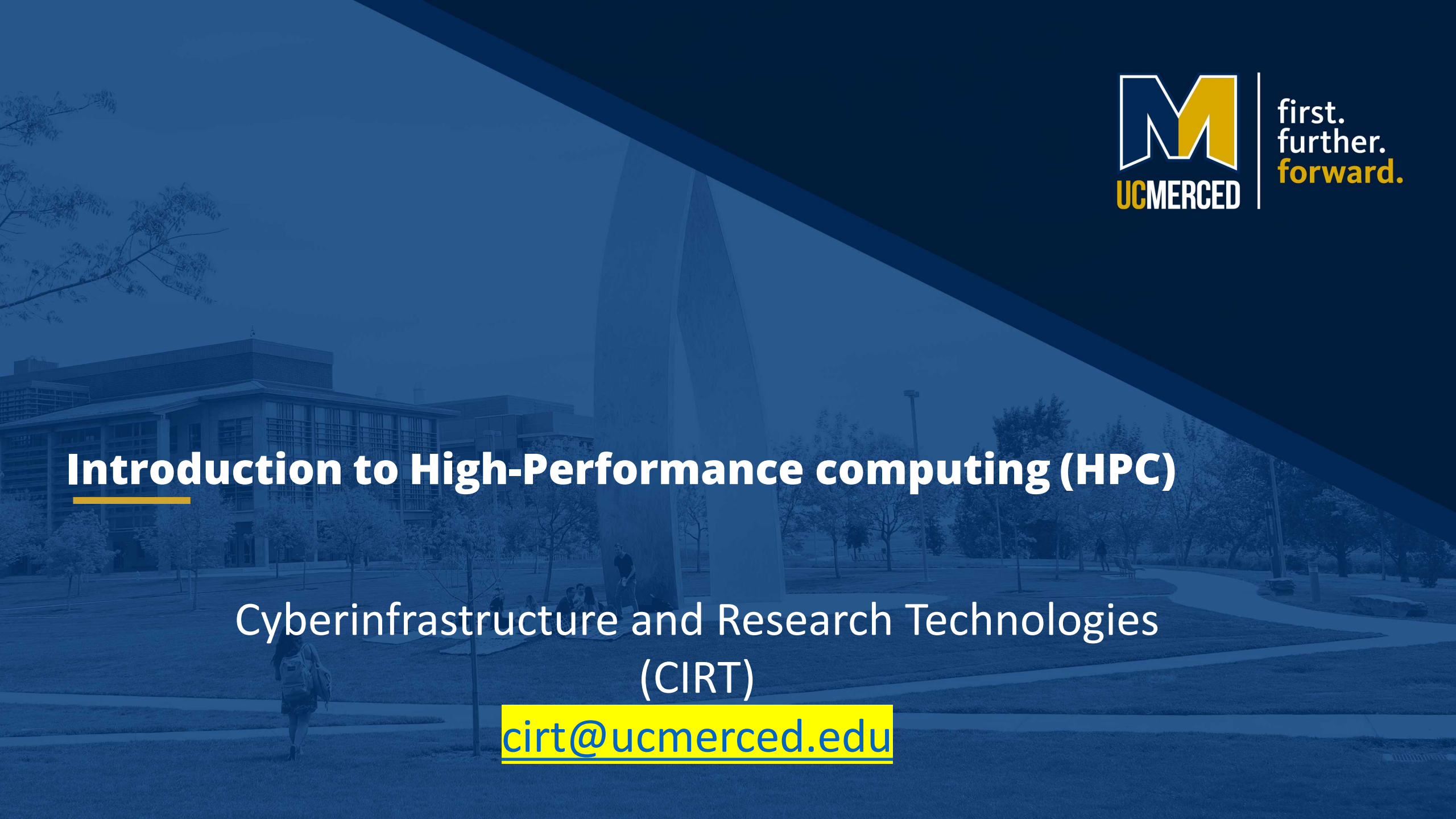


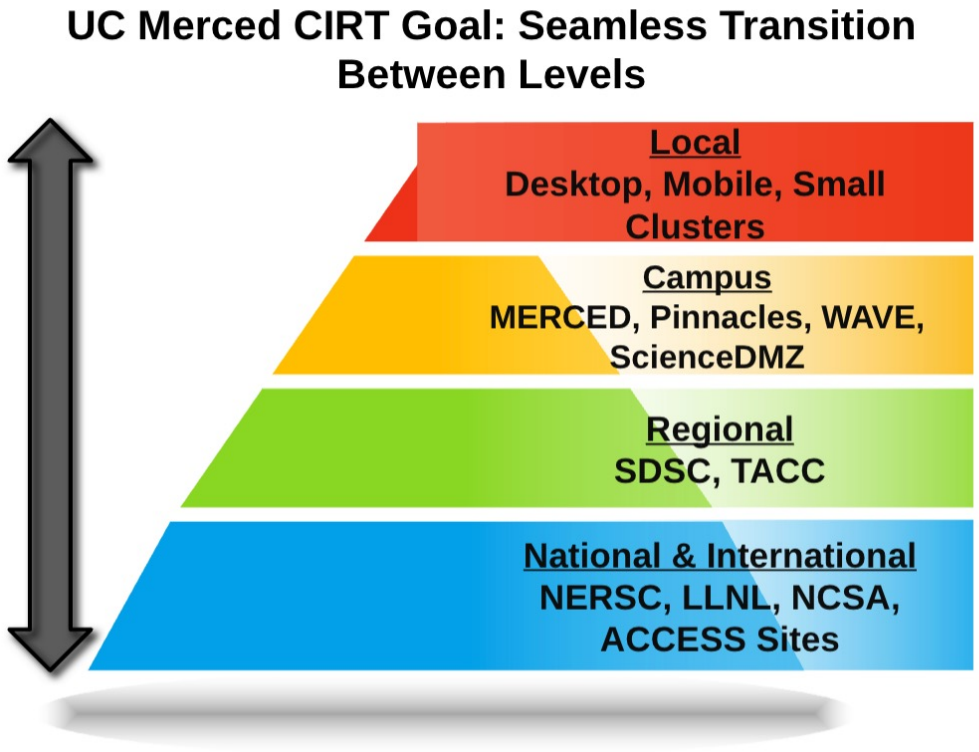
Introduction to High-Performance computing (HPC)

Cyberinfrastructure and Research Technologies (CIRT)
cirt@ucmerced.edu

Today's AGENDA

- What is Supercomputing(HPC)? (10 minutes)
  - Priority 1: Supercomputing terminology
  - Priority 2: Supercomputing at University of California, Merced
- Terminology and HPC Architecture(5 minutes)
- HPC Resources at UC Merced (5 minutes)
  - Campus HPC Structure here @ UC Merced
- What is a Scheduler and Why it is Used?(5 minutes)
  - Slurm Scheduler
- Resource Queues and Limitations (10 Minutes)
- Hands On Training and Q&A(Until end of Training)

CIRT - Goal


UC Merced CIRT Goal: Seamless Transition Between Levels
Local
Desktop, Mobile, Small Clusters
Campus
MERCED, Pinnacles, WAVE, ScienceDMZ
Regional
SDSC, TACC
National & International
NERSC, LLNL, NCSA, ACCESS Sites

What is Supercomputing?

- Supercomputing is the biggest, fastest computing right this minute
- A supercomputer is one of the biggest, fastest computers right this minute
    - So, the definition of supercomputing is constantly changing.

Rule of Thumb: A supercomputer is typically at least 100 times as powerful as a PC.

Jargon:

