# HPC User Environment 1

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HPC User Services

LSU HPC / LONI

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Louisiana State University

Baton Rouge

January 31, 2024

- **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

**LSU**

- **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
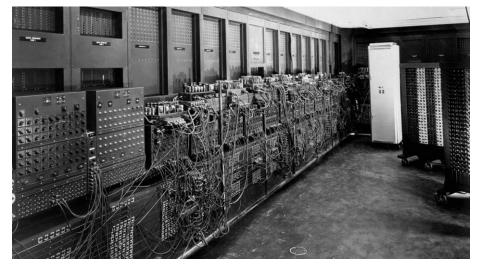
LSU INFORMATION TECHNOLOGY SERVICES

# Outline

**LSU**

- **HPC User Environment 1**

ENIAC, 1945

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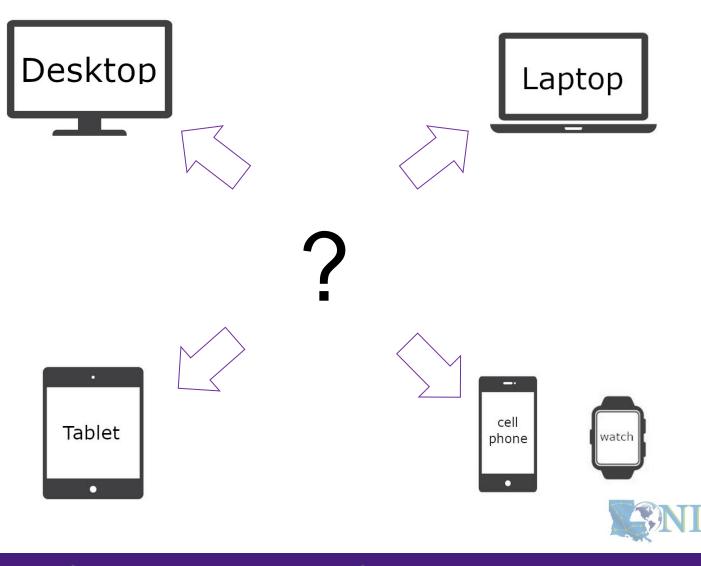
Desktop

Laptop

?

Tablet

cell phone

watch

ENIAC, 1945

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



Desktop
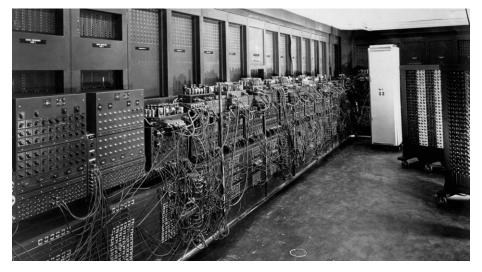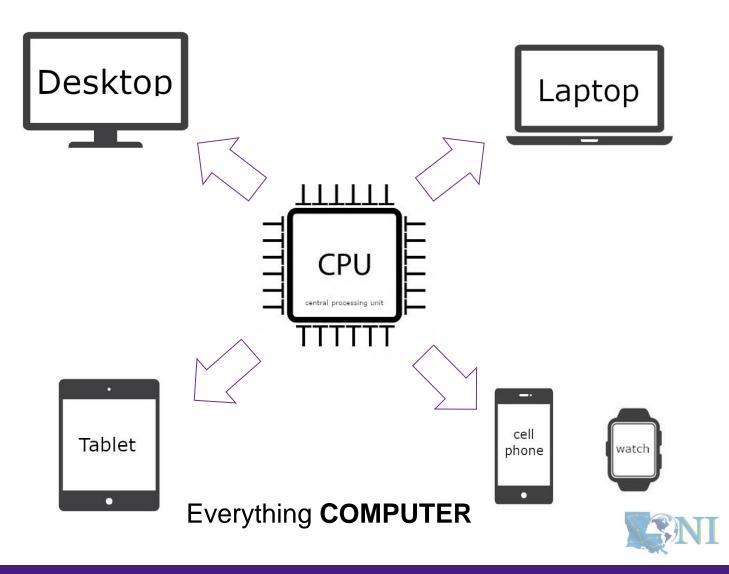
Laptop

