2025 LONI
Scientific Computing Bootcamp

Overview

HPC User Services

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LONI HPC

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June 2 - 4 and June 9 - 11, 2025

Outline

Why Scientific Computing?

Why Parallel?

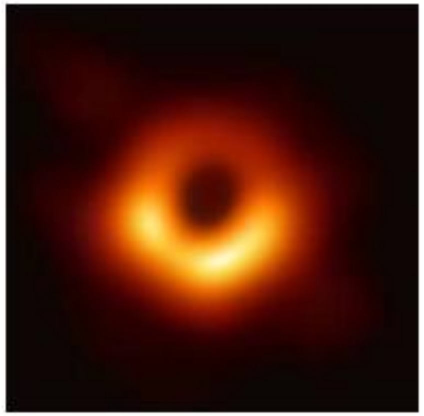
Getting Started with Scientific and Parallel Computing - How to

Introduction to Scientific and Parallel Computing

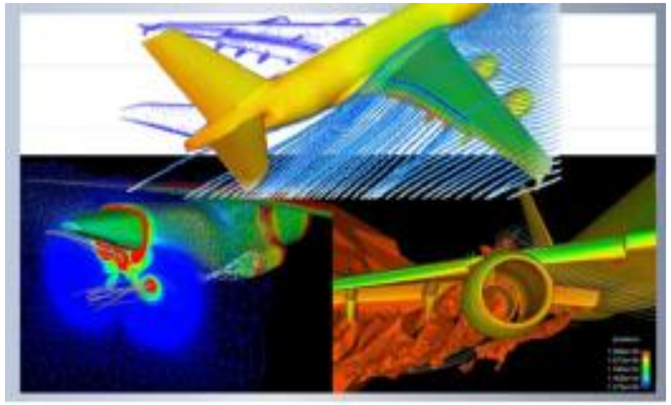
Why Scientific Computing?

Why Scientific Computing?

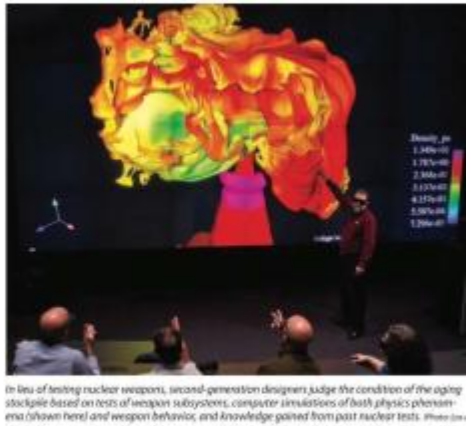
- **Scientific Computing is nowadays:**
  - The “third pillar of science”, in addition to theoretical analysis and experiments for scientific discovery.
- **Sometimes other means are:**
  - Impossible
  - Costly (time, labor and money)
  - Dangerous or undesirable



Astrophysics



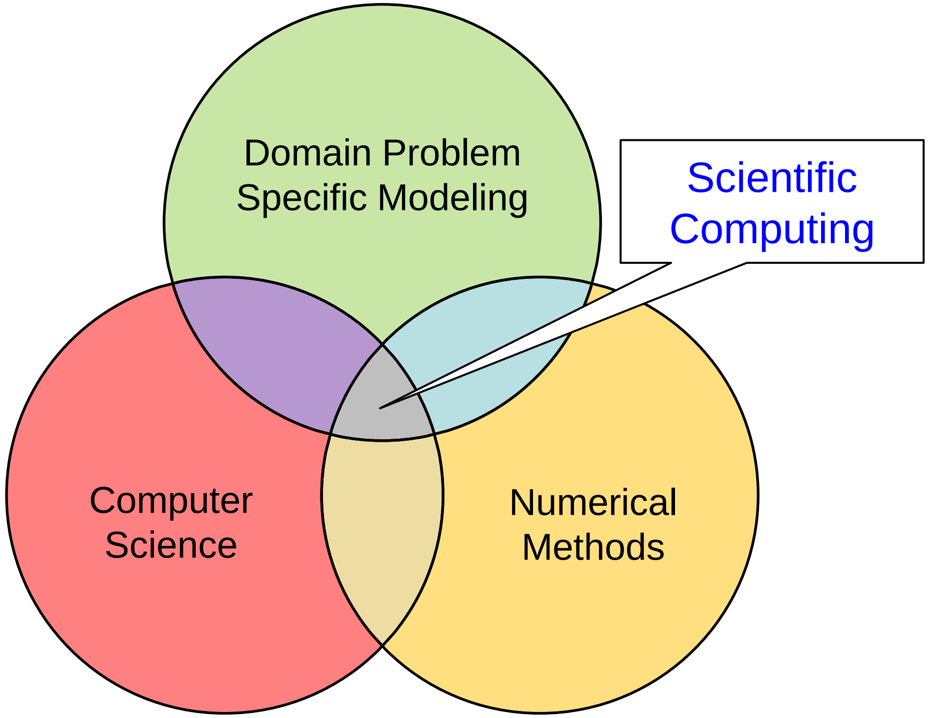
Aircraft design



Nuclear weapon tests

What is Scientific Computing?

- ***"Scientific Computing is the collection of tools, techniques, and theories required to solve on a computer mathematical models of problems in Science and Engineering." –*** *(Golub & Ortega 1992)*
- **It is a rapidly growing multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems.**



Abacus, 2nd century BC

Calculating-Table by Gregor Reisch: Margarita Philosophica, 1503.

How to Conduct Scientific Computing?

- **Scientific theory and algorithm**
  - From your own study/research background
- **Software**
  - General purpose
    - Excel
    - Matlab
    - **Python/R**/Perl/C/Fortran, etc.
  - Dedicated software, such as:
    - Ansys (CFD, Structural/Solid Mechanics/Electronics)
    - Lammps/Gromacs/NAMD/Amber (Molecular Dynamics)
  - Most cases, we need both
- **Hardware**
  - Your laptop/desktop/lab server
  - Cloud Computing
  - Supercomputers
    - HPC

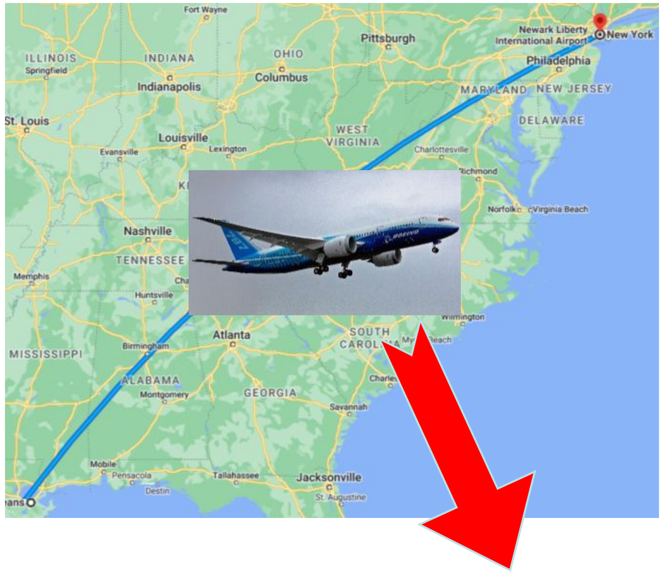
LONI QB3/4 cluster

Introduction to Scientific and Parallel Computing

Why Parallel?

