HPC User Environment 1

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HPC User Services

LSU HPC / LONI

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Louisiana State University

Baton Rouge

September 13, 2023

Outline

- **HPC User Environment 1**

  1. An intro to HPC
  2. Accounts and allocations
  3. Into the cluster
  4. Software environment (modules)

- **HPC User Environment 2**

  1. Queuing system
  2. How to run jobs

Outline

- **HPC User Environment 1**

1. An 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

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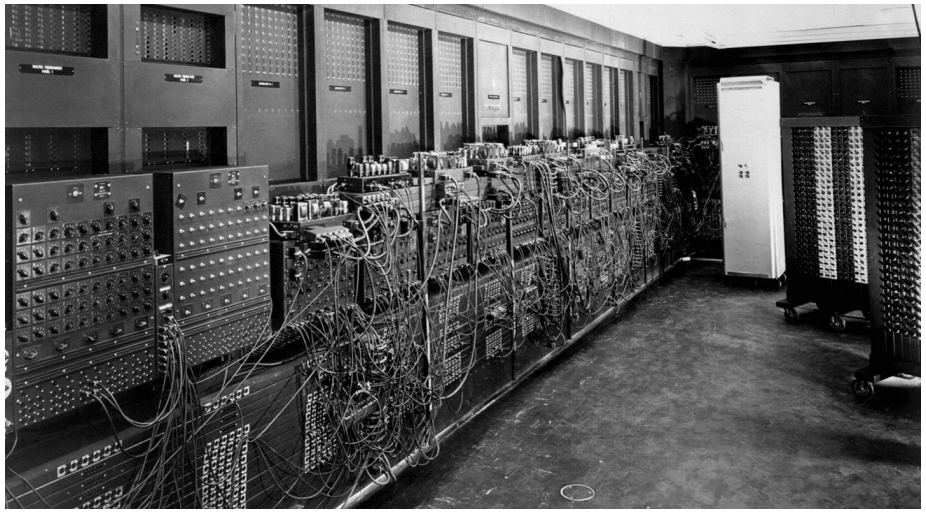
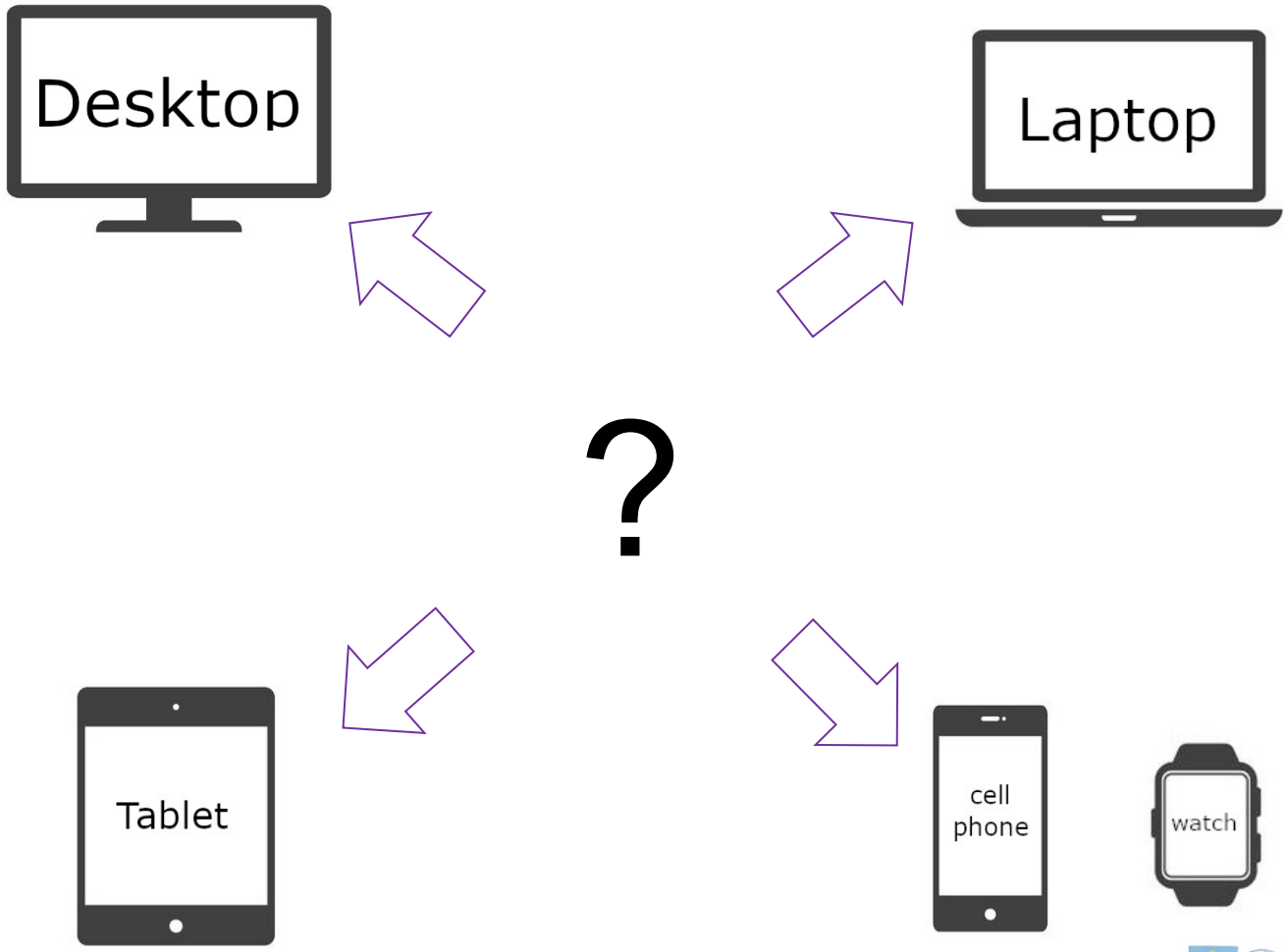
1) Why HPC?

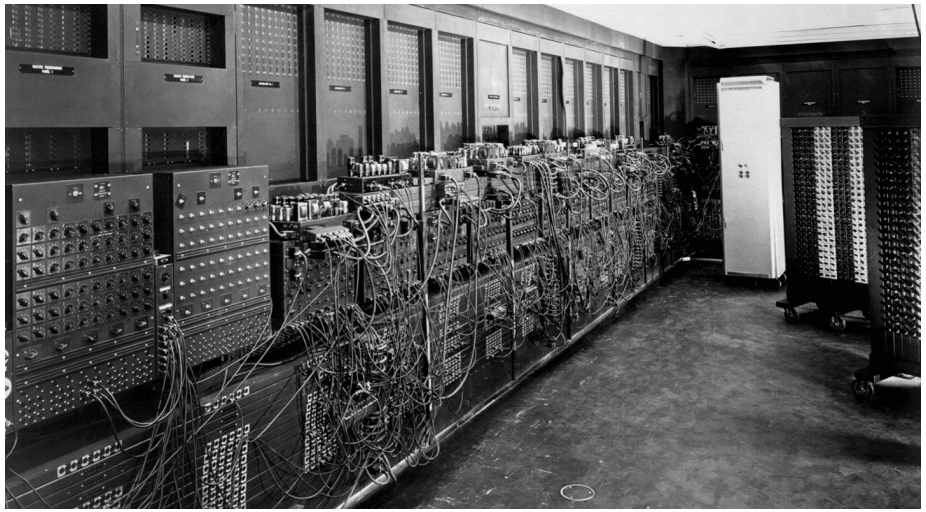


ENIAC, 1945

First all-vacuum tube supercomputer (18000 vacuum tubes), a decimal computer, hard-wired program with dials and switches.



1) Why HPC?



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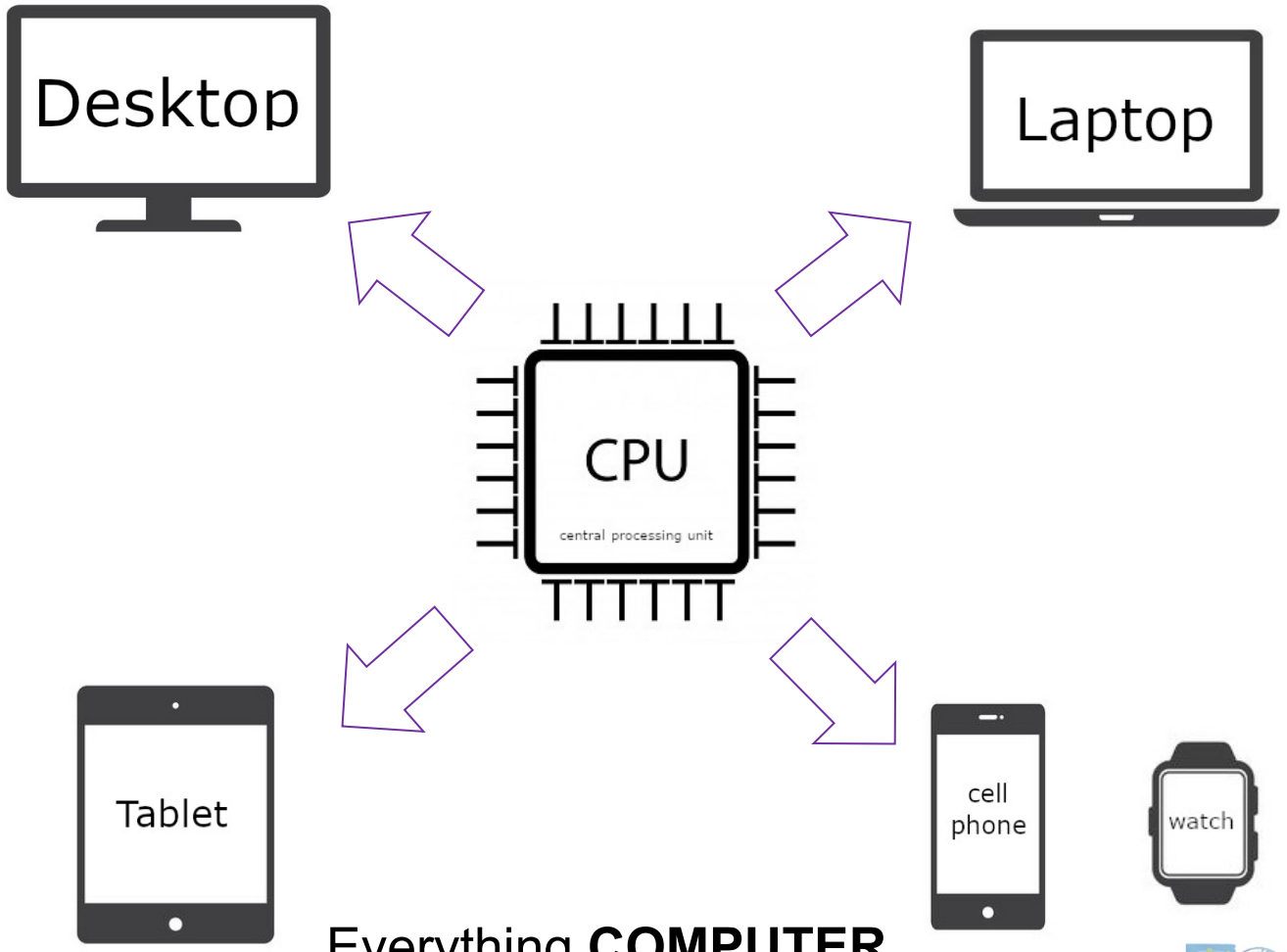
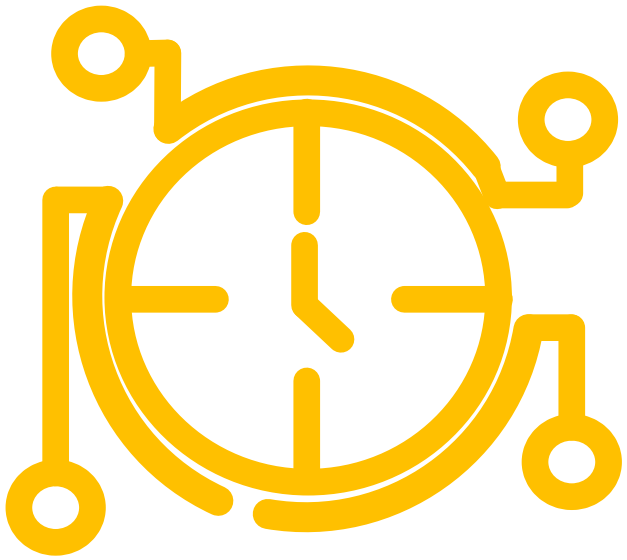


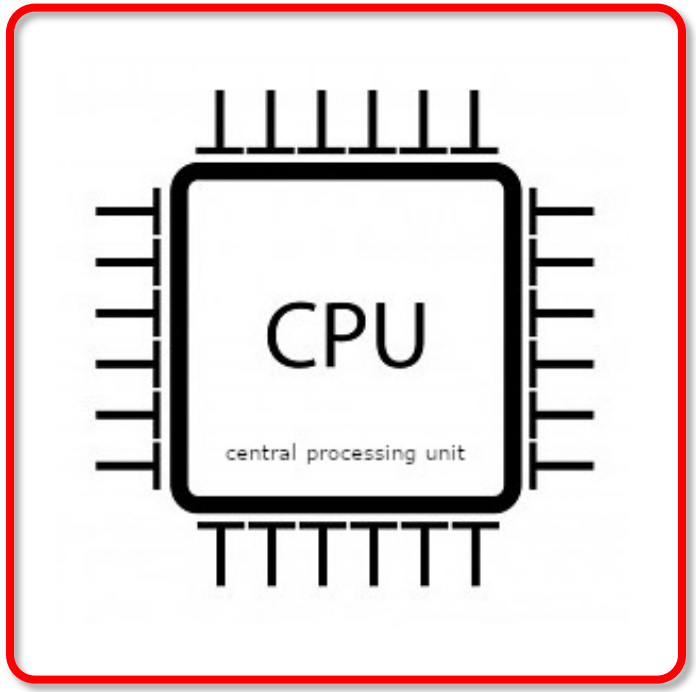
Moor's law – double transistors every two years

