

HPC User Environment 1

Jason Li

HPC User Services

LSU HPC / LONI

sys-help@loni.org

Louisiana State University
Baton Rouge
September 14, 2022







HPC User Environment 1

- 1. Intro to HPC
- 2. Getting started
- 3. Into the cluster
- 4. Software environment (modules)

- 1. Queuing system
- 2. How to run jobs







- 1. Intro to HPC
- 2. Getting started
- 3. Into the cluster
- 4. Software environment (modules)







- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC
- 2. Getting started
 - 1) Accounts
 - 2) Allocation
- 3. Into the cluster
 - 1) Getting connected
 - 2) File system
- 4. Software environment
 - 1) Preinstalled (modules)
 - 2) User installation







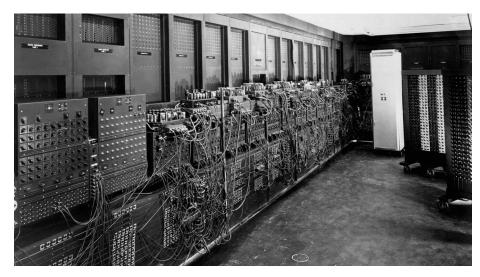
- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC
- 2. Getting started
 - 1) Accounts
 - 2) Allocation
- 3. Into the cluster
 - 1) Getting connected
 - 2) File system
- 4. Software environment
 - 1) Preinstalled (modules)
 - 2) User installation







Everything COMPUTER!



ENIAC, 1945





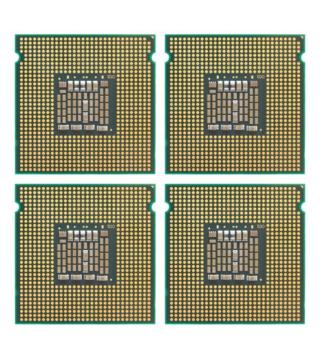




Parallel computing







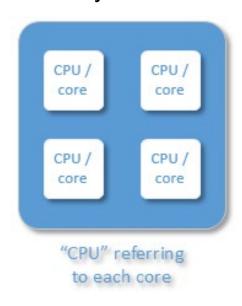


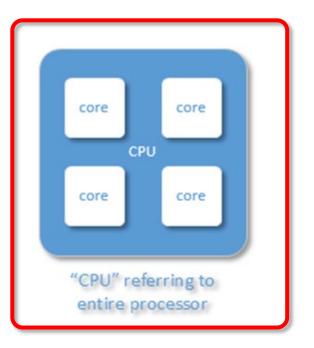




Definition

- "core", "CPU", "processor"
- "core": the basic computation unit
- "processor": could have many cores





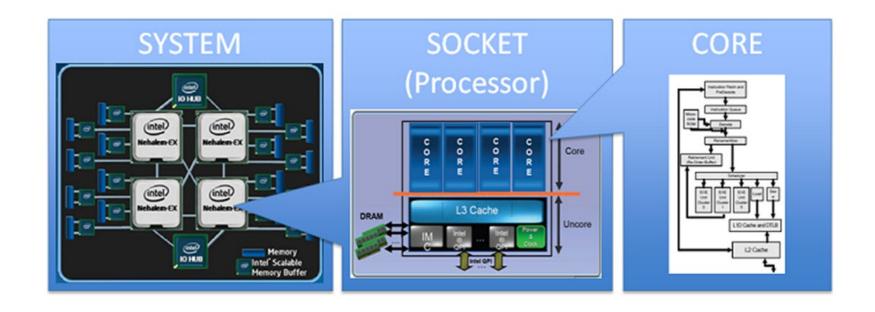
In this training, CPU = processor, which has multiple cores.

(The term "CPU" will not be used)





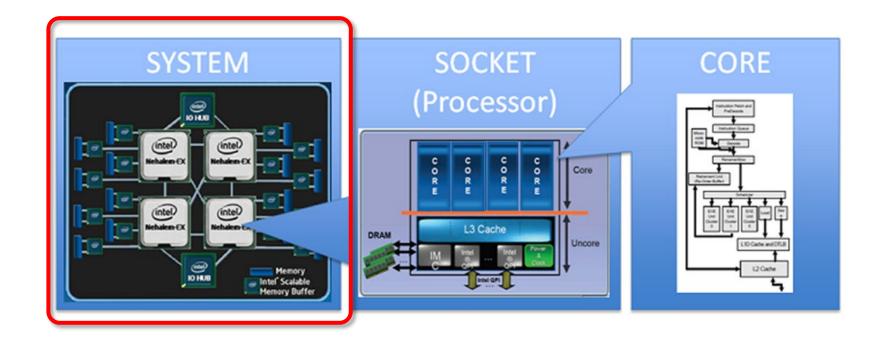








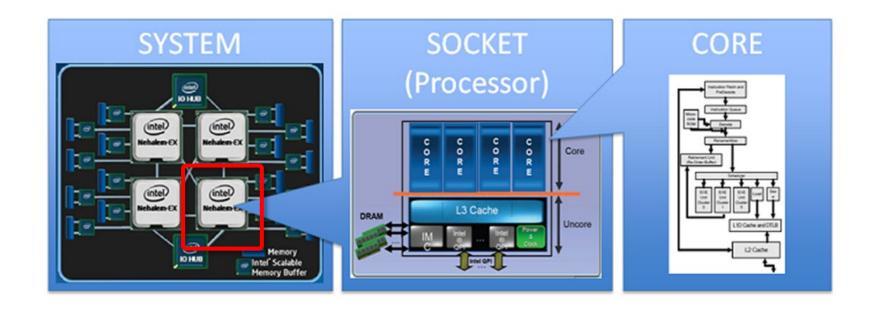








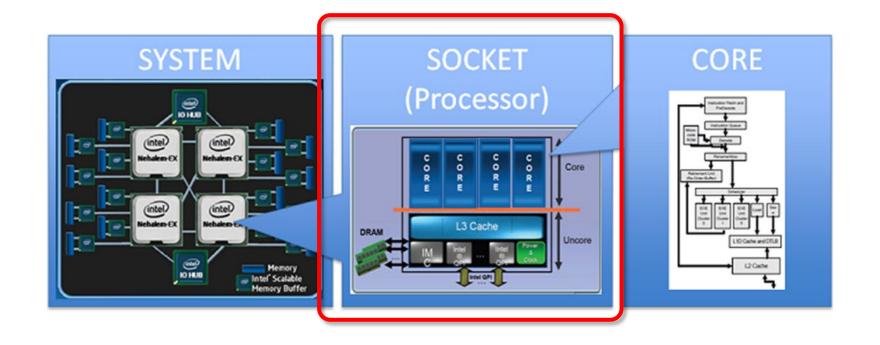








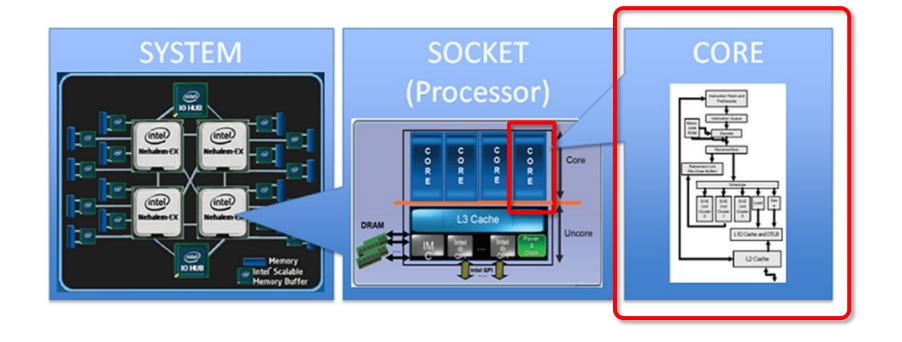










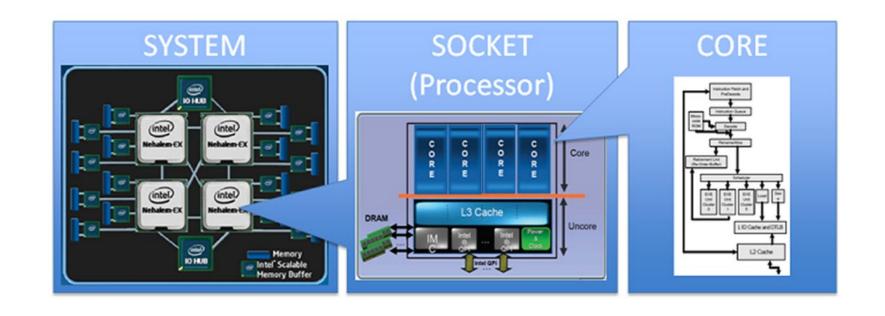








How many cores does this computer have?



4 cores * 4 processors = 16 total cores







- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC
- 2. Getting started
 - 1) Accounts
 - 2) Allocation
- 3. Into the cluster
 - 1) Getting connected
 - 2) File system
- 4. Software environment
 - 1) Preinstalled (modules)
 - 2) User installation







- High Performance Computing (HPC): computation at the cutting edge of modern technology, often done on a --
- Supercomputer: the class of machines that rank among the fastest in the world
 - Rule of thumb: at least 100 times as powerful as a PC





600 mph

60 mph

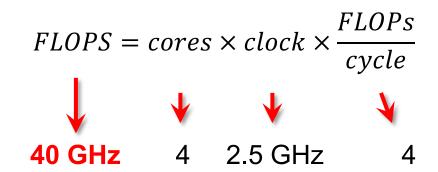
How do we evaluate the performance of HPC?







Performance is measured in Floating Point Operations Per Second (FLOPS)



- Do you know ENIAC's FLOPS? 500
- "The first teraflop desktop PC processor"
 - Intel i9-7980XE (Sep 2017)
 - 18 cores
 - $18 \times 4.4 \ GHz \times 16 = 1267 \ GFLOPS = 1.267 \ TFLOPS$



Computer performance

Name	FLOPS
yottaFLOPS	1024
zettaFLOPS	1021
exaFLOPS	1018
petaFLOPS	1015
teraFLOPS	1012
gigaFLOPS	109
megaFLOPS	106
kiloFLOPS	103







Your smartphone vs. supercomputer 20 years ago

Apple's A16 Bionic (neural engine): 17 TFLOPS

#1 as of Nov 2001 (Top 500 list): 12.3 TFLOPS



Computer performance

Name	FLOPS
yottaFLOPS	1024
zettaFLOPS	1021
exaFLOPS	1018
petaFLOPS	1015
teraFLOPS	1012
gigaFLOPS	109
megaFLOPS	106
kiloFLOPS	103



[1] Apple Event — September 7, https://www.top500.org/lists/top500/2001/11/
[2] Top 500 list, https://www.top500.org/lists/top500/2001/11/







Current (June 2022):

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,730,112	1,102.00	1,685.65	21,100
2	Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
3	LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	1,110,144	151.90	214.35	2,942



[1] Top 500 list, https://www.top500.org/lists/top500/2022/06/







Current (June 2022):

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,730,112	1,102.00	1,685.65	21,100
2	Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
3	LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	1,110,144	151.90	214.35	2,942



[1] Top 500 list, https://www.top500.org/lists/top500/2022/06/







Current (June 2022):

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,730,112	1,102.00	1,685.65	21,100
2	Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
3	LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	1,110,144	151.90	214.35	2,942



[1] Top 500 list, https://www.top500.org/lists/top500/2022/06/







Current (June 2022):

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,730,112	1,102.00	1,685.65	21,100
2	Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
3	LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	1,110,144	151.90	214.35	2,942



[1] Top 500 list, https://www.top500.org/lists/top500/2022/06/







June 2019:

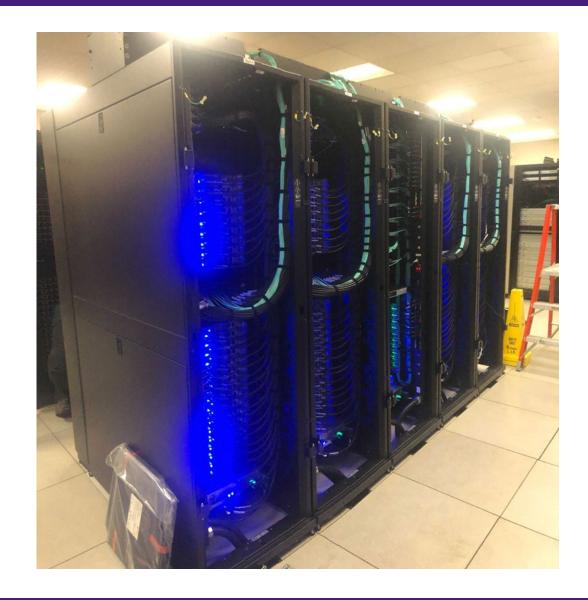
Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
474	QB-2 - Dell C8220X Cluster, Intel Xeon E5- 2680v2 10C 2.8GHz, Infiniband FDR, NVIDIA K20x, DELL EMC Louisiana Optical Network Initiative United States	23,040	1.05	1.47	500





LSU

Inside a cluster:

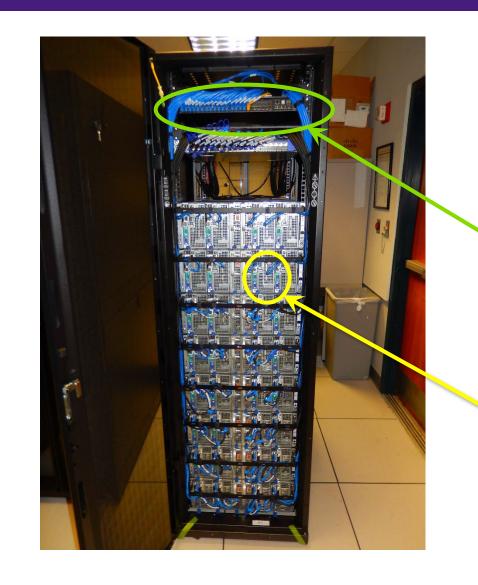








Inside a rack:



Interconnect:
 Infiniband
 Switch

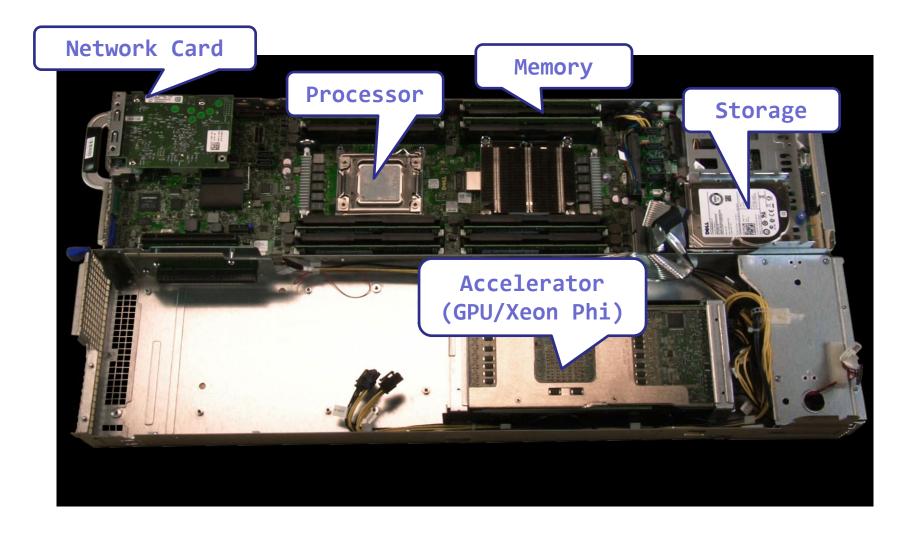
Compute Node







Inside a node:









- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC
- 2. Getting started
 - 1) Accounts
 - 2) Allocation
- 3. Into the cluster
 - 1) Getting connected
 - 2) File system
- 4. Software environment
 - 1) Preinstalled (modules)
 - 2) User installation



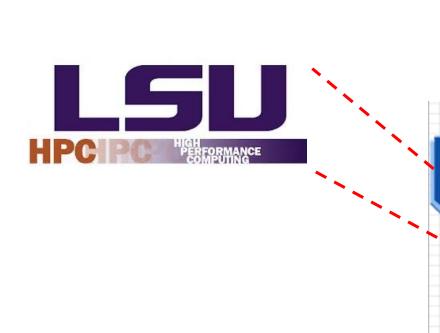


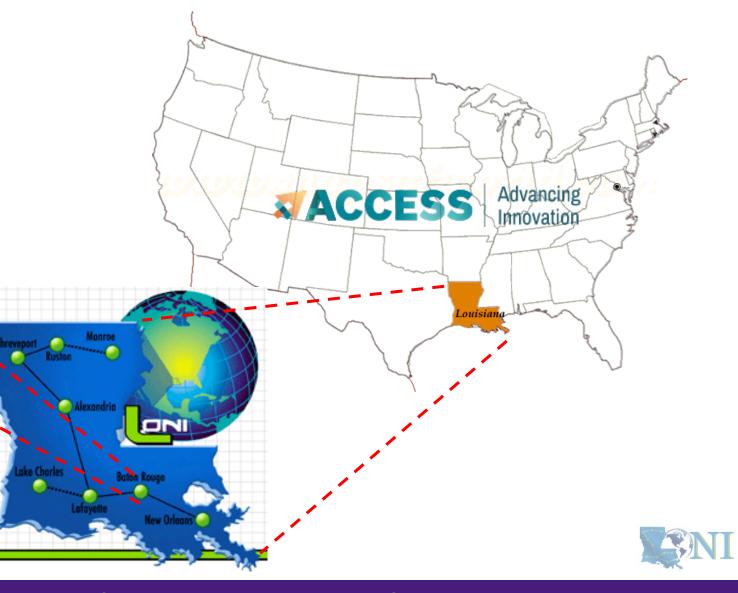


i. University level: LSU HPC

ii. State level: LONI

iii. National level: ACCESS









- i. University level: LSU HPC
 - Available to LSU (Baton Rouge campus) Faculty and their affiliates
 - Administered & supported by HPC@LSU









i. University level: LSU HPC

SuperMIC		
Hostname	smic.hpc.lsu.edu	
Peak Performance/TFlops	925	
Compute nodes	360	
Processor/node	2 10-core	
Processor Speed	2.8 GHz	
Processor Type	Intel Xeon 64bit	
Nodes with Accelerators	360	
Accelerator Type	Xeon Phi 7120P	
OS	RHEL v6	
Vendor		
Memory per node 64 GB		
Detailed Cluster Description		
<u>User Guide</u>		
Available Software		

Deep Bayou		
Hostname	db1.lsu.edu	
Peak Performance/TFlops	257	
Compute nodes	13	
Processor/node	2 24-core	
Processor Speed	2.4 GHz	
Processor Type	Intel Cascade Lake Xeon 64bit	
Nodes with Accelerators	13	
Accelerator Type	2 x NVIDIA Volta V100S	
OS	RHEL v7	
Vendor	Dell	
Memory per node 192 GB		
Detailed Cluster Description		
<u>User Guide</u>		
Available Software		

SuperMike III		
Hostname	mike.hpc.lsu.edu	
Peak Performance/TFlops	1,285	
Compute nodes	183	
Processor/node	2 32-core	
Processor Speed	2.6GHz	
Processor Type	Intel Xeon Ice Lake	
Nodes with Accelerators	8	
Accelerator Type	4 NVIDIA A100	
OS	RHEL v8	
Vendor	Dell	
Memory per node 256/2048 GB		
Detailed Cluster Description		
<u>User Guide</u>		
Available Software		







i. University level: LSU HPC

SuperMIC		
Hostname	smic.hpc.lsu.edu	
Peak Performance/TFlops	925	
Compute nodes	360	
Processor/node	2 10-core	
Processor Speed	2.8 GHz	
Processor Type	Intel Xeon 64bit	
Nodes with Accelerators	360	
Accelerator Type	Xeon Phi 7120P	
OS	RHEL v6	
Vendor		
Memory per node 64 GB		
Detailed Cluster Description		
<u>User Guide</u>		
<u>Available Software</u>		

Deep Bayou		
Hostname	db1.lsu.edu	
Peak Performance/TFlops	257	
Compute nodes	13	
Processor/node	2 24-core	
Processor Speed	2.4 GHz	
Processor Type	Intel Cascade Lake Xeon 64bit	
Nodes with Accelerators	13	
Accelerator Type	2 x NVIDIA Volta V100S	
OS	RHEL v7	
Vendor	Dell	
Memory per node 192 GB		
Detailed Cluster Description		
<u>User Guide</u>		
Available Software		

SuperMike III		
Hostname	mike.hpc.lsu.edu	
Peak Performance/TFlops	1,285	
Compute nodes	183	
Processor/node	2 32-core	
Processor Speed	2.6GHz	
Processor Type	Intel Xeon Ice Lake	
Nodes with Accelerators	8	
Accelerator Type 4 NVIDIA A100		
OS RHEL v8		
Vendor Dell		
Memory per node 256/2048 GB		
Detailed Cluster Description		
<u>User Guide</u>		
Available Software		







i. University level: LSU HPC

SuperMIC	
Hostname	smic.hpc.lsu.edu
Peak Performance/TFlops	925
Compute nodes	360
Processor/node	2 10-core
Processor Speed	2.8 GHz
Processor Type	Intel Xeon 64bit
Nodes with Accelerators	360
Accelerator Type	Xeon Phi 7120P
OS	RHEL v6
Vendor	
Memory per node	64 GB
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

Deep Ba	you
Hostname	db1.lsu.edu
Peak Performance/TFlops	257
Compute nodes	13
Processor/node	2 24-core
Processor Speed	2.4 GHz
Processor Type	Intel Cascade Lake Xeon 64bit
Nodes with Accelerators	13
Accelerator Type	2 x NVIDIA Volta V100S
OS	RHEL v7
Vendor	Dell
Memory per node	192 GB
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

SuperMike III	
Hostname	mike.hpc.lsu.edu
Peak Performance/TFlops	1,285
Compute nodes	183
Processor/node	2 32-core
Processor Speed	2.6GHz
Processor Type	Intel Xeon Ice Lake
Nodes with Accelerators	8
Accelerator Type	4 NVIDIA A100
OS	RHEL v8
Vendor	Dell
Memory per node	256/2048 GB
Detailed Cluster Description	
<u>User Guide</u>	
<u>Available Software</u>	







i. University level: LSU HPC

SuperMIC	
Hostname	smic.hpc.lsu.edu
Peak Performance/TFlops	925
Compute nodes	360
Processor/node	2 10-core
Processor Speed	2.8 GHz
Processor Type	Intel Xeon 64bit
Nodes with Accelerators	360
Accelerator Type Xeon Phi 7120P	
OS	RHEL v6
Vendor	
Memory per node	64 GB
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

Deep Ba	ayou
Hostname	db1.lsu.edu
Peak Performance/TFlops	257
Compute nodes	13
Processor/node	2 24-core
Processor Speed	2.4 GHz
Processor Type	Intel Cascade Lake Xeon 64bit
Nodes with Accelerators	13
Accelerator Type	2 x NVIDIA Volta V100S
OS	RHEL v7
Vendor	Dell
Memory per node	192 GB
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

Superl	Mike III
Hostname	mike.hpc.lsu.edu
Peak Performance/TFlops	1,285
Compute nodes	183
Processor/node	2 32-core
Processor Speed	2.6GHz
Processor Type	Intel Xeon Ice Lake
Nodes with Accelerators	8
Accelerator Type	4 NVIDIA A100
OS	RHEL v8
Vendor	Dell
Memory per node	256/2048 GB
Detailed Cluster Description	
<u>User Guide</u>	
<u>Available Software</u>	







i. University level: LSU HPC

SuperMIC	
Hostname	smic.hpc.lsu.edu
Peak Performance/TFlops	925
Compute nodes	360
Processor/node	2 10-core
Processor Speed	2.8 GHz
Processor Type	Intel Xeon 64bit
Nodes with Accelerators	360
Accelerator Type	Xeon Phi 7120P
OS	RHEL v6
Vendor	
Memory per node	64 GB
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

Deep Ba	ayou
Hostname	db1.lsu.edu
Peak Performance/TFlops	257
Compute nodes	13
Processor/node	2 24-core
Processor Speed	2.4 GHz
Processor Type	Intel Cascade Lake Xeon 64bit
Nodes with Accelerators	13
Accelerator Type	2 x NVIDIA Volta V100S
OS	RHEL v7
Vendor Dell	
Memory per node 192 GB	
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