Introductory Problem

- Fly from New Orleans, LA to New York, NY



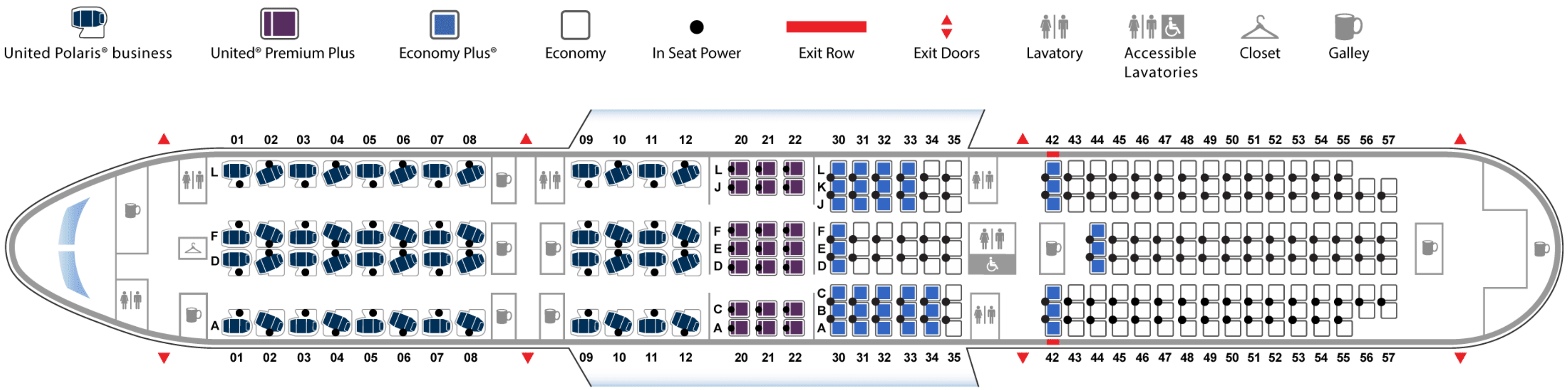
1 (one)
Boeing 787

Distance=1182 miles
Velocity =~600 mph
Time = ~2 hours

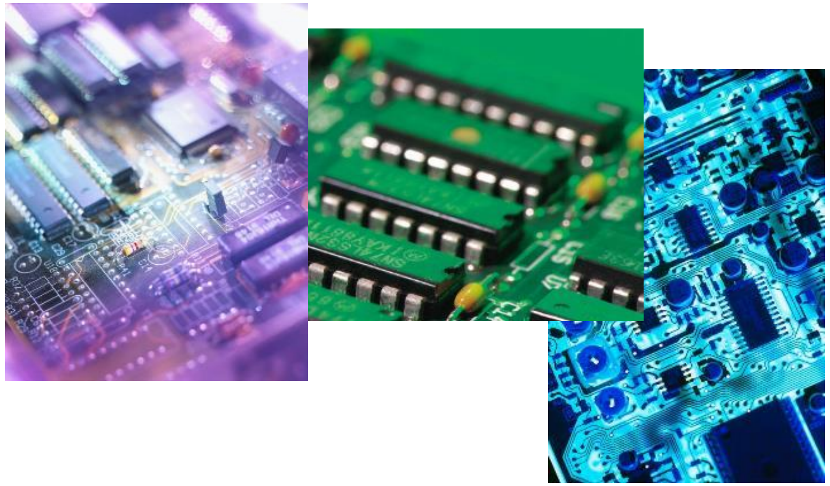
2 (two)
Boeing 787
???

Considering number of seats?