Transistor size – atom size

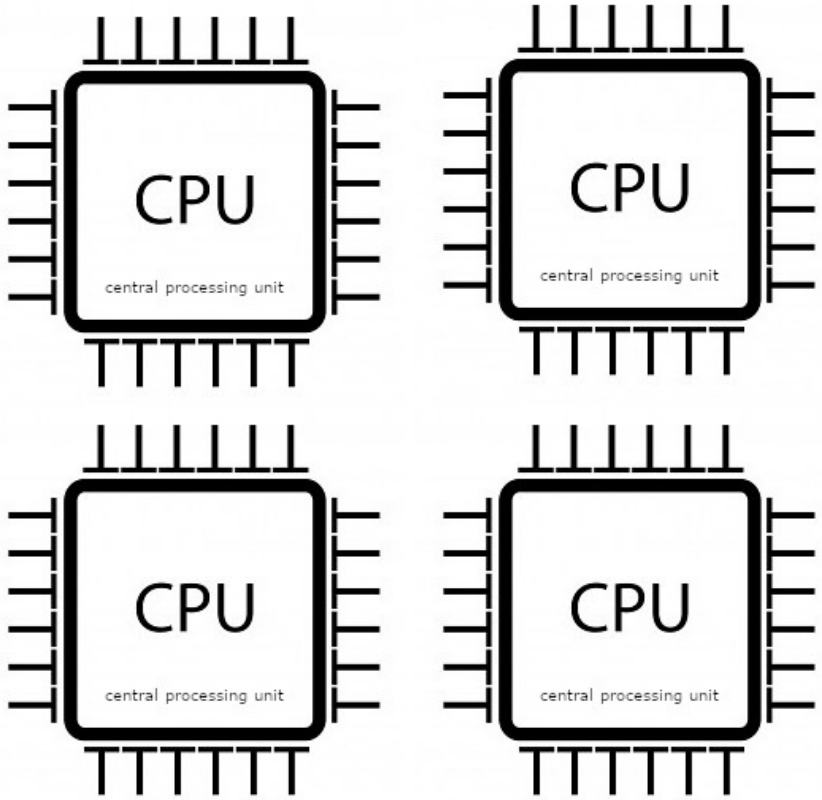


Clock speed? –

cycles per second

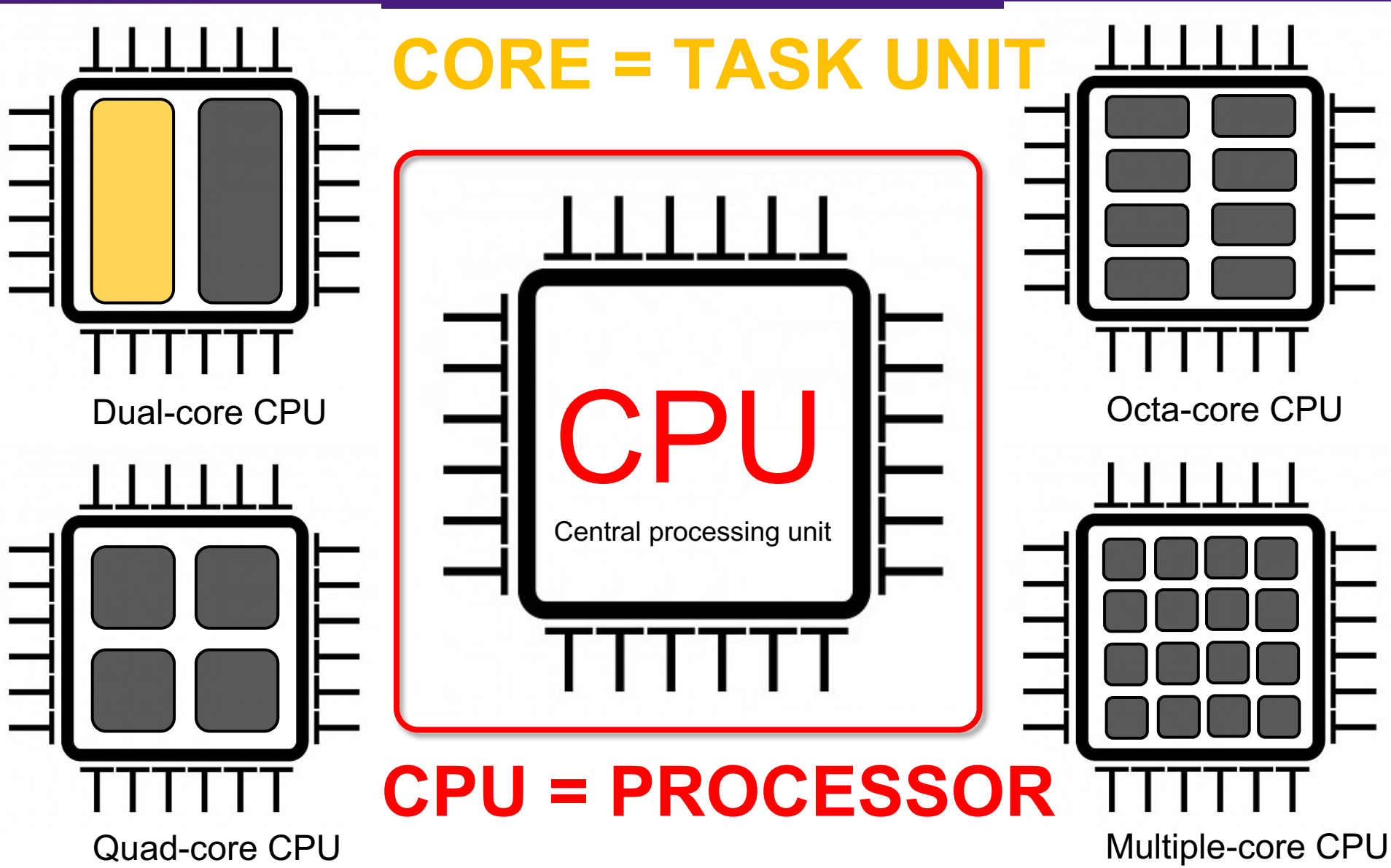


Intel® Core™ i7-1065G7 Processor
8M Cache, up to 3.90 GHz



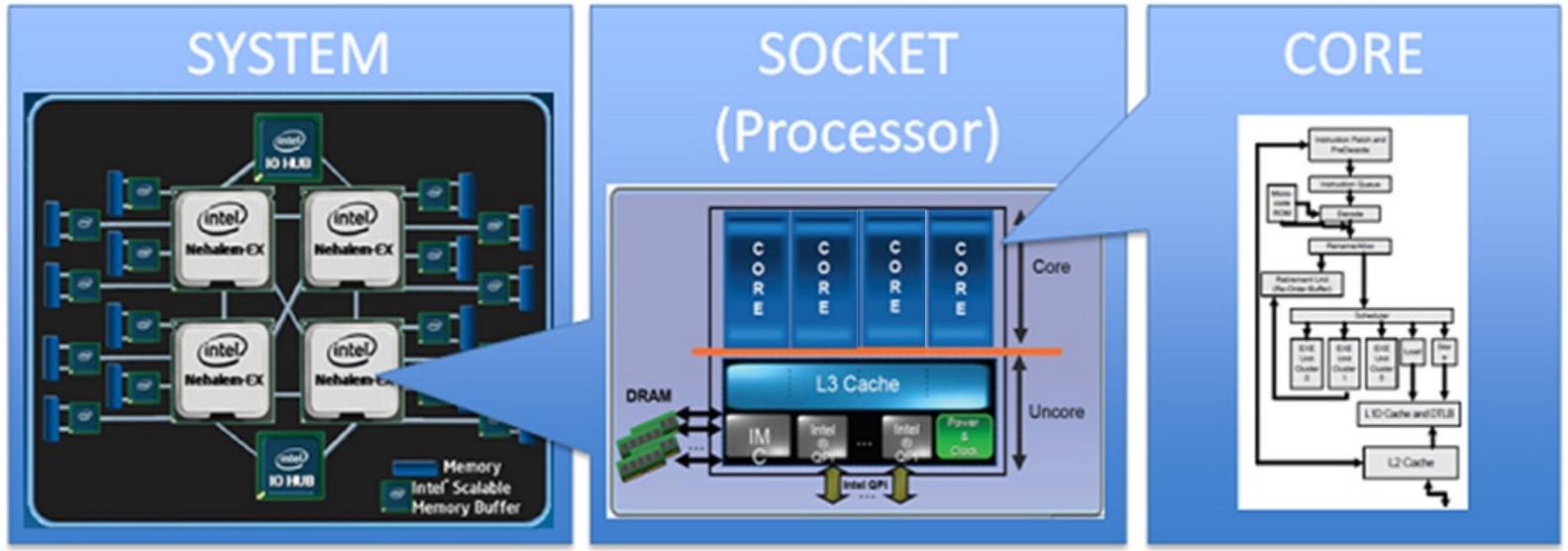
Parallel computing

1) Why HPC?


CORE = TASK UNIT
CPU
Central processing unit
CPU = PROCESSOR
Dual-core CPU
Quad-core CPU
Octa-core CPU
Multiple-core CPU

1) Why HPC?

- How many processors does this computer have?



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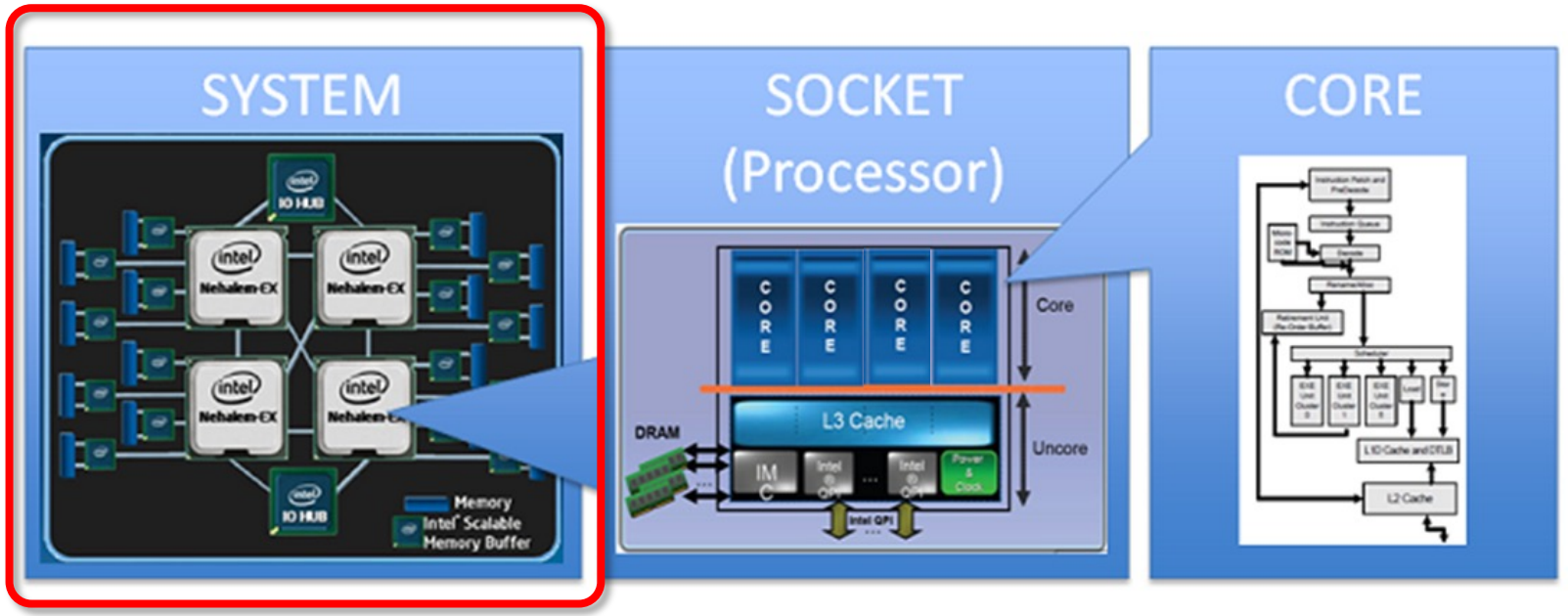

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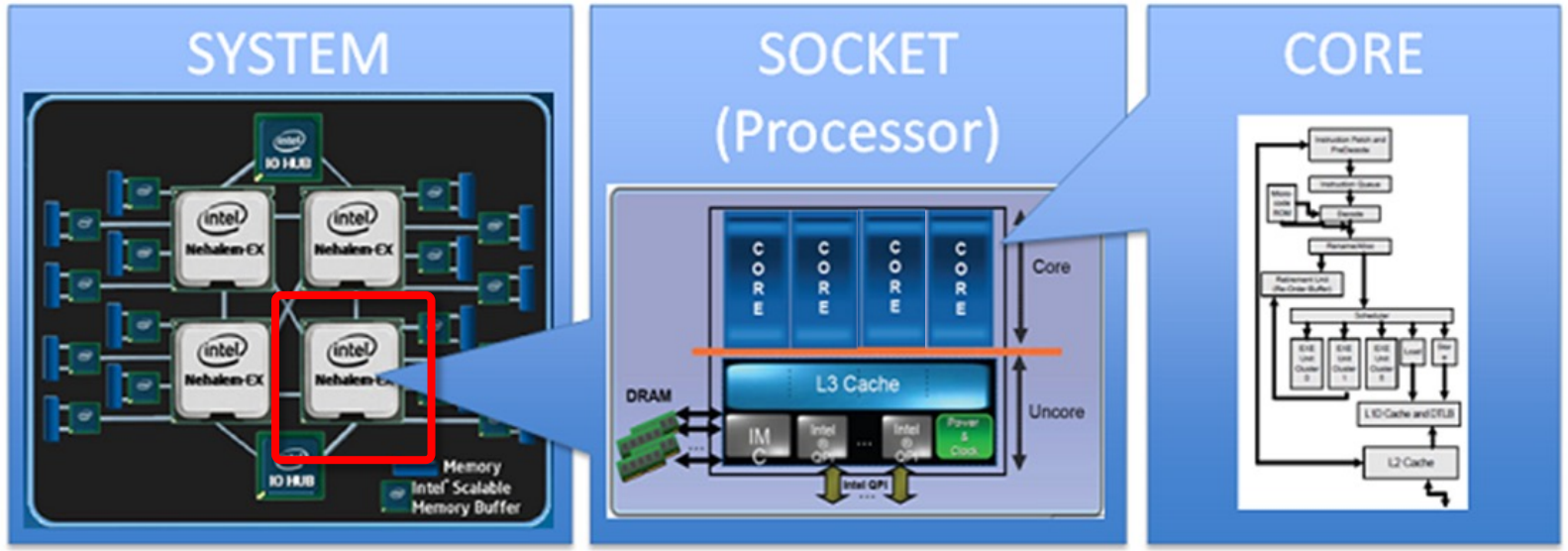
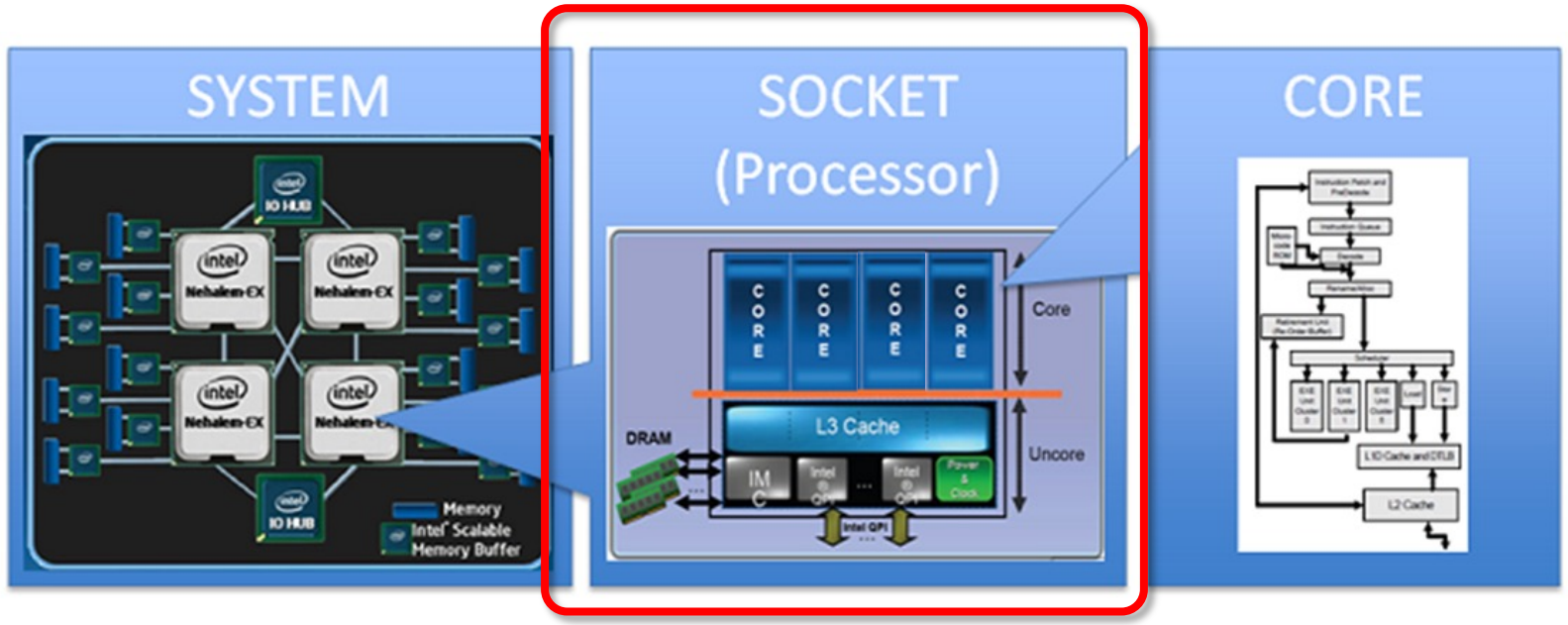


1) Why HPC?