SuperMike III	
Hostname	mike.hpc.lsu.edu
Peak Performance/TFlops	1,285
Compute nodes	183
Processor/node	2 32-core
Processor Speed	2.6GHz
Processor Type	Intel Xeon Ice Lake
Nodes with Accelerators	8
Accelerator Type 4 NVIDIA A100	
OS	RHEL v8
Vendor Dell	
Memory per node 256/2048 GB	
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	







i. University level: LSU HPC

SuperMIC	
Hostname	smic.hpc.lsu.edu
Peak Performance/TFlops	925
Compute nodes	360
Processor/node	2 10-core
Processor Speed	2.8 GHz
Processor Type	Intel Xeon 64bit
Nodes with Accelerators	360
Accelerator Type	Xeon Phi 7120P
OS	RHEL v6
Vendor	
Memory per node 64 GB	
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

Deep Ba	ayou
Hostname	db1.lsu.edu
Peak Performance/TFlops	257
Compute nodes	13
Processor/node	2 24-core
Processor Speed	2.4 GHz
Processor Type	Intel Cascade Lake Xeon 64bit
Nodes with Accelerators	13
Accelerator Type	2 x NVIDIA Volta V100S
OS	RHEL v7
Vendor Dell	
Memory per node 192 GB	
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

SuperMike III		
Hostname	mike.hpc.lsu.edu	
Peak Performance/TFlops	1,285	
Compute nodes	183	
Processor/node	2 32-core	
Processor Speed	2.6GHz	
Processor Type	Intel Xeon Ice Lake	
Nodes with Accelerators	8	
	8 4 NVIDIA A100	
Accelerators	·	
Accelerators Accelerator Type	4 NVIDIA A100	
Accelerator Type OS	4 NVIDIA A100 RHEL v8	
Accelerator Type OS Vendor	4 NVIDIA A100 RHEL v8 Dell 256/2048 GB	
Accelerator Type OS Vendor Memory per node	4 NVIDIA A100 RHEL v8 Dell 256/2048 GB	







i. University level: LSU HPC

SuperMIC	
Hostname	smic.hpc.lsu.edu
Peak Performance/TFlops	925
Compute nodes	360
Processor/node	2 10-core
Processor Speed	2.8 GHz
Processor Type	Intel Xeon 64bit
Nodes with Accelerators	360
Accelerator Type	Xeon Phi 7120P
OS	RHEL v6
Vendor	
Memory per node	64 GB
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

Deep Bayou	
Hostname	db1.lsu.edu
Peak Performance/TFlops	257
Compute nodes	13
Processor/node	2 24-core
Processor Speed	2.4 GHz
Processor Type	Intel Cascade Lake Xeon 64bit
Nodes with Accelerators	13
	13 2 x NVIDIA Volta V100S
Accelerators	2 x NVIDIA Volta
Accelerators Accelerator Type	2 x NVIDIA Volta V100S
Accelerator Type OS	2 x NVIDIA Volta V100S RHEL v7
Accelerator Type OS Vendor	2 x NVIDIA Volta V100S RHEL v7 Dell 192 GB
Accelerator Type OS Vendor Memory per node	2 x NVIDIA Volta V100S RHEL v7 Dell 192 GB

SuperMike III		
Hostname	mike.hpc.lsu.edu	
Peak Performance/TFlops	1,285	
Compute nodes	183	
Processor/node	2 32-core	
Processor Speed	2.6GHz	
Processor Type	Intel Xeon Ice Lake	
Nodes with Accelerators	8	
Accelerator Type	4 NVIDIA A100	
OS	RHEL v8	
Vendor	Dell	
Memory per node	256/2048 GB	
Detailed Cluster Description		
<u>User Guide</u>		
Available Software		







i. University level: LSU HPC

SuperMIC	
Hostname	smic.hpc.lsu.edu
Peak Performance/TFlops	925
Compute nodes	360
Processor/node	2 10-core
Processor Speed	2.8 GHz
Processor Type	Intel Xeon 64bit
Nodes with Accelerators	360
Accelerator Type	Xeon Phi 7120P
OS	RHEL v6
Vendor	
Memory per node	64 GB
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

Deep Bayou	
Hostname	db1.lsu.edu
Peak Performance/TFlops	257
Compute nodes	13
Processor/node	2 24-core
Processor Speed	2.4 GHz
Processor Type	Intel Cascade Lake Xeon 64bit
Nodes with Accelerators	13
	13 2 x NVIDIA Volta V100S
Accelerators	2 x NVIDIA Volta
Accelerators Accelerator Type	2 x NVIDIA Volta V100S
Accelerators Accelerator Type OS	2 x NVIDIA Volta V100S RHEL V/
Accelerators Accelerator Type OS Vendor	2 x NVIDIA Volta V100S RHEL V/ Dell 192 GB
Accelerators Accelerator Type OS Vendor Memory per node	2 x NVIDIA Volta V100S RHEL V/ Dell 192 GB

SuperMike III	
Hostname	mike.hpc.lsu.edu
Peak Performance/TFlops	1,285
Compute nodes	183
Processor/node	2 32-core
Processor Speed	2.6GHz
Processor Type	Intel Xeon Ice Lake
Nodes with Accelerators	8
Accelerator Type	4 NVIDIA A100
OS	RHEL v8
Vendor	Dell
Memory per node	256/2048 GB
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	





[1] http://www.hpc.lsu.edu/resources/hpc/index.php#lsuhpc



i. University level: LSU HPC

SuperMIC	
Hostname	smic.hpc.lsu.edu
Peak Performance/TFlops	925
Compute nodes	360
Processor/node	2 10-core
Processor Speed	2.8 GHz
Processor Type	Intel Xeon 64bit
Nodes with Accelerators	360
Accelerator Type	Xeon Phi 7120P
OS	RHEL v6
Vendor	
Memory per node	64 GB
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

Deep Bayou	
Hostname	db1.lsu.edu
Peak Performance/TFlops	257
Compute nodes	13
Processor/node	2 24-core
Processor Speed	2.4 GHz
Processor Type	Intel Cascade Lake Xeon 64bit
Nodes with Accelerators	13
Accelerator Type 2 x NVIDIA Volta V1 00S	
OS RHEL v7	
Vendor	Dell
Memory per node	192 GB
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

SuperMike III		
Hostname	mike.hpc.lsu.edu	
Peak Performance/TFlops	1,285	
Compute nodes	183	
Processor/node	2 32-core	
Processor Speed	2.6GHz	
Processor Type	Intel Xeon Ice Lake	
Nodes with Accelerators	8	
	8 4 NVIDIA A100	
Accelerators	, i	
Accelerators Accelerator Type	4 NVIDIA A100	
Accelerator Type OS	4 NVIDIA A100 RHEL V8	
Accelerator Type OS Vendor	4 NVIDIA A100 RHEL V8 Dell 256/2048 GB	
Accelerators Accelerator Type OS Vendor Memory per node	4 NVIDIA A100 RHEL v8 Dell 256/2048 GB er Description	





[1] http://www.hpc.lsu.edu/resources/hpc/index.php#lsuhpc



ii. State level: Louisiana Optical Network Infrastructure (LONI)

- State-of-the-art fiber optic network
- Runs throughout Louisiana, connects Louisiana and Mississippi research universities.
- \$40M Optical Network, 10Gb Ethernet over fiber optics.
- Available to LONI subscribers and their affiliates
- Administered & supported by HPC@LSU









ii. State level: Louisiana Optical Network Infrastructure (LONI)

- Subscribers:
 - Louisiana State University
 - Louisiana Tech University
 - LSU Health Sciences Center in New Orleans
 - LSU Health Sciences Center in Shreveport
 - Southern University
 - Tulane University
 - University of Louisiana at Lafayette
 - University of New Orleans
 - Grambling State University
 - Southeastern Louisiana University
 - ...







ii. State level: Louisiana Optical Network Infrastructure (LONI)

QB2	
Hostname	qb2.loni.org
Peak Performance/TFlops	1,474
Compute nodes	504
Processor/node	2 10-Core
Processor Speed	2.8GHz
Processor Type	Intel Ivy Bridge–EP Xeon 64bit
Nodes with Accelerators	480
Accelerator Type	NVIDIA Tesla K20x
OS	RHEL v6
Vendor Dell	
Memory per node 64 GB	
Location	Information Systems Building, Baton Rouge
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	

QB3	
Hostname	qbc.loni.org
Peak Performance/TFlops	857
Compute nodes	202
Processor/node	2 24-Core
Processor Speed	2.4GHz
Processor Type	Intel Cascade Lake Xeon 64bit
Nodes with Accelerators	8
Accelerator Type	NVIDIA Volta V100
OS	RHEL v7
Vendor Dell	
Memory per node	192 GB
Location	Information Systems Building, Baton Rouge
Detailed Cluster Description	
<u>User Guide</u>	
Available Software	





[1] http://www.hpc.lsu.edu/resources/hpc/index.php#loni



- iii. National level: Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS)
 - NSF funded
 - https://access-ci.org/









Summary

	LSU HPC	LONI
Available to	LSU faculty & affiliates	LONI subscribers & affiliates
Clusters	SuperMIC Deep Bayou SuperMike III	QB2 QB3





Outline



HPC User Environment 1

- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC
- 2. Getting started
 - 1) Accounts
 - 2) Allocation
- 3. Into the cluster
 - 1) Getting connected
 - 2) File system
- 4. Software environment
 - 1) Preinstalled (modules)
 - 2) User installation





Getting started



Two things needed to run jobs on our clusters:

1) Account

2) Allocation





Outline



HPC User Environment 1

- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC
- 2. Getting started
 - 1) Accounts
 - 2) Allocation
- 3. Into the cluster
 - 1) What users see?
 - 2) Useful commands & tools
- 4. Software environment
 - 1) Preinstalled (modules)
 - 2) User installation







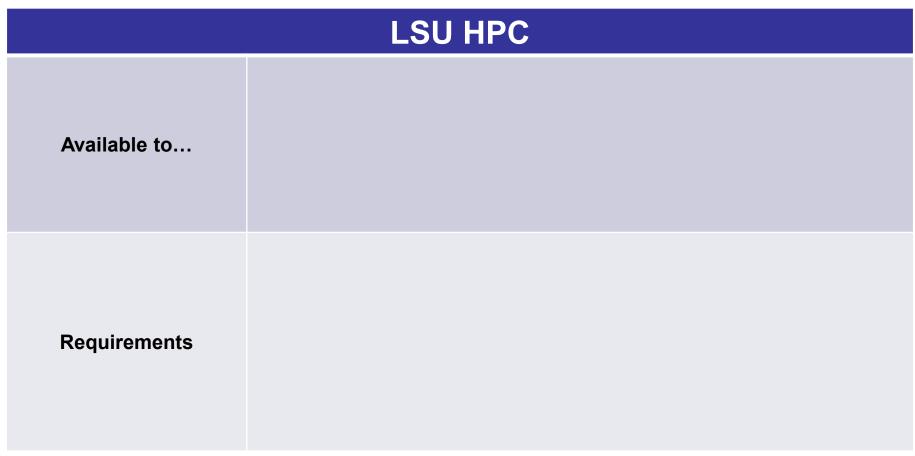
	LSU HPC	LONI
Available to	LSU faculty & affiliates	LONI subscribers & affiliates
Clusters	SuperMIC Deep Bayou SuperMike III	QB2 QB3

- LSU HPC & LONI: distinct systems, distinct accounts
- Having an account on one does not grant the user access to the other















LSU HPC	
Available to	 ✓ Faculty of LSU Baton Rouge campus ✓ Research staff (postdocs, research associates,) ✓ Students (graduate & undergraduate) ✓ Research collaborators (LSU & non-LSU) ✓ Other affiliates
Requirements	







LSU HPC	
Available to	 ✓ Faculty of LSU Baton Rouge campus ✓ Research staff (postdocs, research associates,) ✓ Students (graduate & undergraduate) ✓ Research collaborators (LSU & non-LSU) ✓ Other affiliates
Requirements	 Institutional email (e.g., @lsu.edu) Account sponsor / PI







You are a	Your account sponsor







You are a	Your account sponsor
Full-time faculty @ LSU Baton Rouge campus	Yourself







You are a	Your account sponsor
Full-time faculty @ LSU Baton Rouge campus	Yourself
Graduate student @ LSU doing research	Your advisor