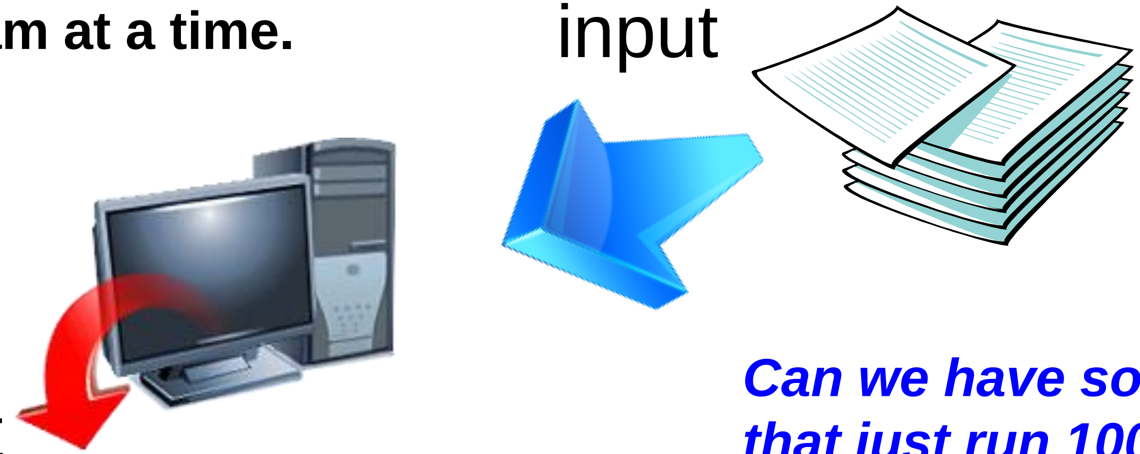
- 787-8 Dreamliner has 248 seats



Some background

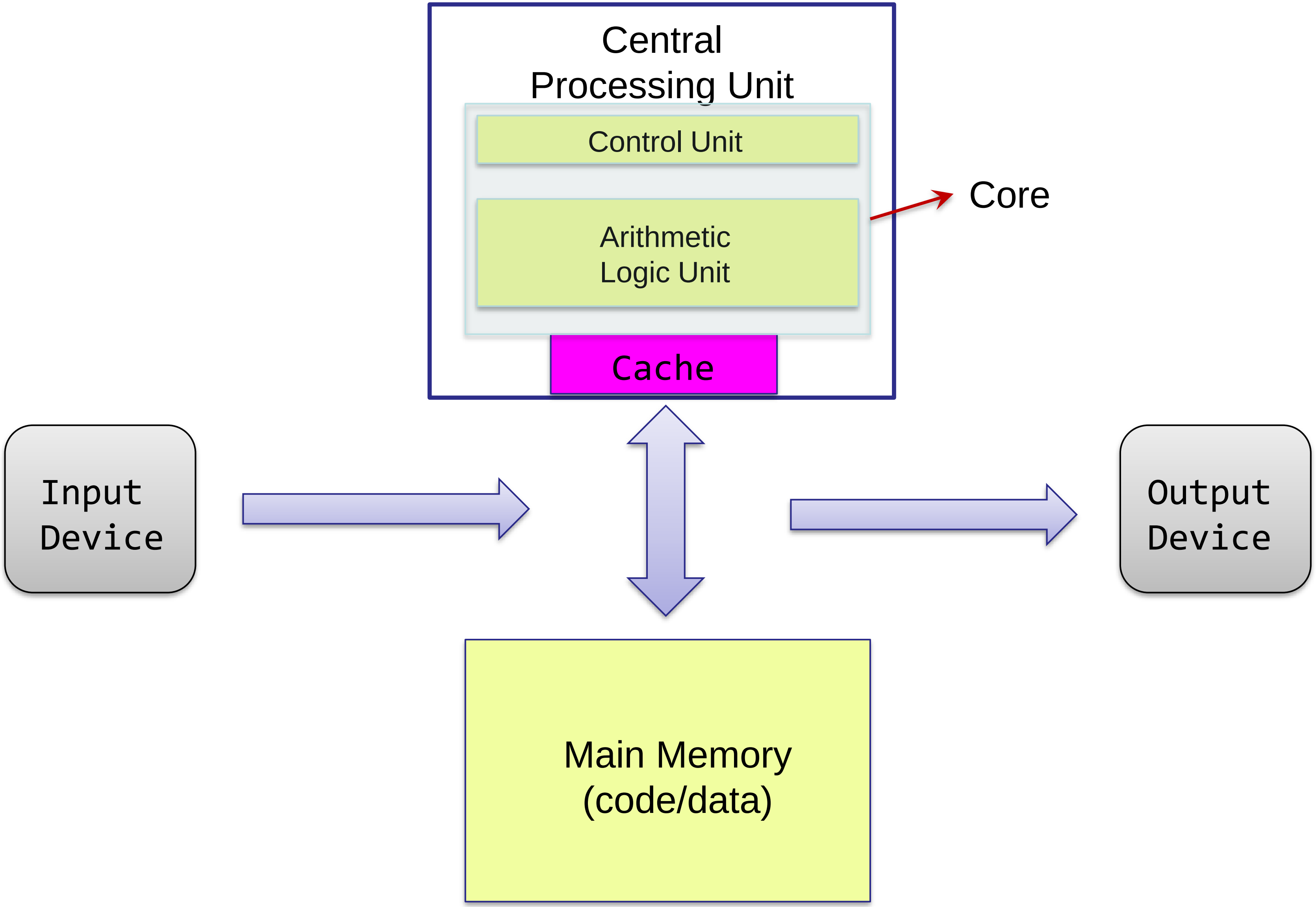


Computer runs one program at a time.



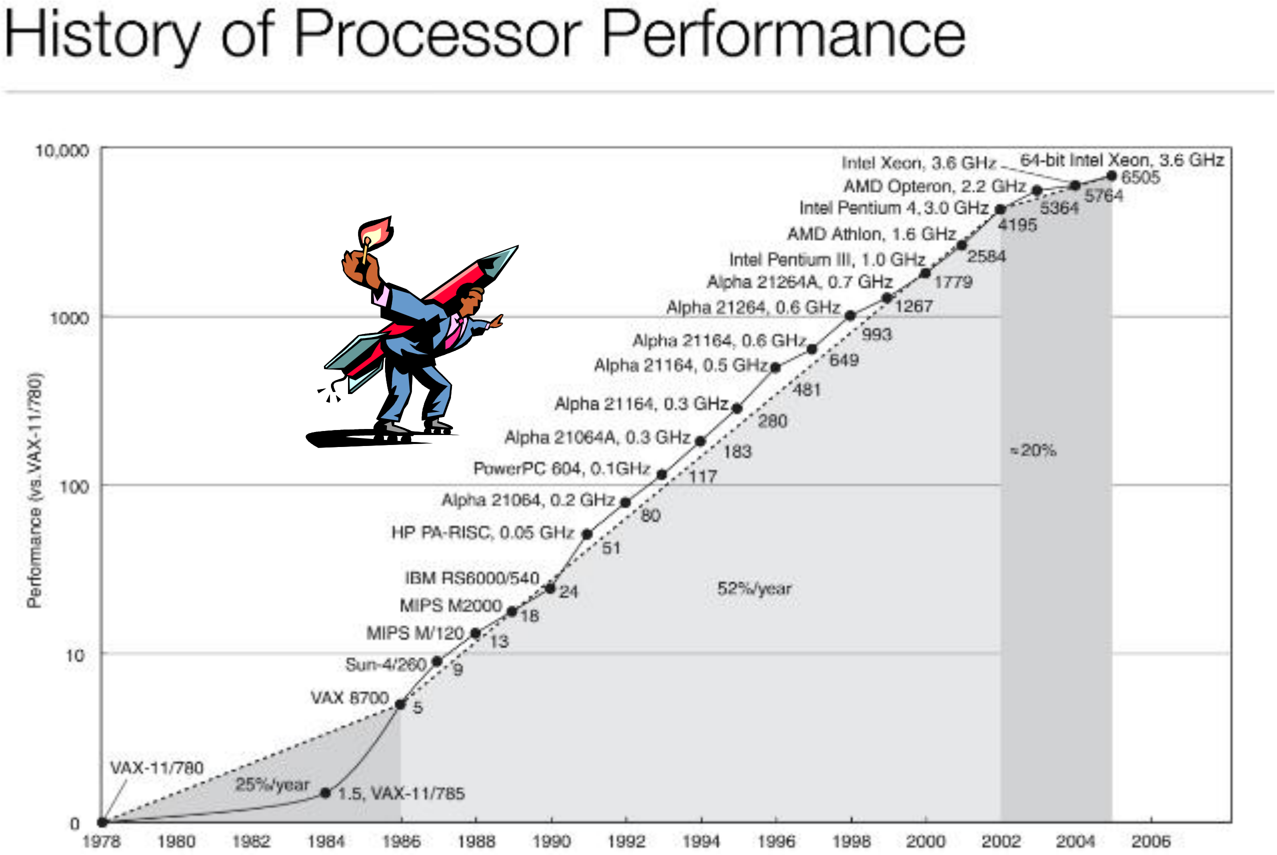
Can we have something that just run 100x faster?

The von Neumann Architecture



Changing Times

- From 1986 - 2002, microprocessors were speeding like a rocket, increasing in performance an average of 50% per year.
- Since then, it's dropped to about 20% increase per year.



