High Performance Computing

An Introduction to NJIT High Performance Computing (HPC) and Services, Session I

April 10, 2024

Outline

- What is NJIT Advanced Research Computing HPC?
- High-Performance Computing (HPC) Concepts
- Hardware Overview
- Data Storage systems
- Getting Started at Advanced Research Computing
- User Environment
- Using Software on HPC
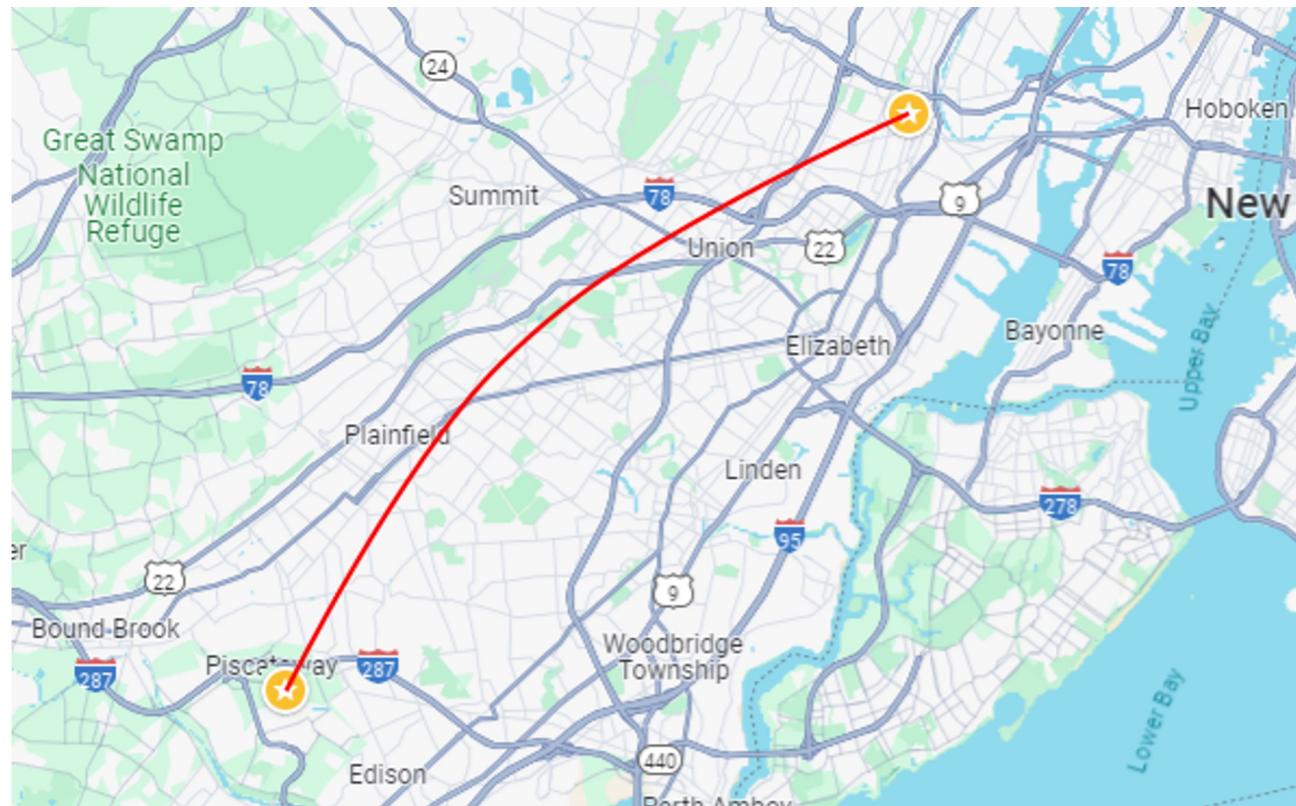
What is the NJIT Advanced Research Computing HPC?

About NJIT HPC

NJIT new high performance computing environment, built through a partnership with DataBank, a leading provider of enterprise-class colocation, connectivity and managed services, is live in DataBank's Piscataway, N.J. data center (EWR2) and will support NJIT's research efforts.