- **How many cores does this computer have?**



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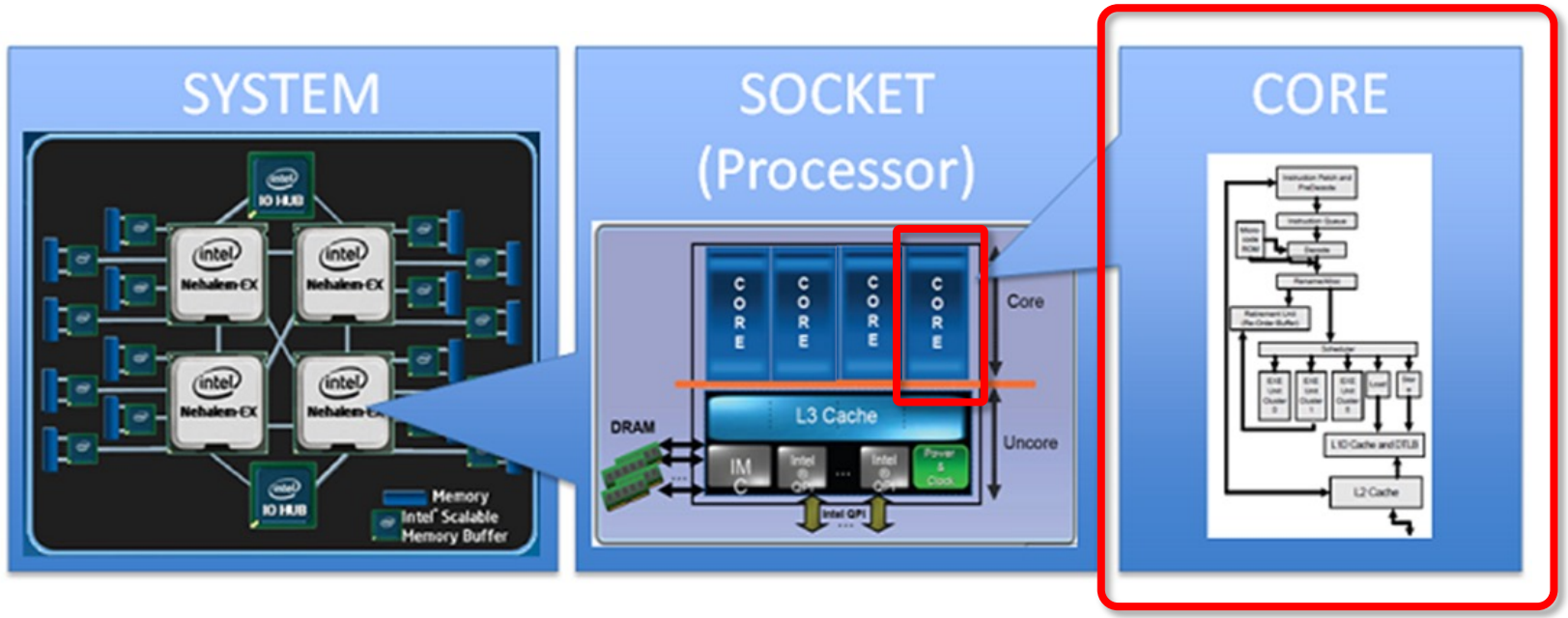

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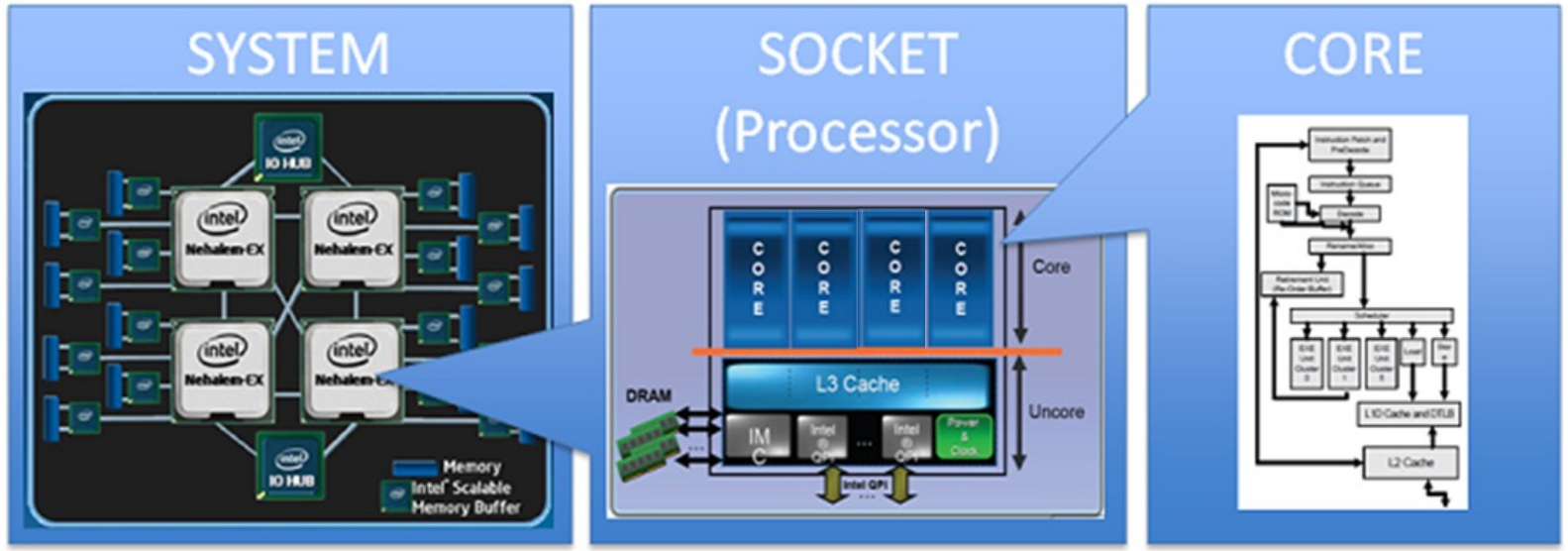

4 cores * 4 processors = 16 total cores

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2) What is HPC?

- **High Performance Computing (HPC): the ability to process data and perform complex calculations at high speeds using the cutting-edge modern technology.**
- **Supercomputer: the class of machines that rank among the fastest in the world.**
  - Rule of thumb: at least 100 times as powerful as a single PC.

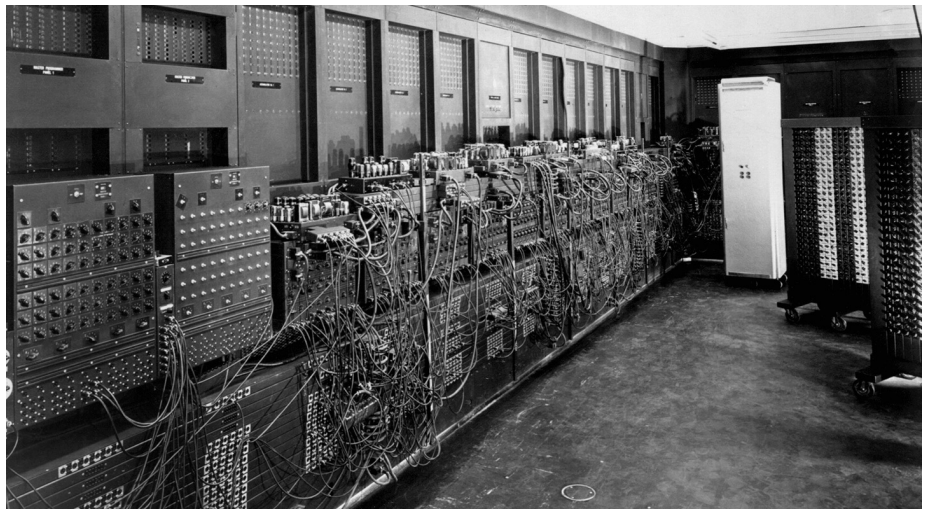
600 mph

60 mph

How do we evaluate the performance of supercomputer?

2) What is HPC?

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



ENIAC FLOPS: 500

$$FLOPS = cores \times clock \times \frac{FLOPs}{cycle}$$

1267 GHz × 18 × 4.4 GHz × 16

1.27 TFLOPS

Computer performance

Name	FLOPS
yottaFLOPS	10^{24}
zettaFLOPS	10^{21}
exaFLOPS	10^{18}
petaFLOPS	10^{15}
teraFLOPS	10^{12}
gigaFLOPS	10^{9}
megaFLOPS	10^{6}
kiloFLOPS	10^{3}

"*The first teraflop desktop PC:* Intel i97980XE (Sep 2017)"

CPU clock rate: 4.4 GHz
CORE: 18 cores
FLOPs per cycle: 16

https://en.wikichip.org/wiki/flops

2) What is HPC?

- **Your smartphone vs. supercomputer 22 years ago**
  - **Apple A16 Bionic** (neural engine): **17 TFLOPS**
  - #1 ASCI WHITE, SP POWER3 375 MHZ: **7.3 (12.3) TFLOPS**
    Total Cores: **8,192**, OS: **AIX**; Vendor: **IBM**
  - #1 **Fujitsu** 105MHz: **0.2 (0.4) TFLOPS**
    Total Cores: **140**, OS: **UXP/V**; Vendor: **Fujitsu**

iPhone 14 Pro (2022)

CPU clock rate: 3.46 GHz
CORE: 6 cores
Transistors: 16 billion
Technology: 4 nm
OS system: iOS

Computer performance

Name	FLOPS
yottaFLOPS	10^{24}
zettaFLOPS	10^{21}
exaFLOPS	10^{18}
petaFLOPS	10^{15}
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megaFLOPS	10^{6}
kiloFLOPS	10^{3}

[1] Apple Event — September 7, https://www.youtube.com/watch?v=ux6zXguiqxM
[2] Top 500 list, https://www.top500.org/lists/top500/2022/11/

2) What is HPC?

Current (November 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 (2021) 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

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2) What is HPC?

LSU

TOP500 SUPERCOMPUTER SITES

Current (June 2022):

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
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2) What is HPC?

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

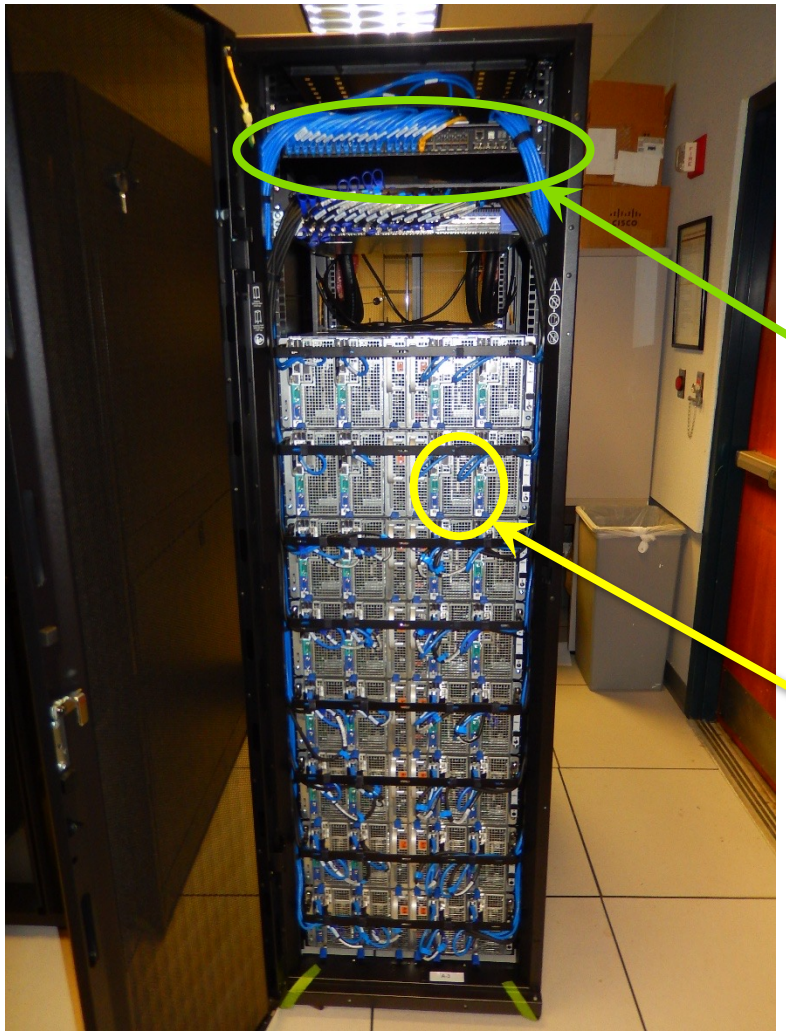
[1] Top 500 list, https://www.top500.org/lists/top500/list/2019/06/?page=5

2) What is HPC?

- **Inside a cluster:**

2) What is HPC?

- **Inside a rack:**

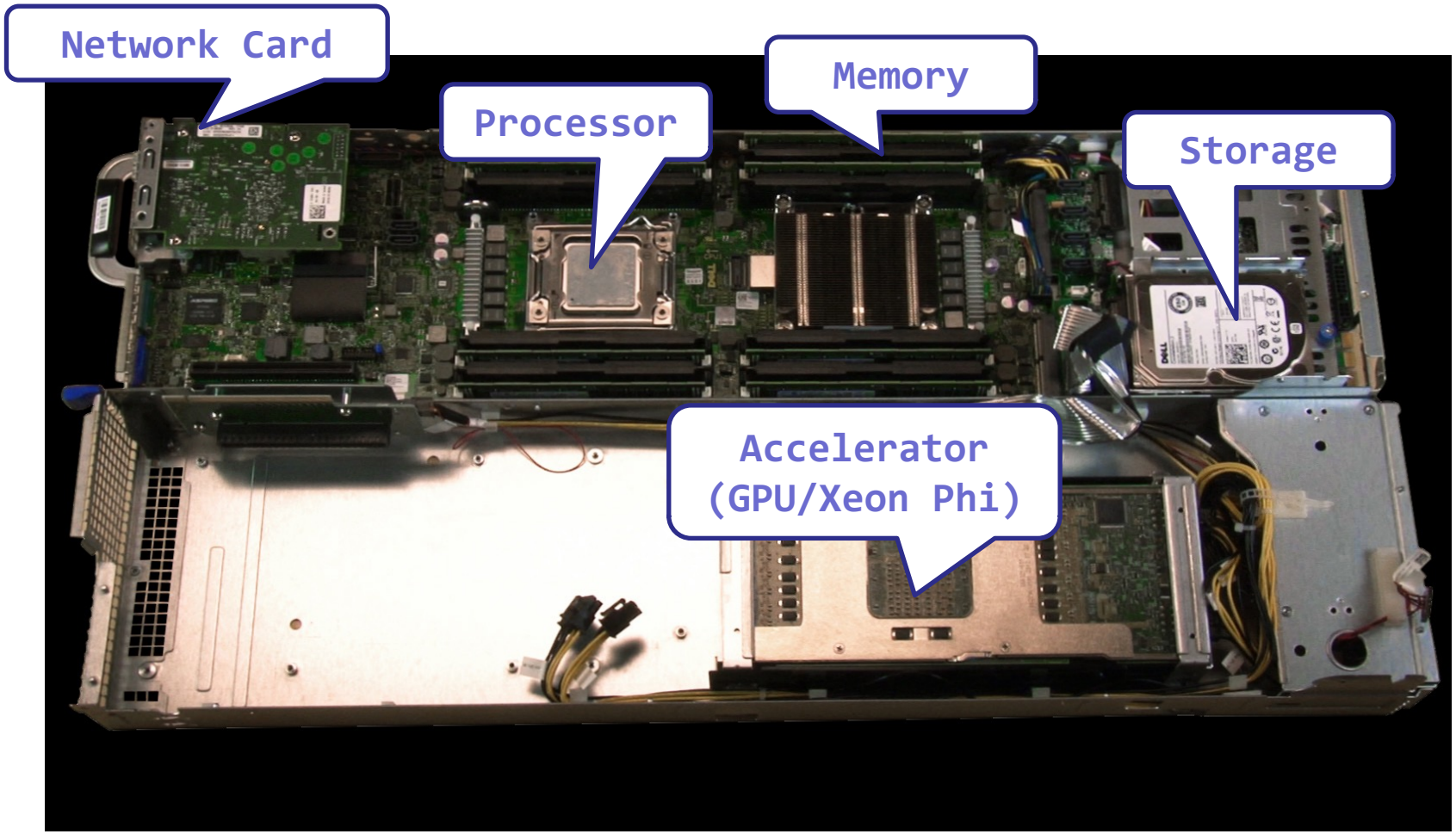


Interconnect: Infiniband Switch

Compute Node

2) What is HPC?

- **Inside a node:**



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3) Our HPC

i. **University level: LSU HPC**
ii. **State level: LONI**
iii. **National level: ACCESS**

Universities of Louisiana State

Louisiana State University Campus, Baton Rouge, LA

Advancing Innovation

Universities of the United States

LSU INFORMATION TECHNOLOGY SERVICES

ACCESS: https://access-ci.org

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	
User Guide	
Available Software	

Deep Bayou	
Hostname	db1.lsu.edu
Peak Performance/TFlops	257
Compute nodes	13
Processor/node	2 24-core
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Processor Type	Intel Cascade Lake Xeon 64bit
Nodes with Accelerators	13
Accelerator Type	2 x NVIDIA Volta V100S
OS	RHEL v7
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SuperMike III	
Hostname	mike.hpc.lsu.edu
Peak Performance/TFlops	1,285
Compute nodes	183
Processor/node	2 32-core
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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

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	
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

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

- State-of-the-art fiber optic network
- Runs throughout Louisiana State, connects Louisiana and Mississippi State 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)

[1] https://loni.org/about/participants/

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	
User Guide	
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	
User Guide	
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/

3) Our HPC

- **Summary**

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

Questions?

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. Intro the cluster
    1) Getting connected
    2) File system
4. Software environment
    1) Preinstalled (modules)
    2) User installation

Two things are 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. Intro the cluster
    1) What users see?
    2) Useful commands & tools
4. Software environment
    1) Preinstalled (modules)
    2) User installation

1) Accounts

	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

1) Accounts

i. Eligibility (LSU HPC)

LSU HPC	
Available to…	
Requirements	

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

i. Eligibility (LSU HPC)

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)

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 (LSU HPC)

You are a …	Your account sponsor

1) Accounts

i. Eligibility (LSU HPC)

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

1) Accounts

i. Eligibility (LSU HPC)

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 (LSU HPC)

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 (LSU HPC)

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 (LSU HPC)

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

1) Accounts

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)

1) Accounts

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

Test1

- **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

Test1

- **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

Test2

- **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

Test2

- **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

1) Accounts

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

1) Accounts

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

1) Accounts

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

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

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 • …	

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

iv. Reset password

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

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

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 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

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."