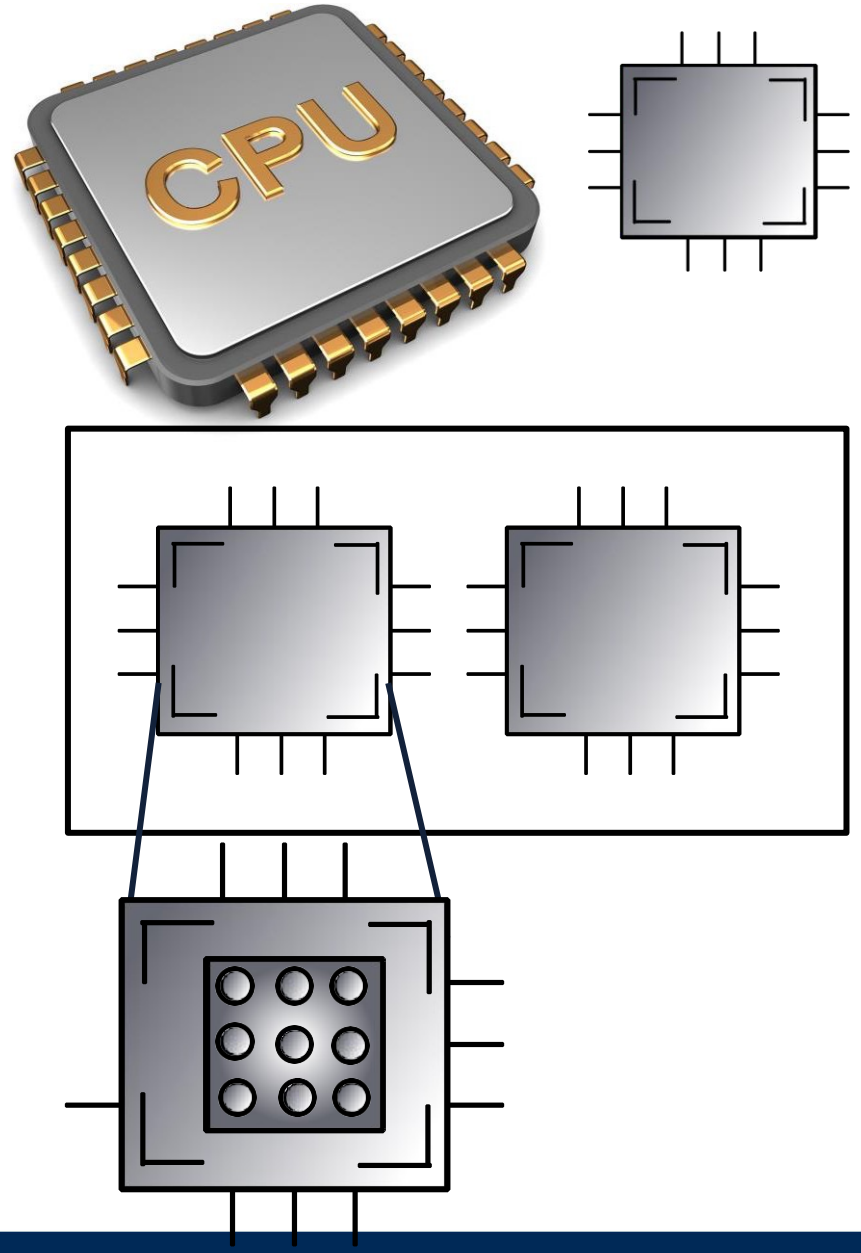
Supercomputing is also known as
High Performance Computing (HPC) or High End Computing (HEC) or Cyberinfrastructure (CI)

I am working at Cyberinfrastructure and Research Technologies (CIRT) team

https://it.ucmerced.edu/CIRT

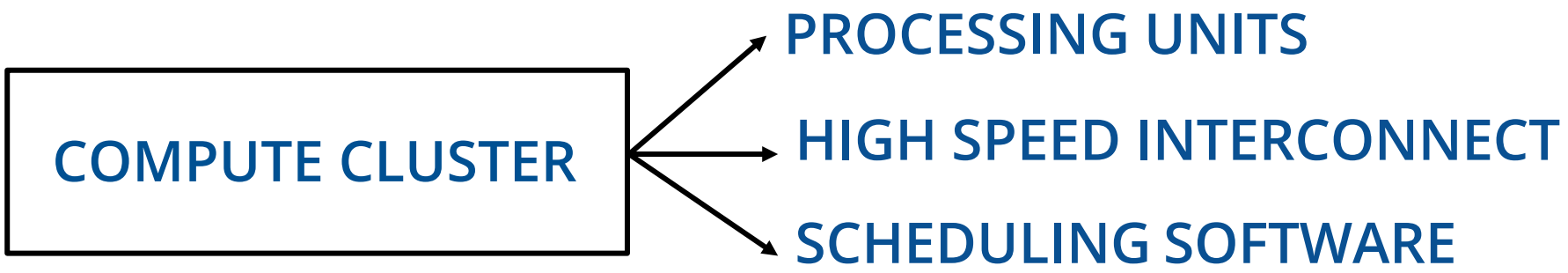
Terminologies

- CPU (processor)
  - Central Processing Unit
- GPU
  - Graphics Processing Unit
  - Deep learning, massive parallelism, 3D rendering…
- Nodes
  - Multiple CPUs
  - CPU nodes
  - GPU nodes
- Cores
  - Processing element
  - 1 CPU may contain multiple cores
  - 1 GPU many smaller specialized cores