The services NJIT HPC provides

- High performance computing services

- Computational science expertise

Service Catalog

Cluster Computing

Built by Dell, the computing environment "Wulver" provides a total of 127 compute nodes or servers

Research Data Storage

High-performance, large capacity data storage spaces that are perfect for a wide variety of research data

Education

High performance computing and networking resources come together to create an exciting and innovative teaching and research environment
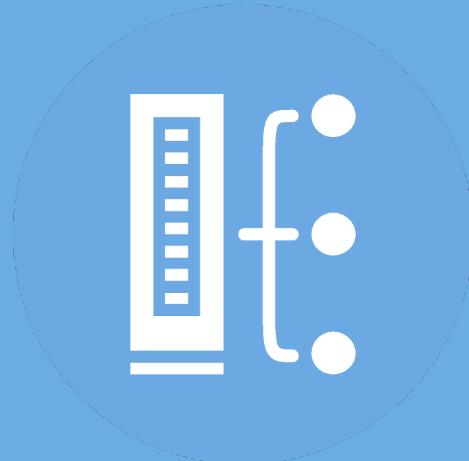
HPC Facilitation Service

Empowering users to perform essential research computing projects through training and effective user support
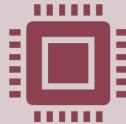
Scientific Software Development

Deep expertise in developing and deploying software

HPC Concepts

Why Use HPC?

Your simulations or analyses take too long on your personal computer

More (faster) cores

Multithreading

Multi-node parallelization (openmpi & intelmpi)

GPU acceleration (NVIDIA's CUDA)

Distributed computing
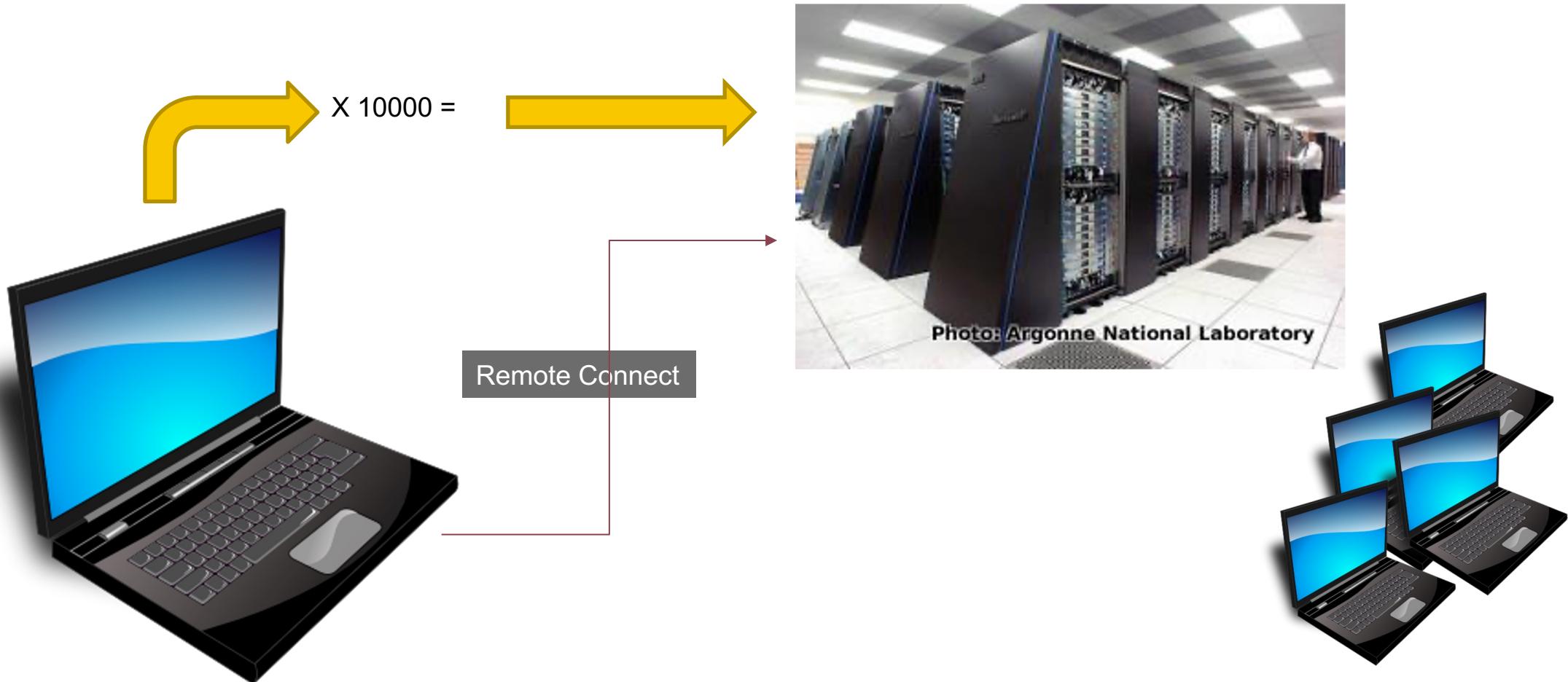
The size of your data is too large to be contained (storage) or accessed (memory) on your computer