You are a	Your account sponsor
Full-time faculty @ LSU Baton Rouge campus	Yourself
Graduate student @ LSU doing research	Your advisor
Outside collaborator	Your LSU collaborator (full-time faculty)







You are a	Your account sponsor
Full-time faculty @ LSU Baton Rouge campus	Yourself
Graduate student @ LSU doing research	Your advisor
Outside collaborator	Your LSU collaborator (full-time faculty)
LSU student taking a course that requires HPC	Your instructor (full-time faculty)







You are a	Your account sponsor
Full-time faculty @ LSU Baton Rouge campus	Yourself
Graduate student @ LSU doing research	Your advisor
Outside collaborator	Your LSU collaborator (full-time faculty)
LSU student taking a course that requires HPC	Your instructor (full-time faculty)
REU student working @ LSU	Your LSU advisor (full-time faculty)







i. Eligibility (LONI)

LONI		
Available to	 ✓ Faculty of LONI subscribers ✓ Research staff (postdocs, research associates,) ✓ Students (graduate & undergraduate) ✓ Research collaborators (@ LONI subscribers / outside) ✓ Other affiliates 	
Requirements	 Institutional email (e.g., @uno.edu) Account sponsor / PI ✓ Full-time faculty & certain research staff @ LONI subscribers × Students, postdocs, research associates (even @ LONI subscribers) × Outside collaborators × HPC staff 	







i. Eligibility (LONI)

You are a	Your account sponsor
Full-time faculty @ LONI subscribers	Yourself
Graduate student during research	Your advisor (faculty @ LONI subscribers)
Outside collaborator	Your collaborator (faculty @ LONI subscribers)
Student taking a course that requires HPC	Your instructor (faculty @ LONI subscribers)
REU student	Your advisor (faculty @ LONI subscribers)







i. Eligibility (Summary)

	LSU HPC	LONI
Available to	 ✓ Faculty of LSU Baton Rouge campus ✓ Research staff (postdocs, research associates,) ✓ Students (graduate & undergraduate) ✓ Research collaborators (LSU & non-LSU) ✓ Other affiliates 	 ✓ Faculty of LONI subscribers ✓ Research staff (postdocs, research associates,) ✓ Students (graduate & undergraduate) ✓ Research collaborators ✓ Other affiliates
Requirements	 Institutional email (e.g., @lsu.edu) Account sponsor / PI Full-time faculty & certain research staff @ LSU Baton Rouge campus Students, postdocs, research associates (even @ LSU) Outside collaborators HPC staff 	 Institutional email (e.g., @uno.edu) Account sponsor / PI Full-time faculty & certain research staff @ LONI subscribers Students, postdocs, research associates (even @ LONI subscribers) Outside collaborators HPC staff



i. Eligibility

- **❖** I can be granted an LSU HPC or LONI account if:
 - a) I am using HPC resource for my research, the account will be sponsored by my advisor (PI)
 - b) I am attending HPC training sessions, the account will be sponsored by the HPC staff
 - c) I am taking a class that requires using HPC resource, the account will be sponsored by the course instructor
 - d) a and b
 - e) a and c
 - f) All of the above







i. Eligibility

- **❖** I can be granted an LSU HPC or LONI account if:
 - a) I am using HPC resource for my research, the account will be sponsored by my advisor (PI)
 - b) I am attending HPC training sessions, the account will be sponsored by the HPC staff
 - c) I am taking a class that requires using HPC resource, the account will be sponsored by the course instructor
 - d) a and b
 - e) a and c
 - f) All of the above







i. Eligibility

- Who may be eligible for LSU HPC accounts? (Choose all that apply)
 - a) Alice, a professor in Europe, who collaborates with Professor X @ LSU Baton Rouge campus and wishes to run simulations
 - b) Bob, recently graduated from LSU and moved to New York for a postdoc position, but is still working with his PhD advisor Professor Y @ LSU Baton Rouge campus to finish their unfinished research
 - c) Charlie, a current undergraduate student @ LSU Baton Rouge campus, who is taking an online Machine Learning course given by Professor Z @ Stanford, and needs practice on a GPU-enabled HPC system







i. Eligibility

- **❖** Who may be eligible for LSU HPC accounts? (Choose all that apply)
 - a) Alice, a professor in Europe, who collaborates with Professor X @ LSU Baton Rouge campus and wishes to run simulations
 - b) Bob, recently graduated from LSU and moved to New York for a postdoc position, but is still working with his PhD advisor Professor Y @ LSU Baton Rouge campus to finish their unfinished research
 - c) Charlie, a current undergraduate student @ LSU Baton Rouge campus, who is taking an online Machine Learning course given by Professor Z @ Stanford, and needs practice on a GPU-enabled HPC system







ii. How to apply

	LSU HPC	LONI
Portal	https://accounts.hpc.lsu.edu/login_request.php	https://allocations.loni.org/login_request.php







ii. How to apply

	LSU HPC	LONI
Portal	https://accounts.hpc.lsu.edu/login_request.php	https://allocations.loni.org/login_request.php



[1] http://www.hpc.lsu.edu/links.php





ii. How to apply

	LSU HPC	LONI
Portal	https://accounts.hpc.lsu.edu/login_request.php	https://allocations.loni.org/login_request.php
Steps	 a) Enter your institutional email and submit b) Check email and open the link (valid for 24 hrs) c) Fill the form (In Contact/Collaborator, enter your d) You will receive a notification when your account Be patient. Do not reset your password if you cannot 	nt is activated once we have verified your credentials







iii. Manage your account

	LSU HPC	LONI
Portal	https://accounts.hpc.lsu.edu	https://allocations.loni.org







iii. Manage your account

	LSU HPC	LONI
Portal	https://accounts.hpc.lsu.edu	https://allocations.loni.org
Things to do	 Change personal information, password, Change default shell (bash / tcsh / ksh / csh / sh) Request / manage / check allocation Request / manage / check storage 	







iv. Reset password

	LSU HPC	LONI
Portal	https://accounts.hpc.lsu.edu/user_reset.php	https://allocations.loni.org/user_reset.php



SN



iv. Reset password

	LSU HPC	LONI
Portal	https://accounts.hpc.lsu.edu/user_reset.php	https://allocations.loni.org/user_reset.php
Steps	 a) Enter your registered email and submit b) Check email and open the link (valid for 24 hrs) c) Enter your new password and submit d) You will receive a confirmation email once your new ** IMPORTANT *** Your new password is NOT available right aw Do NOT submit multiple times 	ew password is approved by our staff vay (wait until you receive confirmation of approval)



[1] http://www.hpc.lsu.edu/links.php





iv. Reset password

Case study

User:

"I have been trying to access my accounts on QB2 via an SSH client, but the connection won't go through. I reset my passwords this weekend and the terminals keep giving me a 'Password Authentication Failed' error message....."

User Services:

"When you send a password reset request, it has to be manually processed for security reason before your new password becomes available."







Reset password

Password security

- Passwords should be changed as soon as your account is activated for added security.
- Password must be at least 12 and at most 32 characters long, must contain 3 of the 4 classes of characters
 - Lowercase letters
 - Uppercase letters
 - **Digits**
 - Special characters (punctuation, spaces, etc.)
- Do not use a word or phrase from a dictionary
- Do not use a word that can be obviously tied to the user (e.g., your name, user name, etc.)
- Do NOT share your password to others, including your advisor!!!!!





Outline



HPC User Environment 1

- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC
- 2. Getting started
 - 1) Accounts
 - 2) Allocation
- 3. Into the cluster
 - 1) Getting connected
 - 2) File system
- 4. Software environment
 - 1) Preinstalled (modules)
 - 2) User installation







Account sponsor

Sponsor what?

Allocation







i. What is allocation?

- A deposit of service units (SU) that users will be charged from to run jobs on our cluster
 - 1 SU = 1 core-hour
 - Example:
 - My allocation: 50,000 SU
 - Running a job: 24 core * 10 hours = 240 SU
 - Balance: 49,760 SU
 - Cannot run jobs after exhausted
- All LSU HPC & LONI clusters requires allocation to run jobs
- Free to users
- But not worthless! (1 SU ≈ \$0.1)







ii. Eligibility

You are a	To get allocation







ii. Eligibility

You are a	To get allocation
Account sponsor / PI*	Submit a request





^{*} Full-time faculty & certain research staff @ LSU / LONI subscribers



ii. Eligibility

You are a	To get allocation
Account sponsor / PI*	Submit a request
Non-account sponsor / non-PI	Join your sponsor's allocation





^{*} Full-time faculty & certain research staff @ LSU / LONI subscribers



iii. Request an allocation (if you are an account sponsor / PI)

	LSU HPC	LONI
Portal	https://accounts.hpc.lsu.edu/allocations.php	https://allocations.loni.org/allocations.php







iii. Request an allocation (if you are an account sponsor / PI)

	LSU HPC	LONI
Portal	https://accounts.hpc.lsu.edu/allocations.php	https://allocations.loni.org/allocations.php
Steps	 a) Log in using your account b) Click on "New Allocation for [Cluster Name]" SuperMIC & SuperMike III share allocations QB2 and QB3 share allocations Deep Bayou has separated allocation c) Fill the form and submit d) Your request will be reviewed, and you will be not 	ified if your allocation is approved







iii. Request an allocation (if you are an account sponsor / PI)

Allocation types





[2] http://www.hpc.lsu.edu/users/lonipolicy.php





iii. Request an allocation (if you are an account sponsor / PI)

Allocation types

Type	Size [SU]	Can be requested	Decisions made on	Activated on	Limited to
Startup	50,000	Any time	Following request		2 active / PI
				Jan 1 Apr 1 Jul 1	
				Oct 1	





[2] http://www.hpc.lsu.edu/users/lonipolicy.php





iii. Request an allocation (if you are an account sponsor / PI)

Allocation types

Туре	Size [SU]	Can be requested	Decisions made on	Activated on	Limited to
Startup	50,000	Any time	Following request		2 active / PI
Research	> 50 000	> 50,000 Sign 1		Jan 1 Apr 1 Jul 1	[LSU HPC] 3,000,000 SU / allocation 5,000,000 SU / PI
Research	> 50,000			decision date Jul 1 Oct 1	[LONI] 6,000,000 SU / allocation 12,000,000 SU / PI





^[2] http://www.hpc.lsu.edu/users/lonipolicy.php





iii. Request an allocation (if you are an account sponsor / PI)

Allocation types

_			Proposal				
Туре	Гуре Size [SU]		Technical merit	Software characteristics	Previous impact and outcome	External funding or LSU demand	# of pages
Startup)	50,000			(Not required)		
	A	>50,000 and ≤300,000	Required	Required	Optional	Optional	4
Research	В	>300,000 and ≤1,000,000	Required	Required	Required	Optional	5
	С	>1,000,000	Required	Required	Required	Required	6





^[2] http://www.hpc.lsu.edu/users/lonipolicy.php





iv. Join an allocation (if you are not an account sponsor / PI)

LSU HPC	LONI
https://accounts.hpc.lsu.edu/allocations.php	https://allocations.loni.org/allocations.php







iv. Join an allocation (if you are not an account sponsor / PI)

	LSU HPC	LONI
Portal	https://accounts.hpc.lsu.edu/allocations.php	https://allocations.loni.org/allocations.php
Steps	 [Method 1: Join by request] a) Log in using your account b) Click on "Join allocation" c) Search for your account sponsor / PI, and click "Join d) Find the desired allocation you wish to join, click "Join e) Your account sponsor / PI will receive an email notifice [Method 2: Ask your PI to add you] a) Ask your PI to log in using his/her account b) Click on "Manage memberships" c) Find the desired allocation, click "Edit -> Add a User" d) Search for your account, click "Add to [Allocation name 	n" oation and approve your request



* HPC staff CANNOT add you to allocations! Must be approved by your PI!





iv. Join an allocation (if you are not an account sponsor / PI)

Case study

User:

"Hi, my PI recently applied for an allocation on SuperMIC and was approved (see forwarded email below). However, I do not see that this allocation is available for my use in https://accounts.hpc.lsu.edu/balances.php. When will I be able to access the allocation?"

