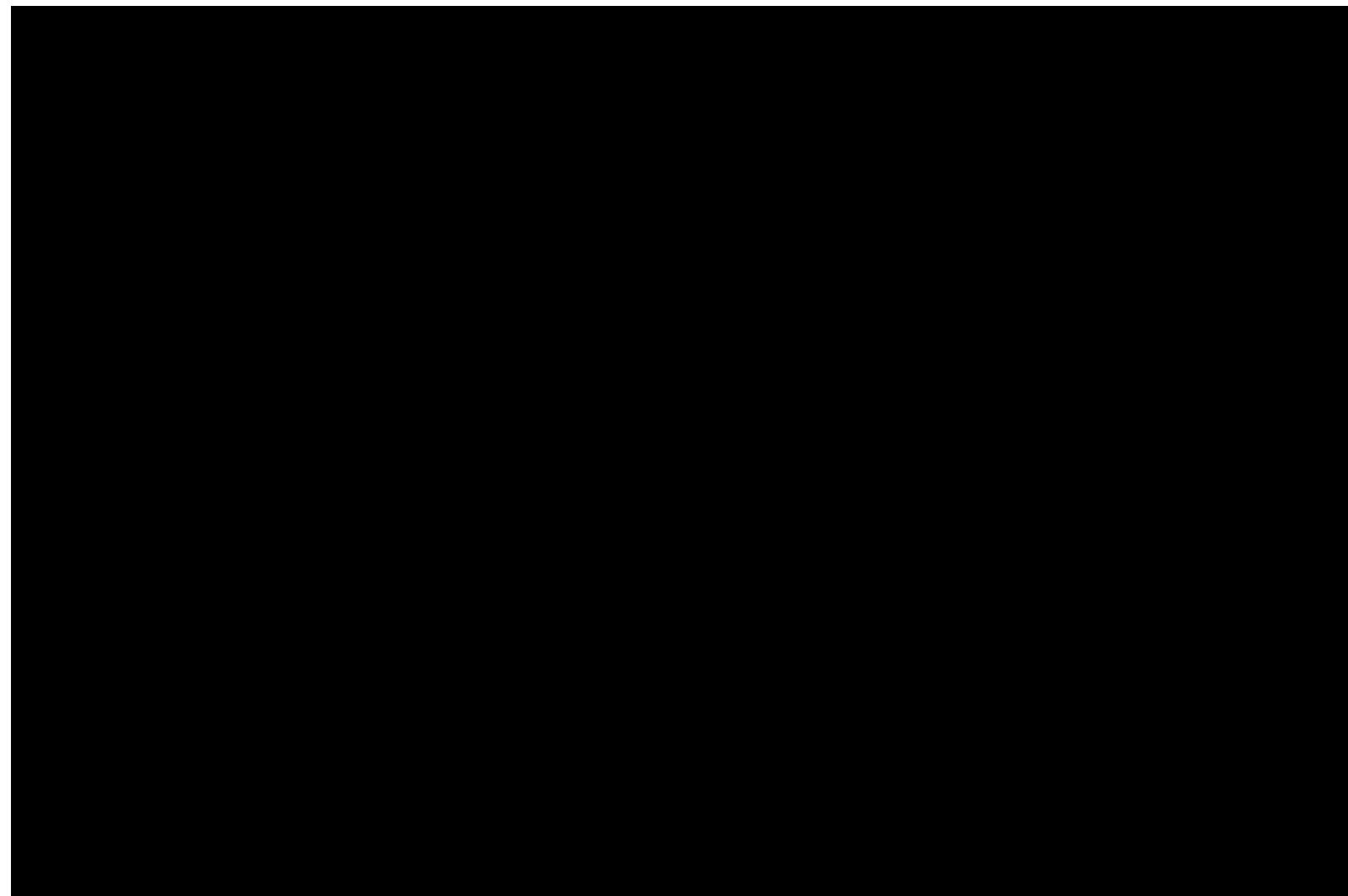
Develop new imaging and 3D reconstruction systems to capture high-resolution dynamics of plant growth.



