System Overview

Jason Li

HPC User Services

LSU HPC / LONI

sys-help@loni.org

Louisiana State University

Baton Rouge

July 27, 2022

Outline

- **System Overview**

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

Outline

- **System Overview**

1. 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

- **System Overview**

1. 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

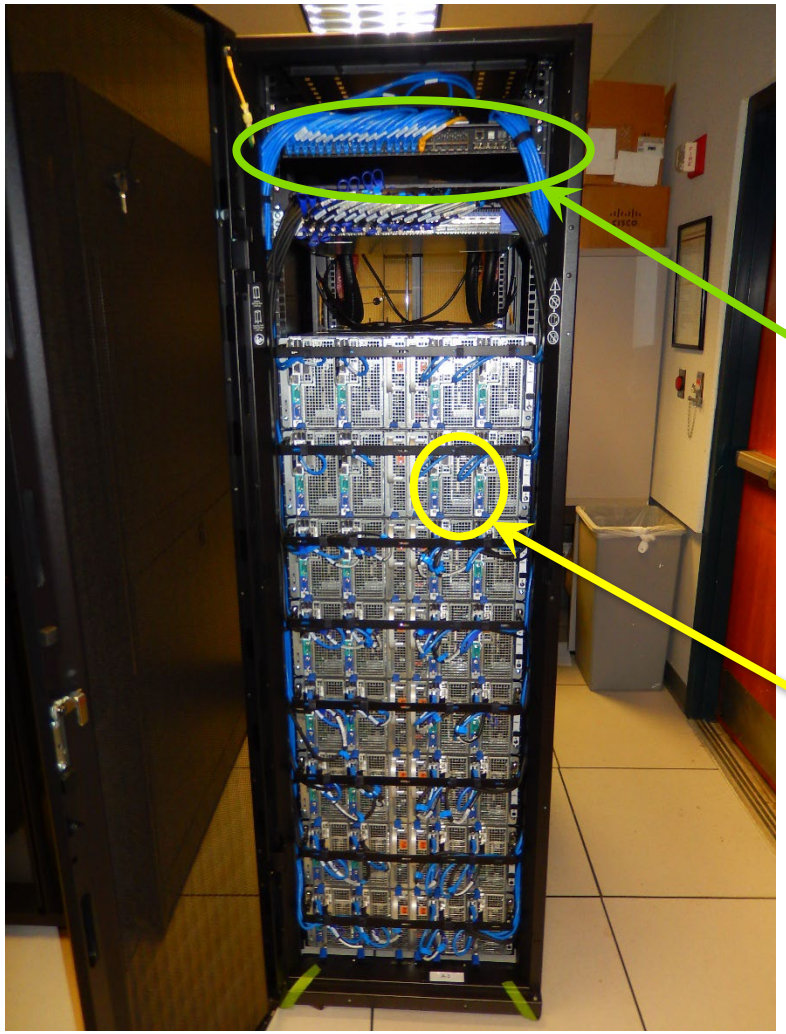
1) Look into the cluster

- **Inside a cluster:**

  SuperMike III

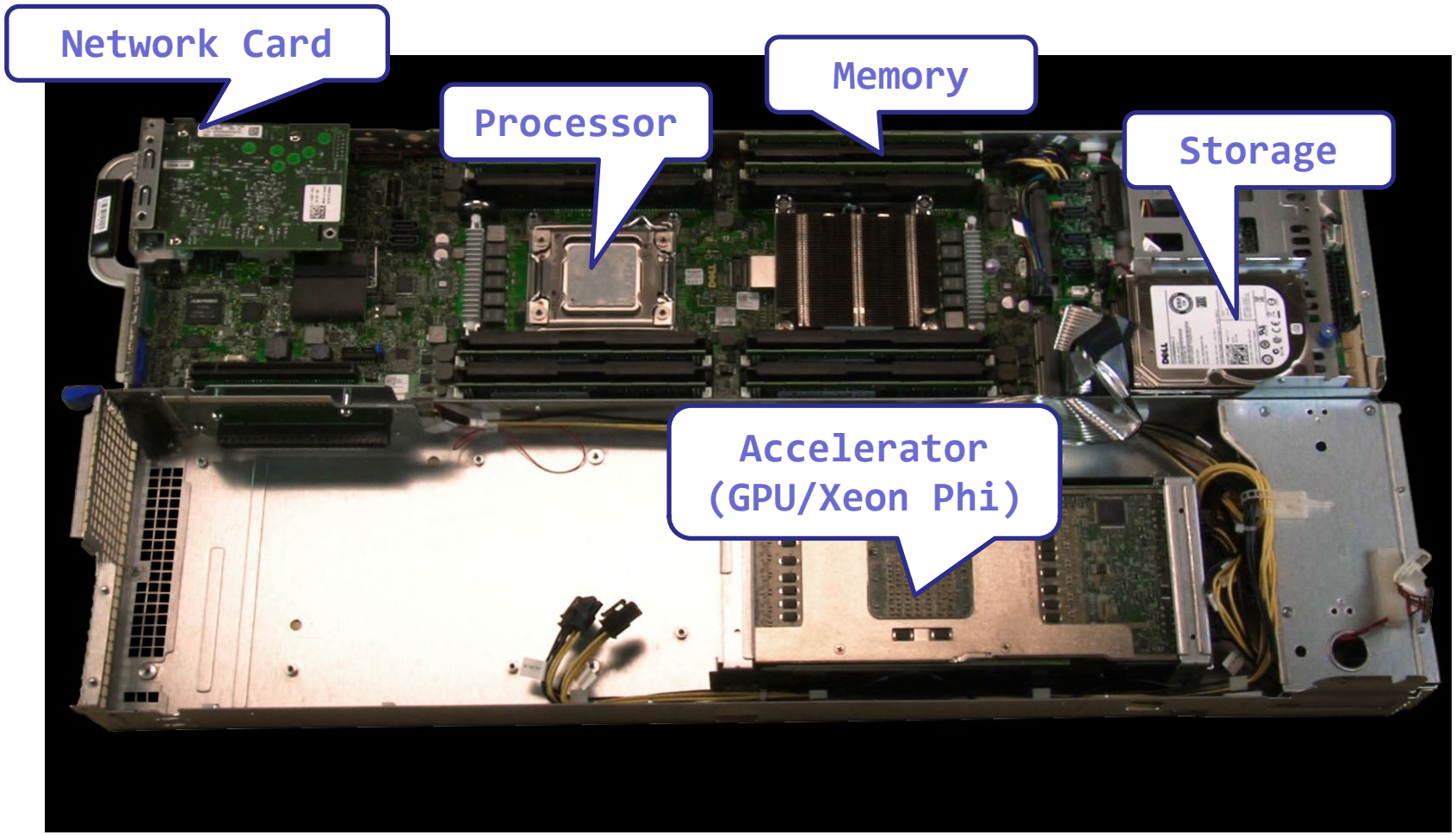
1) Look into the cluster

- **Inside a rack:**



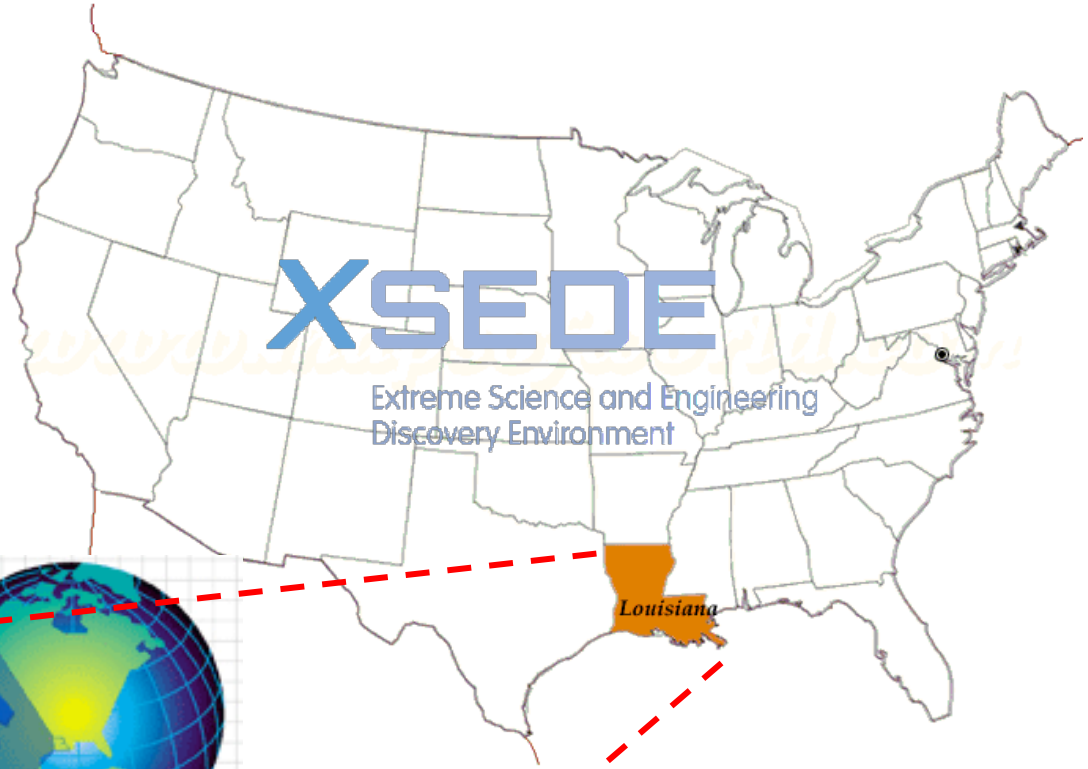
1) Look into the cluster

- **Inside a node:**



2) HPC specs

- University level: LSU HPC
- State level: LONI
- National level: XSEDE



2) HPC specs

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

2) HPC specs

- **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	
User Guide	
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	
User Guide	
Available Software	

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

2) HPC specs

- **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	
User Guide	
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	
User Guide	
Available Software	

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

2) HPC specs

- **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	
User Guide	
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	
User Guide	
Available Software	

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

2) HPC specs

- **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	
User Guide	
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	
User Guide	
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	
User Guide	
Available Software	

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

2) HPC specs

- **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	
User Guide	
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	
User Guide	
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	
User Guide	
Available Software	

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

2) HPC specs

- **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	
User Guide	
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	
User Guide	
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	
User Guide	
Available Software	

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

2) HPC specs

- **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	
User Guide	
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	
User Guide	
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	
User Guide	
Available Software	

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

2) HPC specs

- **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	
User Guide	
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	
User Guide	
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	
User Guide	
Available Software	

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

Outline

- **System Overview**

1. 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

Two things needed to run jobs on our clusters:

1) Account

2) Allocation

Outline

- **System Overview**

1. 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) Accounts

	LSU HPC
Available to…	LSU faculty & affiliates
Clusters	SuperMIC Deep Bayou **SuperMike III**

1) Accounts

i. Eligibility

LSU HPC	
Available to…	
Requirements	

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

1) Accounts

i. Eligibility

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	

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

1) Accounts

i. Eligibility

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** ✓ Full-time faculty & certain research staff @ LSU Baton Rouge campus × Students, postdocs, research associates (even @ LSU) × Outside collaborators × HPC staff

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

1) Accounts

i. Eligibility

You are a …	Your account sponsor

1) Accounts

i. Eligibility

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

1) Accounts

i. Eligibility

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

1) Accounts

i. Eligibility

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)

1) Accounts

i. Eligibility

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)

1) Accounts

i. Eligibility

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)

1) Accounts

ii. How to apply

	LSU HPC
Portal	https://accounts.hpc.lsu.edu/login_request.php
Steps	

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

1) Accounts

ii. How to apply

	LSU HPC
Portal	https://accounts.hpc.lsu.edu/login_request.php
Steps	

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

ii. How to apply

	LSU HPC
Portal	https://accounts.hpc.lsu.edu/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 **account sponsor**'s full name) and submit d) You **will receive a notification** when your account is activated once we have verified your credentials • Be patient. Do not reset your password if you cannot log in yet.