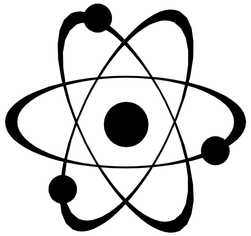
Limitation:

2 GHz Consumer
4 GHz Server

Source:
http://www.cs.columbia.edu/~sedwards/classes/2012/3827-spring/

A Little Physics Problem

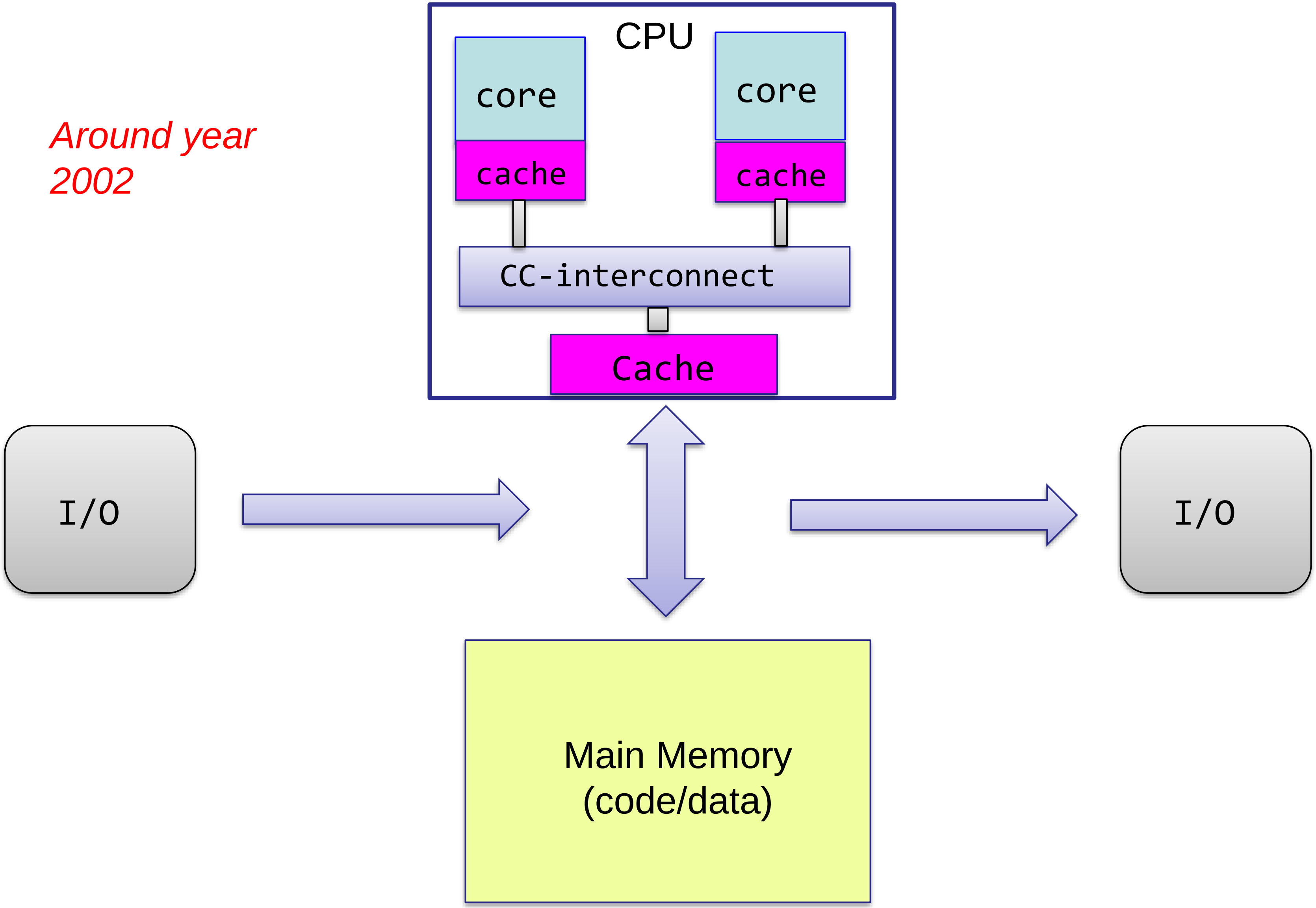
- **Smaller transistors = faster processors.**
- **Faster processors = increased power consumption.**
- **Increased power consumption = increased heat.**
- **Increased heat = unreliable processors.**



- **Solution:**
  - Move away from single-core systems to multicore processors.
  - “core” = central processing unit (CPU)
  - Introducing parallelism
    - ***What if your problem is also not CPU dominant?***