Research at HCC

Examples: Advanced Image Analysis for High-Throughput Phenotyping of Plants

Profs. Harkamal Walia and Hongfeng Yu



Research at HCC

Examples: New Forms of Media Arts by leveraging ML and AI

Prof. Robert Twomey

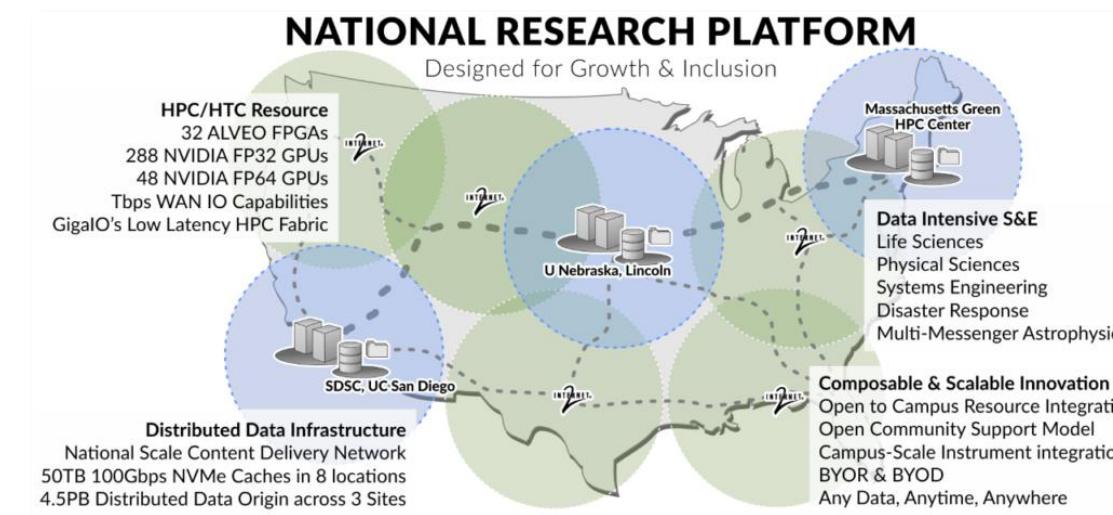
Experiment with new forms of media arts and explore how ML and AI can extend human perception and imagination using the Crane system at HCC

- Include a neural network trained on children's artwork, a ML-generated visual essay reflecting on the historical concept of the sublime, and a live performance of an AI-written radio play.
- Incorporate creative applications of these technologies into classes
- Train students to be “computation artists,” developing fluency with ML and compute-intensive workflows



Research at HCC

Examples:



<https://www.hpcwire.com/off-the-wire/nrp-accelerating-science-with-bold-national-research-platform/>



Faculty invited to learn about National Agricultural Producers Data Cooperative

by Geltner Simmons | IANR Media



<https://news.unl.edu/newsrooms/today/article/faculty-invited-to-learn-about-national-agricultural-producers-data/>

UNL PI: Prof. Derek Weitzel

Husker team takes leading role at CERN's Large Hadron Collider

UNIVERSITY RECEIVES \$51M NSF GRANT TO ADVANCE SUBATOMIC PHYSICS RESEARCH

by Tiffany Lee | Research and Economic Development



Chele Chandler | University Communication
Ilya Kravchenko, Dan Claes, Frank Goff and Ken Bloom are members of the University of Nebraska Department of Physics and Astronomy who collaborate with partners at the European Organization for Nuclear Research, known as CERN. Their work involves CERN's Large Hadron Collider, an image of which is behind the researchers in this photo.