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

1) Accounts

iii. Manage your account

	LSU HPC
Portal	https://accounts.hpc.lsu.edu
Things to do	

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

iii. Manage your account

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

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

1) Accounts

iv. Reset password

	LSU HPC
Portal	https://accounts.hpc.lsu.edu/user_reset.php
Steps	

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

iv. Reset password

	LSU HPC
Portal	https://accounts.hpc.lsu.edu/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 password is approved by our staff ** IMPORTANT ** • Your new password is NOT available right away (wait until you receive confirmation of approval) • Do NOT submit multiple times

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

iv. 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

- **System Overview**

1. 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

2) Allocation

2) 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 clusters requires allocation to run jobs
- **Free** to users
- But not worthless! (**1 SU ≈ $0.1**)

2) Allocation

ii. Eligibility

You are a …	To get allocation …

2) Allocation

ii. Eligibility

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

* Full-time faculty & certain research staff @ LSU

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

2) Allocation

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

	LSU HPC
Portal	https://accounts.hpc.lsu.edu/allocations.php
Steps	

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

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

	LSU HPC
Portal	https://accounts.hpc.lsu.edu/allocations.php
Steps	a) Log in using your account b) Click on "New Allocation for [Cluster Name]" • SuperMIC & SuperMike III share allocations • Deep Bayou has separated allocation c) Fill the form and submit d) Your request will be reviewed, and you will be notified if your allocation is approved

[1] http://www.hpc.lsu.edu/links.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…

[1] http://www.hpc.lsu.edu/users/hpcpolicy.php
[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	Jan 1 Apr 1 Jul 1 Oct 1	2 active / PI

[1] http://www.hpc.lsu.edu/users/hpcpolicy.php
[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	Jan 1 Apr 1 Jul 1 Oct 1	2 active / PI
Research	> 50,000	> 1 month before decision date	Jan 1 Apr 1 Jul 1 Oct 1		**[LSU HPC]** 3,000,000 SU / allocation 5,000,000 SU / PI

[1] http://www.hpc.lsu.edu/users/hpcpolicy.php
[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]	Proposal				
			Technical merit	Software characteristics	Previous impact and outcome	External funding or LSU demand	# of pages
Startup		50,000	(Not required)				
Research	**A**	>50,000 and ≤300,000	Required	Required	Optional	Optional	4
	B	>300,000 and ≤1,000,000	Required	Required	Required	Optional	5
	C	>1,000,000	Required	Required	Required	Required	6

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

2) Allocation

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

	LSU HPC
Portal	https://accounts.hpc.lsu.edu/allocations.php
Steps	

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

	LSU HPC
Portal	https://accounts.hpc.lsu.edu/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 Projects" d) Find the desired allocation you wish to join, click “Join” e) Your account sponsor / PI will receive an email notification and approve your request **[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]”

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

Summary

Two things needed to run jobs on our clusters:

1) Account

2) Allocation

Outline

- **System Overview**

1. 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

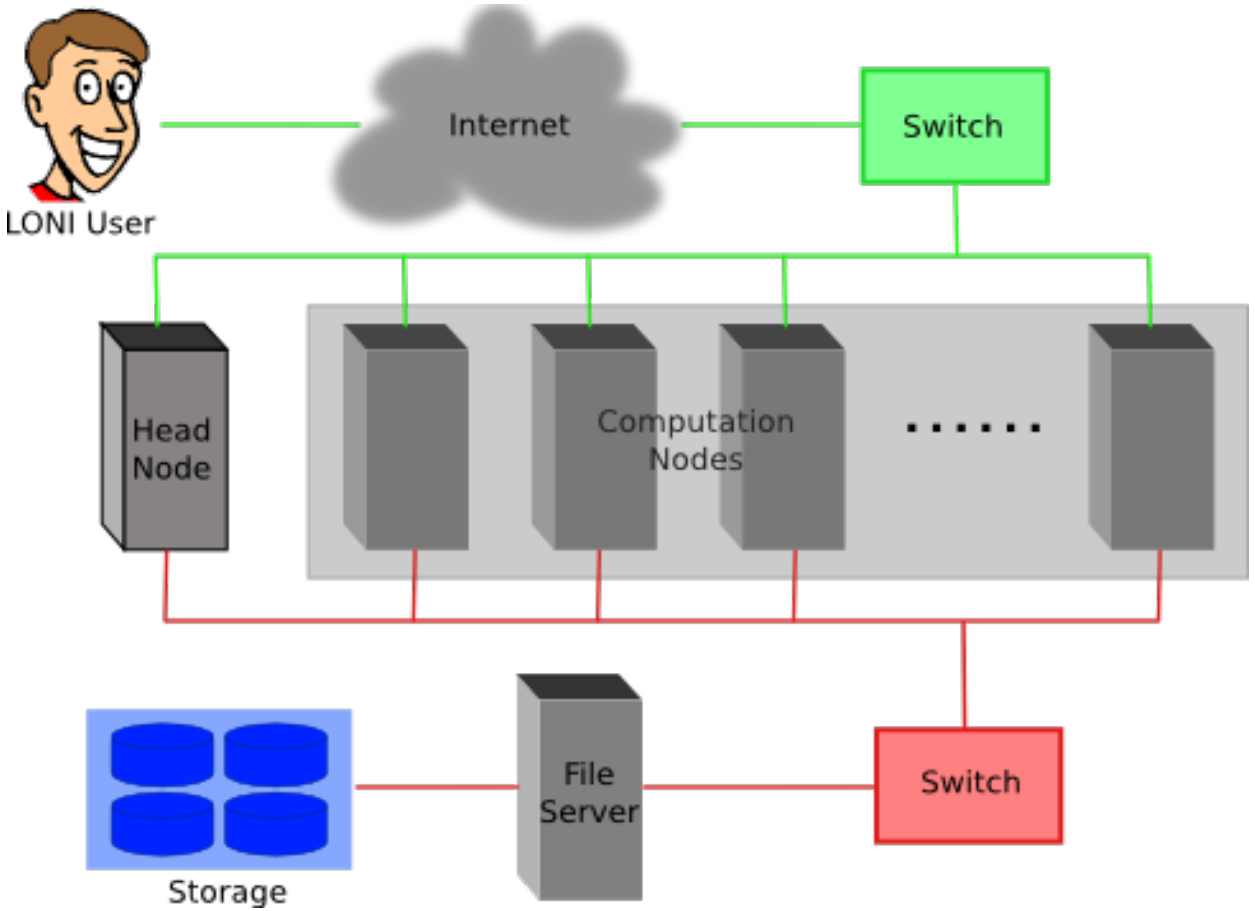
- **System Overview**

1. 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) Getting connected

i. General architecture

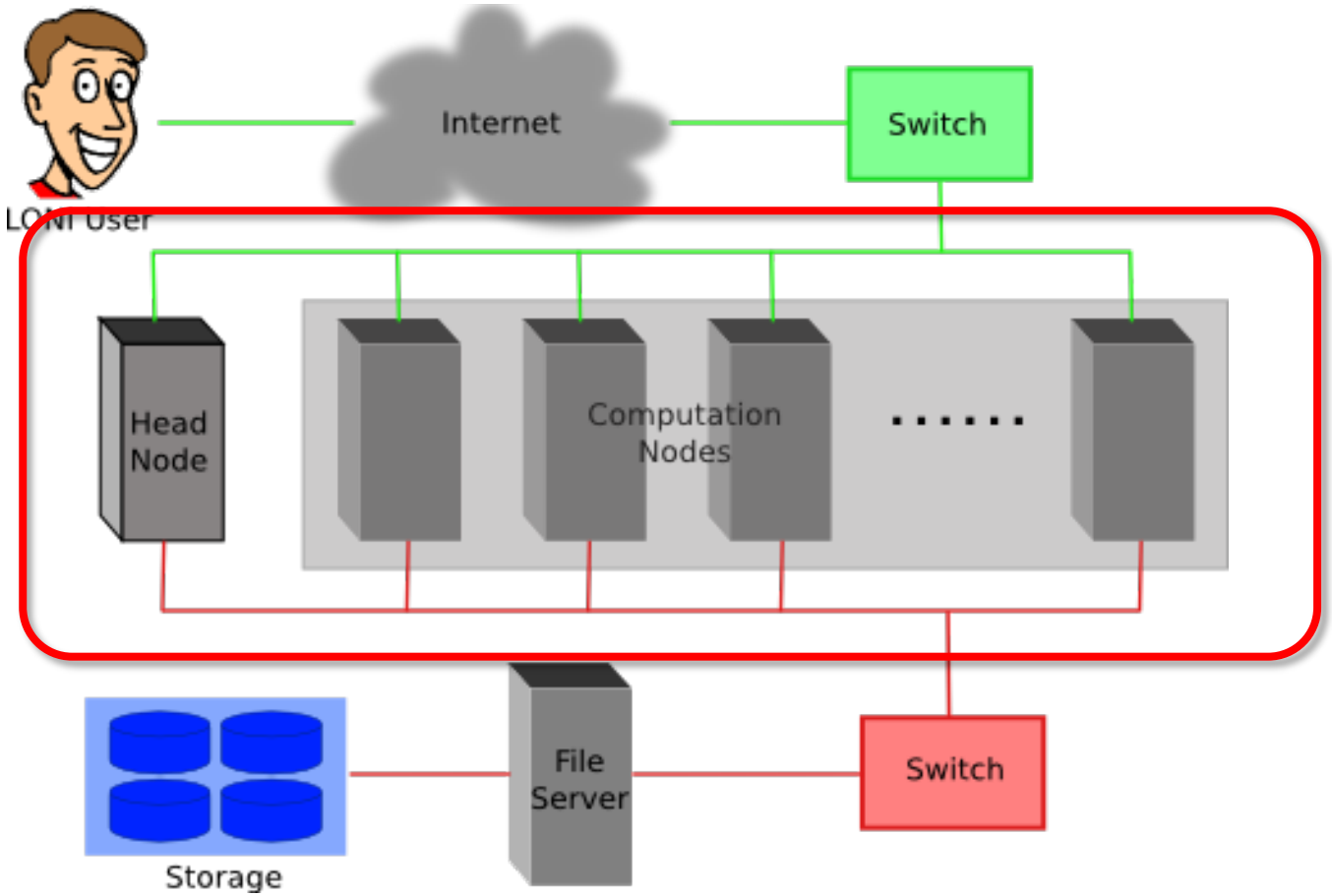
- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously



1) Getting connected

i. General architecture

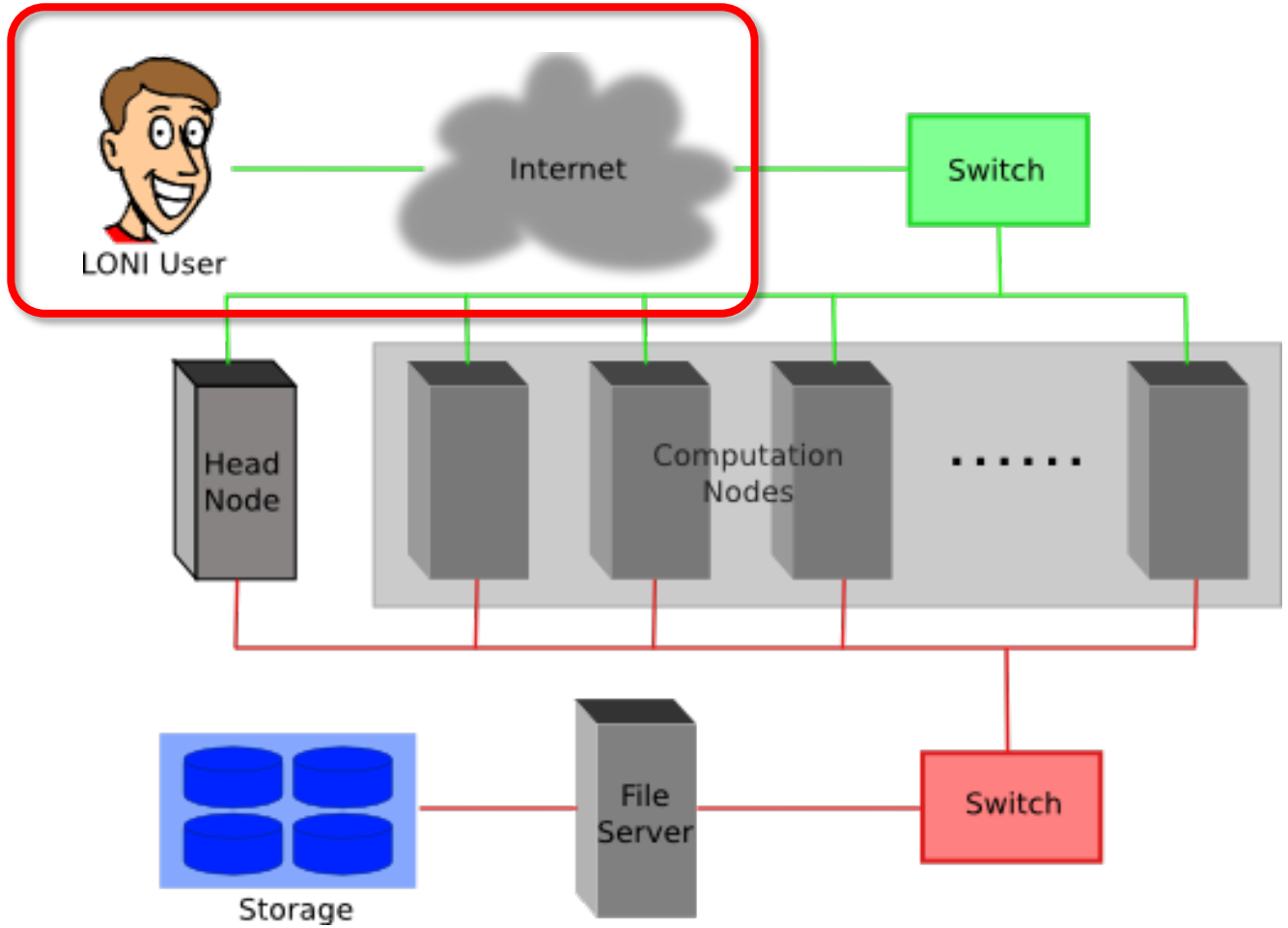
- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously



1) Getting connected

i. General architecture

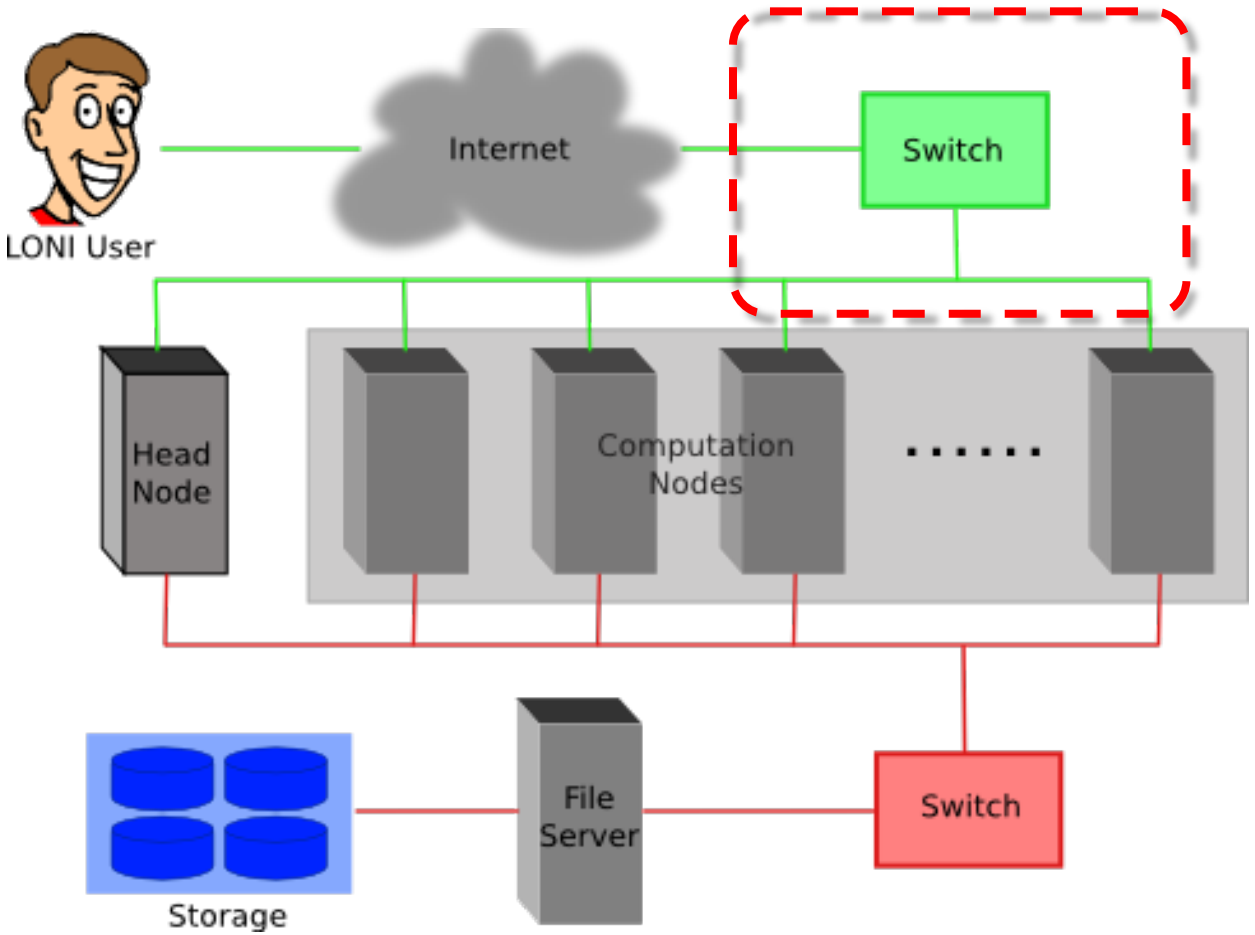
- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously



1) Getting connected

i. General architecture

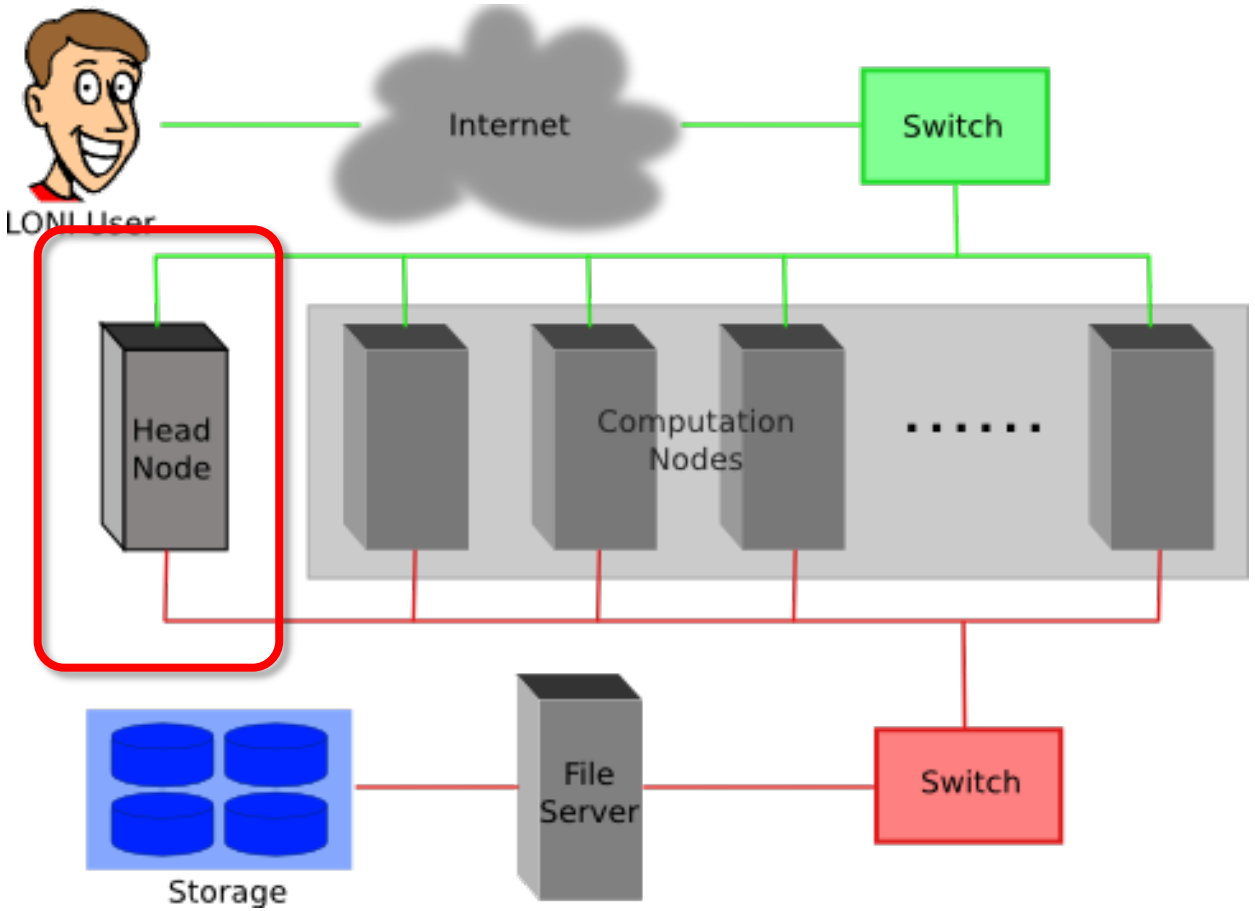
- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously



1) Getting connected

i. General architecture

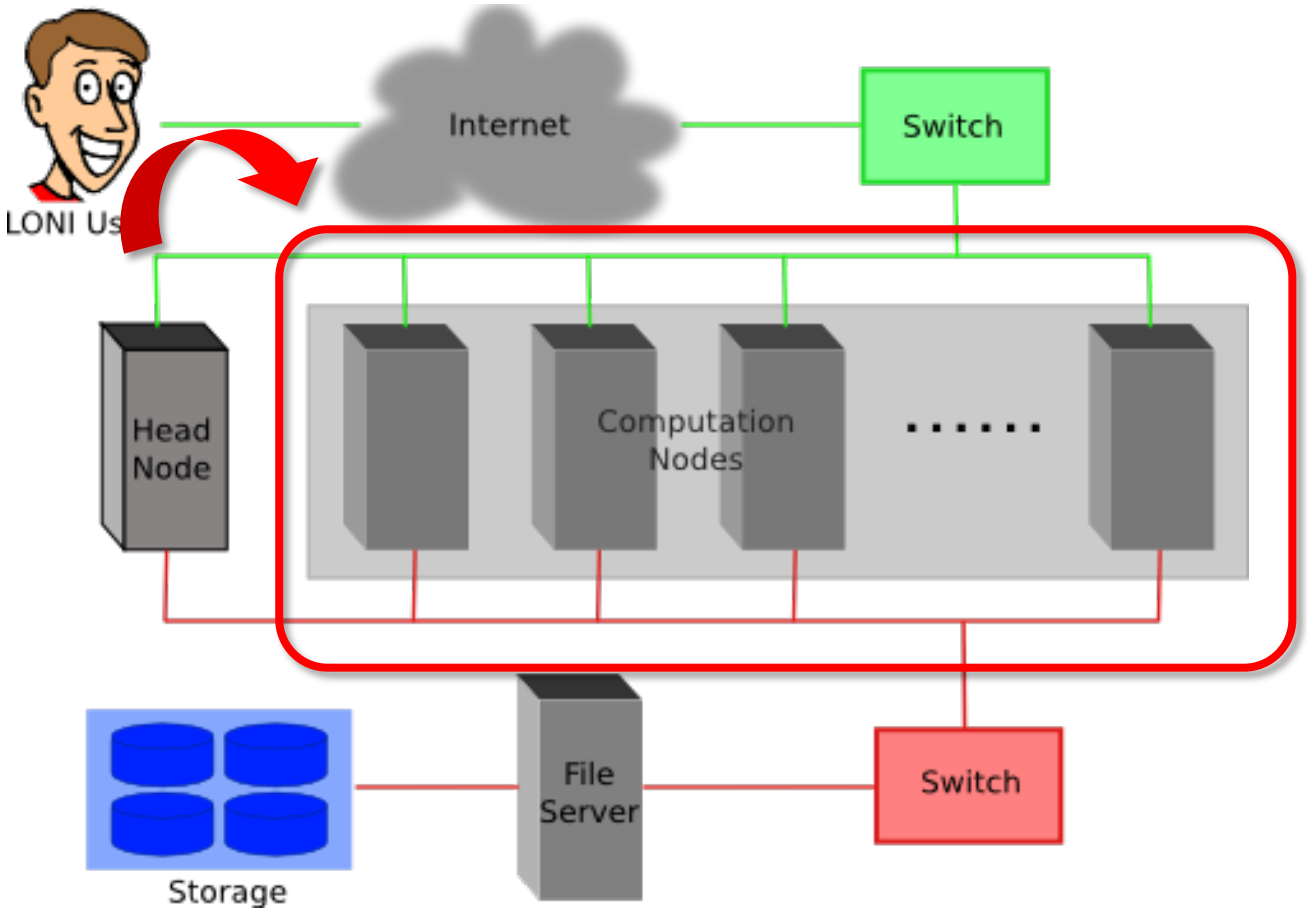
- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously



1) Getting connected

i. General architecture

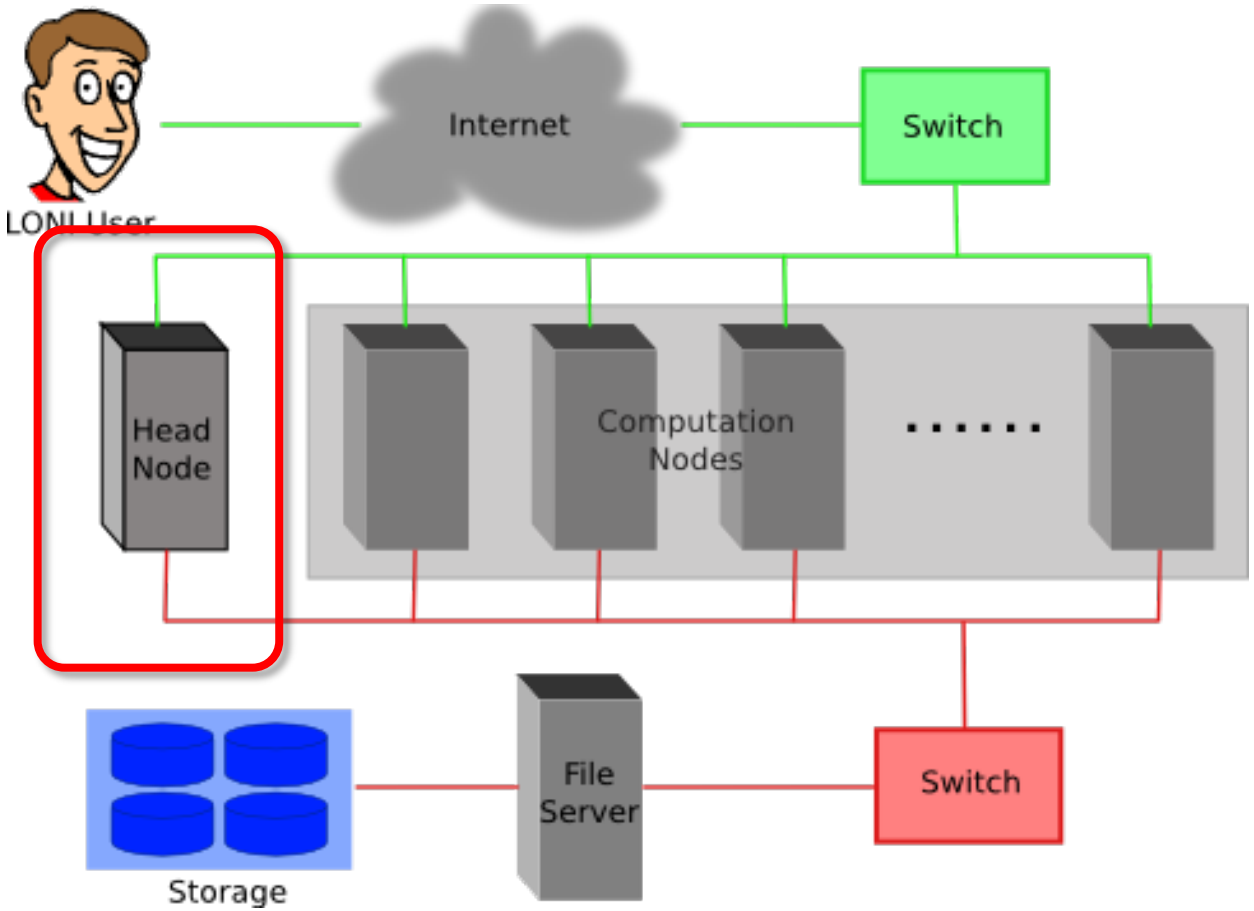
- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously



1) Getting connected

i. 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)

Your OS …	Tool you need …

ii. Logging in

Secure Shell (SSH)

Your OS …	Tool you need …
Linux / Mac	Terminal

ii. Logging in

Secure Shell (SSH)

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

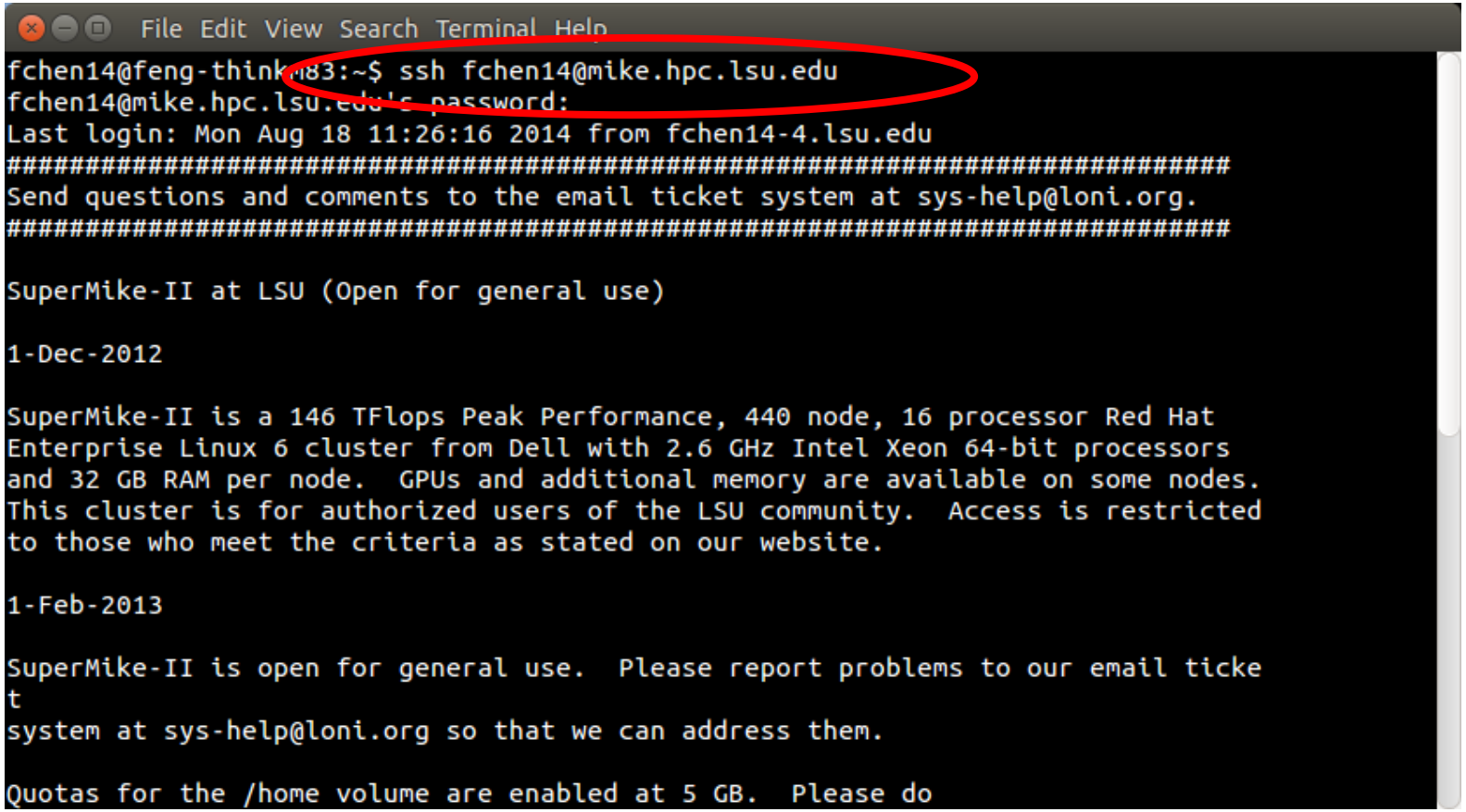
ii. Logging in

Secure Shell (SSH)

Cluster		Address
LSU HPC	SMIC	smic.hpc.lsu.edu
	Deep Bayou	db1.hpc.lsu.edu
	SuperMike III	mike.hpc.lsu.edu