The von Neumann Architecture

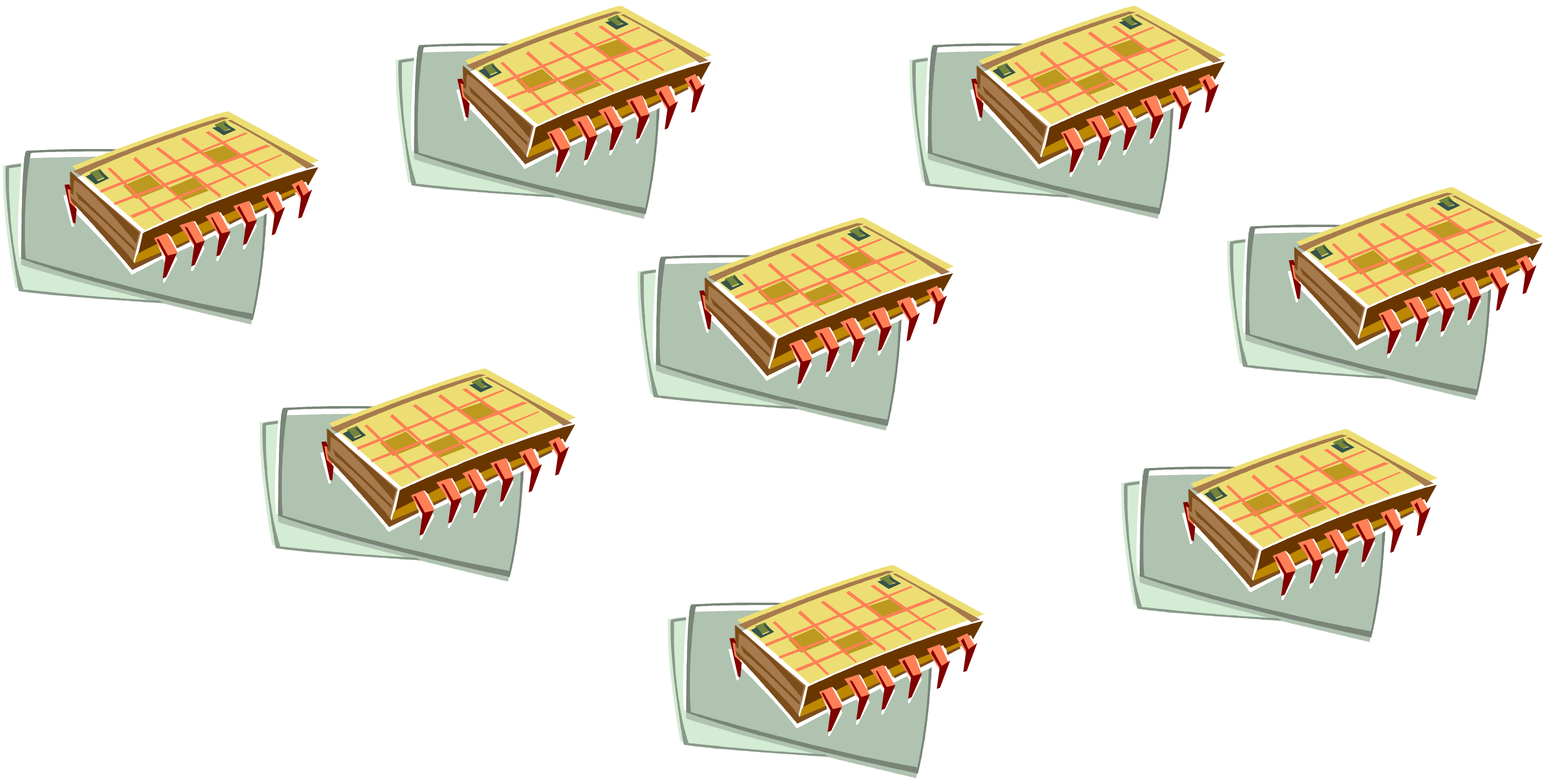
Around year 2002



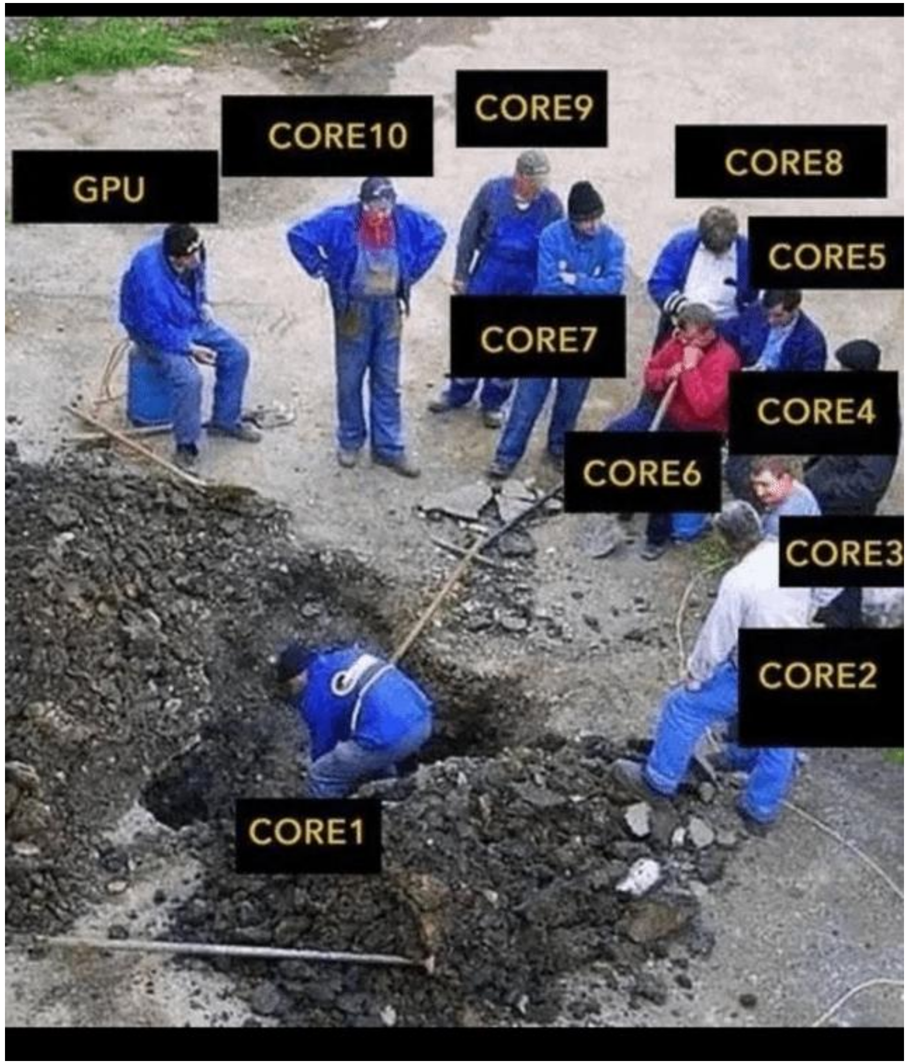
LSU INFORMATION TECHNOLOGY SERVICES

An intelligent solution

- Instead of designing and building faster microprocessors, put multiple processors on a single integrated circuit.

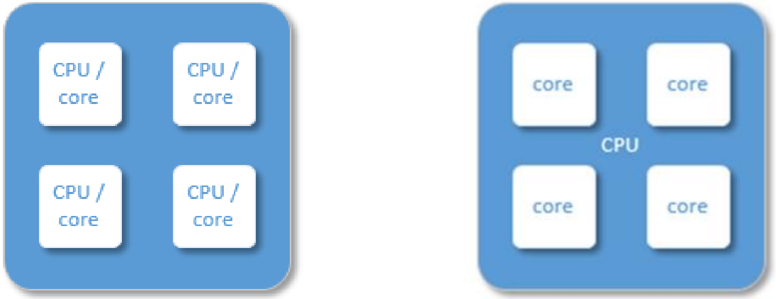


Scenario to Avoid



Core, CPU, Processor?

- A core is usually the basic computation unit.
- A CPU may have one or more cores to perform tasks at a given time.