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

- **HPC User Environment 1**

1. Intro to HPC
   1) Why HPC?
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   3) Our HPC
2. Getting started
   1) Accounts
   2) Allocation
3. Intro 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 & LONI 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 / LONI subscribers

2) Allocation

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

2) Allocation

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

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

2) Allocation

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 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
					[LONI] 6,000,000 SU / allocation 12,000,000 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	LONI
Portal	https://accounts.hpc.lsu.edu/allocations.php	https://allocations.loni.org/allocations.php

2) Allocation

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 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!**

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

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 -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

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

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    1) Preinstalled (modules)
    2) User installation

1) Getting connected

i. General architecture

Term	Definition

1) Getting connected

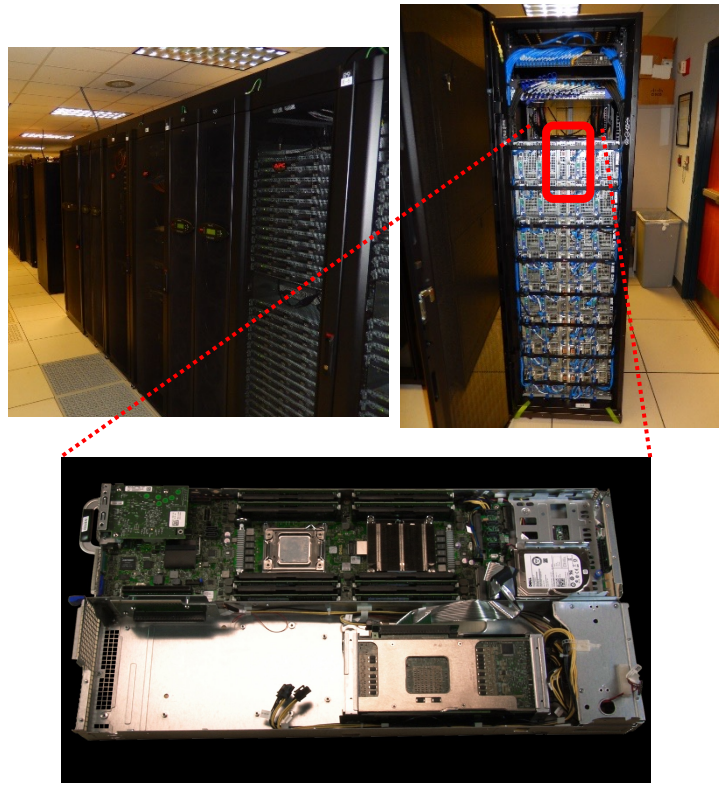
i. General architecture

Term	Definition
Cluster	A set of connected computer nodes that work together. (*E.g., QB2*)

1) Getting connected

i. General architecture

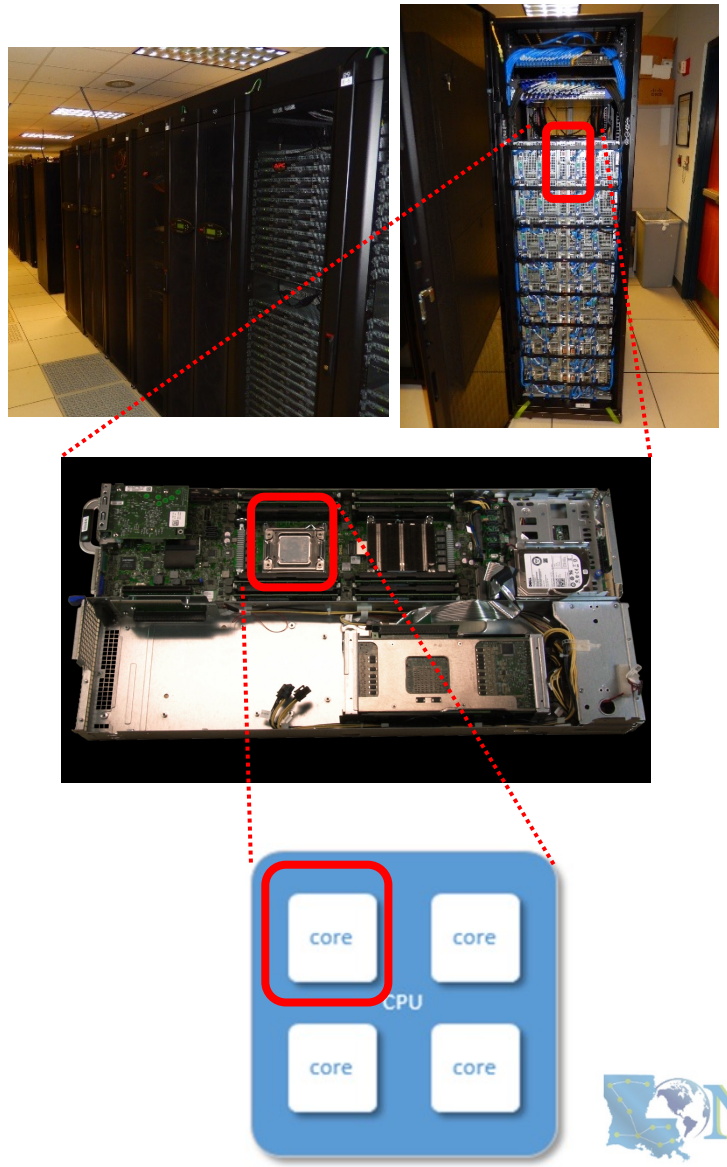
Term	Definition
Cluster	A set of connected computer nodes that work together. (*E.g., QB2*)
Node	A single, named host machine in the cluster. (*E.g., qb010*)



1) Getting connected

i. General architecture

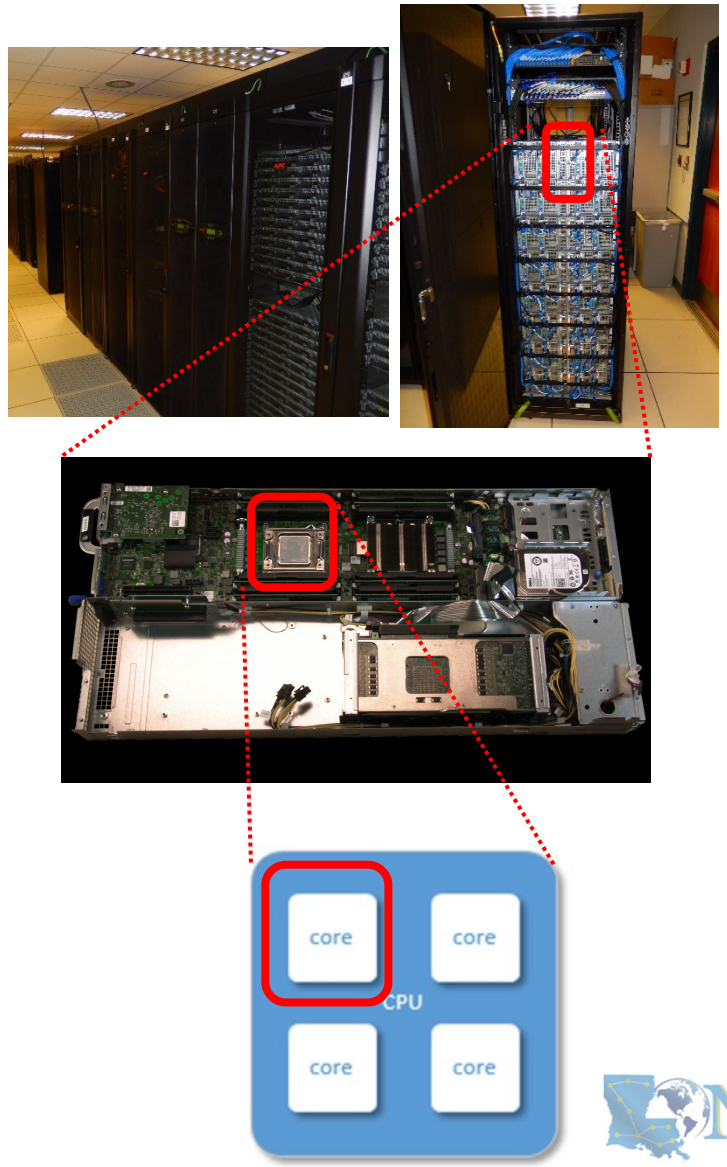
Term	Definition
Cluster	A set of connected computer nodes that work together. (*E.g., QB2*)
Node	A single, named host machine in the cluster. (*E.g., qb010*)
Core	The basic computation unit in a processor. *(E.g.* , QB2 has two 10-core processors → 20 cores)



1) Getting connected

i. General architecture

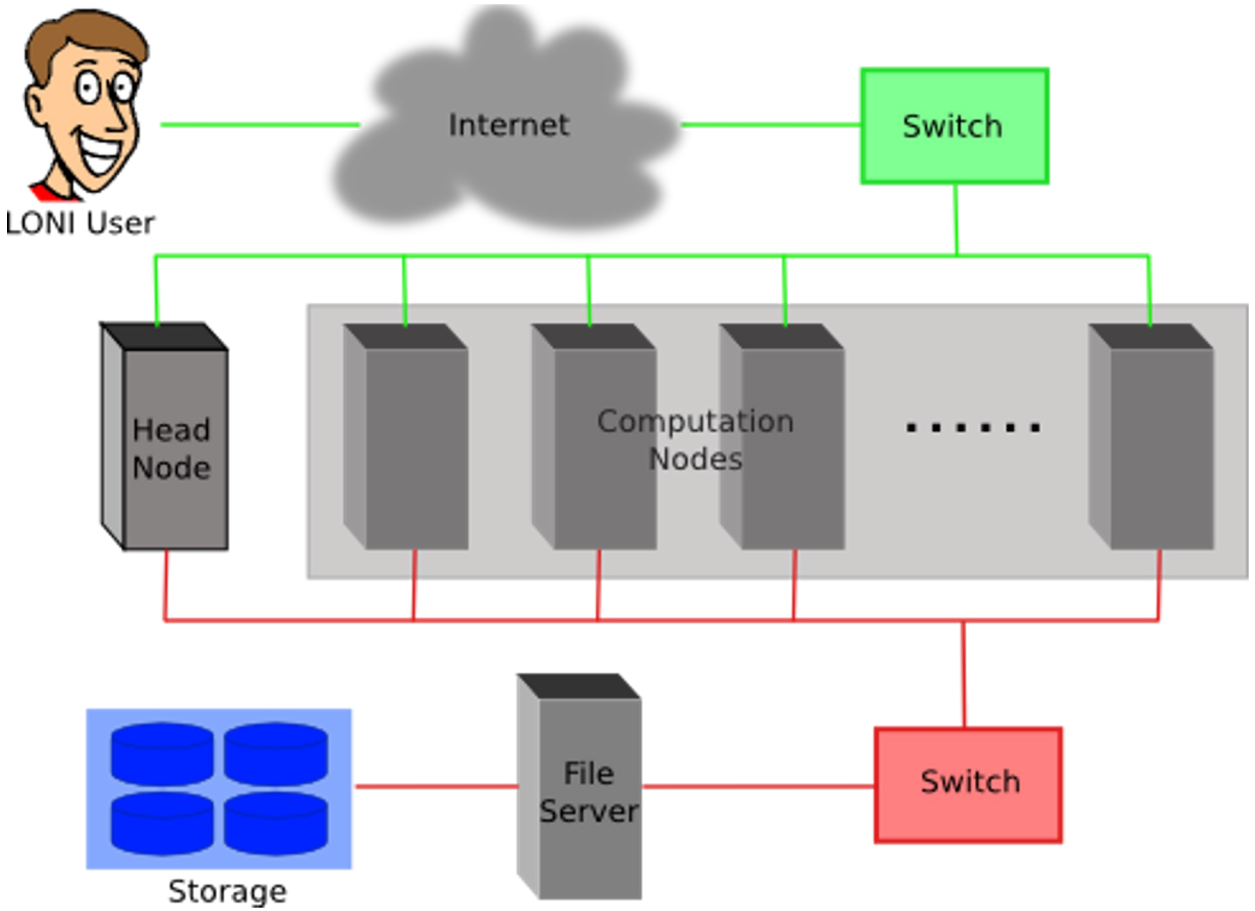
Term	Definition
Cluster	A set of connected computer nodes that work together. (*E.g., QB2*)
Node	A single, named host machine in the cluster. (*E.g., qb010*)
Core	The basic computation unit in a processor. (*E.g.* , QB2 has two 10-core processors → 20 cores)
Job	A user's request to use a certain amount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



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
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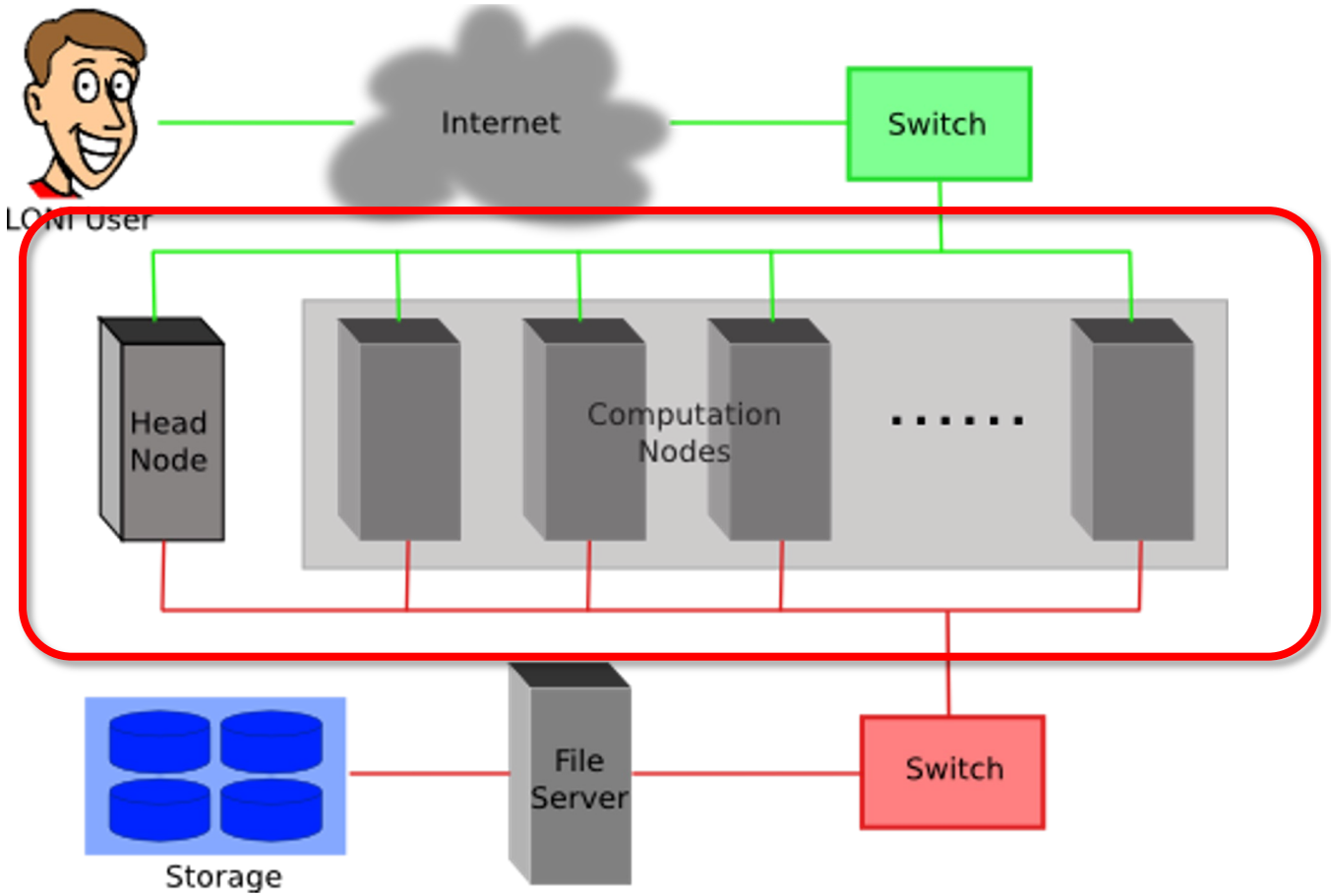
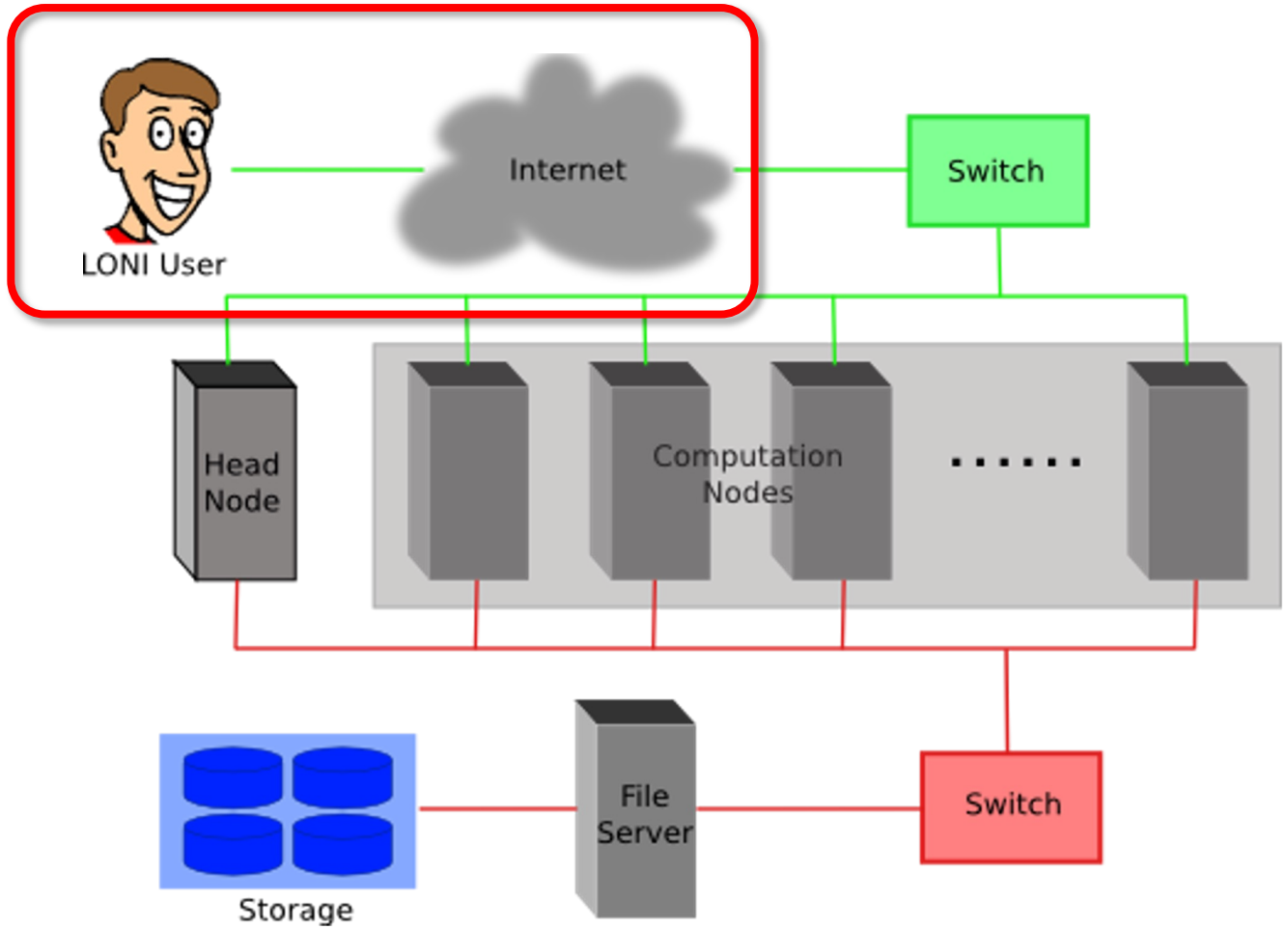