User Services:

"You should either request to join your PI's allocation through the user portal, or ask your PI to add you to the allocation"





Summary



Test

- **❖** What are the <u>TWO</u> things required to run jobs on our clusters?
 - a) An active myLSU account
 - b) An active LSU HPC / LONI account
 - c) An active LSU HPC / LONI allocation
 - d) A valid payment method (credit card / bank account / check / cash ...) to pay for the services

3. Into the cluster





Summary



Test

- **❖** What are the <u>TWO</u> things required to run jobs on our clusters?
 - a) An active myLSU account
 - b) An active LSU HPC / LONI account
 - c) An active LSU HPC / LONI allocation
 - d) A valid payment method (credit card / bank account / check / cash ...) to pay for the services





Break time!



- Login to one of the user portals (LSU HPC or LONI) with your HPC username and password.
 Update your email and phone number (for practice).
 - LSU HPC: https://accounts.hpc.lsu.edu
 - LONI: https://allocations.loni.org
- Download MobaXterm (if you are Windows user)
- Review commands in Linux and the vim editor





Break time!



	Cheat sheet of Commands in Linux
history	Command history
mkdir	Make a folder
ls	List a folder -a List all files including hidden -I Shows files with a long listing format
cd	Change directory
pwd	Show current directory
ср	Сору
rm	Remove files (CAREFUL!)
Up arrow (↑)	Move back in history
Tab	Fill in unique file name
Tab Tab	Press tab twice, show all available file names





Break time!



Cheat sheet of vim editor

- vi (name of file)
- Commands in VI
 - i enter insert mode (-- INSERT -- shows in the bottom left corner)
 - esc exits insert mode, back to the command mode
 - dd -> deletes line
 - u -> Undo
 - Shift Z shift Z or :wq -> saves and exits VI
 - :q! -> exit without saving
 - : (some number) -> moves through file to row #
 - /(indicator) -> search
 - Use N to find Next
 - [(page up)] (page down)
- NO CAPS (for example :q! is not :Q!)





Outline



HPC User Environment 1

- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC
- 2. Getting started
 - 1) Accounts
 - 2) Allocation
- 3. Into the cluster
 - 1) Getting connected
 - 2) File system
- 4. Software environment
 - 1) Preinstalled (modules)
 - 2) User installation







Term	Definition







Term	Definition
Cluster	A set of connected computer nodes that work together. (<i>E.g.</i> , <i>QB2</i>)





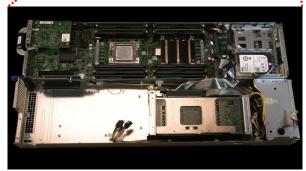






Term	Definition
Cluster	A set of connected computer nodes that work together. (E.g., QB2)
Node	A single, named host machine in the cluster. (<i>E.g., qb010</i>)



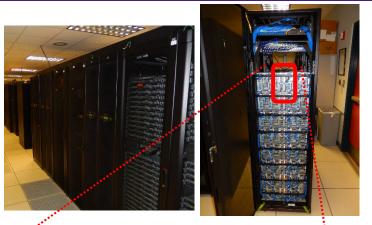


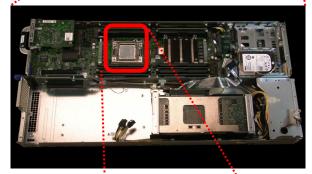


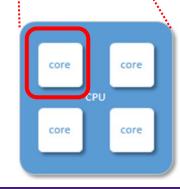




Term	Definition
Cluster	A set of connected computer nodes that work together. (<i>E.g.</i> , <i>QB2</i>)
Node	A single, named host machine in the cluster. (<i>E.g., qb010</i>)
Core	The basic computation unit in a processor. (E.g., QB2 has two 10-core processors \rightarrow 20 cores)





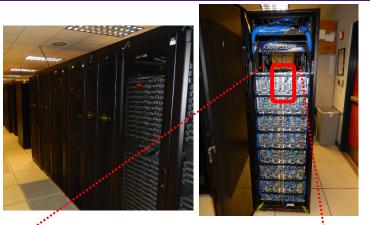


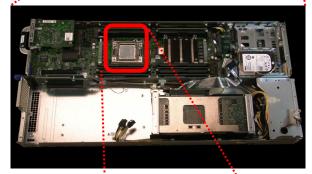


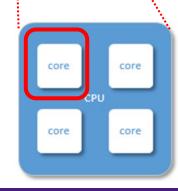




Term	Definition
Cluster	A set of connected computer nodes that work together. (<i>E.g., QB2</i>)
Node	A single, named host machine in the cluster. (<i>E.g., qb010</i>)
Core	The basic computation unit in a processor. (E.g., QB2 has two 10-core processors \rightarrow 20 cores)
Job	A user's request to use a certain amount of resources for a certain amount of time on cluster for his/her work.





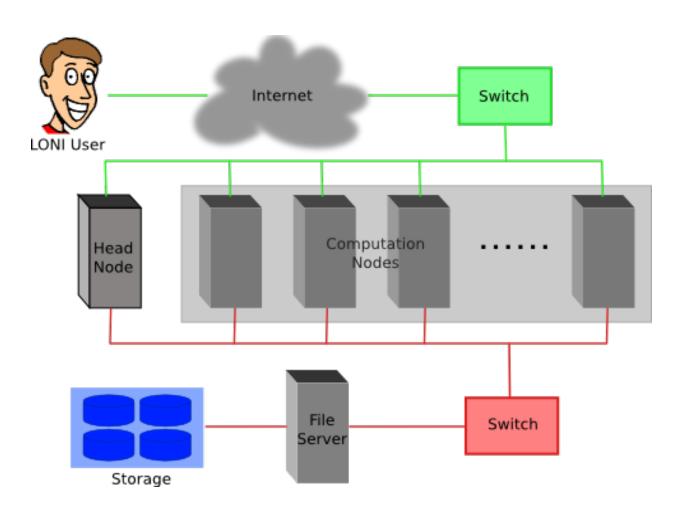








- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously

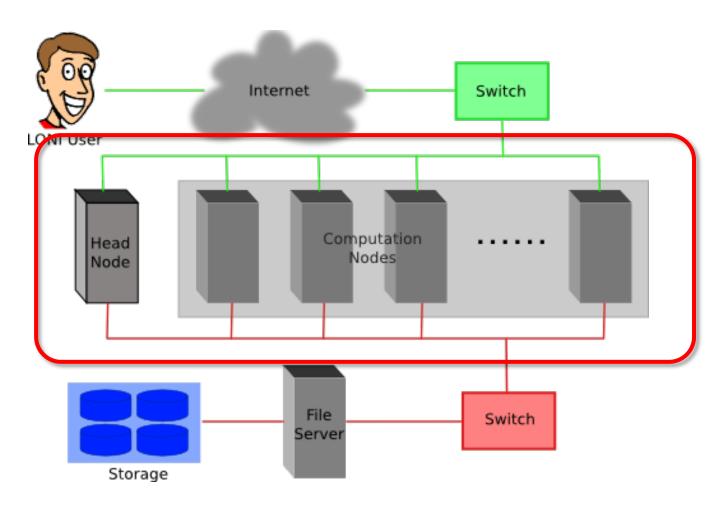








- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously

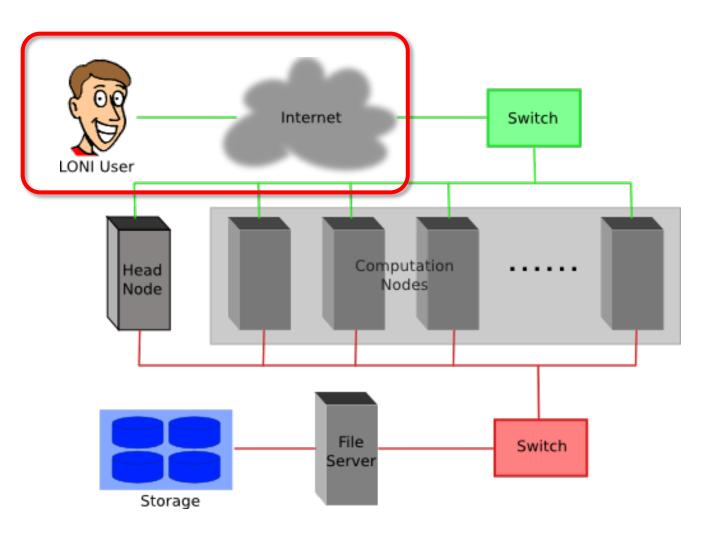








- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously

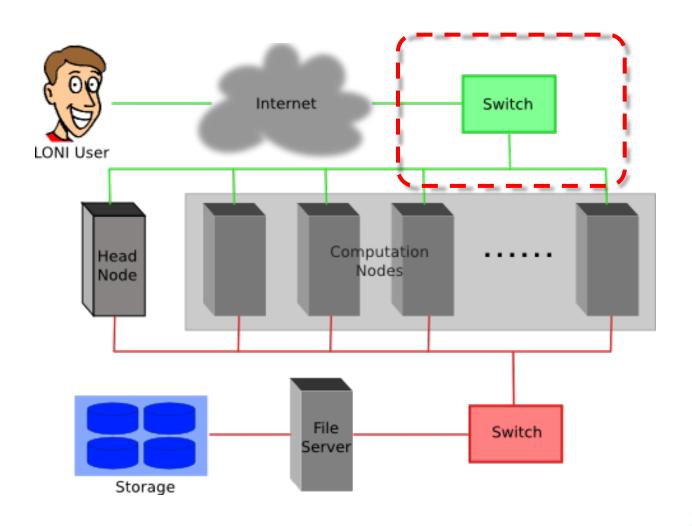








- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously

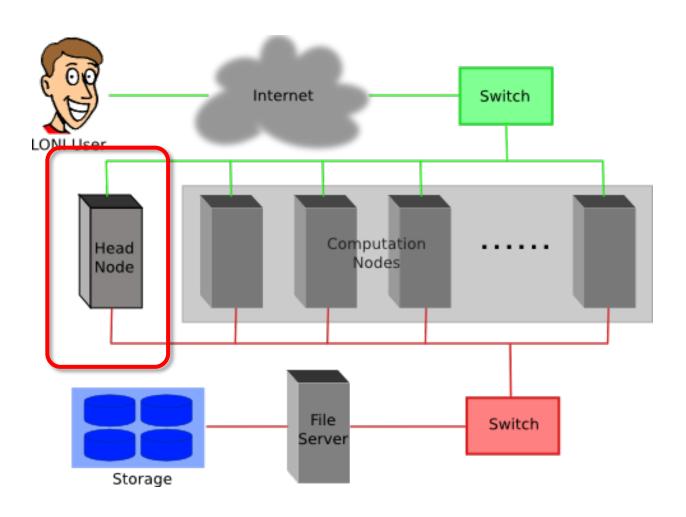








- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously

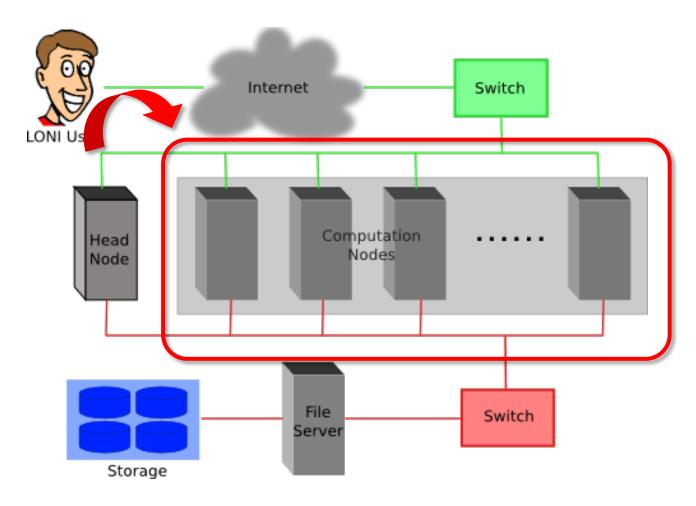








- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously





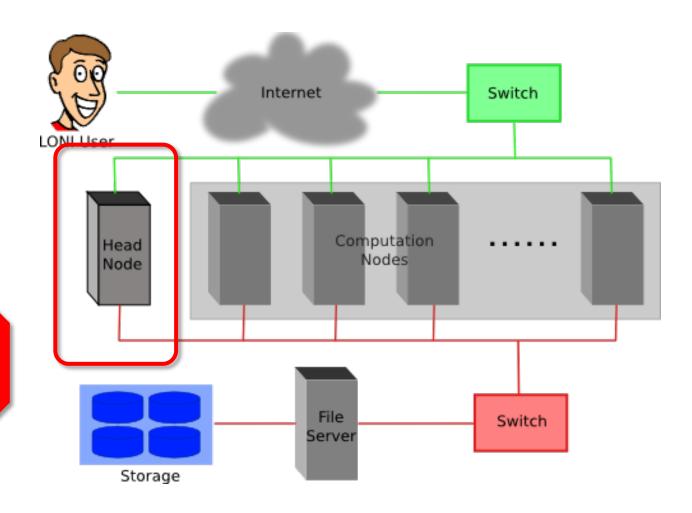




General architecture

- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously

DO NOT RUN **JOBS ON HEAD** NODE!!!