PI: Prof. Ken Bloom

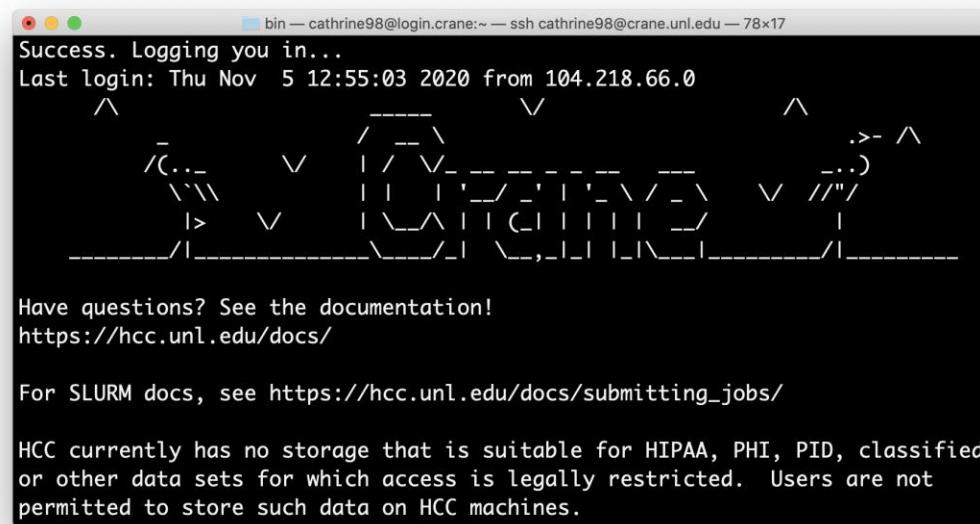
<https://news.unl.edu/newsrooms/today/article/husker-team-takes-leading-role-at-cerns-large-hadron-collider/>

PI: Prof. Jennifer Clarke

HCC OnDemand

Traditional Access

- HCC runs primarily LINUX clusters
 - Traditional interface is a BASH Shell
 - Users interact via a text-based prompt
 - Submit jobs via a (SLURM) script
 - Results written to a file that users must know how to read and/or edit
 - Limited interactive functionality

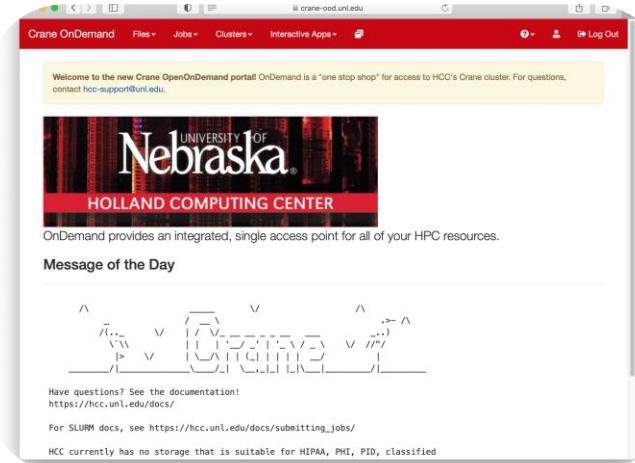


OPEN

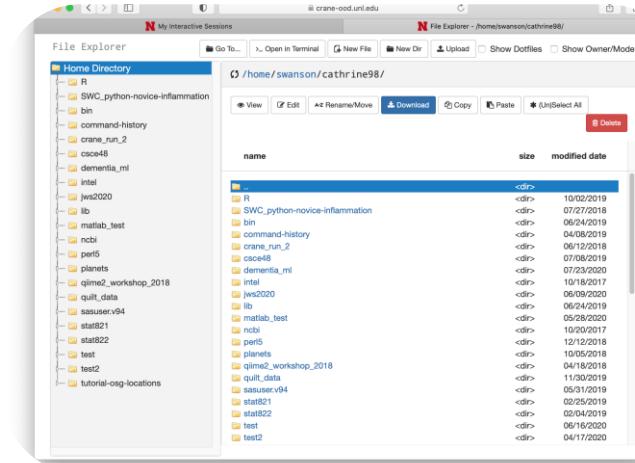
onDemand

- Web-based access to supercomputers
 - Fully featured, interactive GUI
 - Open Source - developed by the Ohio Supercomputing Center
 - Available on Crane and Swan
 - No installation required
 - Only a web browser and HCC account