1) Getting connected

i. General architecture

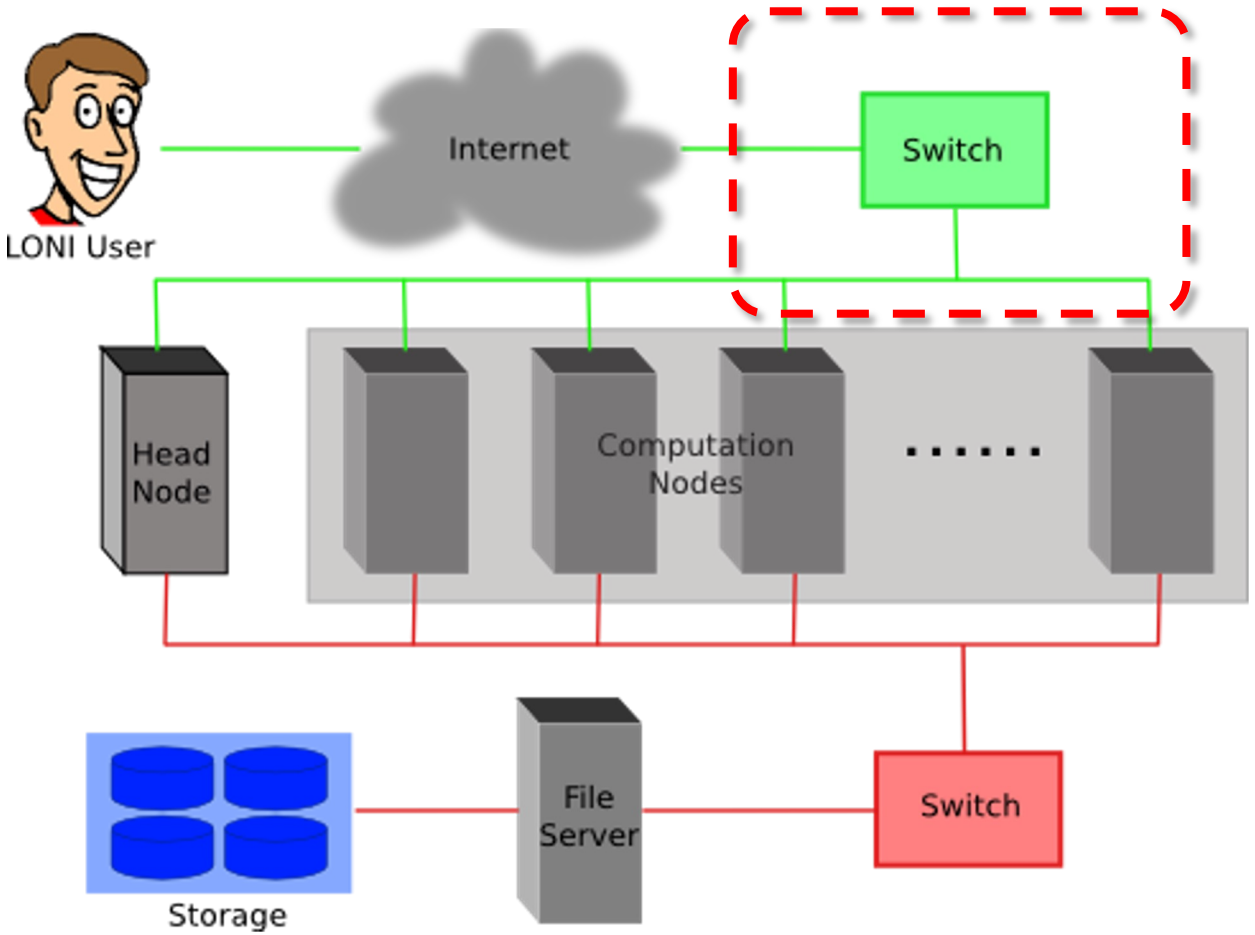
- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously



1) Getting connected

i. General architecture

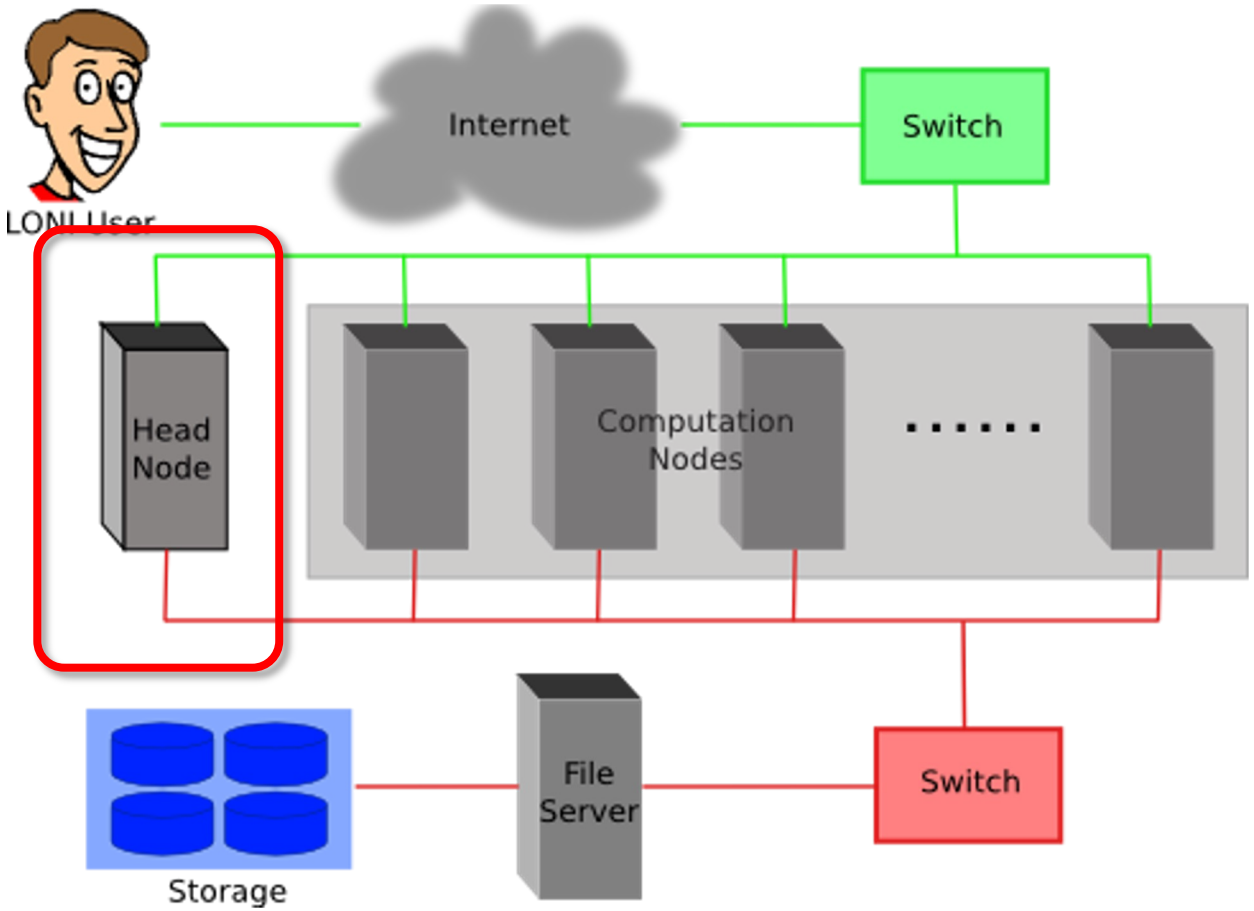
- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously



1) Getting connected

i. General architecture

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



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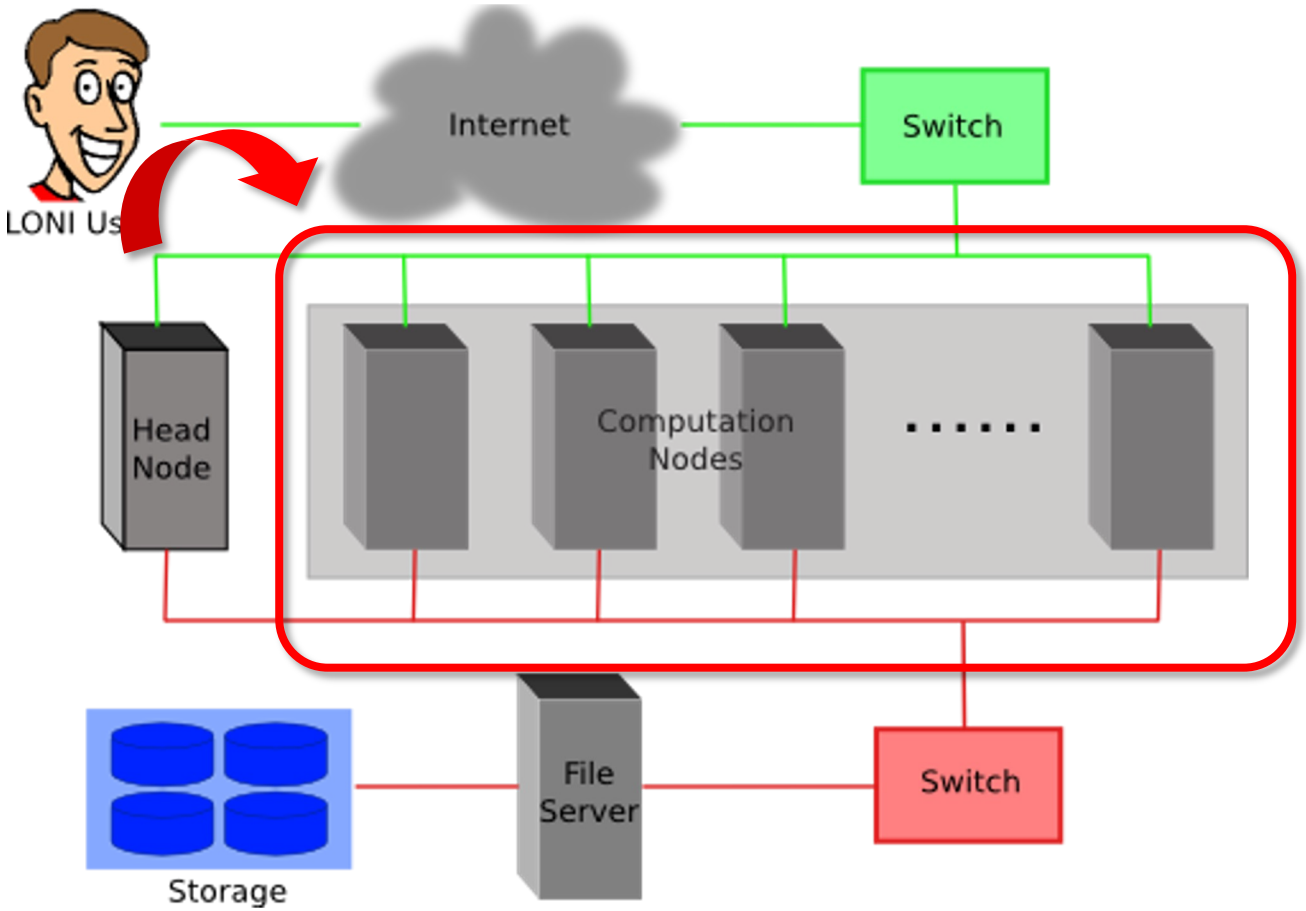

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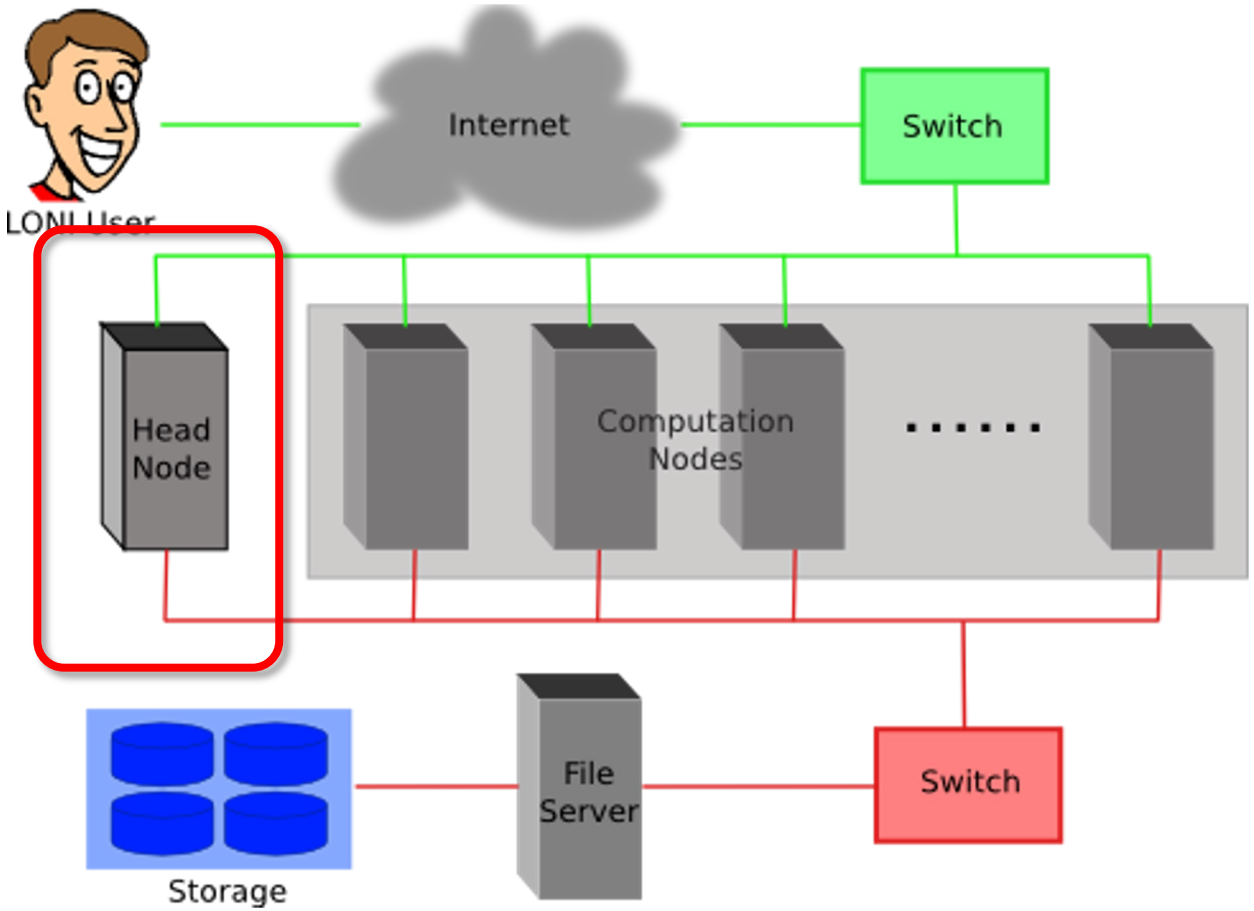

DO NOT RUN JOBS ON HEAD NODE!!!