ii. Logging in

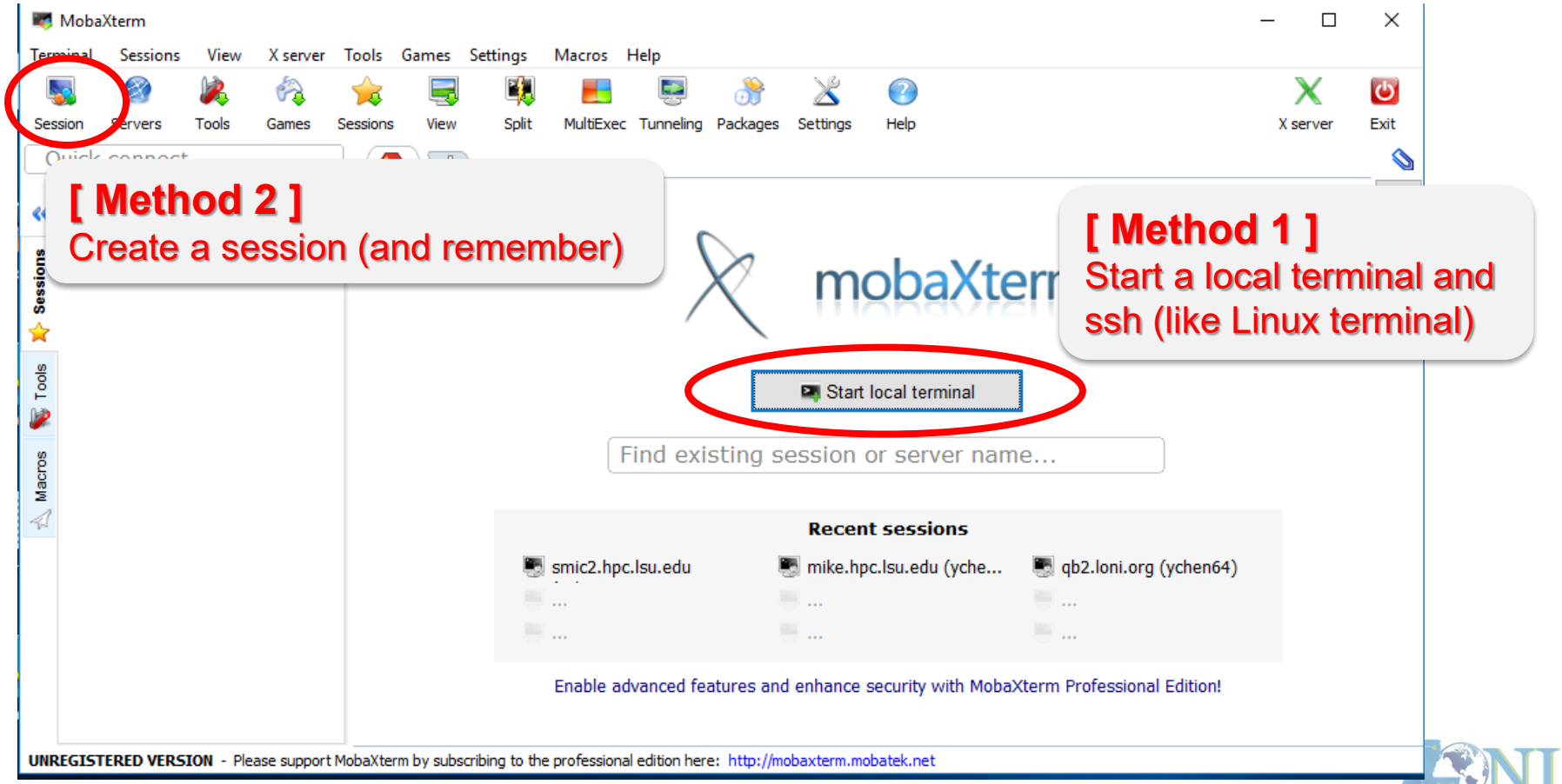
a) Linux / Mac



ii. Logging in

b) Windows

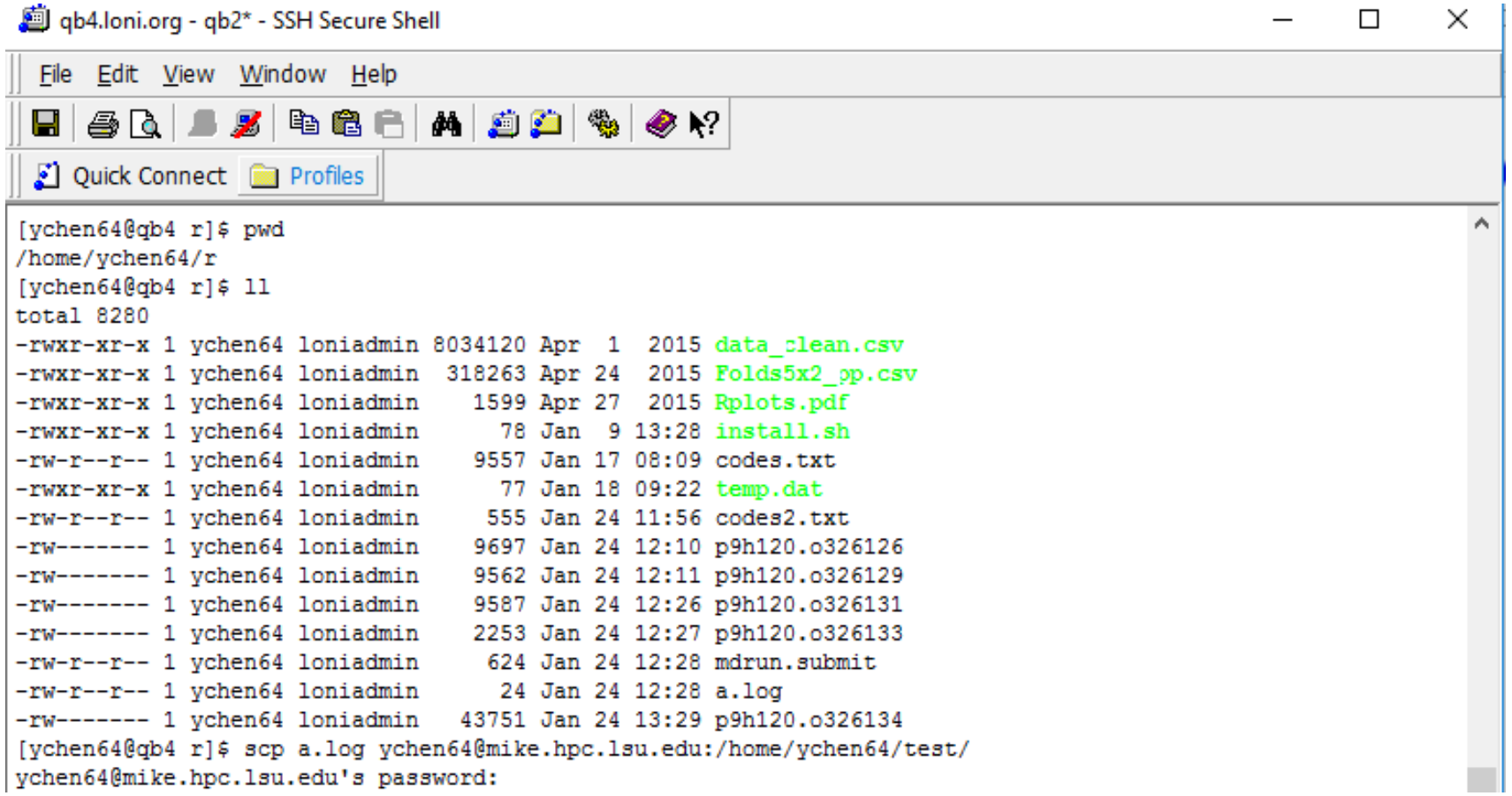
- MobaXterm



ii. Logging in

b) Windows

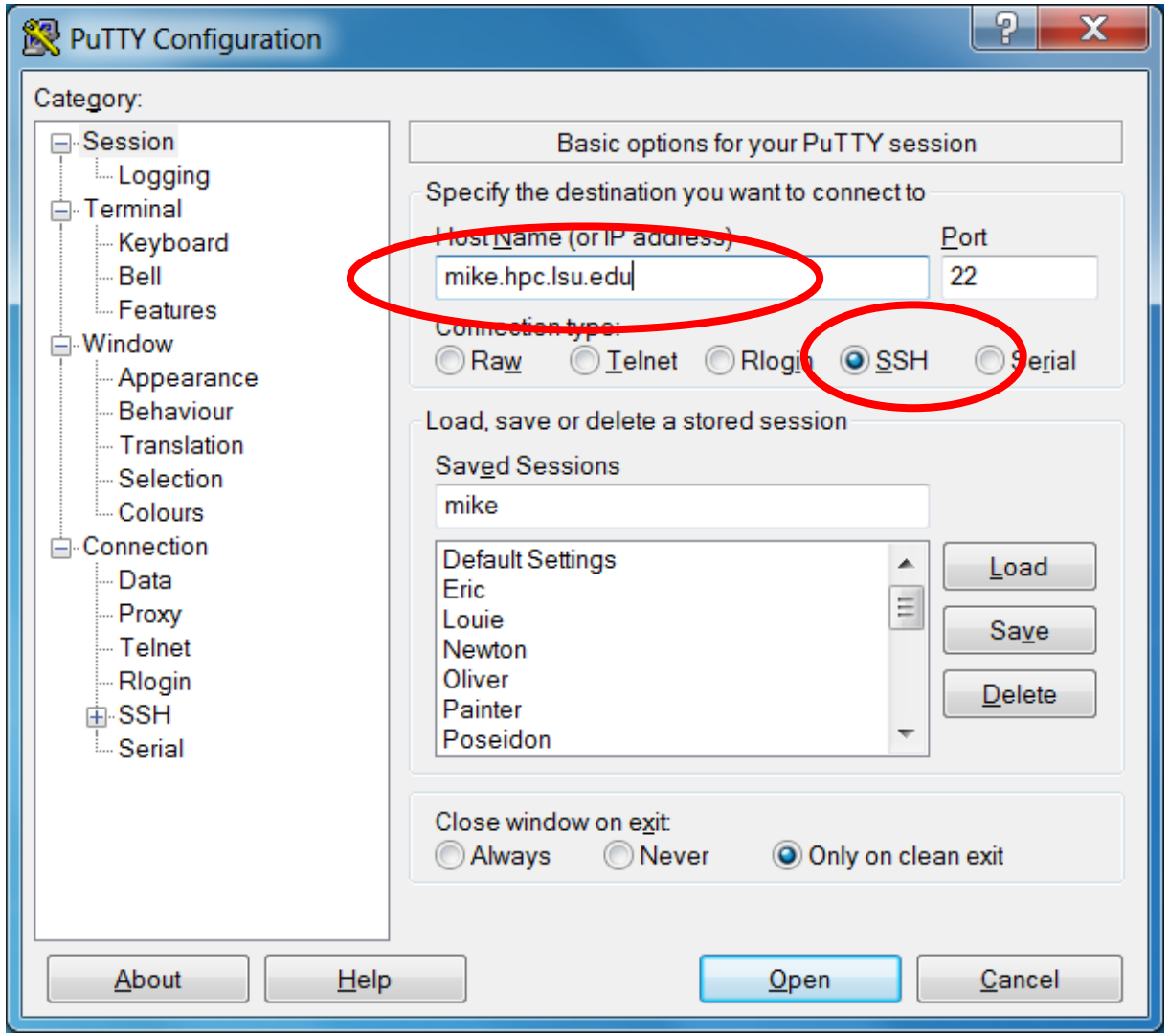
- SSH Secure Shell



ii. Logging in

b) Windows

- Putty



ii. Logging in

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

ii. Logging in

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

You are using…		To enable X11 forwarding…

ii. Logging in

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

You are using…	To enable X11 forwarding…
Linux / Mac	ssh **–X** username@server.address

ii. Logging in

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

You are using…		To enable X11 forwarding…
Linux / Mac		ssh **–X** username@server.address
Windows		

ii. Logging in

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

You are using…		To enable X11 forwarding…
Linux / Mac		ssh **–X** username@server.address
Windows	**MobaXterm**	Enabled by default (can be disabled in “Advanced SSH Settings”)

ii. Logging in

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

You are using…		To enable X11 forwarding…
Linux / Mac		ssh **–X** username@server.address
Windows	**MobaXterm**	Enabled by default (can be disabled in “Advanced SSH Settings”)
	Putty	a) Connection → SSH → X11 → Enable X11 forwarding b) Install X server (*e.g.* Xming)