HCC OnDemand

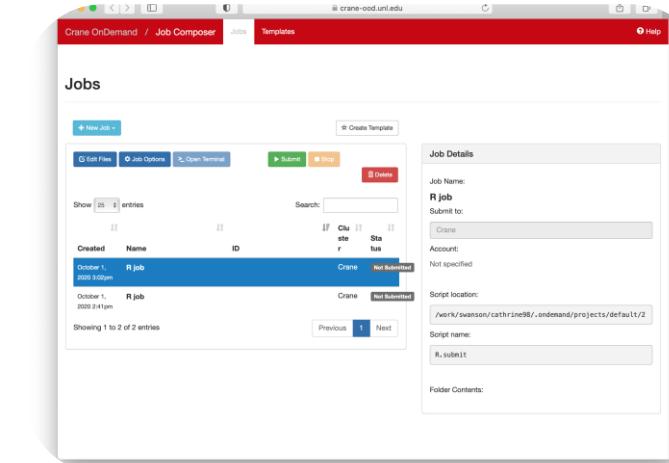


Plugin-free Web Interface



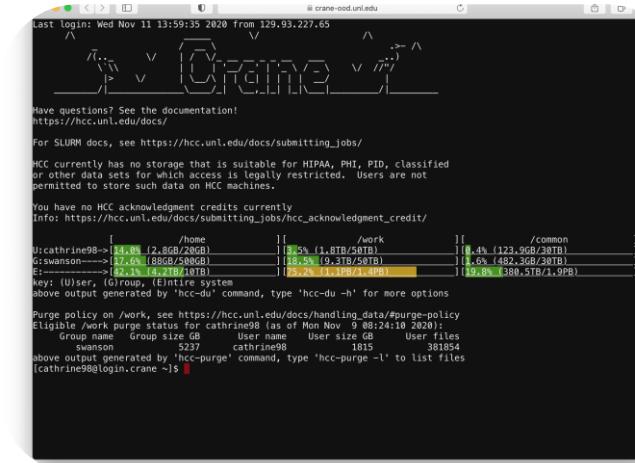
File Explorer

- Easy File Management
- Download and Upload capability



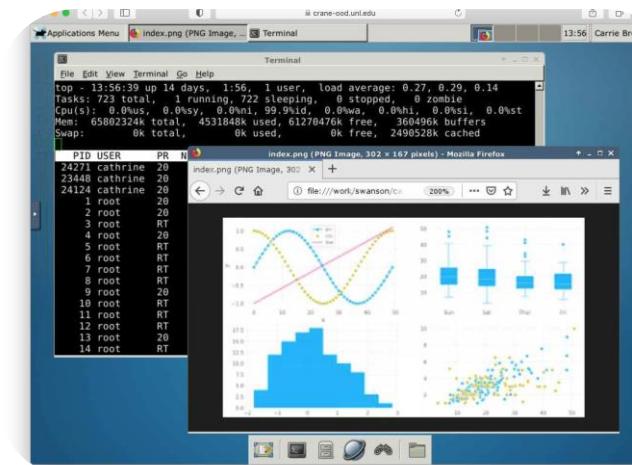
Job Composer

- Assisted submit script creation
- Active job monitoring

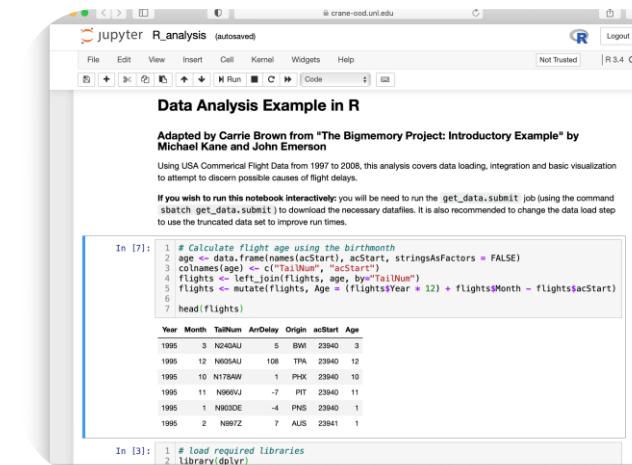


Shell Access

- Traditional Bash CLI interface

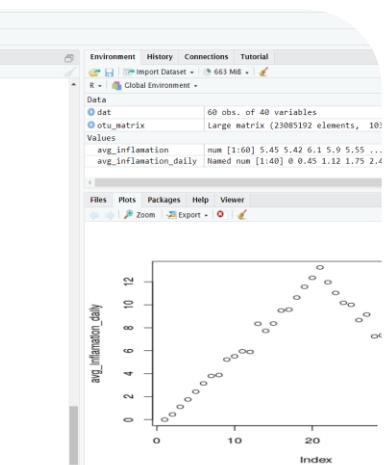


Interactive Desktop



Jupyter Notebook

- Integrative code/markdown documents
- Python/R/Matlab



Applications

- R Studio Server
- Matlab
- COSMOL
- Freesurfer

HCC Anvil

Specify the details for launching an instance.

The chart below shows the resources used by this project in relation to the project's quotas.