ii. Logging in

Secure Shell (SSH)







ii. Logging in

Secure Shell (SSH)

Tool you need







ii. Logging in

Secure Shell (SSH)

Tool you need
Terminal







ii. Logging in

Secure Shell (SSH)

Your OS	Tool you need
Linux / Mac	Terminal
Windows	MobaXterm SSH Secure Shell Putty







ii. Logging in

Secure Shell (SSH)

Your OS	Tool you need	
Linux / Mac	Terminal	
Windows	MobaXterm SSH Secure Shell Putty	
A web browser *	Open OnDemand (OOD) * (https://ondemand.smic.hpc.lsu.edu)	

- * Only on SMIC at the moment
 - Several frequently used applications
 - Must via a wired connection from LSU Baton Rouge campus (or via VPN)







ii. Logging in

Secure Shell (SSH)

Cluster		Address	
	SMIC	smic.hpc.lsu.edu	
LSU HPC	Deep Bayou	db1.hpc.lsu.edu	
	SuperMike III	mike.hpc.lsu.edu	
LONI	QB-2	qb.loni.org	
LONI	QB-3	qbc.loni.org	

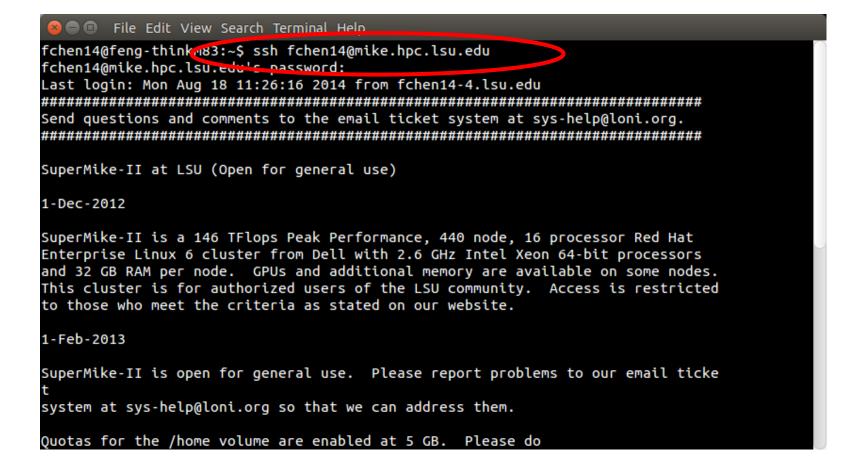






ii. Logging in

a) Linux / Mac

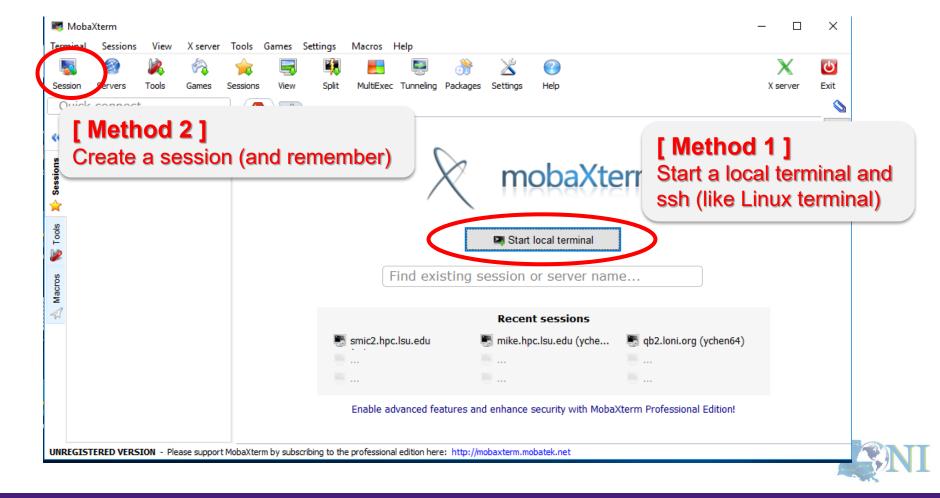








- b) Windows
 - MobaXterm







- b) Windows
 - SSH Secure Shell

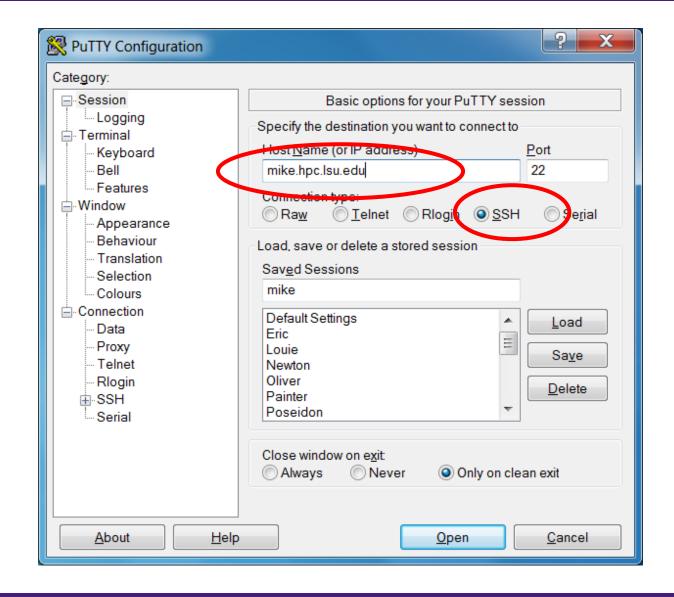
```
qb4.loni.org - qb2* - SSH Secure Shell
                                                                                                    ×
 File Edit View Window Help
    Quick Connect Profiles
[vchen64@qb4 r]$ pwd
/home/vchen64/r
[ychen64@qb4 r]$ 11
total 8280
-rwxr-xr-x 1 ychen64 loniadmin 8034120 Apr 1 2015 data clean.csv
-rwxr-xr-x 1 ychen64 loniadmin 318263 Apr 24 2015 Folds5x2 op.csv
-rwxr-xr-x 1 ychen64 loniadmin
                             1599 Apr 27 2015 Rplots.pdf
-rwxr-xr-x 1 ychen64 loniadmin
                              78 Jan 9 13:28 install.sh
-rw-r--r-- 1 ychen64 loniadmin
                             9557 Jan 17 08:09 codes.txt
                              77 Jan 18 09:22 temp.dat
-rwxr-xr-x 1 ychen64 loniadmin
-rw-r--r-- 1 ychen64 loniadmin
                              555 Jan 24 11:56 codes2.txt
                              9697 Jan 24 12:10 p9h120.o326126
-rw----- 1 ychen64 loniadmin
-rw----- 1 ychen64 loniadmin
                                9562 Jan 24 12:11 p9h120.o326129
                                9587 Jan 24 12:26 p9h120.o326131
-rw----- 1 ychen64 loniadmin
                               2253 Jan 24 12:27 p9h120.o326133
-rw----- 1 ychen64 loniadmin
-rw-r--r-- 1 ychen64 loniadmin
                              624 Jan 24 12:28 mdrun.submit
-rw-r--r-- 1 vchen64 loniadmin
                                  24 Jan 24 12:28 a.log
                              43751 Jan 24 13:29 p9h120.o326134
-rw----- 1 ychen64 loniadmin
[ychen64@qb4 r]$ scp a.log ychen64@mike.hpc.lsu.edu:/home/ychen64/test/
vchen64@mike.hpc.lsu.edu's password:
```







- b) Windows
 - Putty









- ❖ Special note: X11 forwarding
 - Enables graphic user interface (GUI)







- ❖ Special note: X11 forwarding
 - Enables graphic user interface (GUI)

You are using		To enable X11 forwarding	







- ❖ Special note: X11 forwarding
 - Enables graphic user interface (GUI)

You are using	To enable X11 forwarding	
Linux (e.g., Ubuntu)	ssh –X username@server.address	







- ❖ Special note: X11 forwarding
 - Enables graphic user interface (GUI)

You are using	To enable X11 forwarding	
Linux (e.g., Ubuntu)	ssh –X username@server.address	
Mac	a) Install X server (e.g. XQuartz)b) ssh -X username@server.address	







- ❖ Special note: X11 forwarding
 - Enables graphic user interface (GUI)

You are using		To enable X11 forwarding		
Linux (e.g., Ubuntu)		ssh –X username@server.address		
Mac		a) Install X server (<i>e.g.</i> XQuartz)b) ssh -X username@server.address		
Windows				







- ❖ Special note: X11 forwarding
 - Enables graphic user interface (GUI)

You are using		To enable X11 forwarding	
Linux (e.g., Ubuntu)		ssh –X username@server.address	
Mac		a) Install X server (e.g. XQuartz)b) ssh -X username@server.address	
Windows	MobaXterm	Enabled by default (can be disabled in "Advanced SSH Settings")	
VVIIIUUWS			







- ❖ Special note: X11 forwarding
 - Enables graphic user interface (GUI)

You are using		To enable X11 forwarding	
Linux (e.	g., Ubuntu)	ssh –X username@server.address	
Mac		a) Install X server (e.g. XQuartz)b) ssh -X username@server.address	
Mindowo	MobaXterm	Enabled by default (can be disabled in "Advanced SSH Settings")	
Windows	Putty	 a) Install X server (e.g. Xming) b) Connection → SSH → X11 → Enable X11 forwarding 	







Useful commands		
who	Check who is on the node	
balance / showquota	Check allocation balance	
history	Command history	
mkdir	Make a folder	
ls	List a folder -a List all files including hidden -l Shows files with a long listing format	
cd	Change directory	
pwd	Show current directory	
ср	Сору	
rm	Remove files (CAREFUL!)	
Up arrow (↑)	Move back in history	
Tab	Fill in unique file name	
Tab Tab	Press tab twice, show all available file names	





Outline



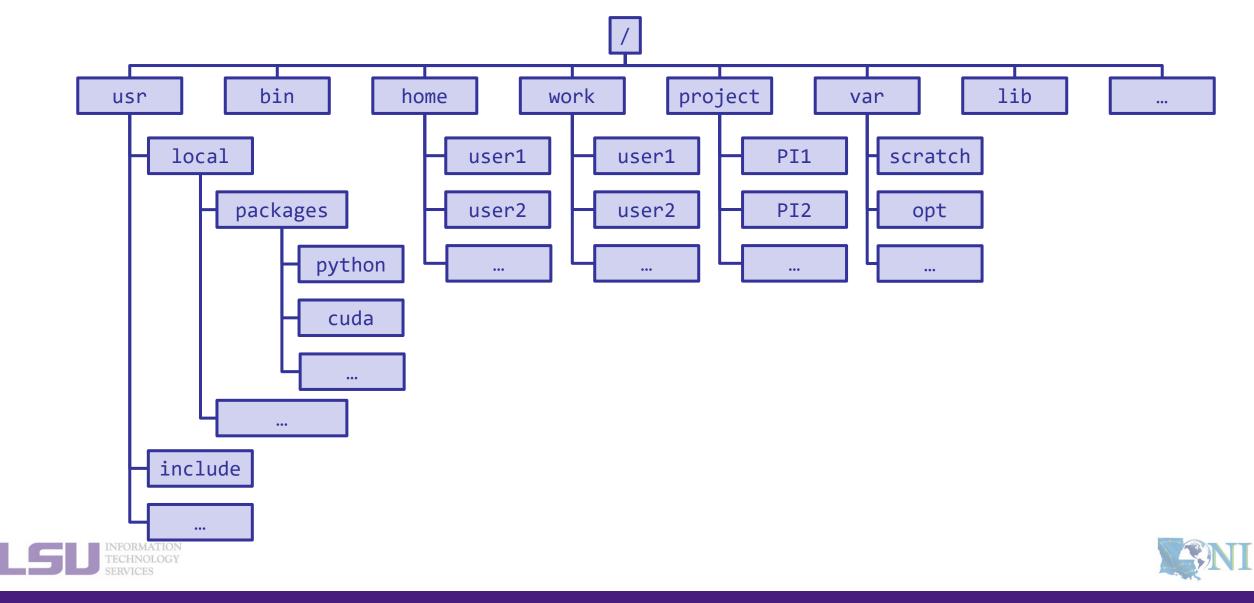
HPC User Environment 1

- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC
- 2. Getting started
 - 1) Accounts
 - 2) Allocation
- 3. Into the cluster
 - 1) Getting connected
 - 2) File system
- 4. Software environment
 - 1) Preinstalled (modules)
 - 2) User installation