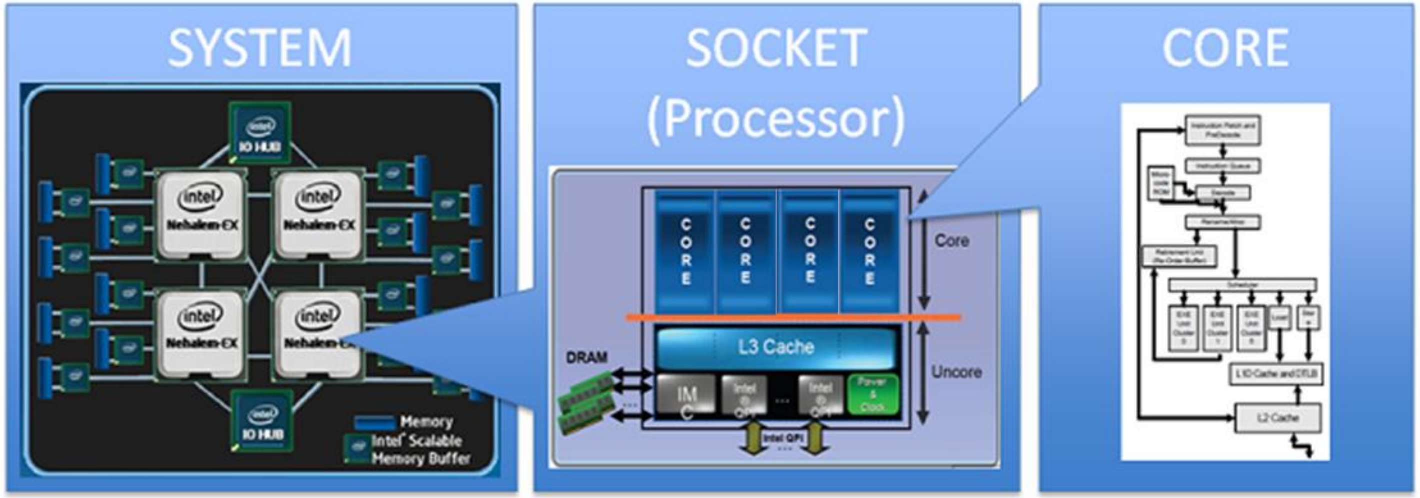
"CPU" referring to each core

"CPU" referring to entire processor

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

Case study – core and processor

- How many cores does this computer have?



- 4 cores * 4 processors = 16 total cores

Concluding Remarks

- **The laws of physics have brought us to the multi-core era.**
- **Serial programs typically don't benefit from the multi-core architecture.**
- **To get speedup, your code needs to be able to make use of multiple cores.**

What is HPC

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

600 mph **60 mph**

- **How do we evaluate the performance of HPC?**

Measure HPC performance-FLOPS

- **Performance is measured in *Floating Point Operations Per Second* (FLOPS or flop/s)**
- $FLOPS = cores \times clock \times \frac{FLOPs}{cycle}$
  - Most processors today can do 4 FLOPs per clock cycle. Therefore a single-core 2.5-GHz processor has a theoretical performance of 10 billion FLOPs = 10 GFLOPs
  - Dual core, quad core? (Intel i3, i5, i7)

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}

- **Question:**
  - A 4-core 2.5GHz desktop, each core can do 16 floating point operations per cycle
  - What is the FLOPs of my desktop?
  - Answer=4x2.5x16=160 GFlops

Supercomputing on a Cell Phone?

- **Hex-core processors are coming to your phone**
  - Nvidia, TI, QualComm…
  - Processing power in the neighborhood of 50 GigaFLOPS
  - Would make the top 500 supercomputer list 20 years ago
  - What is your phone's FLOPS?
    - According to Apple, that iPhone 13 pro's A15 Bionic chip is capable of 15.8 trillion operations per second (TFLOPS).
    - Compare to ENIAC (500 FLOPS)
    - Compare to top 500 in June 2001

      #1 (12.3 TFLOPS)

Computer performance

Name	FLOPS
yottaFLOPS	10^{24}
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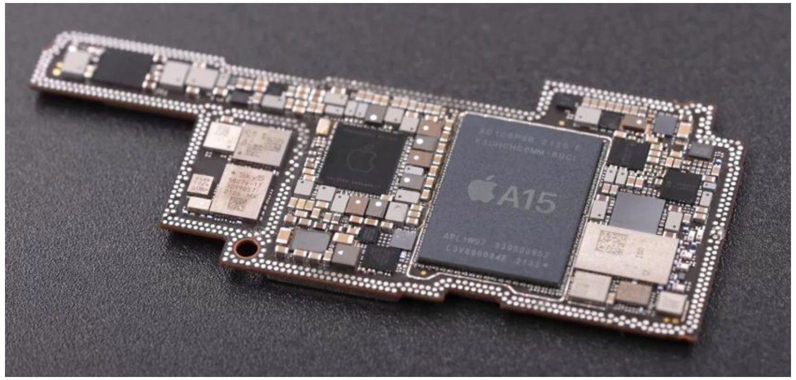


The Top 500 List

- The TOP500 project provides a list of 500 fastest super-computers in the world ranked by their LINPACK performance.
- Semi-annually published (in the public domain)
- November, 2024 list

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**El Capitan** - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States	11,039,616	1,742.00	2,746.38	29,581
2	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE Cray OS, HPE DOE/SC/Oak Ridge National Laboratory United States	9,066,176	1,353.00	2,055.72	24,607
3	**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	9,264,128	1,012.00	1,980.01	38,698

Introduction to Scientific and Parallel Computing

LONI HPC Resources

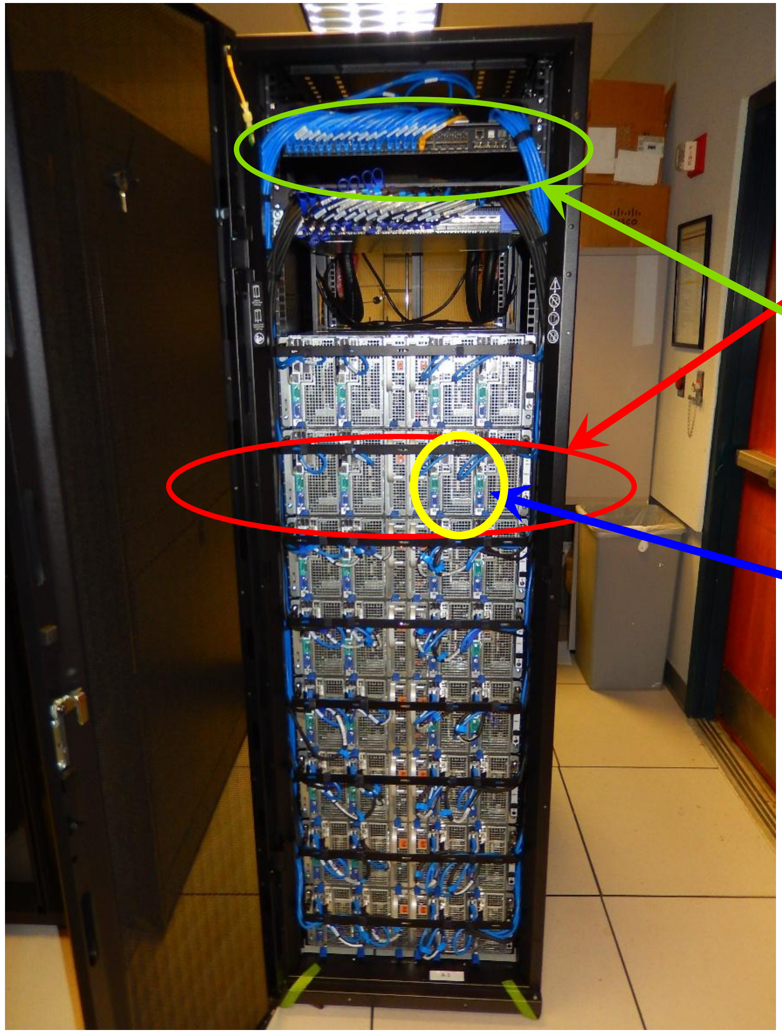
Our HPC

ii. **State level HPC Resource: 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**