Instance Name	CPUs	Memory
VM Name Here	1	2GB
Name	general.small	
VCPUs	1	
Root Disk	20 GB	
Ephemeral Disk	0 GB	
Total Disk	20 GB	
RAM	2,048 MB	

Flavor Details

Instance Name	CPUs	Memory
general.small	1	2GB
general.medium	1	3.8GB
general.large	2	7.5GB
general.xlarge	4	15GB
general.2xlarge	8	30GB
general.4xlarge	16	60GB

High-Memory Instances

Instance Name	CPUs	Memory
memory.large	2	15GB
memory.xlarge	4	30GB

Project Limits

We recommend high memory instances for high performance databases, genome assembly and analysis.

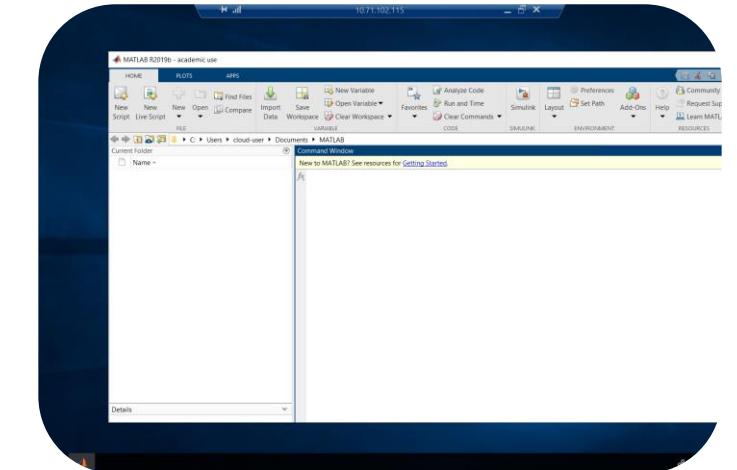
Image Name	Number of Instances	Number of VCPUs	Total RAM
Select Image	39 of 80 Used	174 of 200 Used	635,888 of 1,000,000 MB Used