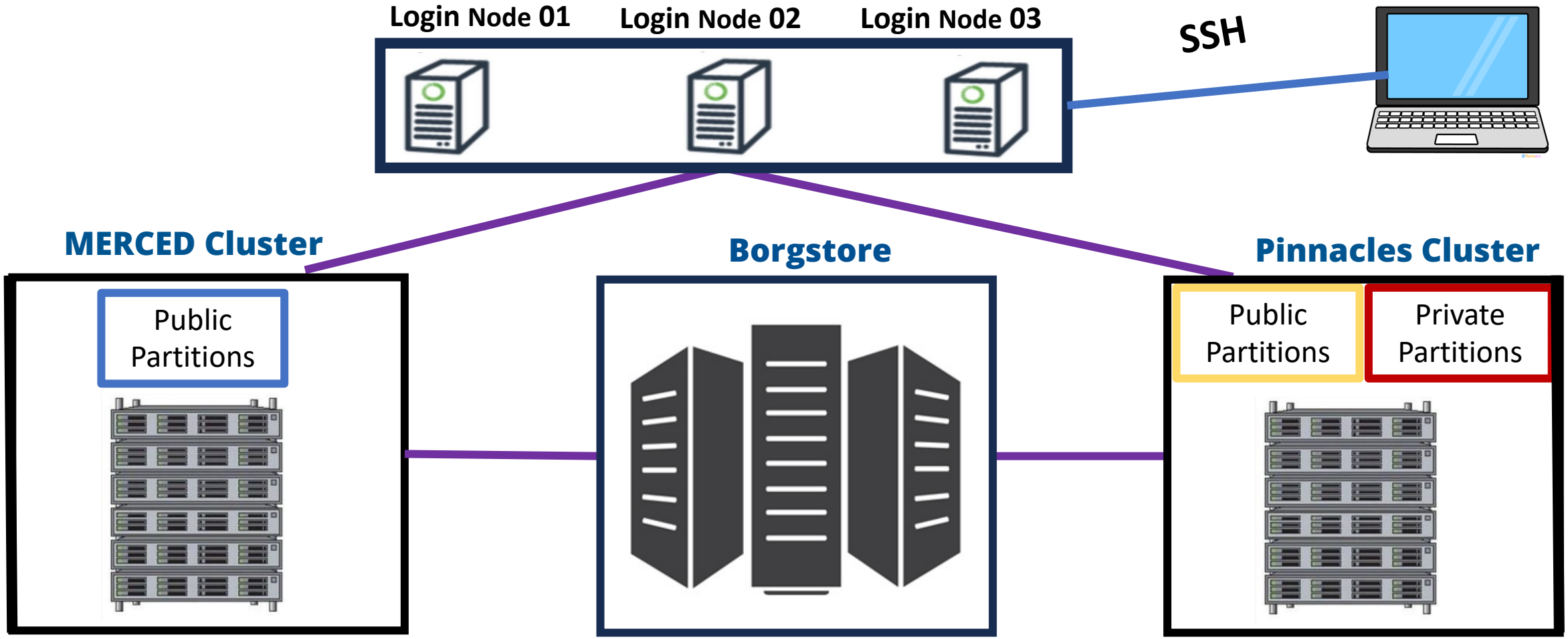
HPC Architecture

- Machines with large number of CPUs and memory
- High-speed interconnect
- Scheduling software



HPC Architecture

= High Speed Interconnect & SLURM scheduling software



Cluster Partitions

Use sinfo command to see all the partitions on the cluster.

Pinnacles Public Partitions

Public Queues	Max Wall Time	Default Time	Max Nodes per Job	Max # of jobs that can be submitted
^test	1 hour	5 min.	2 nodes	1
bigmem	3 days	1 hr	2 nodes	2
gpu	3 days	1 hr	2 nodes	4
*short	6 hours	1 hr	4 nodes	12
medium	1 day	6 hrs	4 nodes	6
long	3 days	1 day	4 nodes	3

MERCED Public Partitions

Public Queues	Max Wall Time	Default Time	Max Nodes per Job	Max # of submitted jobs
bigmem	5 days	1 hr	2 nodes	6
test^	1 hour	5 min.	2 nodes	1
*compute	5 days	1 hr	2 nodes	6

All projects on the cluster have:

- **Equal priority**
- **Each member of the project gets equal priority on the partitions.**