CPU
central processing unit

Tablet

cell phone

watch

Everything **COMPUTER**

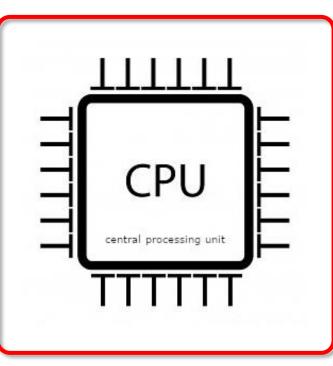# Moor's law – double transistors every two years

**Transistor size – atom size**

## Clock speed? –
**cycles per second**
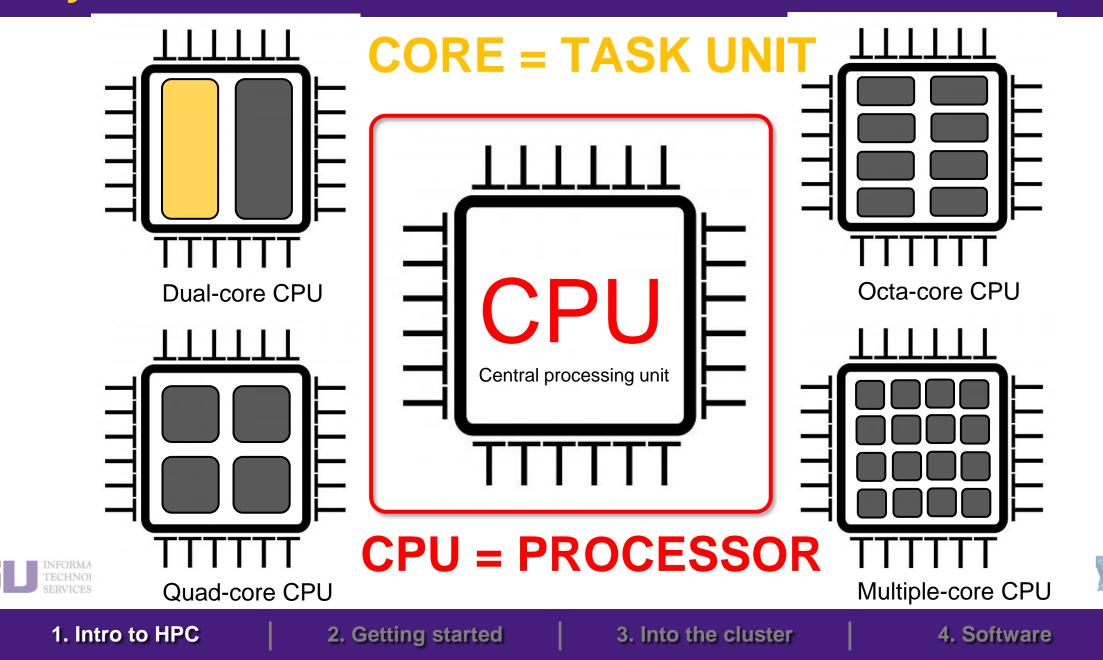
Intel® Core™ i7-1065G7 Processor
8M Cache, up to 3.90 GHz
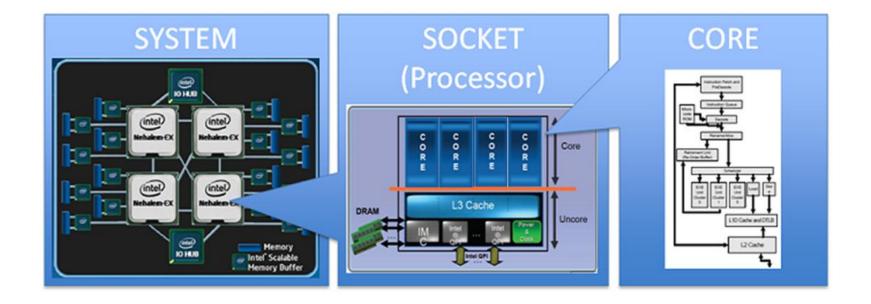
**Parallel computing**