Large memory nodes: 512GB; 2 TB

Distributed computing

Project storage: TBs range

You need a particular software or package for your work

What is the difference between your laptop and a supercomputer?

X 10000 =

Remote Connect

Photo: Argonne National Laboratory

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HPC Terminology

Compute Node

Equivalent to a high-end workstation, part of a cluster

Compute Cluster

A group of computers (nodes) connected by a high-speed network, forming a supercomputer

Core

A processor (CPU), multiple cores per processor chip

Graphical Processing Unit (GPU)

A separate multi-core processor that can handle many small calculations

Memory

Holds data that is being calculated on, as well as computational instructions

Memory types

Shared memory is local to one node and several process

Distributed memory is on multiple nodes

Each core has an associated amount of memory

Standard nodes: ~4 GB/core

Huge memory nodes: ~15 GB/core

Storage

Storage: different types of "disk" for different needs

$HOME directory — Limited quota: not intended for primary storage

Project storage — Long term storage
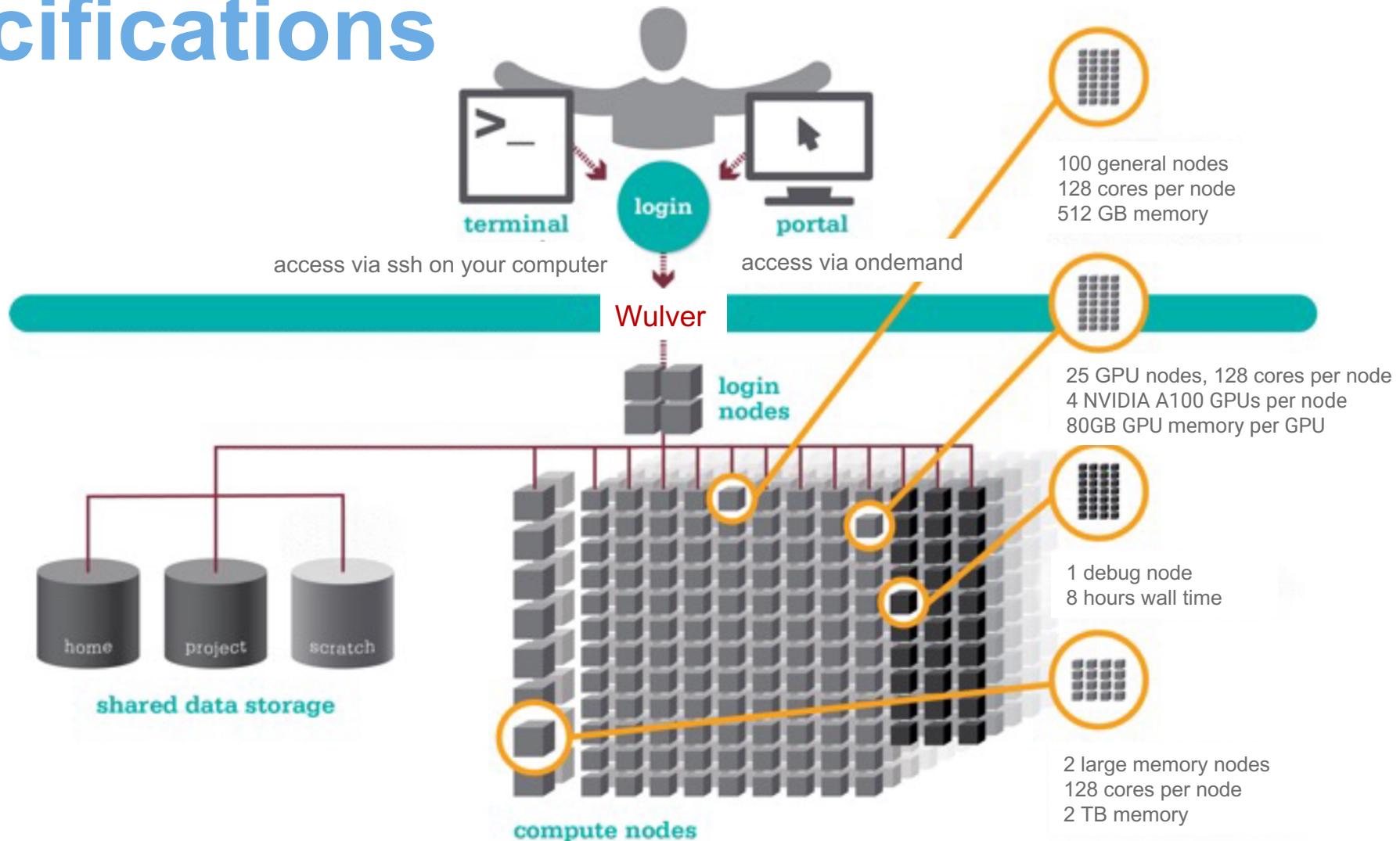
Shared scratch — Short-term storage only