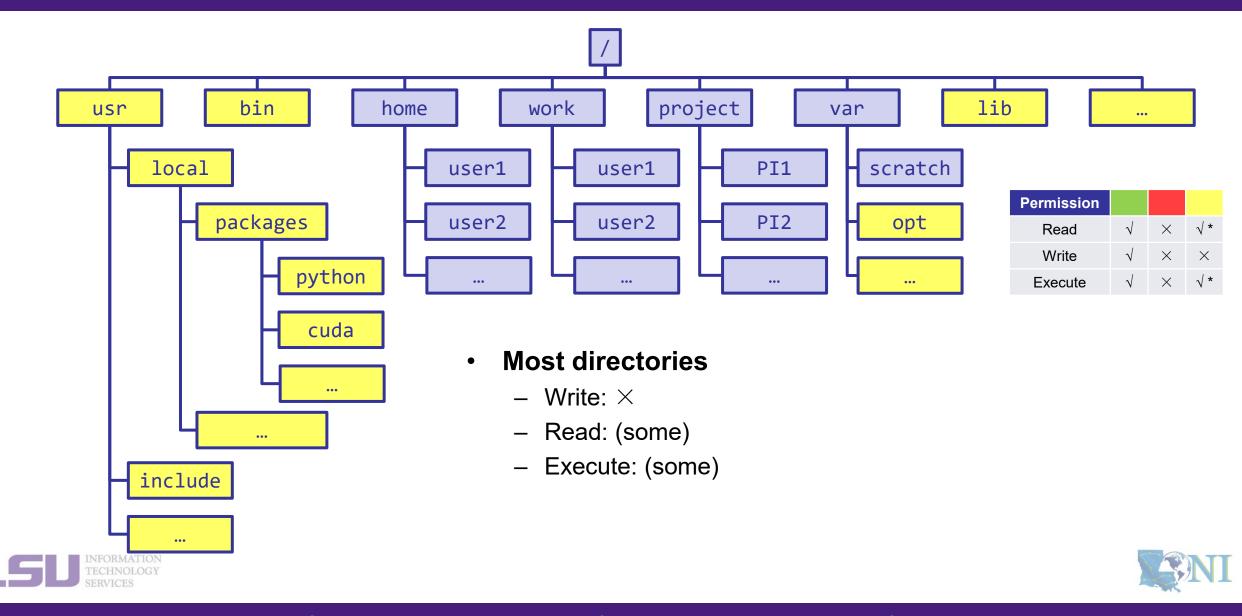




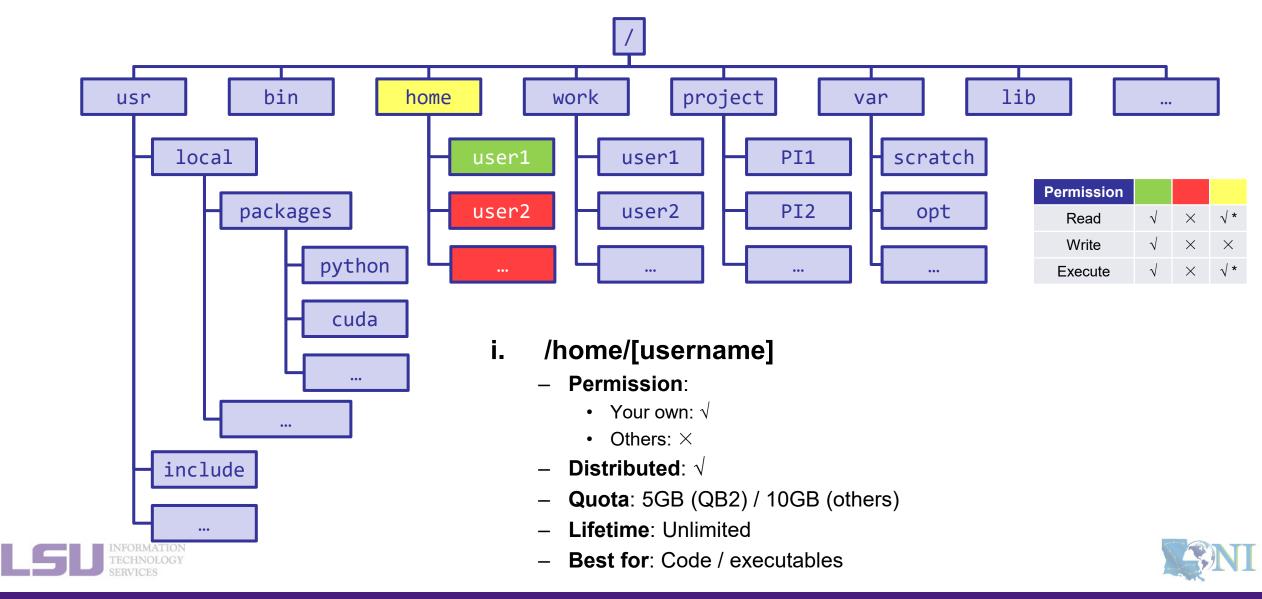




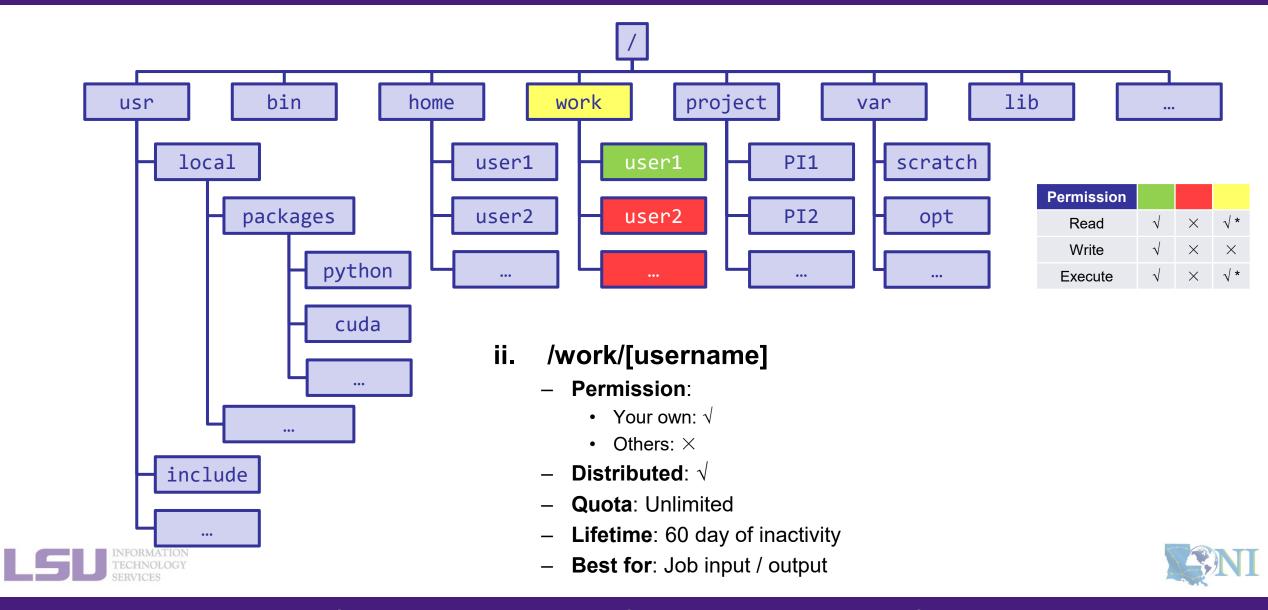




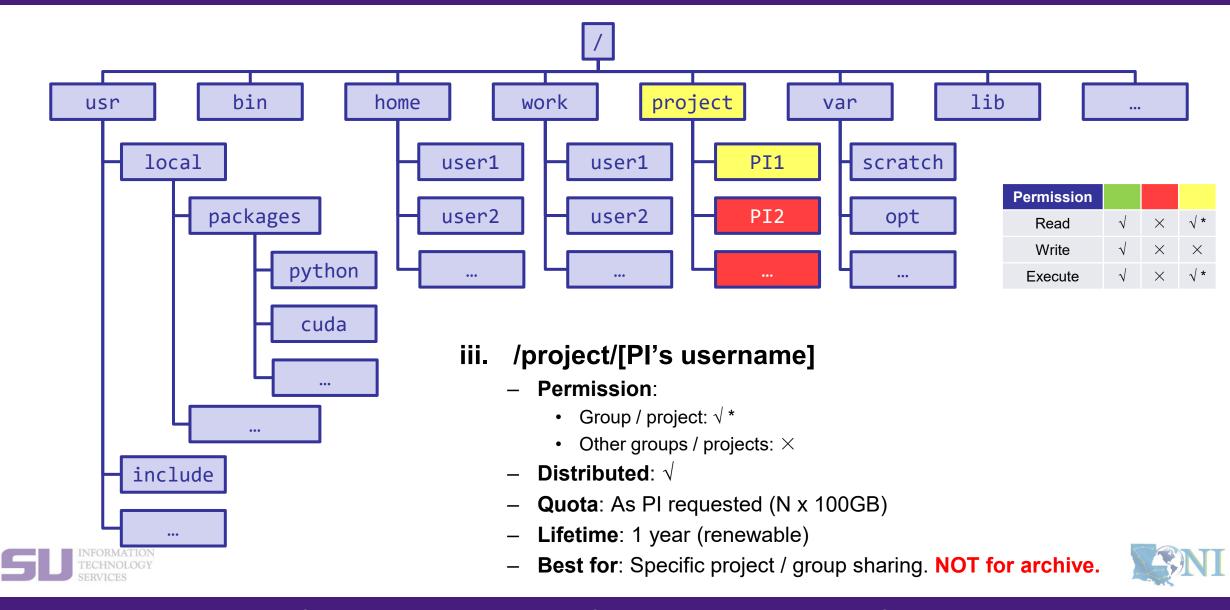




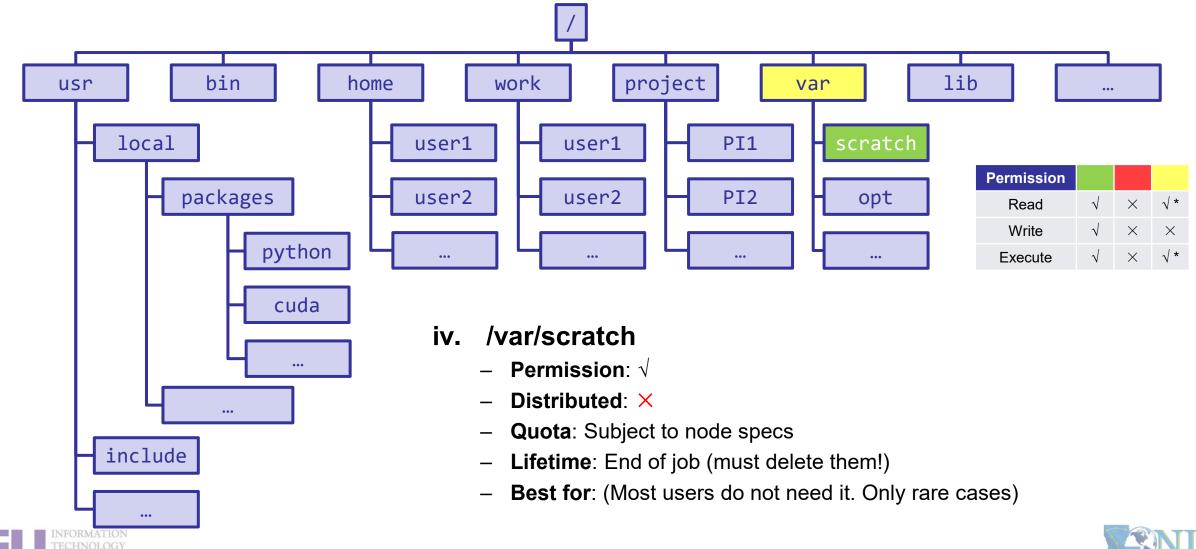
















File system summary

Directory (folder)	Distributed	Throughput	Lifetime	Quota	Best for
/home/[username]	V	Low	Unlimited	5GB (QB2) 10GB (others)	Code / executables
/work/[username]	V	High	60 days of inactivity	Unlimited	Job input/output
/project/[Pi's username]	√	Medium / High	1 year (renewable)	As PI requested (N x 100GB)	Specific project / group sharing. NOT for archive!
/var/scratch	×	High	End of job	Subject to node specs	(Most users do not need it. Only rare cases)