ii. Logging in

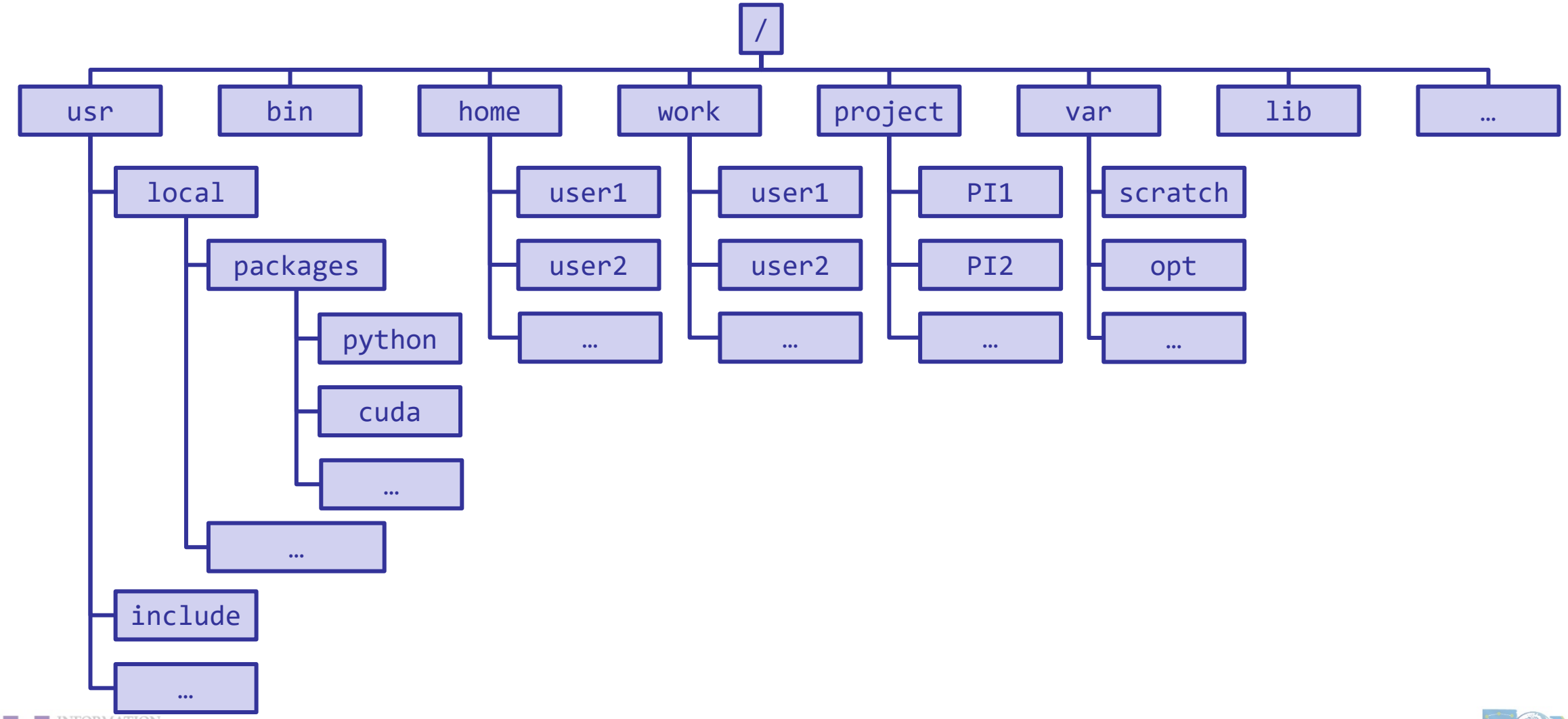
Useful commands	
who	Check who is on the node
balance / showquota	Check allocation balance
history	Command history
mkdir	Make a folder
ls	List a folder -a List all files including hidden -l Shows files with a long listing format
cd	Change directory
pwd	Show current directory
cp	Copy
rm	Remove files (CAREFUL!)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

Outline

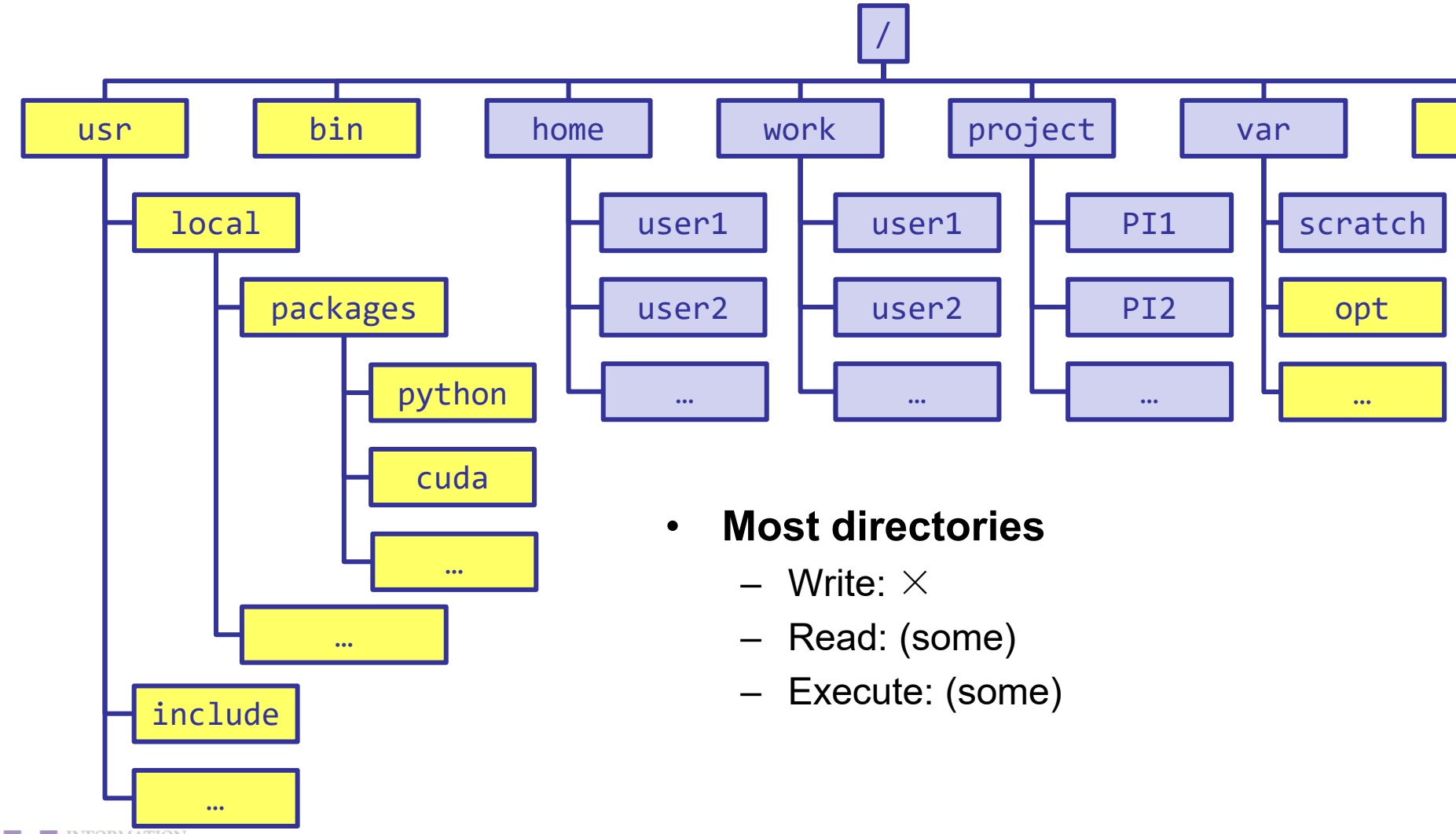
- **System Overview**

1. 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

2) File system



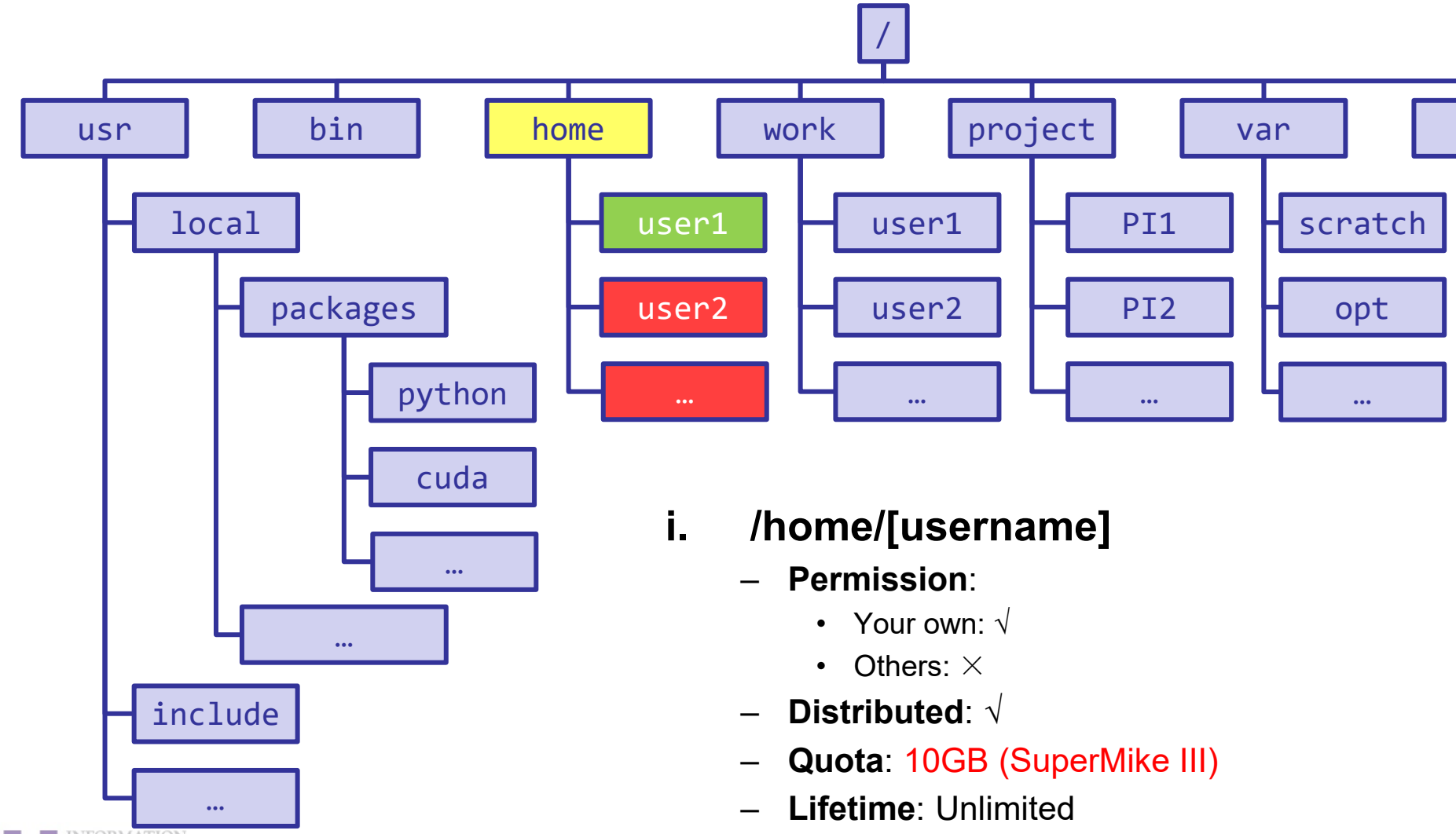
2) File system



Permission			
Read	√	×	√*
Write	√	×	×
Execute	√	×	√*

- **Most directories**
  - Write: ×
  - Read: (some)
  - Execute: (some)