Hardware Overview

Wulver Cluster Specifications

terminal   login   portal

access via ssh on your computer   access via ondemand

Wulver

login nodes

shared data storage

home   project   scratch

compute nodes

100 general nodes
128 cores per node
512 GB memory

25 GPU nodes, 128 cores per node
4 NVIDIA A100 GPUs per node
80GB GPU memory per GPU

1 debug node
8 hours wall time

2 large memory nodes
128 cores per node
2 TB memory

hpc.njit.edu/clusters/get_started_on_Wulver

Login Nodes – Usage

- Purpose
  - Submit jobs to batch system
  - Edit files
  - Manage your files
  - Interactive work – small scale
- Limits
  - 20GB memory
  - CPU usage is limited to 25% per user
- **Use the batch system for serious computing**
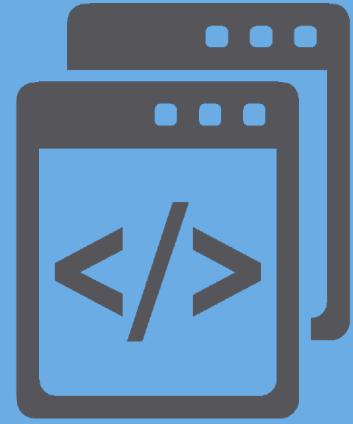
Data Storage Systems

Research Data Storage

- **Home**
  - Store your small sized files here.
  - 50GB per user
  - Backed up
- **Project**
  - Store the large files here.
  - 2TB/PI Group,
  - Backed up
  - Additional storage can be purchased if needed.
- **Archive**
  - Long term storage, by request

- **Scratch**
  - Temporary storage, not backed up
  - Files will be deleted once they 30 days old.
  - Users need to move the important files to project before deletion.
  - Quota per PI group: 10 TB
- **Research**
  - Storage on Lochness, 500GB/PI
  - Are remounted on Wulver

hpc.njit.edu/clusters/get_started_on_Wulver/#wulver-filesystems

Filesystem	Purpose	Quota	Backed-Up?	Purged?
Home ($HOME)	Non-research such as profile, history	50GB	Yes, daily	No
Project (/project/$PI_UCID/$LOGIN/)	Active research by groups.	2 TB/ PI Group	Yes, daily	No
Scratch (/scratch/PI_UCID/$LOGIN)	Temporary space for intermediate results, downloads, checkpoints, and such. MOVE YOUR RESULTS & IMPORTANT FILES TO /project or /research	10 TB/ PI Group	No	Yes – 30 days
Compute (/tmp)	Very high speed temporary storage	Varies (~1 TB)	No	Yes – after job ends
Research (/research/PI_UCID)	Long term archive. Users can buy as much as they need. Existing purchases/quotas will be kept over from Lochness.		Yes, daily	TBD

https://hpc.njit.edu/clusters/get_started_on_Wulver/#wulver-filesystems

Getting Started at Wulver

Getting Access to Wulver

- Getting a Login
  - Faculty can obtain a login to NJIT's HPC by sending an email to hpc@njit.edu
  - Students can obtain a login either by asking their faculty adviser to contact on their behalf
  - For course requiring HPC resources students need to contact their course instructor.