Supercomputer Cluster Racks

Inside A Cluster Rack

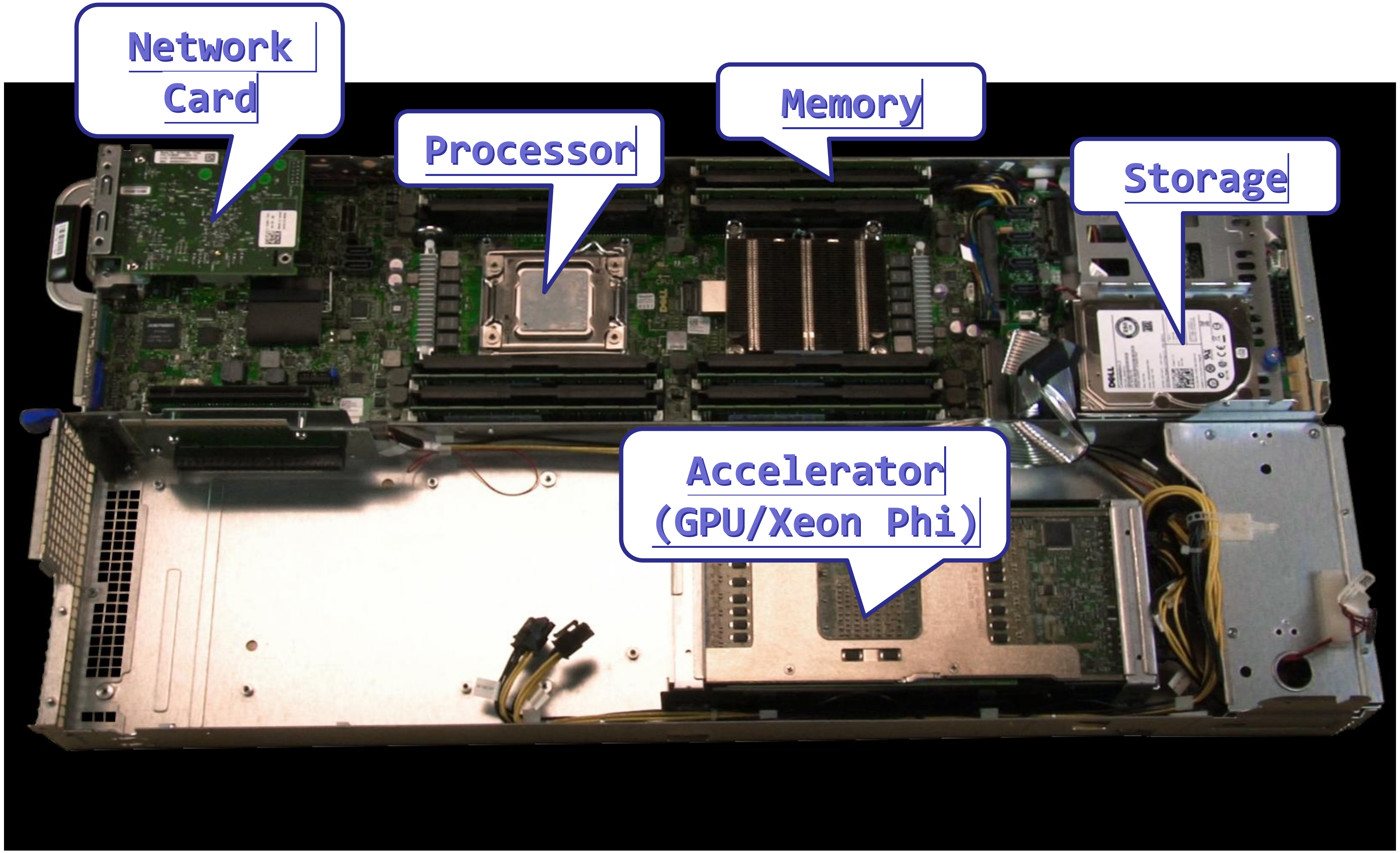


Rack

Interconnect: Infiniband Switch

Compute Node

Inside A Compute Node



Available LONI HPC Resources

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
Online June 15, 2020	

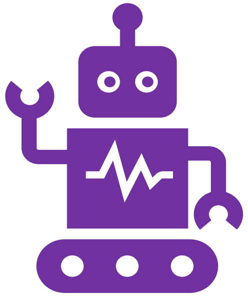
QB4	
Hostname	qbd.loni.org
Peak Performance/TFlops	4,300
Compute nodes	547
Processor/node	2 32-Core
Processor Speed	2.6GHz
Processor Type	Intel Ice Lake Xeon 64bit
Nodes with Accelerators	62
Accelerator Type	NVIDIA Ampere A100
OS	RHEL v8
Vendor	Dell
Memory per node	256/512/2048 GB
Location	Information Systems Building, Baton Rouge
Online Summer, 2024	

Ref: http://hpc.loni.org/resources/hpc/index.php

Our *Free* Service for LSU and LONI Researchers

User support on LONI/LSU HPC resources

Research computing training classes



Application support
Trouble shooting

Grant proposal support

Our Goals

- Provide reliable HPC computing resources.
- Provide a high level of expertise, technical support and knowledge domain consulting and training in order to enable better leverage of computing resources.
- Provide both existing and emerging HPC solutions that enable them to expand their research opportunities and capabilities.
- Respond to researchers’ changing software requirements.