2) File system

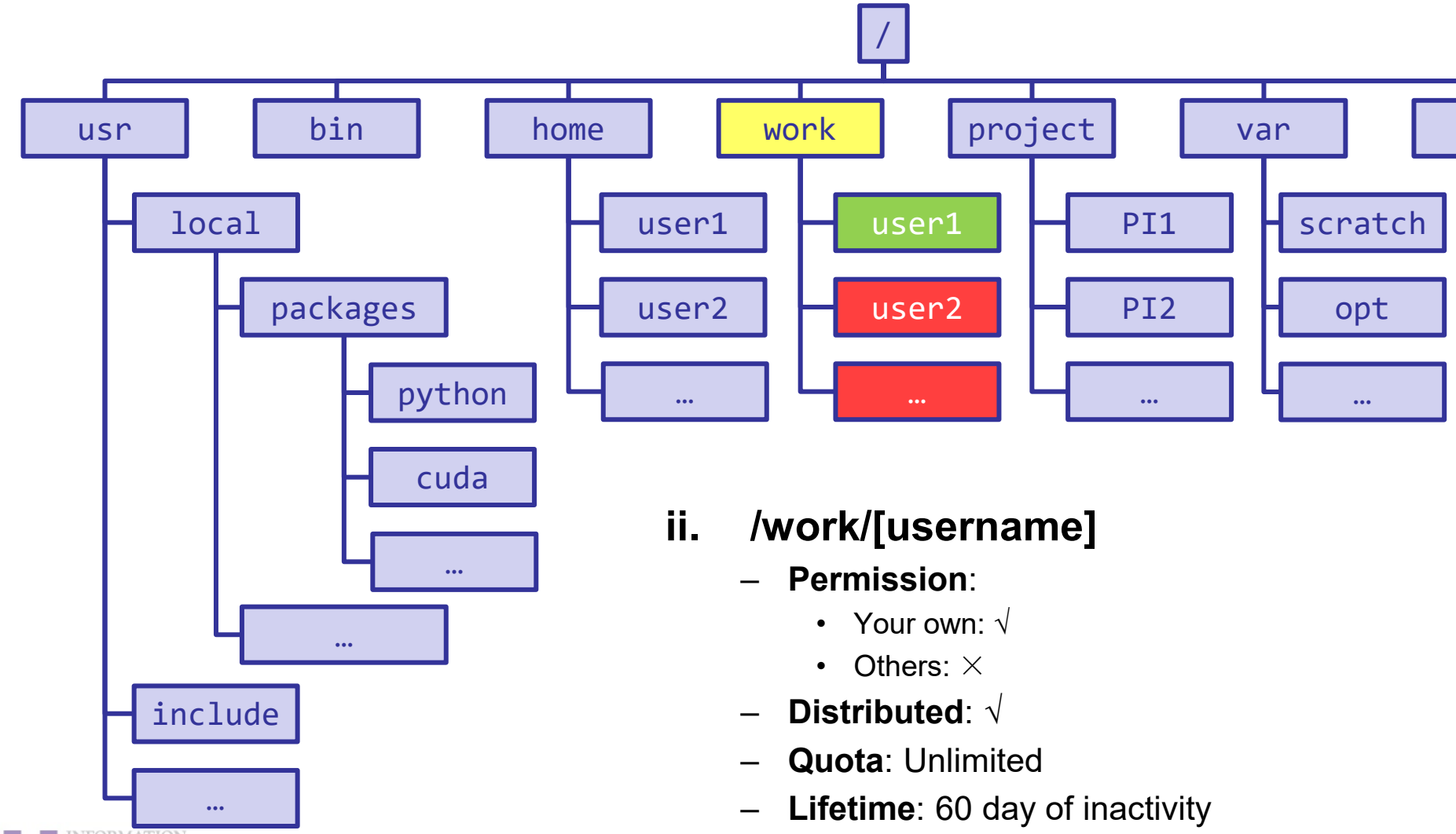


Permission			
Read	√	×	√ *
Write	√	×	×
Execute	√	×	√ *

i. /home/[username]

- **Permission**:
  - Your own: √
  - Others: ×
- **Distributed**: √
- **Quota**: 10GB (SuperMike III)
- **Lifetime**: Unlimited
- **Best for**: Code / executables

2) File system

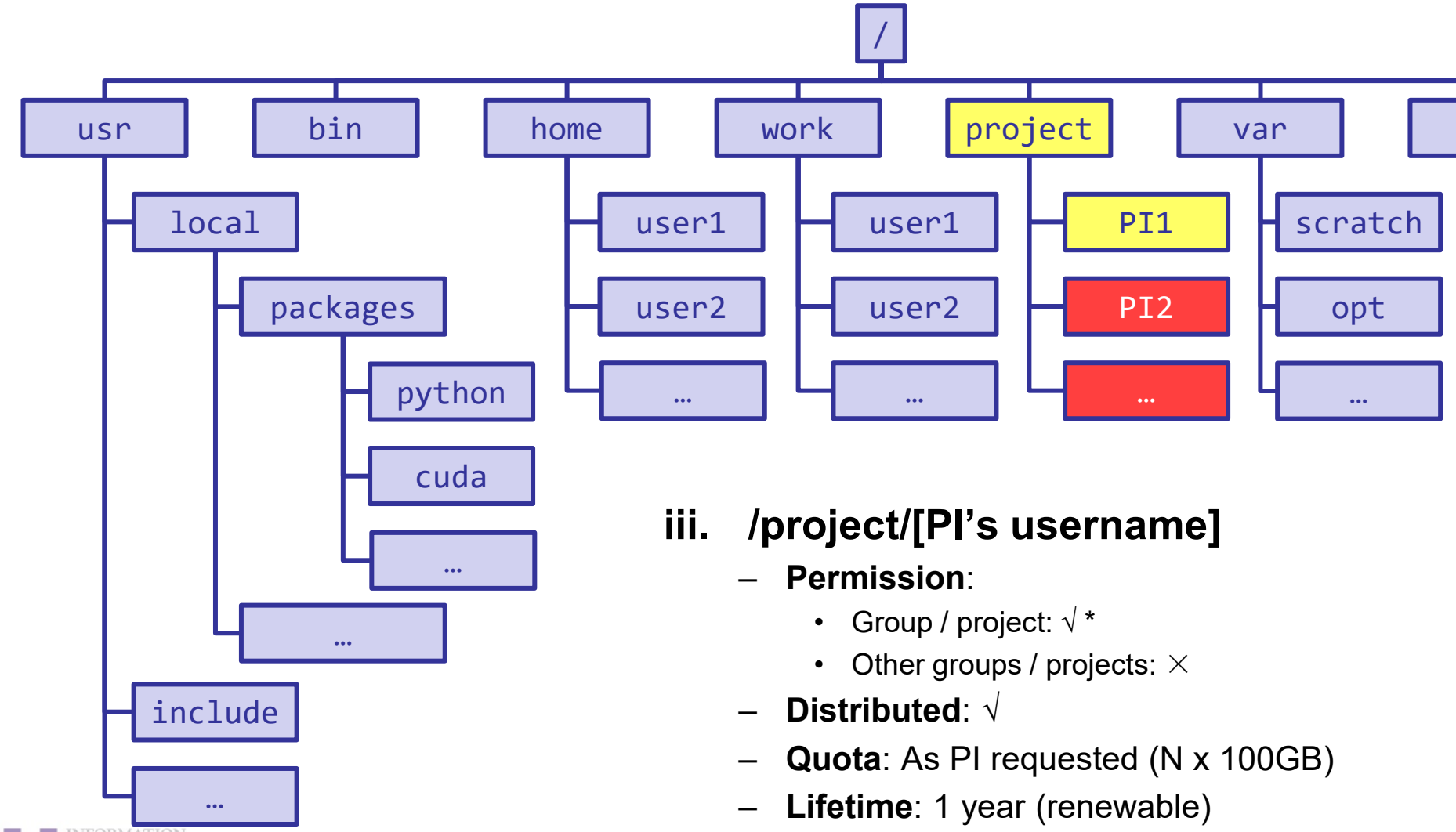


Permission			
Read	√	×	√ *
Write	√	×	×
Execute	√	×	√ *

ii. /work/[username]

- **Permission**:
  - Your own: √
  - Others: ×
- **Distributed**: √
- **Quota**: Unlimited
- **Lifetime**: 60 day of inactivity
- **Best for**: Job input / output

2) File system

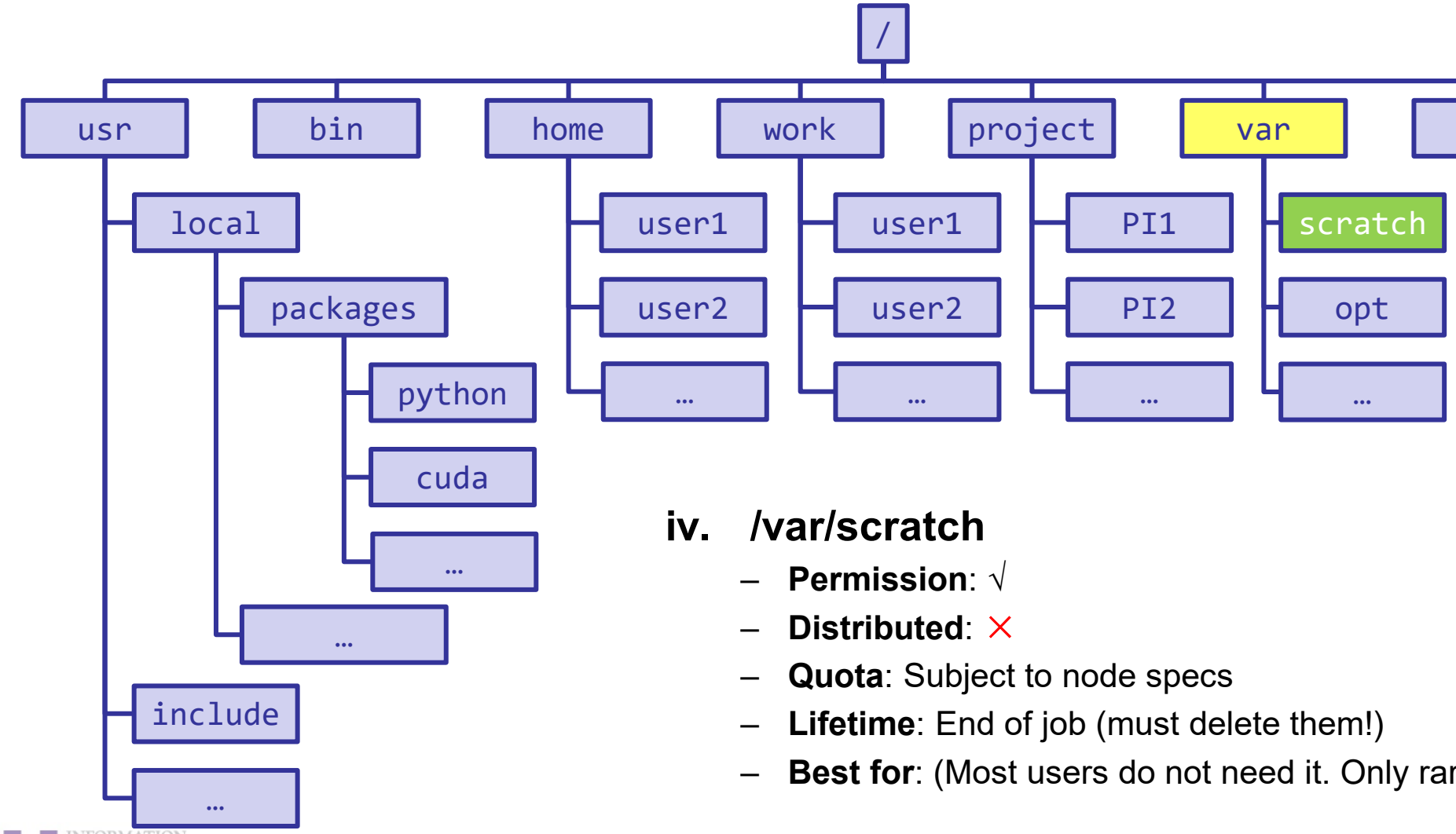


Permission			
Read	√	×	√ *
Write	√	×	×
Execute	√	×	√ *

iii. /project/[PI's username]

- **Permission**:
  - Group / project: √ *
  - Other groups / projects: ×
- **Distributed**: √
- **Quota**: As PI requested (N x 100GB)
- **Lifetime**: 1 year (renewable)
- **Best for**: Specific project / group sharing. **NOT for archive.**

2) File system



Permission			
Read	√	×	√ *
Write	√	×	×
Execute	√	×	√ *

iv. /var/scratch

- **Permission**: √
- **Distributed**: ×
- **Quota**: Subject to node specs
- **Lifetime**: End of job (must delete them!)
- **Best for**: (Most users do not need it. Only rare cases)

File system summary

Directory (folder)	Distributed	Throughput	Lifetime	Quota	Best for
/home/[username]	√	Low	Unlimited	5GB (SMIC & QB2) 10GB (others)	Code / executables
/work/[username]	√	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**
  - SuperMike III **share /work and /project directories** with SMIC
  - **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**