Tips

- Neither /work nor /project is for long-term storage
- /work directory will be created 1 hour after the first cluster login
- /project directory: Only PI w/ active allocations can apply! (See appendix or contact us)
- Never write output to your home directory!
- Check current disk quota and usage: balance / showquota







File transfer

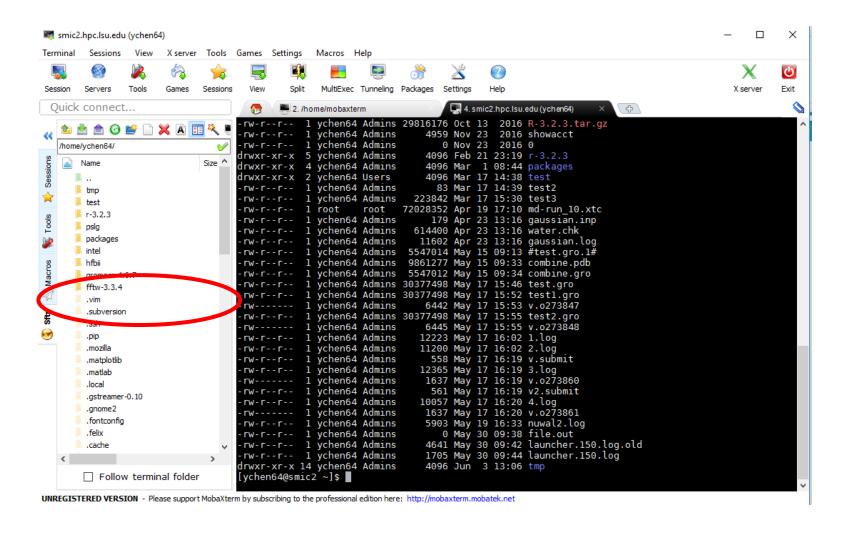
Commands		
scp / rsync	 From/to a Unix/Linux/Mac machine (including between the clusters) Syntax: scp <options> <source/> <destination></destination></options> rsync <options> <source/> <destination></destination></options> 	
wget	From a download link on a website (usually opened with a web browser)Syntax: wget <link/>	







File transfer







Outline



HPC User Environment 1

- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC
- 2. Getting started
 - 1) Accounts
 - 2) Allocation
- 3. Into the cluster
 - 1) Getting connected
 - 2) File system
- 4. Software environment
 - 1) Preinstalled (modules)
 - 2) User installation





Outline



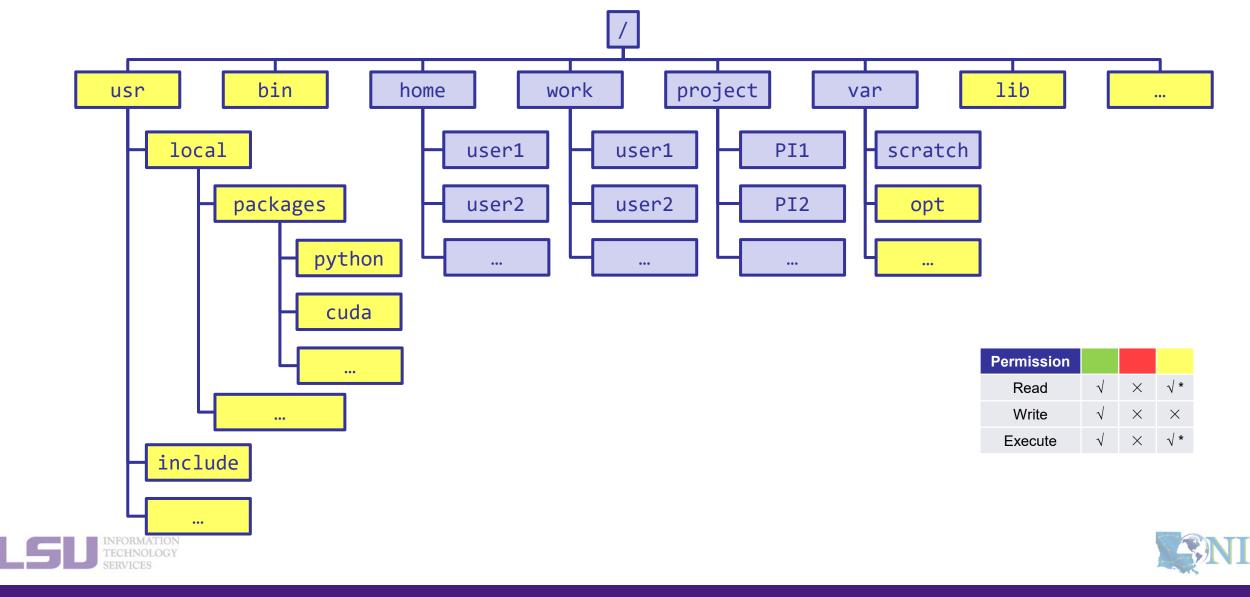
HPC User Environment 1

- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC
- 2. Getting started
 - 1) Accounts
 - 2) Allocation
- 3. Into the cluster
 - 1) Getting connected
 - 2) File system
- 4. Software environment
 - 1) Preinstalled (modules)
 - 2) User installation

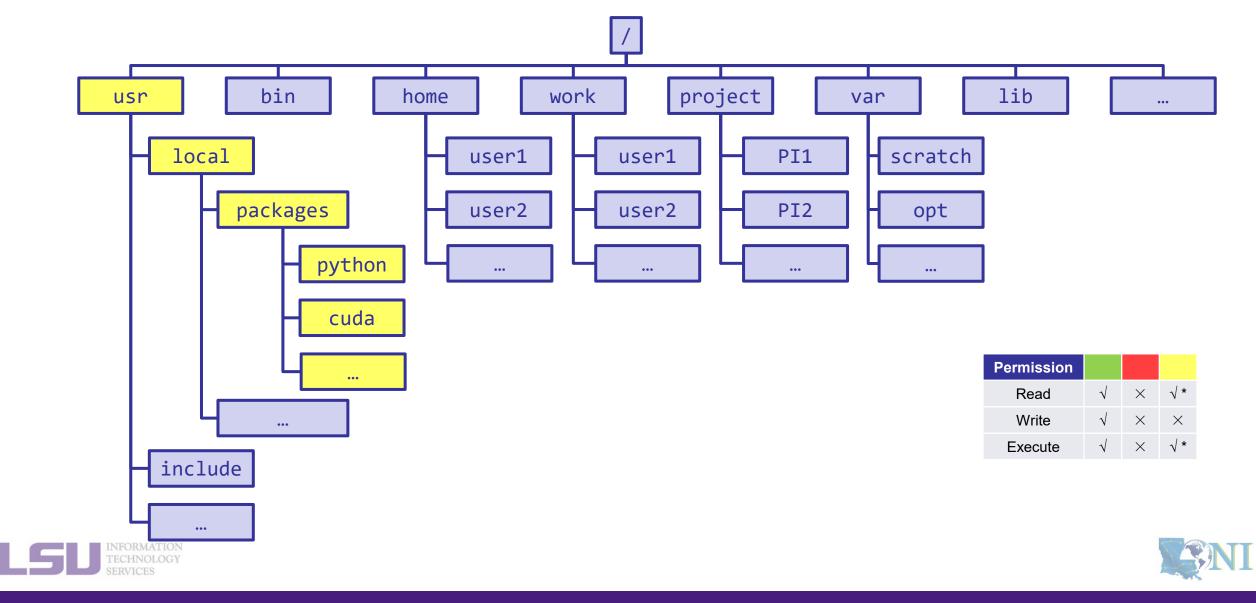














Modules

- Softwares that are can be loaded / unloaded on demand.
- List of modules preinstalled system-wide: https://www.hpc.lsu.edu/docs/guides/index.php

Category	Modules
Mathematical & utility	FFTW, HDF5, NetCDF, PETSc
Applications	Amber, CPMD, NWChem, NAMD, Gromacs, R, LAMMPS
Visualization	VisIt, VMD, GaussView
Programming Tools	Totalview, DDT, TAU







Modules

Useful commands		
module available (module av)	List available modules on the cluster	
module list (module li)	List currently loaded modules	
module load [module name]	Load module(s)	
module unload [module name]	Unload module(s)	
module swap [module 1] [module 2]	Unload a Module 1 and load Module 2	
module purge	Unload all modules	
module display [module name]	Display module information and all environmental variables changes when loaded	







Modules

– Auto-load modules: ~/.modules





Outline



HPC User Environment 1

- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC
- 2. Getting started
 - 1) Accounts
 - 2) Allocation
- 3. Into the cluster
 - 1) Getting connected
 - 2) File system
- 4. Software environment
 - 1) Preinstalled (modules)
 - 2) User installation







You can't	You can

3. Into the cluster







You can't	You can
yum / apt-getsudo (!!!)	







You can't	You can
yum / apt-getsudo (!!!)	 Build from source Use virtual environment (e.g., conda) * Advanced methods (e.g., Singularity) * Ask HPC staff for help







Recommended paths:

- a) /home (for yourself)
- b) /project (for group sharing or large applications)





Summary



- Two types of software packages:
 - Preinstalled (modules)
 - User installed





3. Into the cluster

Take home message



HPC User Environment 1

- 1. Intro to HPC
 - 1) Why HPC?
 - 2) What is HPC?
 - 3) Our HPC

→ LSU HPC (SMIC, Deep Bayou, SuperMike III) / LONI (QB2, QB3)

- 2. Getting started
 - 1) Accounts

→ Need an account sponsor! Most likely a faculty

2) Allocation

→ Request a new one or join an existing one

- 3. Into the cluster
 - 1) Getting connected
- → Logging in via SSH; Do NOT run jobs on head node

- → Know your /home, /work, /project
- 4. Software environment
 - 1) Preinstalled

- → Use modules
- 2) User installation
- → No sudo or yum





Next week



HPC User Environment 2

- 1. Queuing system
- 2. How to run jobs





Contact us



Contact user services

Email Help Ticket: sys-help@loni.org

Telephone Help Desk: +1 (225) 578-0900





Appendix 1. Applying for storage allocation (/project)



- Storage allocation ≠ computing allocation (what we talked about today)
- PI can apply for extra disk space on the /project volume for you and his/her entire research group if
 - your research requires some files to remain on the cluster for a fairly long period of time; and
 - their size exceeds the quota of the /home
- The unit is 100 GB
- Storage allocations are good for 1 year, but can be extended based on the merit of the request
- Examples of valid requests
 - I am doing a 12-month data mining project on a large data set
 - The package I am running requires 10 GB of disk space to install
- Examples of invalid requests
 - I do not have time to transfer the data from my scratch space to my local storage and I need a temporary staging area





Appendix 2. Create your own module key



• An example of a simple module file (~/my_module/gitkey):

```
#%Module
proc ModulesHelp { } {
    puts stderr { my compiled version of git.
    }
}
module-whatis {version control using git}
set GIT_HOME /home/fchen14/packages/git-master/install
prepend-path PATH $GIT_HOME/bin
```

Add the path to the key to the MODULEPATH environment variable:

```
$ export MODULEPATH=~/my_module:$MODULEPATH
```

Then try to use:

```
$ module load gitkey
$ which git
$ module unload gitkey
$ which git
```