HPC Clusters Physical Setup

- MERCED and Pinnacles Computing Clusters are located at Borg Cube

Pinnacles Specs

- 40 CPU & 8 GPU Nodes
- 4 BigMem Nodes
  - 1 TB RAM

CPU Compute Nodes

- CPU – 2 Intel 28 core Xeon Gold 6330
- 256 GB RAM

Merced Specs

CPU Compute Nodes

- Multigenerational Nodes
  - Haswell, Broadwell, Skylake
  - 128GB/256GB of Ram

Infiniband Architecture

- InfiniBand (IB) networking communications
- RDMA (Remote Direct Memory Access)

- 10GigE has 5-6 times the latency of IB

- IB has 3.7x the throughput of 10GigE

Slurm Scheduler

Scheduling is the method by which work specified by some means is assigned to resources that complete the work. A scheduler is what carries out the scheduling activity.

Slurm Scheduler has three key functions.

1. Allocates exclusive and/or non-exclusive access to resources (compute nodes) to users for some duration of time so they can perform work.
2. Provides a framework for starting, executing, and monitoring work (normally a parallel job) on the set of allocated nodes.
3. Arbitrates contention for resources by managing a queue of pending work.

Computing Workspace & Resources

Shared Filesystem

Folder	Space
/home/<UCMID>/data	500G
/home/<UCMID>/scratch	500G
/home/<UCMID>/	70G

Commonly Used Commands in HPC

Below is just a brief list. More commands with different purposes can be found on our HPC Documentation Website and on other resources on the web.

UNIX Commands

Command	Use	Command	Use
pwd	Print current Directory	cat	Print contents onto terminal
ls	List sub-content	nano <file>	Open simple text editor
rm <file>	Permanently Delete File	mkdir	Create new directory
mv <file>/directory	Move file to another file	help	Comprehensive list of commands

SLURM Commands

Command	Use
sbatch <job.file>	Submit job onto Computing Cluster
scancel <job ID>	Cancel Job
squeue	Displays all running/pending jobs
sinfo	Presents partition information

Guest Account Login: (During the session you will be given a guest login information)

Otherwise, you can use your own account for this practice session

1. ssh guest0##@login.rc.ucmerced.edu
    1. “**ucm_Pinnacles**” - Password
2. To see the available modules that are installed use the following:

   module avail
3. Copy the practice files: (always use the Tab key from keyboard to help you for autocompletion)

   cp -r /home/avilla49/hpc_training/ .

Note: The folder will have two subfolders with some sample scripts, user can play around with them

Job Submission Script

```
#! /bin/bash
#SBATCH   --nodes=1
#SBATCH   --ntasks=1
#SBATCH -p test
#SBATCH --time=0-00:15:00    # 15 minutes
#SBATCH --output=my_%j.stdout
#SBATCH --job-name=test
#SBATCH --export=ALL

whoami
```

Submitting the job.

sbatch sample.sub

Simple Job Submission Demo

- Run single python job

  Python_test1.py

- Check the status of the job using “squeue –u username” or “squeue --me” commands

Getting Help and Office Hours

Troubleshooting a Job:
https://ucmerced.github.io/hpc_docs/#/Manage_job

Requesting Support Via ServiceNow Ticket System:
https://ucmerced.service-now.com/servicehub?id=sh_new

HPC Office Hours

WHERE? **Online & In-person(ACS 365)**
WHEN? **Every Friday from 11:30 am – 1pm**

Other Resources

Login MOTD
CIRT Website
HPC Documentation page

Additional Resources

- Slurm overview - https://slurm.schedmd.com/documentation.html
- Slurm sbatch - https://slurm.schedmd.com/sbatch.html
- Slurm sinfo - https://slurm.schedmd.com/sinfo.html
- Slurm squeue - https://slurm.schedmd.com/squeue.html
- Requesting help from CIRT - https://it.ucmerced.edu/services?field_service_service_catalog_tid=5
- HPC Documentation https://github.com/ucmerced/merced-cluster/wiki/

Diverse Research Groups on Campus

- Natural Sciences – Soil Biogeochemistry, Biological Physics Theory and Computation, Theoretical Atomic and Molecular Physics, Applied Mathematics, Quantum Chemistry, Quantitative Systems Biology

- Engineering – Tribology, Machine Learning, Fault tolerance/resilience in
  large-scale parallel and distributed systems, power-aware computing

- Social Sciences Humanities and Arts- Evolution of Communication, Neural Networks, Vocal Motor Control, Mesoamerican Indigenous literatures and cultures, Central American and Latina/o cultural studies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