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

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Secure Shell (SSH)

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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)

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

ii. Logging in

Secure Shell (SSH)

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

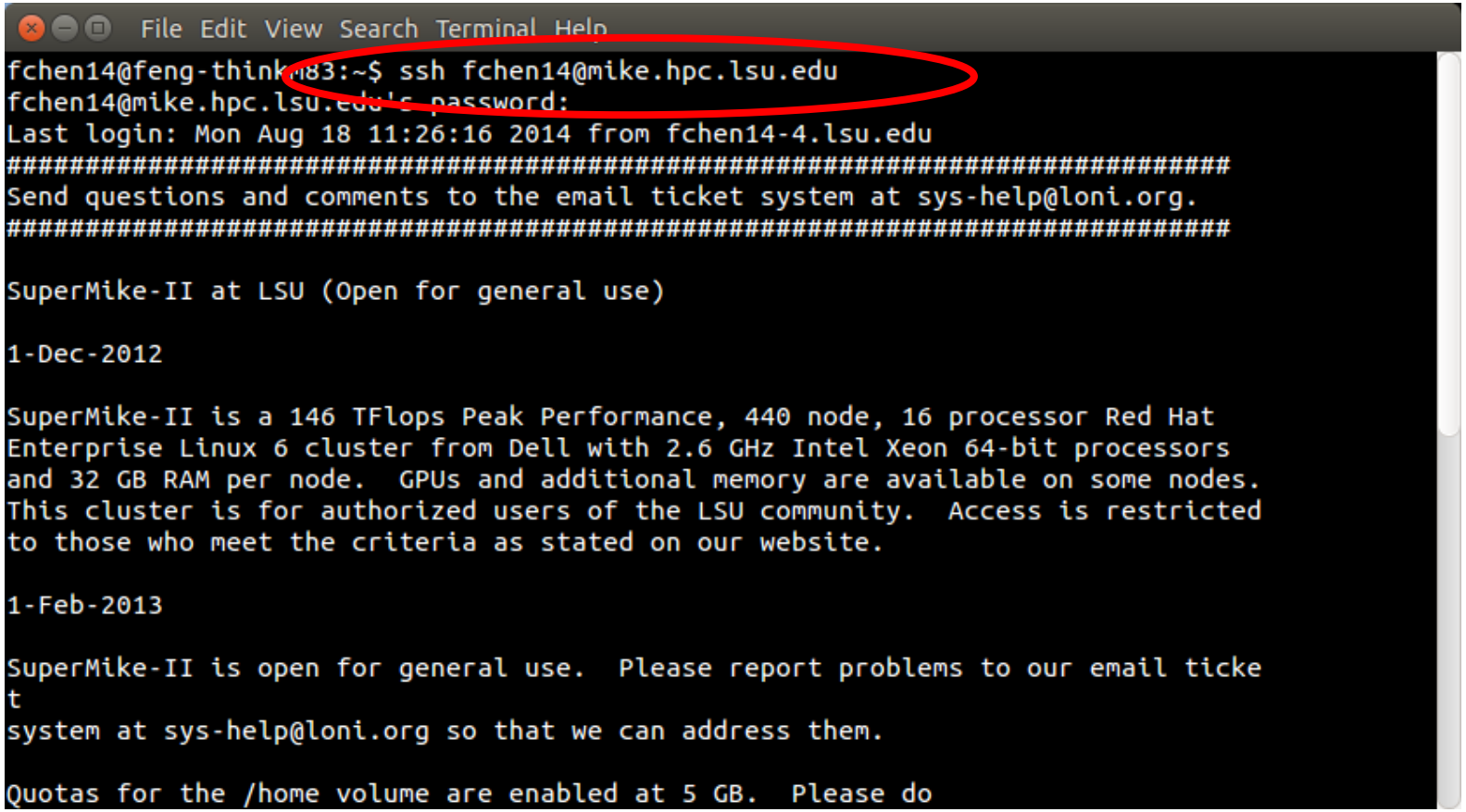
ii. Logging in

```
ssh -X username @ remote host address
```

1) Getting connected

ii. Logging in

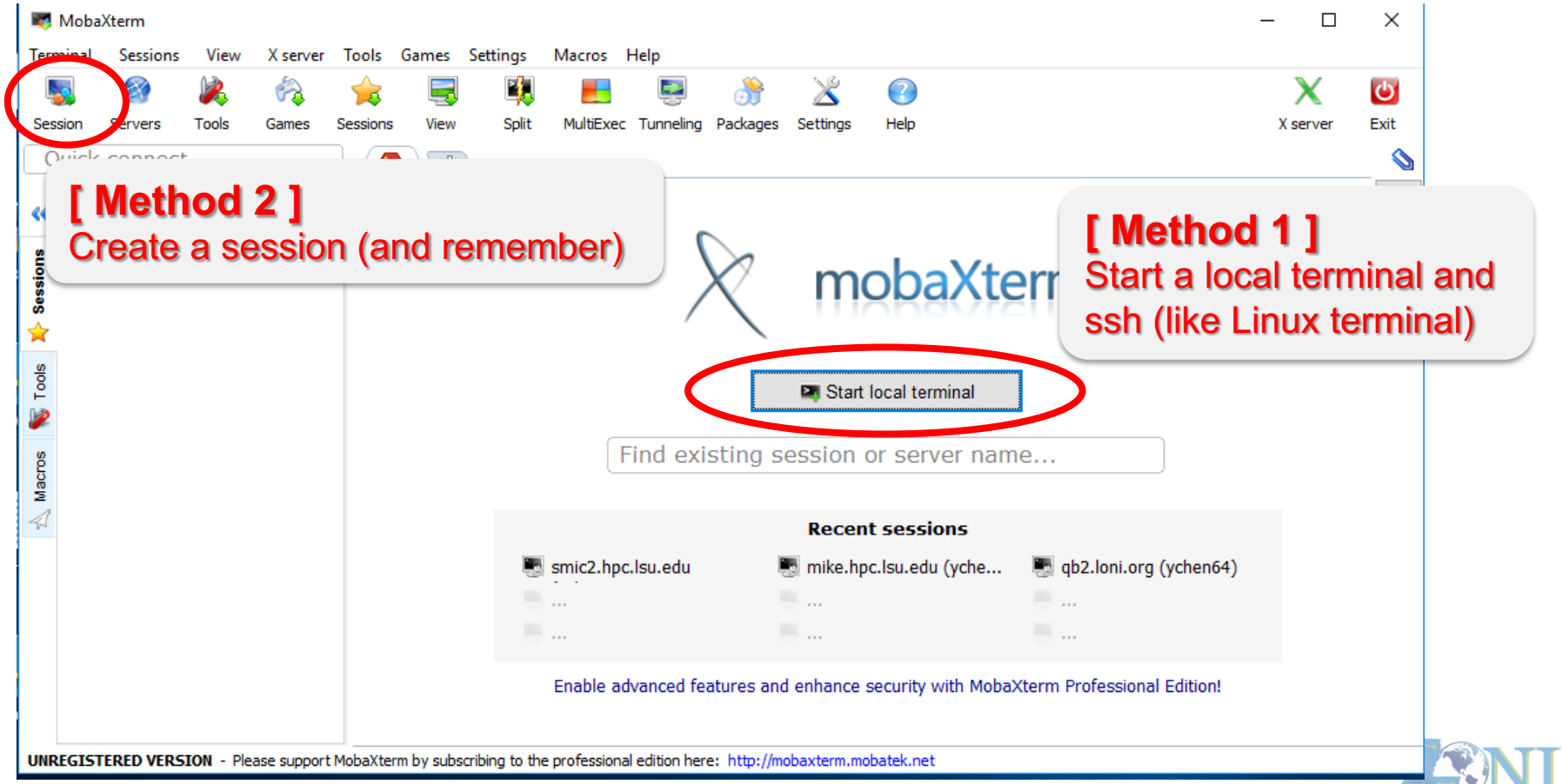
a) Linux / Mac



ii. Logging in

b) Windows

- MobaXterm

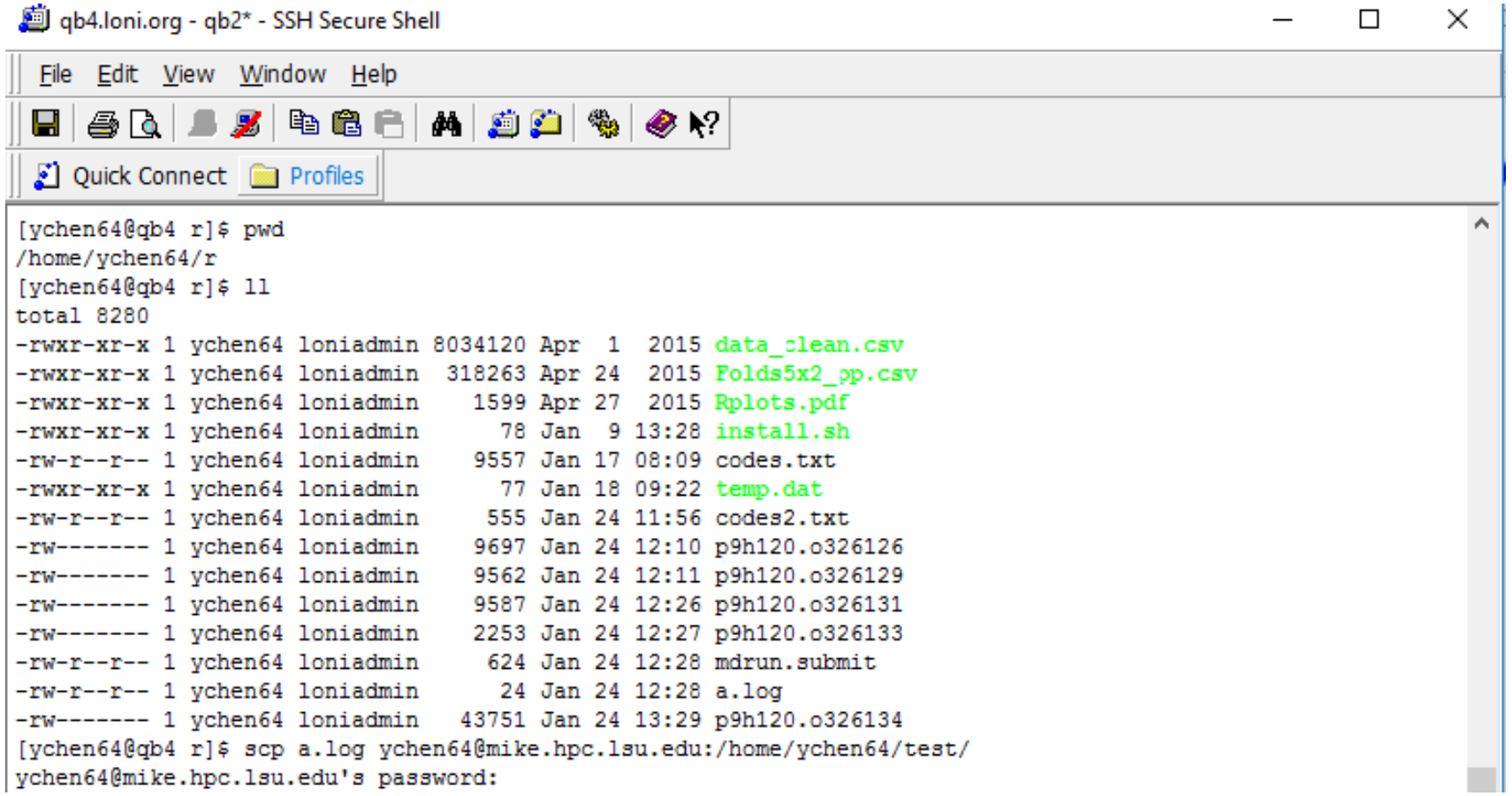


1) Getting connected

ii. Logging in

b) Windows

- SSH Secure Shell

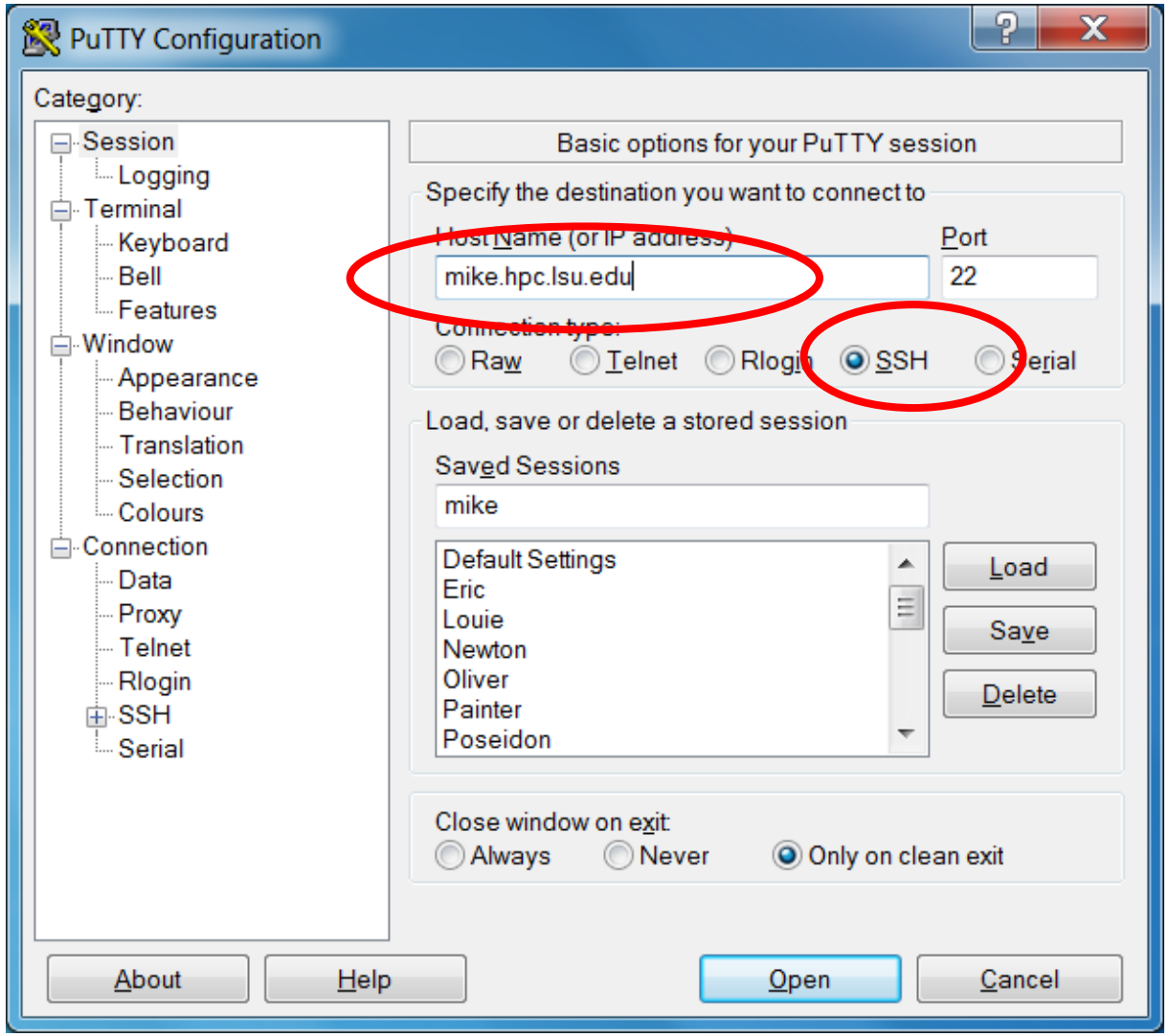


1) Getting connected

ii. Logging in

b) Windows

- Putty



ii. Logging in

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

ii. Logging in

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You are using…	To enable X11 forwarding…

ii. Logging in

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

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  - 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

ii. Logging in

❖ 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	

ii. Logging in

- Special note: **X11 forwarding**
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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”)

ii. Logging in

❖ 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")
	Putty	a) Install X server (*e.g.* Xming) b) Connection → SSH → X11 → Enable X11 forwarding