**CORE = TASK UNIT**

Dual-core CPU

## CPU
Central processing unit

Octa-core CPU

Quad-core CPU

Multiple-core CPU

**CPU = PROCESSOR**

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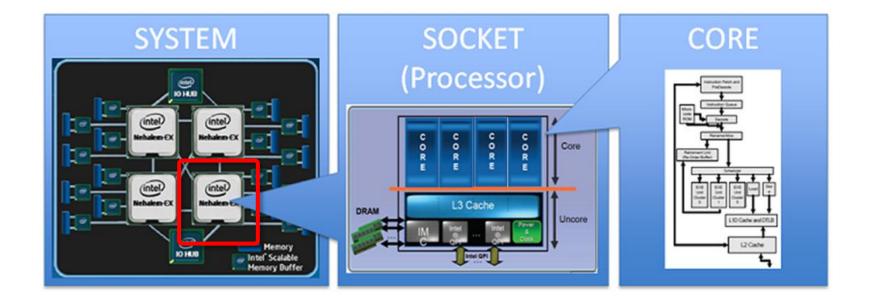
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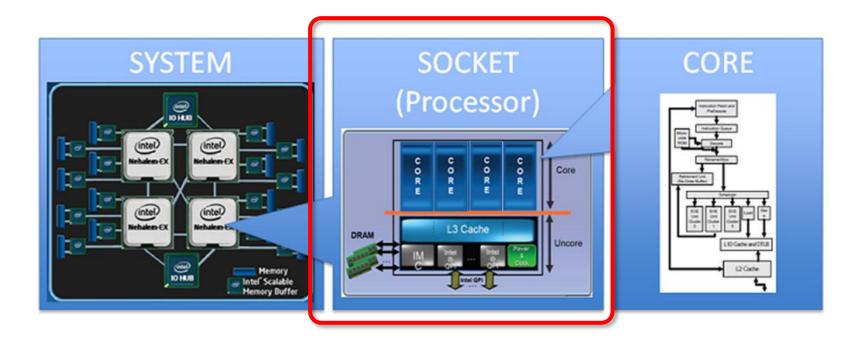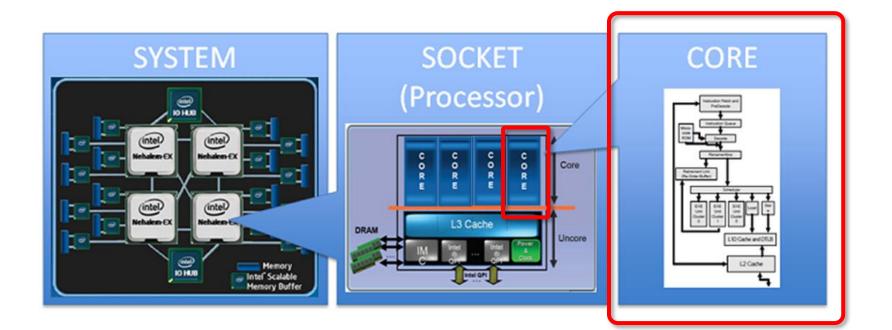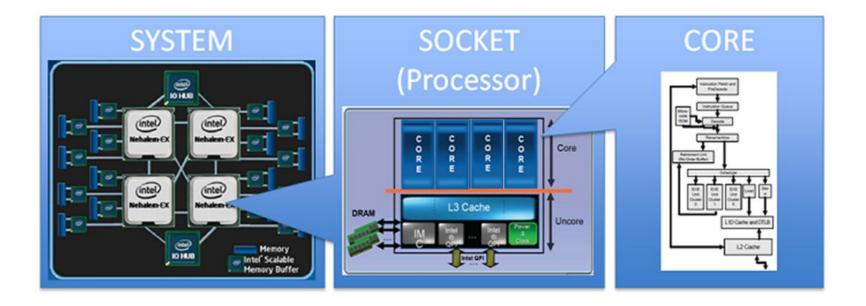
- **How many cores does this computer have?**