Simple VM Creation

Multiple “flavors” / Instance Types

Multiple Operating Systems

- Windows 10 / Ubuntu / Centos / Fedora



Preconfigured Software Install

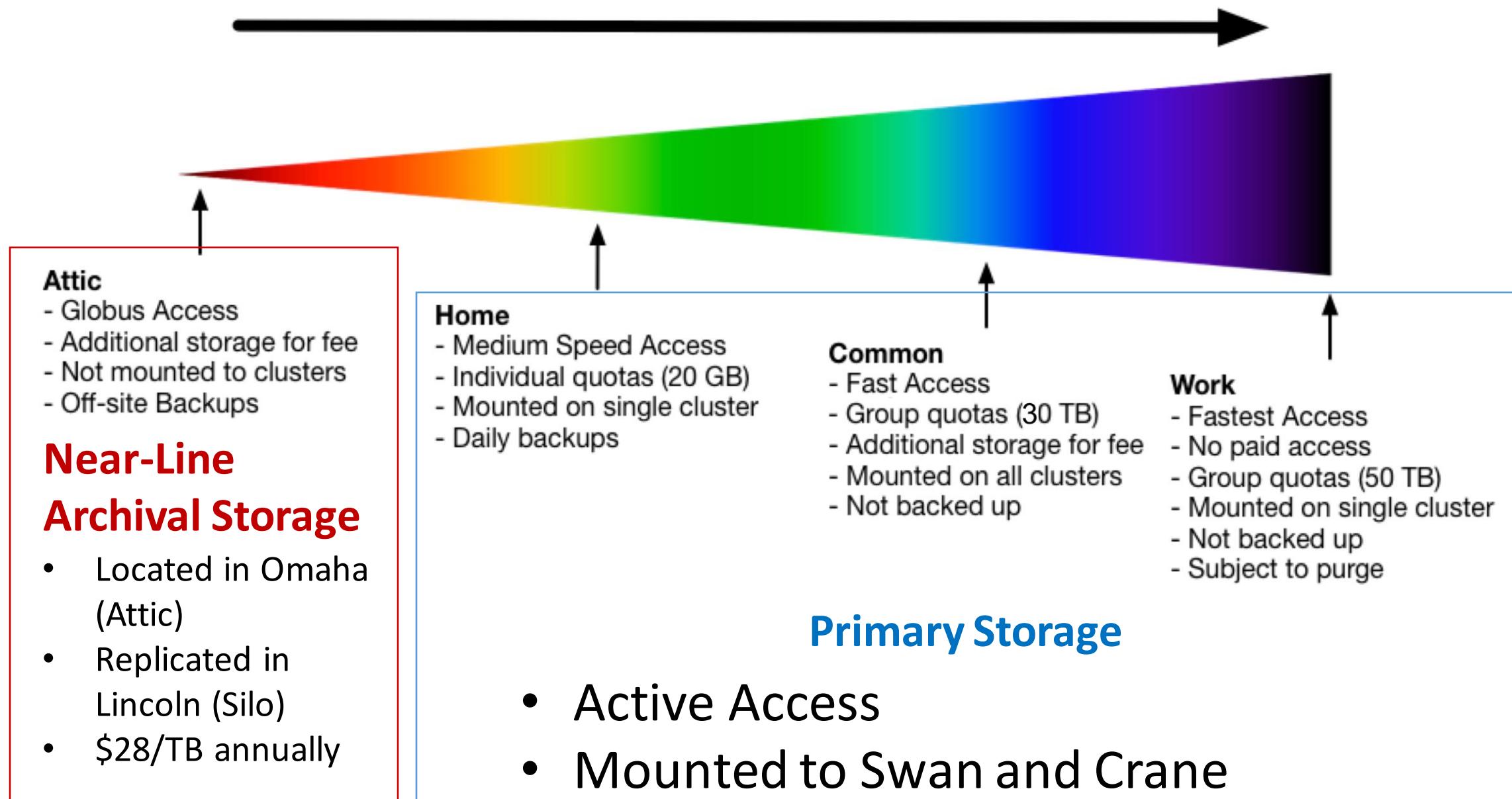
- Windows 10 with Mathematica / Matlab
- Linux with Xfce Desktop Environment