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

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    2) Allocation
3. Into the cluster
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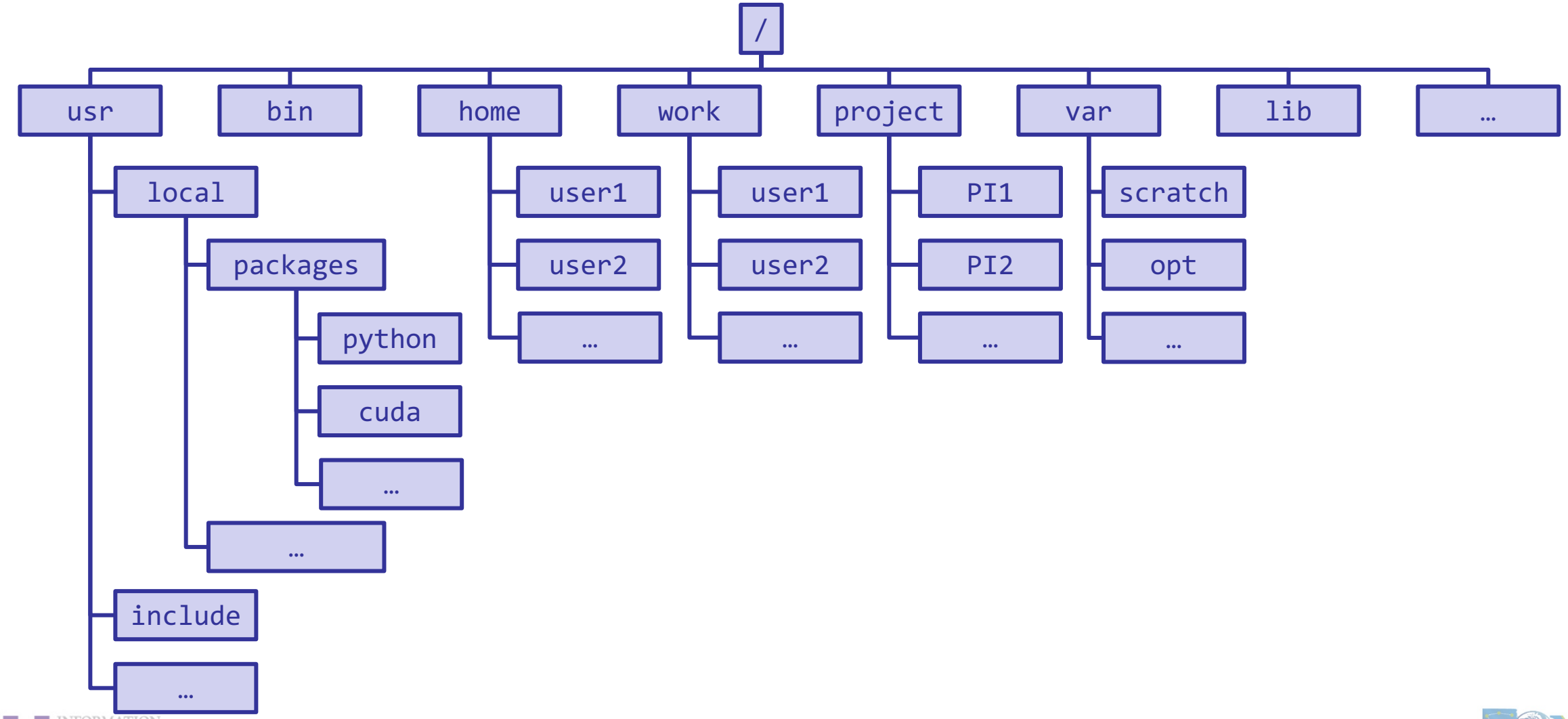
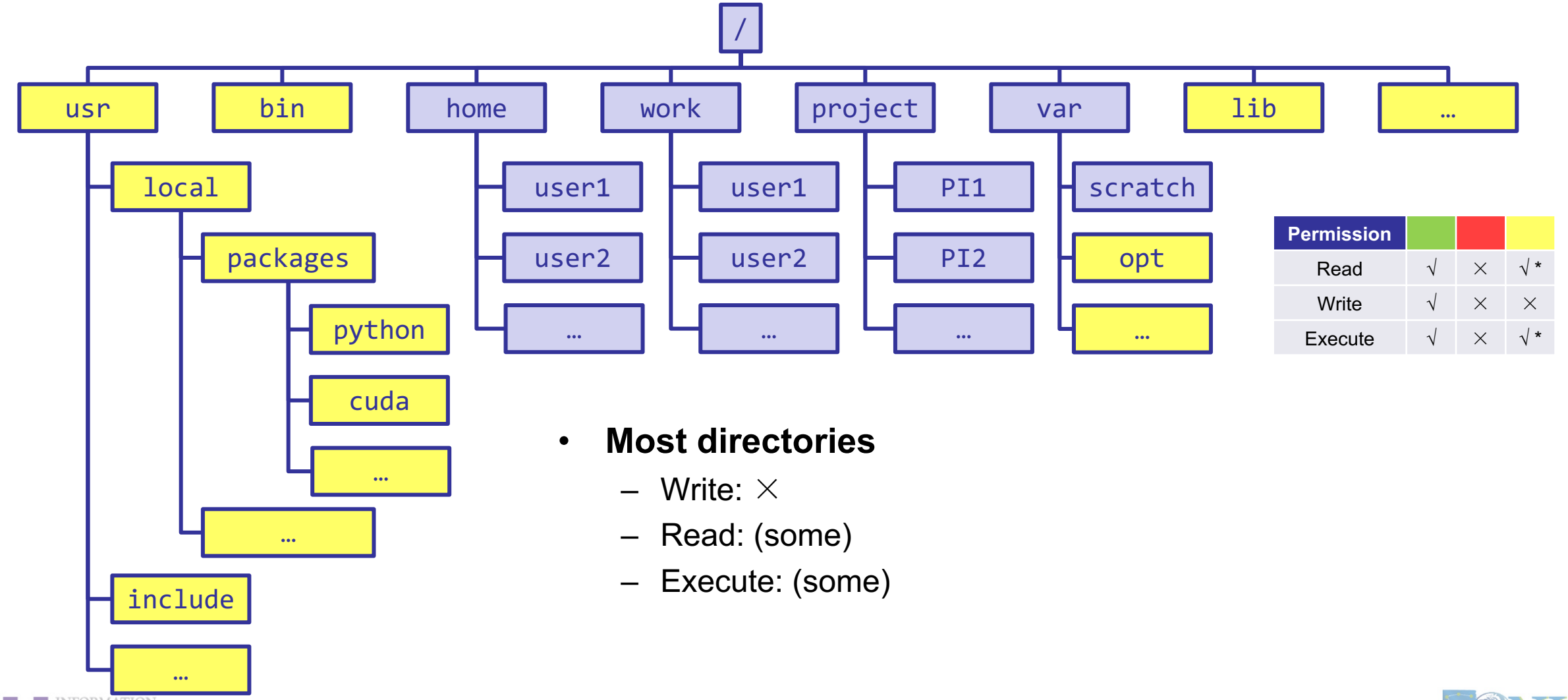
    2) File system
4. Software environment
    1) Preinstalled (modules)
    2) User installation

2) File system



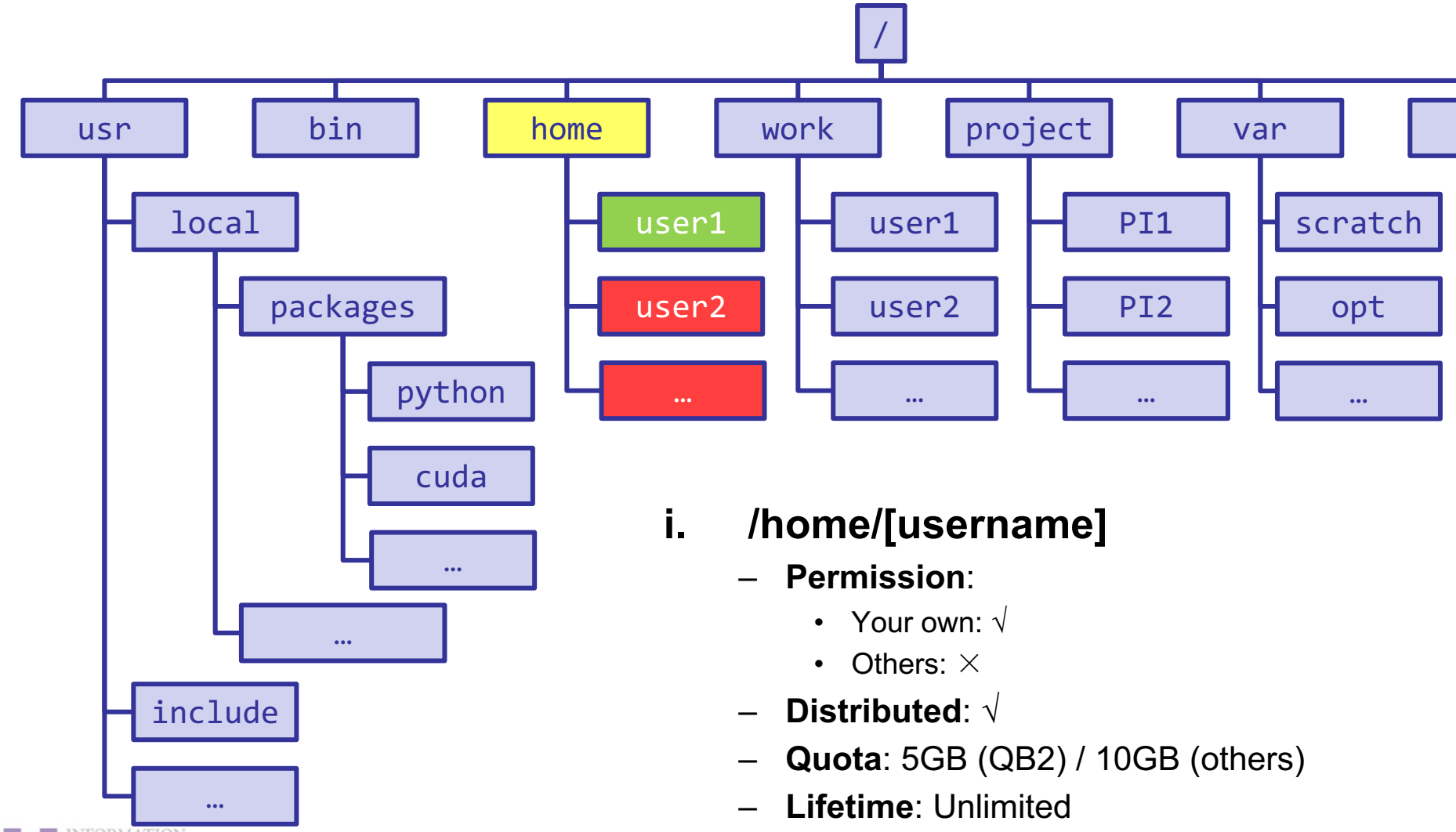
2) File system



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

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

2) File system

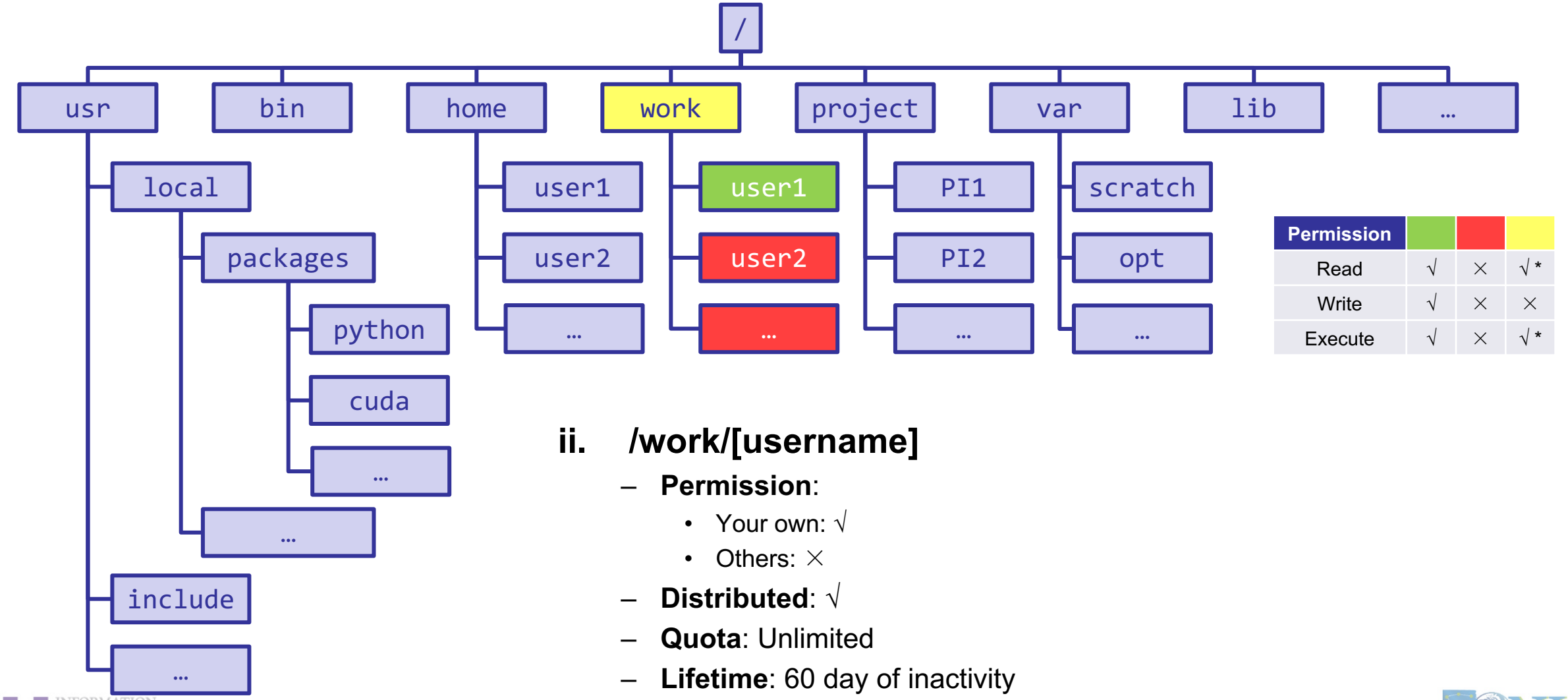


Permission			
Read	√	×	√ *
Write	√	×	×
Execute	√	×	√ *

i. /home/[username]

- **Permission**:
  - Your own: √
  - Others: ×
- **Distributed**: √
- **Quota**: 5GB (QB2) / 10GB (others)
- **Lifetime**: Unlimited
- **Best for**: Code / executables

2) File system

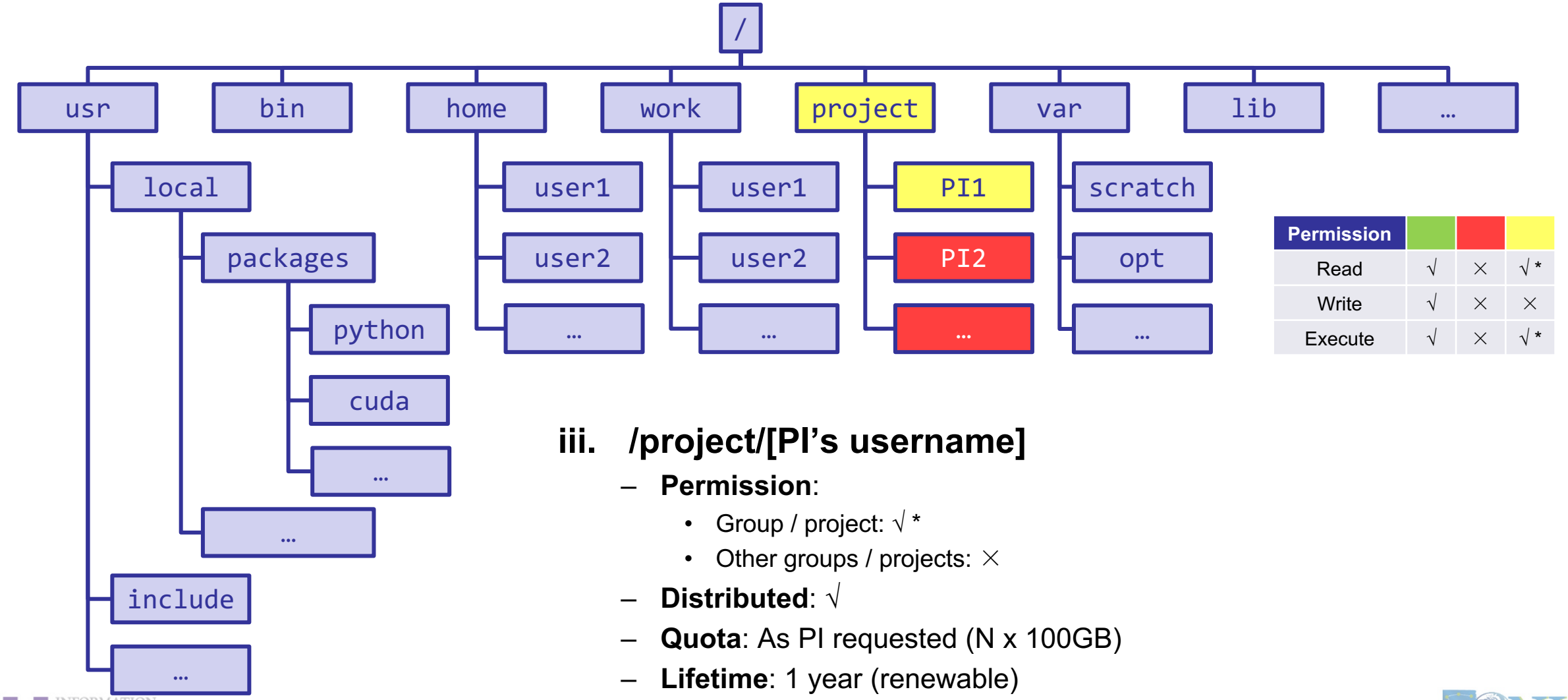


Permission			
Read	√	×	√ *
Write	√	×	×
Execute	√	×	√ *

ii. /work/[username]