**4 cores * 4 processors = 16 total cores**

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**LSU**

- **HPC User Environment 1**

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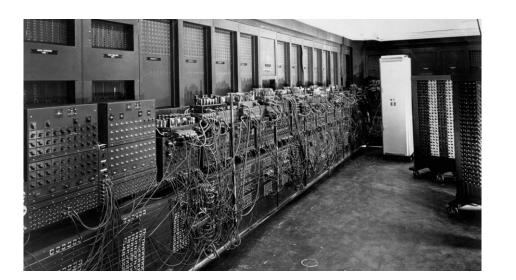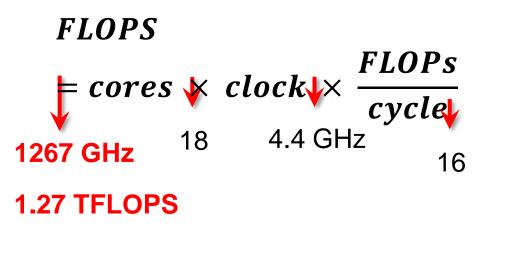
- **Performance is measured in Floating Point Operations Per Second (FLOPS)**

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

**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 | $10^{3}$ |

**ENIAC FLOPS:** **500**

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

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

- **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**

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

**Current (November 2023):**

| Rank | Syste | 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 | 8,699,904 | 1,194.00 | 1,679.82 | 22,703 |
| 2 | **Aurora** - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States | 4,742,808 | 585.34 | 1059.33 | 24,687 |
| 3 | **Eagle** - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Microsoft Azure United States | 1,123,200 | 561.20 | 846.84 | - |

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**TOP 500** SUPERCOMPUTER SITES

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**LONI**

**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<br>Louisiana Optical Network Initiative<br>United States | 23,040 | 1.05 | 1.47 | 500 |

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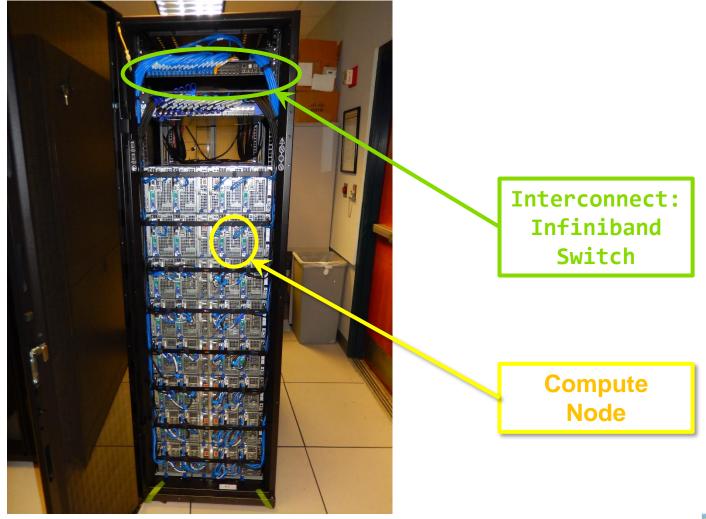
- **Inside a cluster:**

- **Inside a rack:**



**Interconnect: Infiniband Switch**

**Compute Node**

- **Inside a node:**

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

Universities of Louisiana State



LSU HPC

Louisiana State University Campus, Baton Rouge, LA

ACCESS | Advancing Innovation

Universities of the United States

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

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| 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)**

Louisiana State University

Louisiana Tech University

University of New Orleans

Southern University

Tulane University

University of Louisiana at Lafayette

Xavier University of Louisiana

The LONI Institute
www.institute.loni.org

[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/

- **Summary**

|  | LSU HPC | LONI |
|---|---|---|
| **Available to…** | LSU faculty & affiliates | LONI subscribers & affiliates |
| **Clusters** | SuperMIC<br>Deep Bayou<br>SuperMike III | QB2<br>QB3 |

Questions?