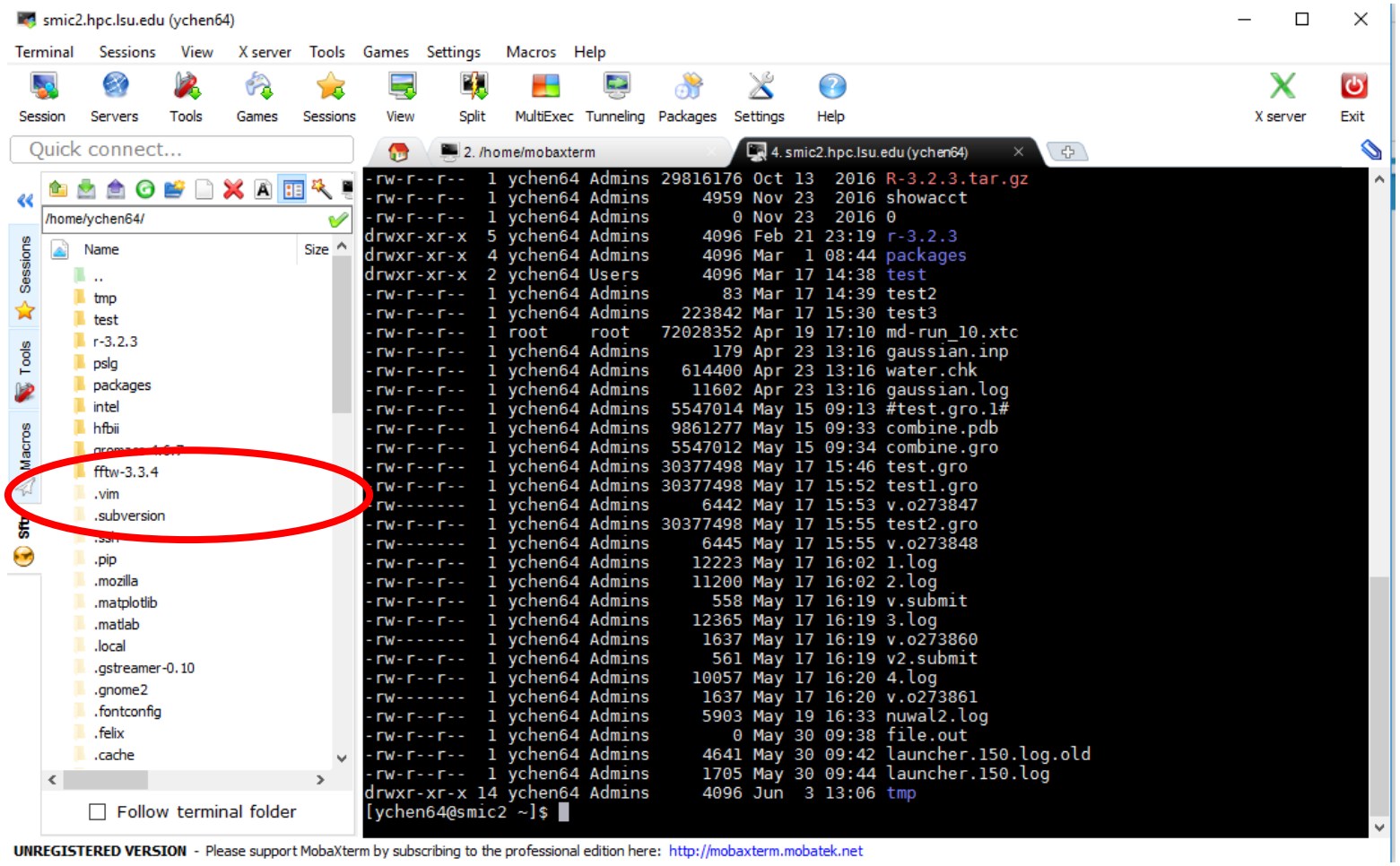
2) File system

- **File transfer**

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

2) File system

- **File transfer**



Outline

- **System Overview**

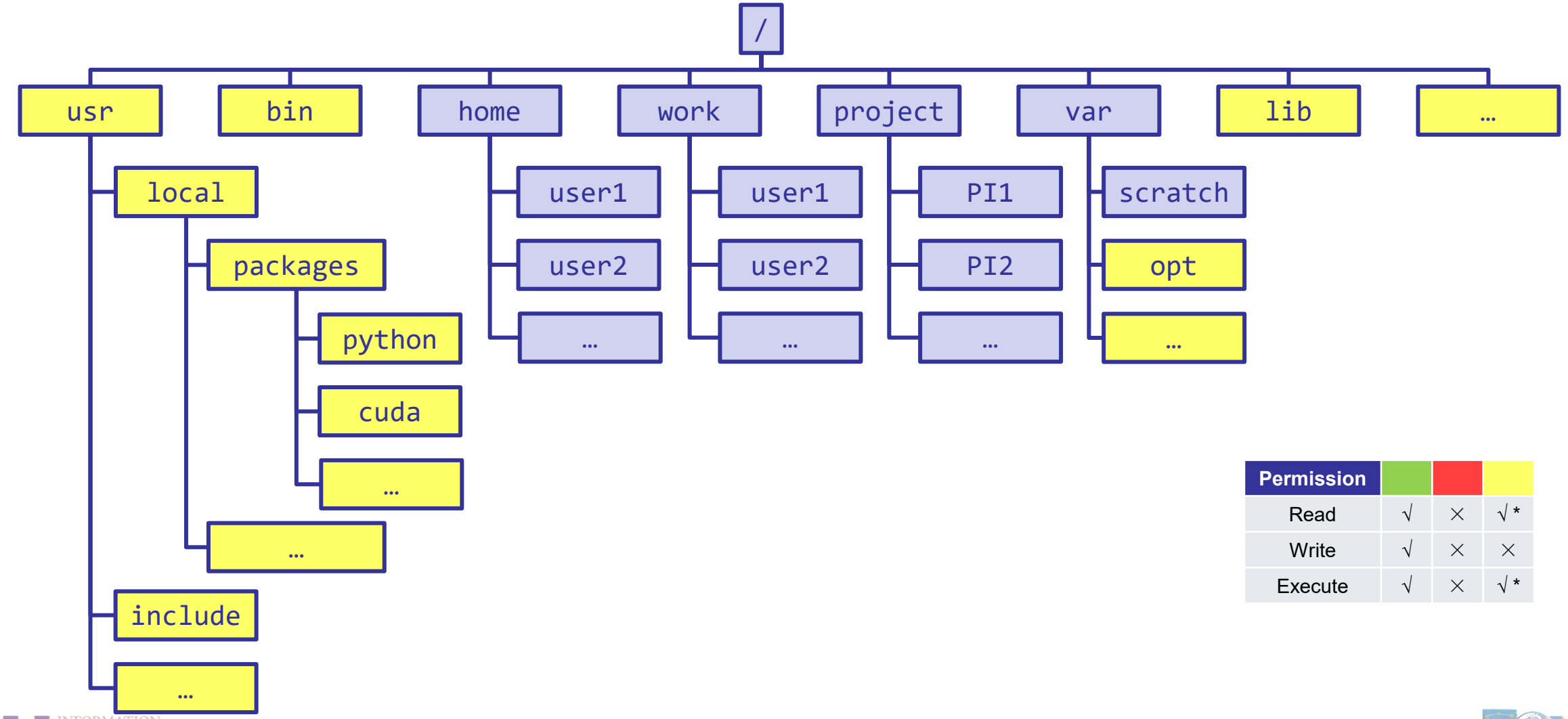
1. Our HPC
2. Getting started
    1) Accounts
    2) Allocation
3. Into the cluster
    1) Getting connected
    2) File system
4. Software environment
    1) Preinstalled (modules)
    2) User installation

Outline

- **System Overview**

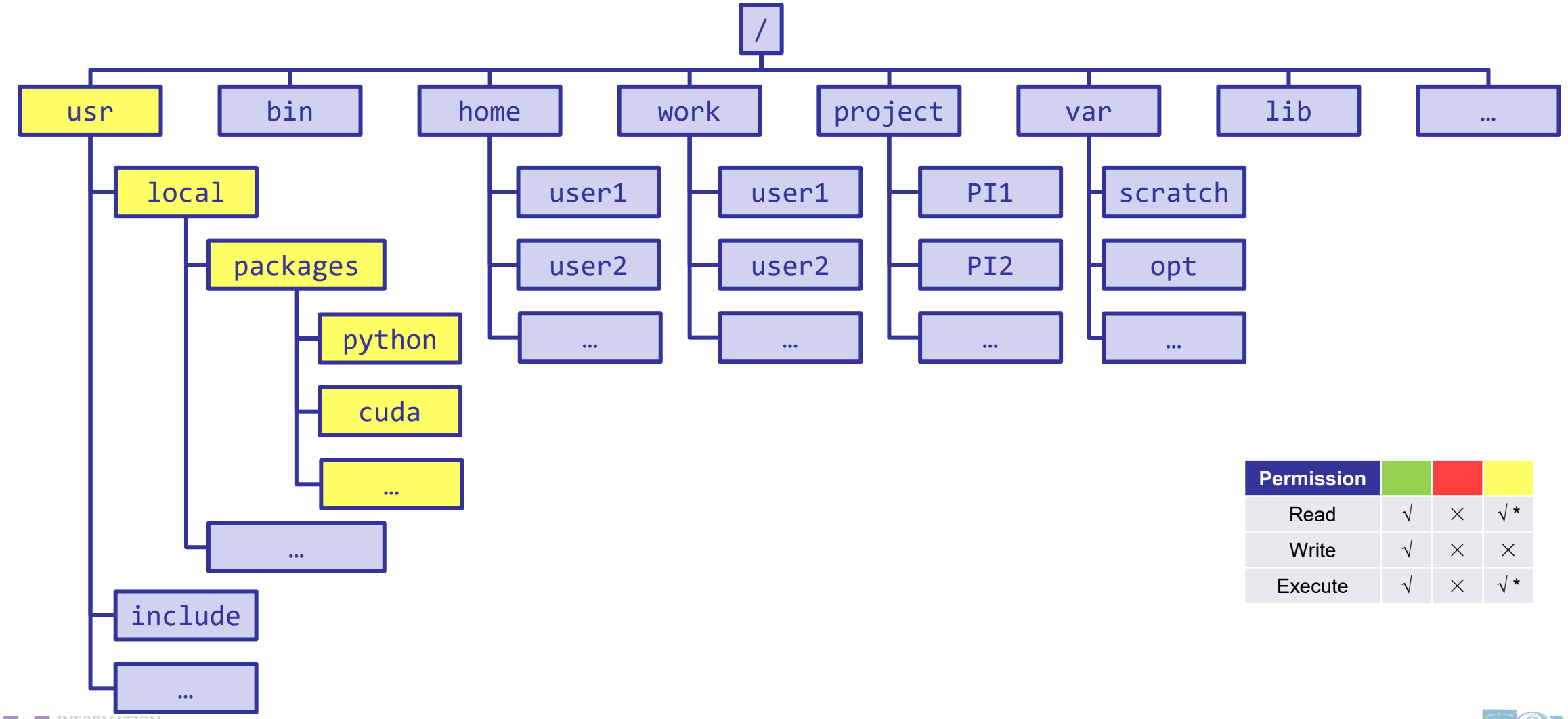
1. Our HPC
2. Getting started
    1) Accounts
    2) Allocation
3. Into the cluster
    1) Getting connected
    2) File system
4. Software environment
    1) Preinstalled (modules)
    2) User installation

1) Preinstalled (modules)



Permission			
Read	√	×	√ *
Write	√	×	×
Execute	√	×	√ *

1) Preinstalled (modules)



Permission			
Read	√	×	√ *
Write	√	×	×
Execute	√	×	√ *

1) Preinstalled (modules)

- **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…
Applications	Amber, NAMD, Gromacs, R, LAMMPS ...
Parallelization	Intel MPI, MPICH, MVAPICH2, OpenMPI, …

1) Preinstalled (modules)

- **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

1) Preinstalled (modules)

- **Modules**
  - Auto-load modules: **~/.modules**

Outline

- **System Overview**

1. 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

2) User installation

You can't…	You can…

2) User installation

You can't…	You can…
• yum / apt-get • sudo (!!!) • …	

2) User installation

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

[1] http://www.hpc.lsu.edu/training/archive/tutorials.php

2) User installation

- **Recommended paths:**

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

Summary

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

Take home message

- **System Overview**

1. Our HPC → **Specs of SuperMike III**
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**
   2) File system → **Know your /home, /work, /project**
4. Software environment
   1) Preinstalled (modules) → **Use modules**
   2) User installation → **No sudo or yum**

Coming up next

- **10:15 – 10:30**
  - Break
- **10:30 – 11:30**
  - Job management with Slurm
- **11:30 – 12:30**
  - Performance benchmarks and tuning
- **12:30 – 02:00**
  - Lunch break
- **02:00 – 04:00**
  - Q & A + On-ramp sessions (breakout sessions)

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
```