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

2) File system

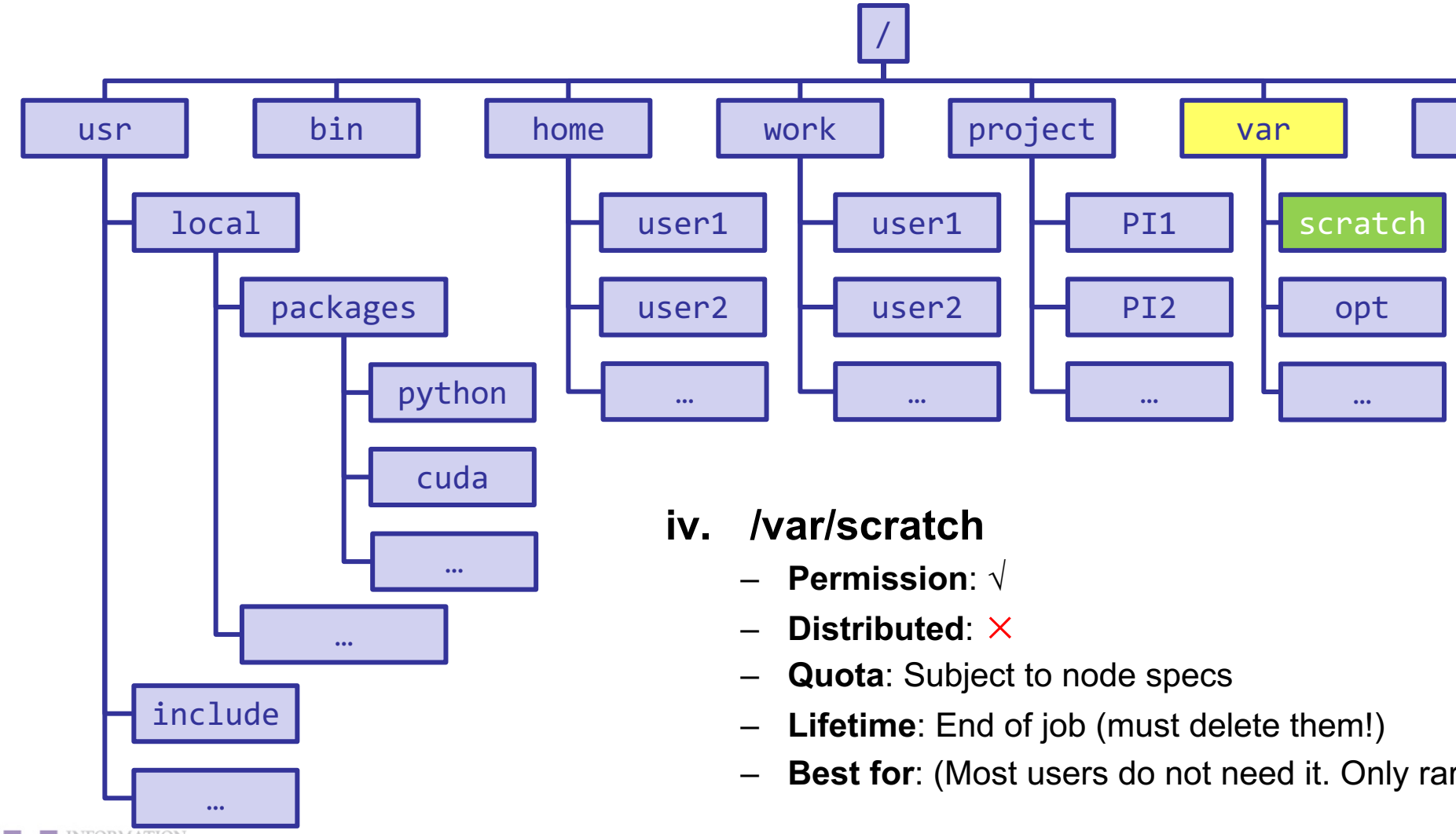


Permission			
Read	√	×	√ *
Write	√	×	×
Execute	√	×	√ *

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)

2) File system

File system summary

Directory (folder)	Distributed	Throughput	Lifetime	Quota	Best for
/home/[username]	√	Low	Unlimited	5GB (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**
  - **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**

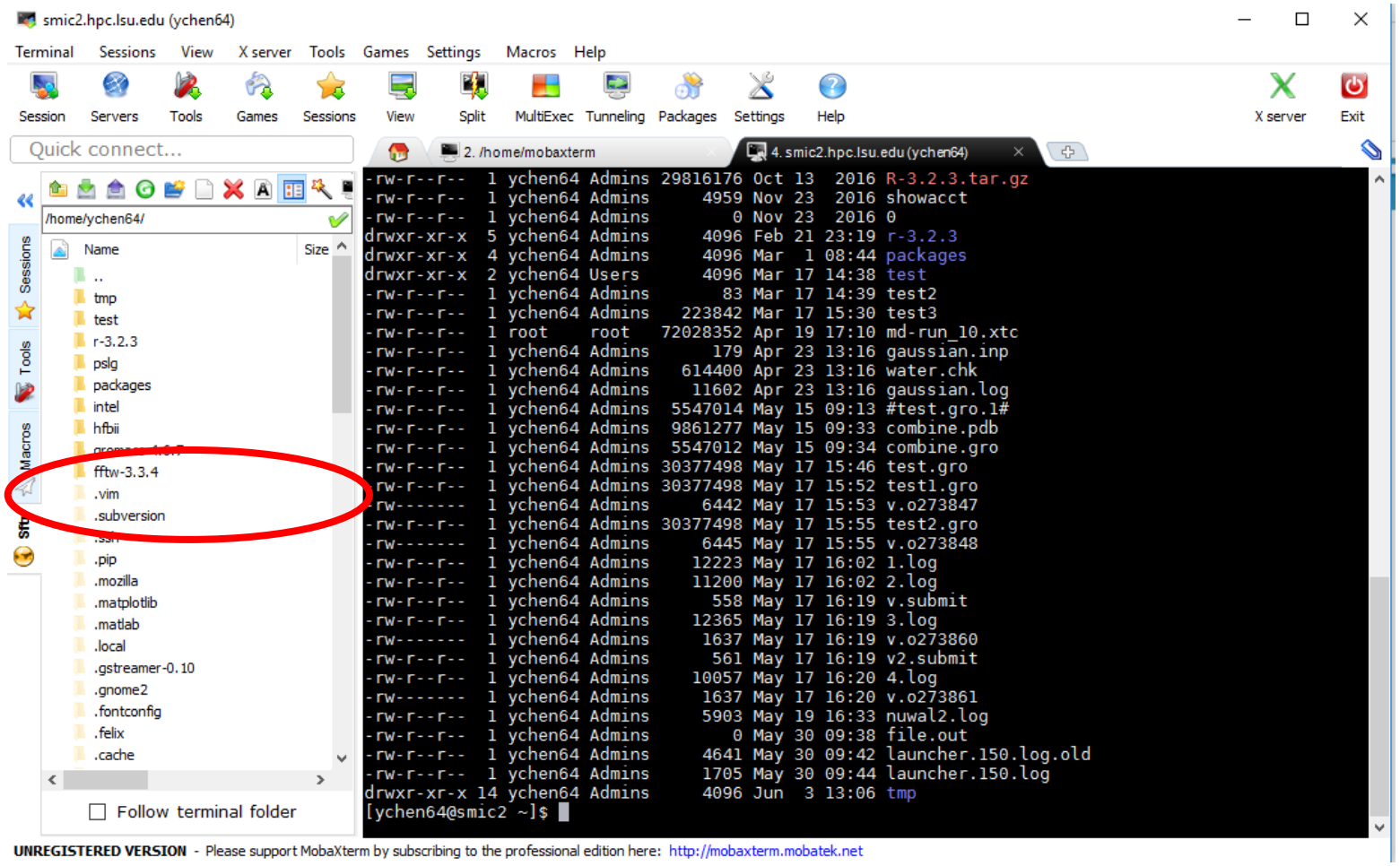
2) File system

- **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**



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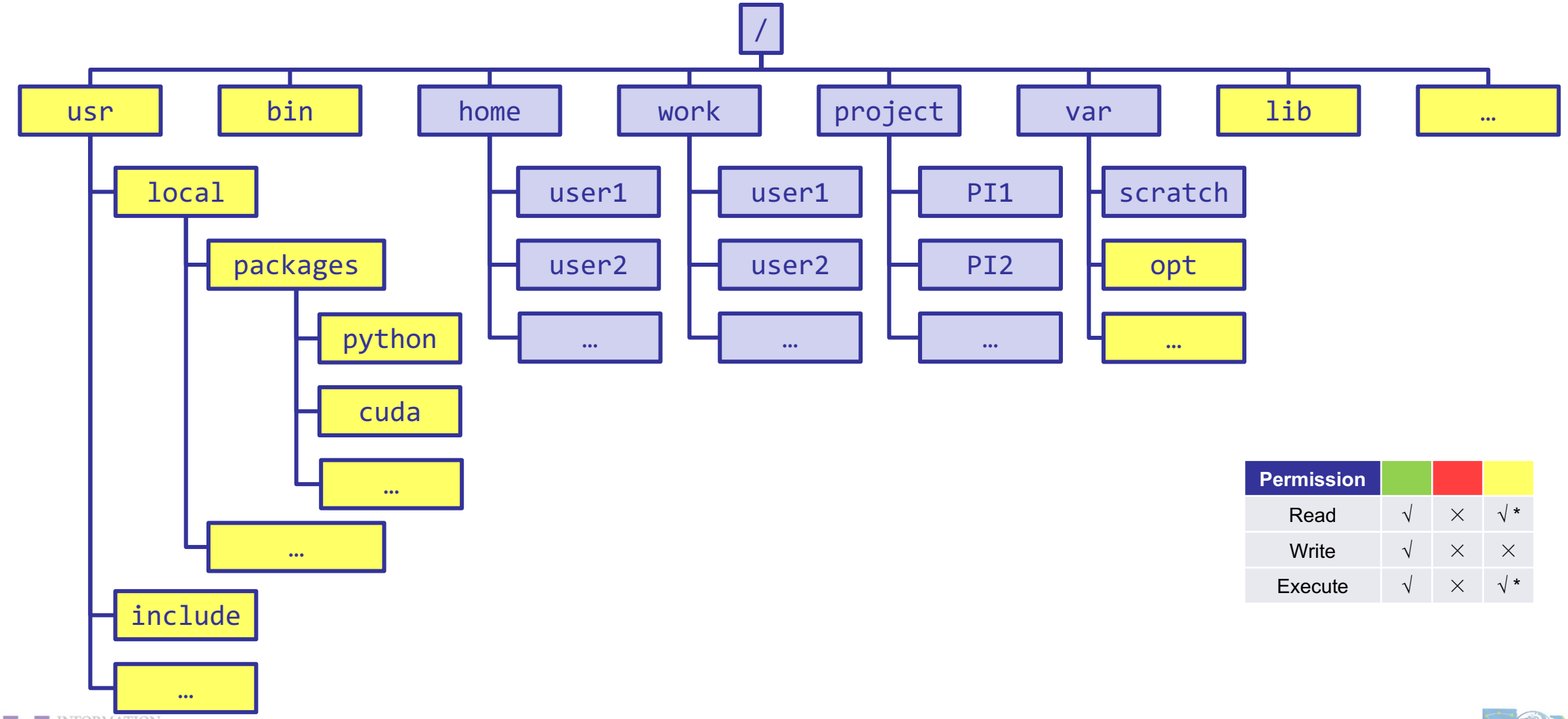
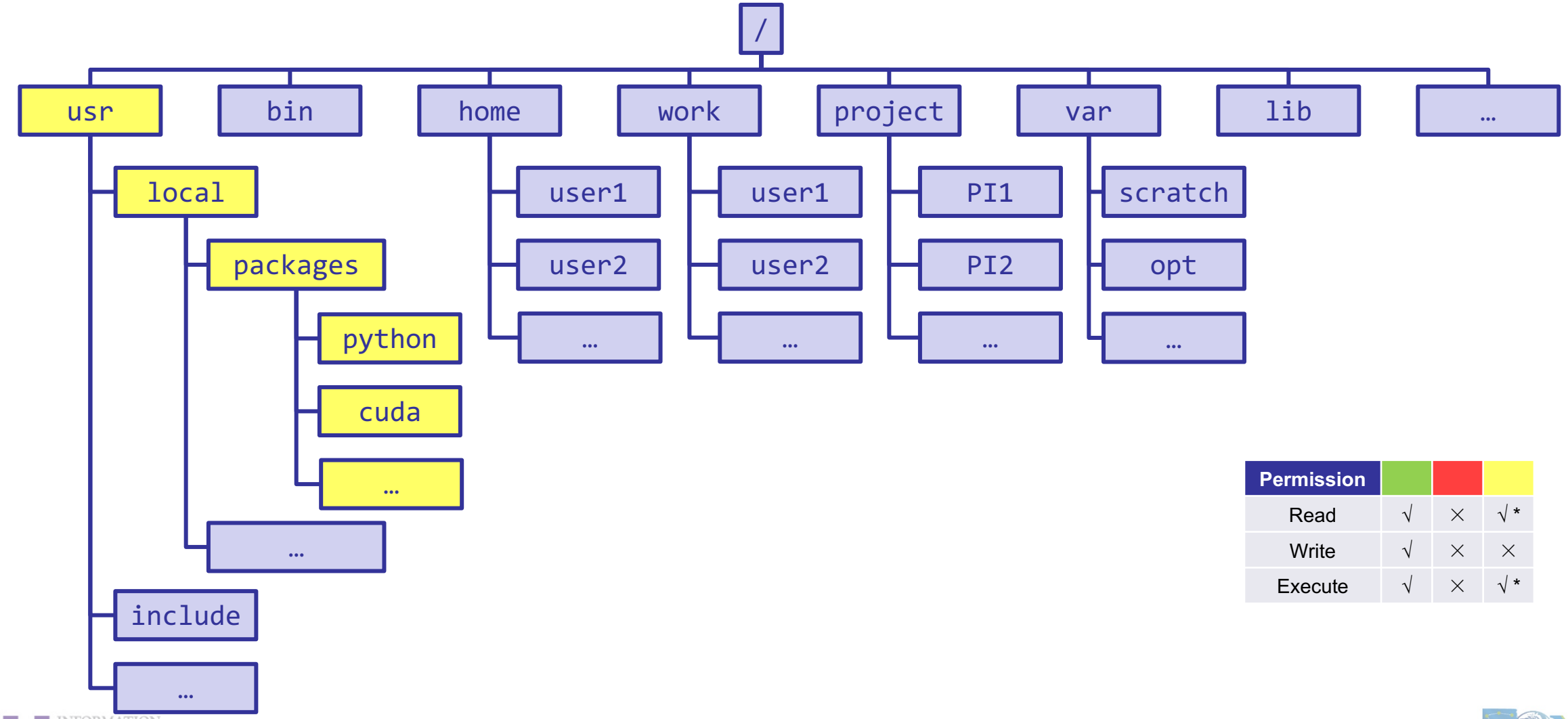
1) Preinstalled (modules)



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

1) Preinstalled (modules)



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

1) Preinstalled (modules)

- **Modules**
  - Software that 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 …

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**

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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

- **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**
   2) File system → **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
```

References

- 1. https://www.4freephotos.com/CPU-schematic-6037.html
- 2. https://en.wikipedia.org/wiki/Apple_A16#/media/File:Apple_A16.jpg
- 2. https://www.cpu-monkey.com/en/cpu-apple_a16_bionic