# Outline

**LSU**

- **HPC User Environment 1**

**Two things are needed to run jobs on our clusters**

**1) Account**                          **2) Allocation**

# Outline

- **HPC User Environment 1**

# 1) Accounts

| | LSU HPC | LONI |
|---|---|---|
| **Available to…** | LSU faculty & affiliates | LONI subscribers & affiliates |
| **Clusters** | SuperMIC<br>Deep Bayou<br>SuperMike III | QB2<br>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<br>✓ Research staff (postdocs, research associates, …)<br>✓ Students (graduate & undergraduate)<br>✓ Research collaborators (LSU & non-LSU)<br>✓ 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<br>✓ Research staff (postdocs, research associates, …)<br>✓ Students (graduate & undergraduate)<br>✓ Research collaborators (LSU & non-LSU)<br>✓ Other affiliates |
| **Requirements** | • **Institutional email** (*e.g.*, @lsu.edu)<br>• **Account sponsor / PI**<br>   ✓ <u>Full-time faculty & certain research staff @ LSU Baton Rouge campus</u><br>   ✗ Students, postdocs, research associates (even @ LSU)<br>   ✗ Outside collaborators<br>   ✗ 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<br>✓ Research staff (postdocs, research associates, …)<br>✓ Students (graduate & undergraduate)<br>✓ Research collaborators (@ LONI subscribers / outside)<br>✓ Other affiliates |
| **Requirements** | • **Institutional email** (*e.g.*, @uno.edu)<br>• **Account sponsor / PI**<br>  ✓ <u>Full-time faculty & certain research staff @ LONI subscribers</u><br>  ✕ Students, postdocs, research associates (even @ LONI subscribers)<br>  ✕ Outside collaborators<br>  ✕ 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) |

## i. Eligibility (Summary)

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

## i. Eligibility (Summary)

| | LSU HPC | LONI |
|---|---|---|
| **Available to…** | ✓ Faculty of LSU Baton Rouge campus<br>✓ Research staff (postdocs, research associates, …)<br>✓ Students (graduate & undergraduate)<br>✓ Research collaborators (LSU & non-LSU)<br>✓ Other affiliates | ✓ Faculty of LONI subscribers<br>✓ Research staff (postdocs, research associates, …)<br>✓ Students (graduate & undergraduate)<br>✓ Research collaborators<br>✓ Other affiliates |
| **Requirements** | • In...  edu)<br>• A...<br><br>✗ Students, postdocs, research associates (even @ LSU)<br>✗ Outside collaborators<br>✗ HPC staff | ...research staff @<br><br>✗ Students, postdocs, research associates (even @ LONI subscribers)<br>✗ Outside collaborators<br>✗ HPC staff |

**NOTE: The account username should not contain the COMMON words. It may contain part of your names.**

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

## 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** |
| | | |

## 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<br><br>b) Check email and open the link (valid for 24 hrs)<br><br>c) Fill the form (In **Contact/Collaborator**, enter your **account sponsor**'s full name) and submit<br><br>d) You **will receive a notification** when your account is activated once we have verified your credentials<br><br>   • Be patient. Do not reset your password if you cannot log in yet. | |

[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 |
| | | |

[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, …<br><br>• Change **default shell** (bash / tcsh / ksh / csh / sh)<br><br>• Request / manage / check allocation<br><br>• Request / manage / check storage<br><br>• … | |

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

**LSU**

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<br><br>b) Check email and open the link (valid for 24 hrs)<br><br>c) Enter your new password and submit<br><br>d) You will receive a confirmation email once your new password is approved by our staff<br><br>**\*\* IMPORTANT \*\***<br>• Your new password is **NOT** available right away (wait until you receive confirmation of approval)<br>• Do **NOT** submit multiple times | |

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

**LSU**

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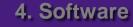
- **User Services:**
  "When you send a password reset request, it has to be manually processed for security reason before your new password becomes available."

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**

**LSU**

**Account sponsor** $\xrightarrow{\text{Sponsor what?}}$ **Allocation**
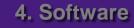
## i. What is allocation?

- 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

**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 / LONI subscribers

LSU INFORMATION TECHNOLOGY SERVICES

LONI

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

## 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<br><br>b) Click on "New Allocation for [Cluster Name]"<br> • SuperMIC & SuperMike III share allocations<br> • QB2 and QB3 share allocations<br> • Deep Bayou has separated allocation<br><br>c) Fill the form and submit<br><br>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… |
|---|---|---|---|---|---|
| | | | | | |
| | | | | | |
| | | | | | |

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<br>Apr 1<br>Jul 1<br>Oct 1 | |