Job Priorities

- Standard Priority (`--qos=standard`)
  - Faculty PIs are allocated 300,000 Service Units (SU) per year on request at no cost
  - Additional SUs may be purchased at a cost of $0.005/SU.
  - The minimum purchase is 50,000 SU ($500)
  - Wall time maximum - 72 hours

- Low Priority (`--qos=low`)
  - Not charged against SU allocation
  - Wall time maximum - 72 hours
  - Jobs can be preempted by those with higher and standard priority jobs when they are in the queue

- High Priority (`--qos=high_$PI`)
  - Not charged against SU allocation
  - Wall time maximum - 72 hours – can be increased based on PI's request
  - Only available to contributors
  - `listqos` – To see the list of high priority queues

Usage Charges

- Charges are in terms of SU (Service Units) core hours
- Services, e.g. compute and storage
- PI will be charged if requesting more space in Project

Partition	Nodes	Cores /Node	CPU	GPU	Memory	SU charge
--partition=general	100	128	2.5G GHz AMD EPYC 7763 (2)	NA	512 GB	1 SU per hour per cpu
--partition=debug	1	4	2.5G GHz AMD EPYC 7763 (2)	NA	512 GB	No charges, must be used with --qos=debug
--partition=gpu	25	128	2.0 GHz AMD EPYC 7713 (2)	NVIDIA A100 GPUs (4)	512 GB	3 SU per hour per cpu
--partition=bigmem	2	128	2.5G GHz AMD EPYC 7763 (2)	NA	2 TB	1.5 SU per hour per cpu

Check SU and Quota usage

- quota_info $LOGNAME

  Usage for account: xy1234

  SLURM Service Units (CPU Hours): 277557 (300000 Quota)

  PROJECT Storage: 867 GB (of 2048 GB quota)

  User ab1234 Usage: 11 GB (No quota)
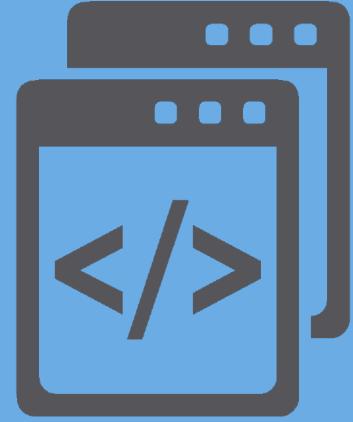
  SCRATCH Storage: 791 GB (of 10240 GB quota)

  User ab1234 Usage: 50 GB (No quota)

  HOME Storage ab1234 Usage: 0 GB (of 50 GB quota)

Wulver Maintenance

- Wulver will be temporarily out of service for maintenance once a month, specifically on the 2nd Tuesday, to perform updates, repairs, and upgrades.
- During the maintenance period, the logins will be disabled
- Jobs that do not end before the maintenance window begins will be held until the maintenance is complete

User Environment

Linux Operating System

- "UNIX-like"
- Widely used in HPC
- Mostly command-line
- Choice of shells (bash is default)
- Freely distributable, open-source software
- **Tutorials available: https://www.hostinger.com/tutorials/linux-commands**
- www.linux.org

Basic Linux Shell Commands

List of basic shell commands	
cd	rm
mkdir	echo
pwd	export
ln	alias
ls	grep
cp	scp
mv	rsync
cat	man

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Available software on Wulver

- **General programming software (∮ licensed)**
  - gnu compilers and debugger
  - ∮ Intel compilers
  - ∮ ANSYS
  - ∮ COMSOL
  - ∮ MATLAB
  - ∮ VASP
  - Python
  - MD software - GROMACS, LAMMPS
  - CFD – OpenFOAM
  - Visualization Software – ParaView, ∮ Tecplot

Do you use a specific software package?
- Open source software packages can be installed
- If you have a license, we can help you use it on Wulver

https://hpc.njit.edu/Software

Resources to get your questions answered

Getting Started: Access to Wulver

List of Software: Wulver Software

HOW TOs: Conda Documentation

      Installing Python packages via Conda

Request Software: HPC Software Installation

Contact: Please visit HPC Contact

Open a ticket: email to hpc@njit.edu

Consult with Research Computing Facilitator: Facilitator Calendar Appointment

System updates

- Read Message of the Day on login

- Visit NJIT HPC News

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