VMs Accessed through SSH or RDP

HCC Storage Options

- Faster File Access (higher bandwidth / IOPS)
- Ease of Access
- Diminishing Redundancy (backups)



File Transfers

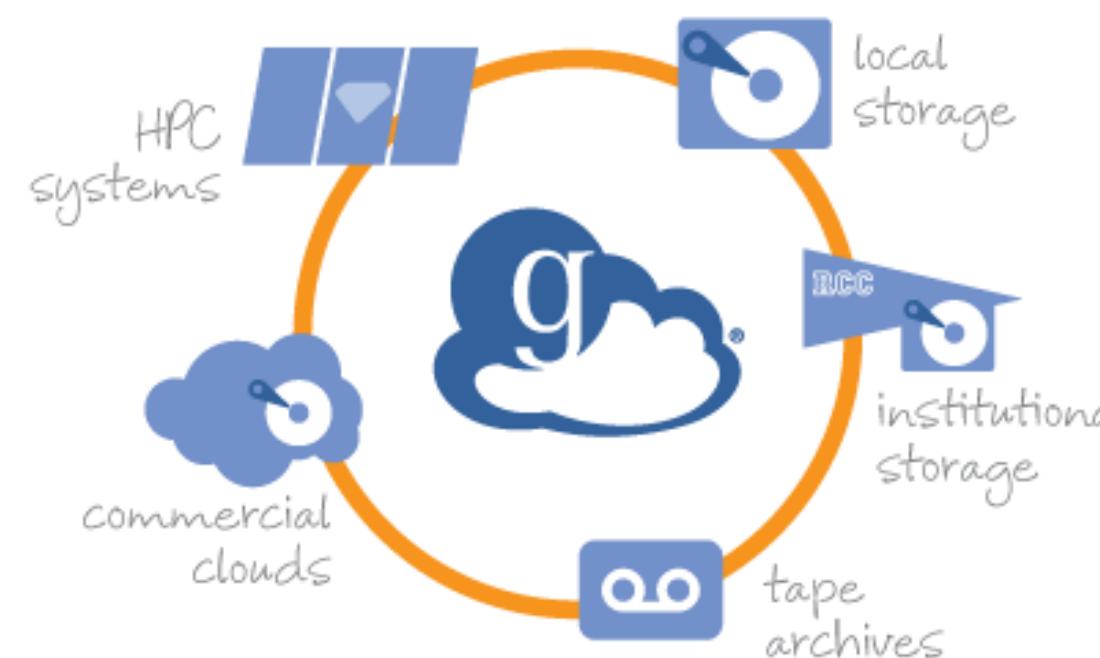
Traditional Access

CLI Tools

- scp, sftp, rsync

GUI Tools

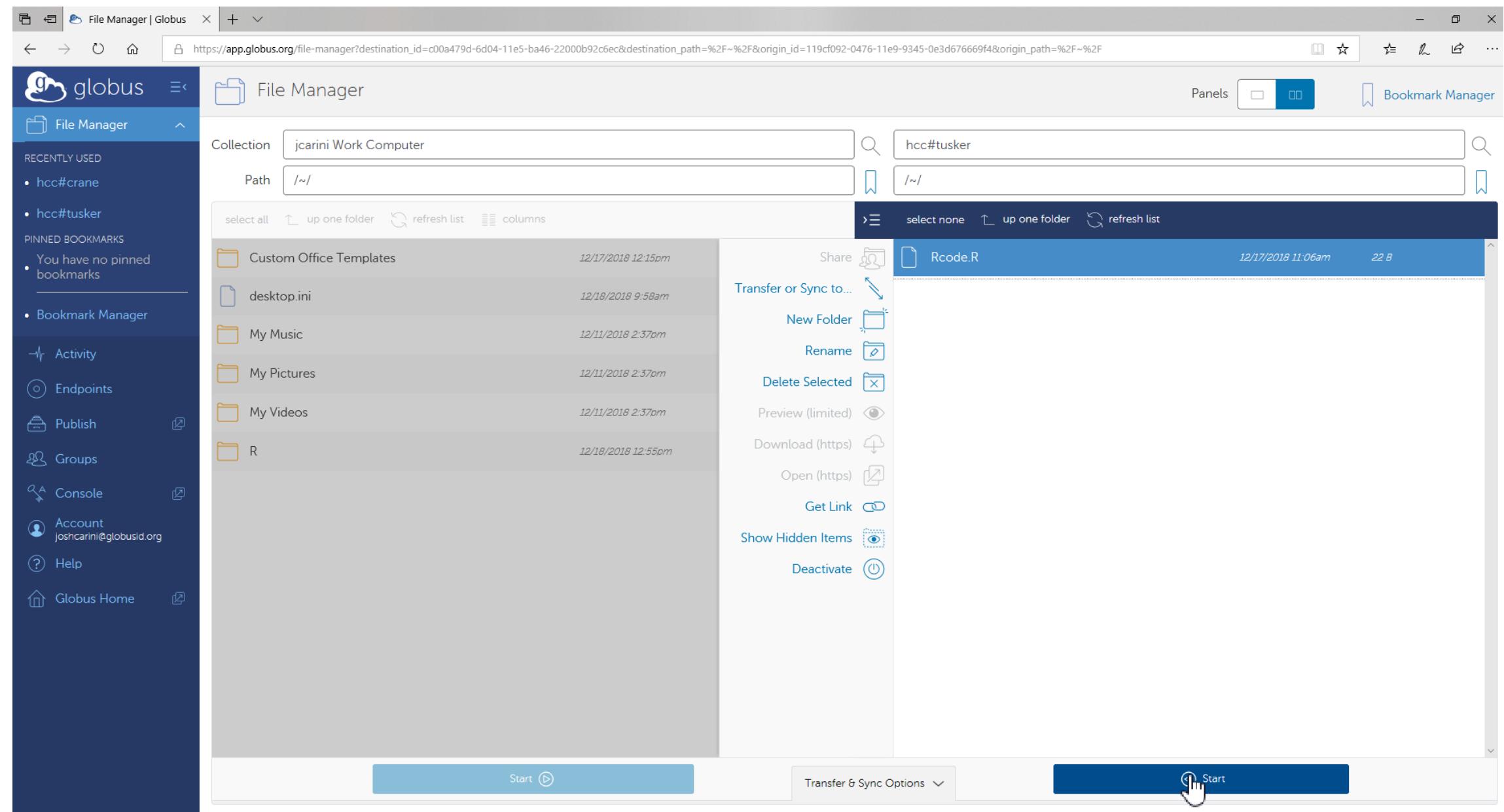
- WinSCP, CyberDuck, FileZilla



Globus Connect

- Research Data Management service
- Developed by UChicago
- Web-based user portal
- File transfers between established endpoints and personal machines (with the Globus Connect client)
- User configured shared endpoints for ease of collaboration
- Configured to utilize HCC's high speed transfer nodes
- Integrated with UNL OneDrive

Globus Connect



HCC Support

Documentation:

- Written documentation to guide users through all aspects of HCC.
 - hcc.unl.edu/docs
- Examples of traditional usage of HPC Resources.
 - <https://github.com/unlhcc/job-examples>

Support:

- Email based support
 - hcc-support@unl.edu
- Open Office Hours:
 - Tuesdays and Thursdays from 2-3PM
 - Currently held via Zoom
go.unl.edu/HCCHelp
- One on One Appointments

Training:

- HCC Workshops:
 - June Workshop Series (Every June)
 - Kickstart (Currently every fall)
- Carpentries:
 - Host Software Carpentry workshops, commonly Python and R.
- Classroom and Group Tutorials
 - Provide tutorials to classes and groups on a per-request basis.

Thank You!

- University of Nebraska
- Nebraska Research Initiative
- OneIT
- NSF, EPSCoR, DOE, NIH