[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<br>Apr 1<br>Jul 1<br>Oct 1 | 2 active / PI |
| **Research** | > 50,000 | > 1 month before decision date | Jan 1<br>Apr 1<br>Jul 1<br>Oct 1 | | **[ LSU HPC ]**<br>3,000,000 SU / allocation<br>5,000,000 SU / PI<br>**[ LONI ]**<br>6,000,000 SU / allocation<br>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 |
| **Research** B | >300,000 and ≤1,000,000 | Required | Required | Required | Optional | 5 |
| **Research** 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

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** |
| | | |

## 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 ]**<br>a)  Log in using your account<br>b)  Click on "Join allocation"<br>c)  Search for your account sponsor / PI, and click "Join Projects"<br>d)  Find the desired allocation you wish to join, click "Join"<br>e)  Your account sponsor / PI will receive an email notification and approve your request<br><br>**[ Method 2: Ask your PI to add you ]**<br>a)  Ask your PI to log in using his/her account<br>b)  Click on "Manage memberships"<br>c)  Find the desired allocation, click "Edit -> Add a User"<br>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"
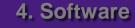
- **Test**

❖ **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

- **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

- 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!

**LSU**
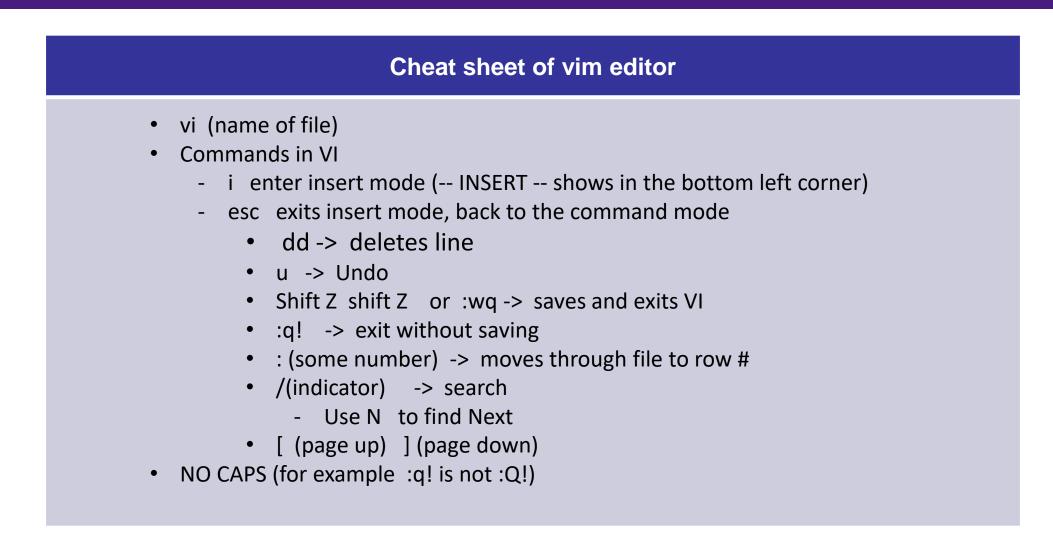
| Cheat sheet of Commands in Linux | |
|---|---|
| history | Command history |
| mkdir | Make a folder |
| ls | List a folder<br>    -a    List all files including hidden<br>    -l    Shows files with a long listing format |
| cd | Change directory |
| pwd | Show current directory |
| cp | Copy |
| rm | 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!

**LSU**

## 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**

## i. General architecture

| Term | Definition |
|------|------------|
|      |            |
|      |            |
|      |            |
|      |            |

i. **General architecture**

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

## 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*) |
| | |
| | |

**LSU**

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)* |
|  |  |

## 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. |

## 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**

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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 |
|  |  |
|  |  |

ii.   Logging in

## Secure Shell (SSH)

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

## ii. Logging in

### Secure Shell (SSH)

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

* • Only on SMIC and SuperMike 3 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

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## ii. Logging in

### a) Linux / Mac

## ii.   Logging in

b)   Windows

- MobaXterm



[ Method 2 ]
Create a session (and remember)

[ Method 1 ]
Start a local terminal and ssh (like Linux terminal)

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)

**LSU**

## 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 (e.g., Ubuntu) | ssh **–X** username@server.address |
| | |
| | |
| | |

**LSU**

## 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) <br> b)  ssh **–X** username@server.address |
|  |  |
|  |  |

# 1) Getting connected

**LSU**

## ii. Logging in

❖ Special note: **X11 forwarding**
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| Windows | |

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## 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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| Windows | **MobaXterm** | **Enabled by default**<br>(can be disabled in "Advanced SSH Settings") |
| | | |

## ii. Logging in

❖ Special note: **X11 forwarding**
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| You are using… | | To enable X11 forwarding… |
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| Linux (e.g., Ubuntu) | | ssh **–X** username@server.address |
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| Windows | **MobaXterm** | **Enabled by default**<br>(can be disabled in "Advanced SSH Settings") |
| Windows | Putty | a) Install X server (*e.g.* Xming)<br>b) Connection → SSH → X11 → Enable X11 forwarding |

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## 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<br>        -a    List all files including hidden<br>        -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 |

- **HPC User Environment 1**

# 2) File system

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

| Permission | | | |
|---|---|---|---|
| Read | √ | ✕ | √* |
| Write | √ | ✕ | ✕ |
| Execute | √ | ✕ | √* |

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

| Permission | | | |
|---|---|---|---|
| Read | √ | × | √* |
| Write | √ | × | × |
| Execute | √ | × | √* |

| Permission | | | |
|---|---|---|---|
| Read | √ | × | √* |
| Write | √ | × | × |
| Execute | √ | × | √* |

ii. **/work/[username]**
- **Permission**:
  - Your own: √
  - Others: ×
- **Distributed**: √
- **Quota**: Unlimited
- **Lifetime**: 60 day of inactivity
- **Best for**: Job input / output

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.**

**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)

| Permission | | | |
|---|---|---|---|
| Read | √ | ✗ | √* |
| Write | √ | ✗ | ✗ |
| Execute | √ | ✗ | √* |

## File system summary

| Directory (folder) | Distributed | Throughput | Lifetime | Quota | Best for |
|---|---|---|---|---|---|
| **/home/[username]** | √ | Low | Unlimited | 5GB (QB2)<br>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.<br>**NOT for archive!** |
| **/var/scratch** | × | High | End of job | Subject to node specs | (Most users do not need it.<br>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)<br><br>• Syntax:<br>   - `scp <options> <source> <destination>`<br>   - `rsync <options> <source> <destination>` |
| wget | From a download link on a website (usually opened with a web browser)<br><br>• Syntax:<br>   - `wget <link>` |

- **File transfer**

- **HPC User Environment 1**

- **HPC User Environment 1**

| Permission | | | |
|---|---|---|---|
| Read | √ | × | √* |
| Write | √ | × | × |
| Execute | √ | × | √* |

- **Modules**
    - Software that <span style="color:red">can be loaded / unloaded</span> on demand.
    - List of modules <span style="color:red">preinstalled system-wide</span>: 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**

- **HPC User Environment 1**

| You can't… | You can… |
|------------|----------|
|            |          |

# 2) User installation
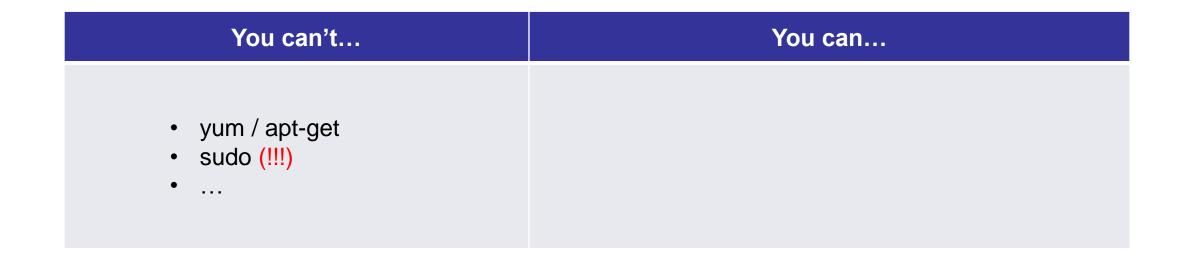
| You can't… | You can… |
|:---:|:---:|
| • yum / apt-get<br>• sudo (!!!)<br>• … | |

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

[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)

- **Two types of software packages:**

  - Preinstalled (modules)
  - User installed

- **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**

- **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

- **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

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