Usual Way of Getting Started

- **Understand the basic usage of popular scientific computing programming tools**
  - **Python**
- **One application of the programming tools**
  - **Deep Learning**

Introduction to Scientific and Parallel Computing

Bootcamp Logistics

Agenda

- **Day 1**
  - Introduction to Python
- **Day 2**
  - Intermediate Python
- **Day 3**
  - Getting Started with MATLAB: From Python to AI Integration
- **Day 4**
  - Exploring Deep Neural Networks: A Beginner's Guide
- **Day 5**
  - NVidia Deep Learning Institute: Fundamentals of Deep Learning
- **Day 6**
  - Introduction to Large Language Models (LLMs)

- **Our source code repository:**
  - https://github.com/lsuhpchelp/loniscworkshop2025
  - Computing Environment - **Google Colab**
    - **See** https://colab.research.google.com/notebooks

Lectures and Hands-on sessions

- **Morning sessions 9am-12noon**
  - **Lecture**

- **Afternoon sessions 1pm-4pm**
  - **Lecture/Exercise**

- **Although recordings will be available, we strongly recommend you try to follow the live session.**

- **Lunch:**
  - **12 noon**

Google Colaboratory

- **Colaboratory, or "Colab" for short, allows you to write and execute Python (or R) in your browser, with**
  - Zero configuration required
  - Free access to GPUs
  - Easy sharing

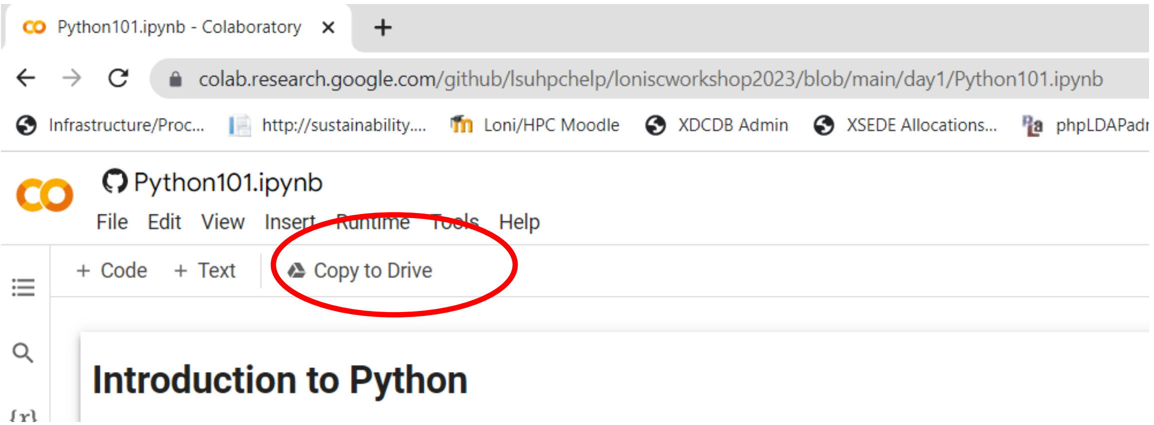
- **Allows you to focus on learning the Python (or R) language itself instead of working on installing and configuring a programming environment.**

  - Ref: https://colab.research.google.com/notebooks/intro.ipynb

Open Colab Notebook from Github

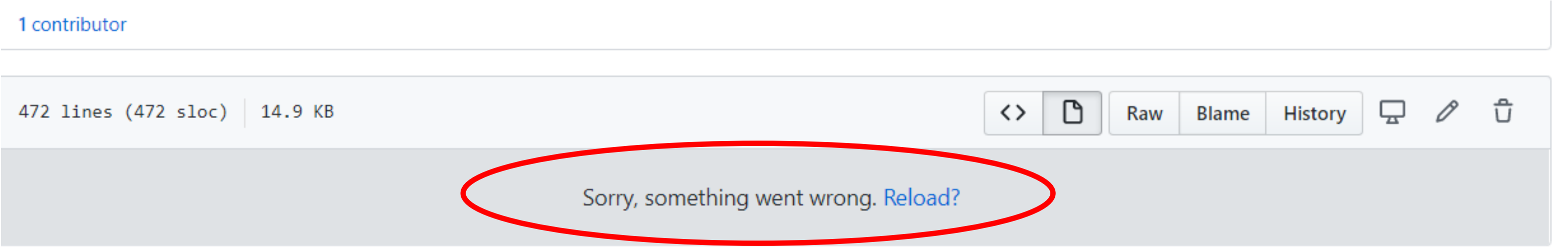
- **Open the below link:**
  - https://github.com/lsuhpchelp/loniscworkshop2025/blob/main/day1/Python101.ipynb
  - Or navigate yourself in the github repo:
    - https://github.com/lsuhpchelp/loniscworkshop2025.git
    - Select "`day1 > Python101.ipynb`"
- **Click the “Open in Colab” link:**

- **After the Colab notebook is laid out, you need one more step, save the Colab notebook to your google drive by “COPY TO DRIVE”, or you will be editing the notebook in “Playground” (read only) mode:**

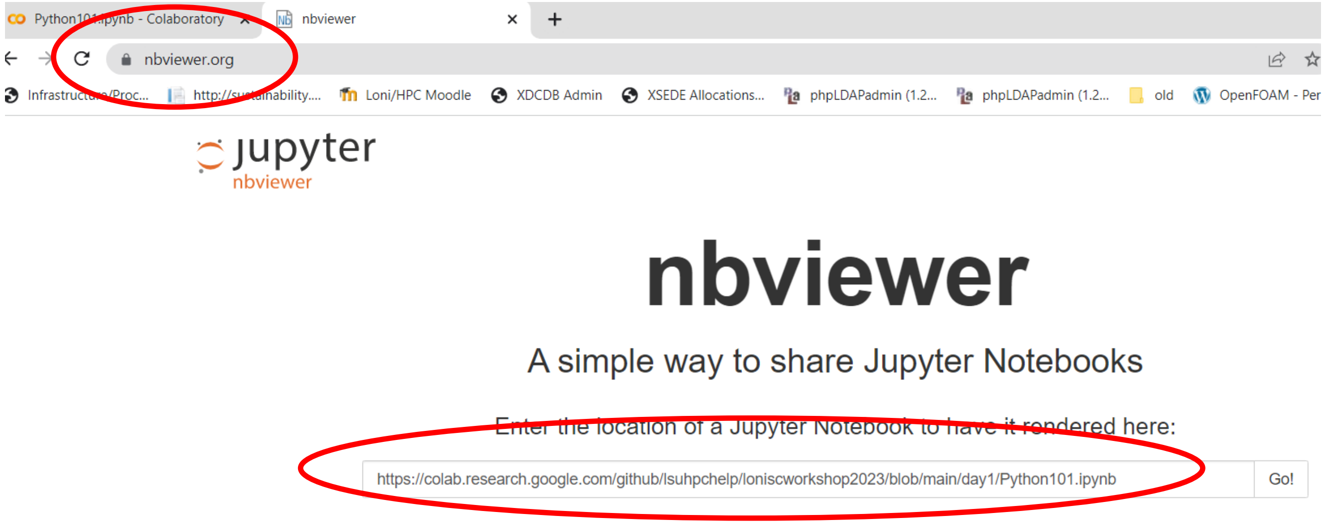


Possible Bug of Github (Rarely seen recently)

- **In case of the “Something went wrong, try again later?”**

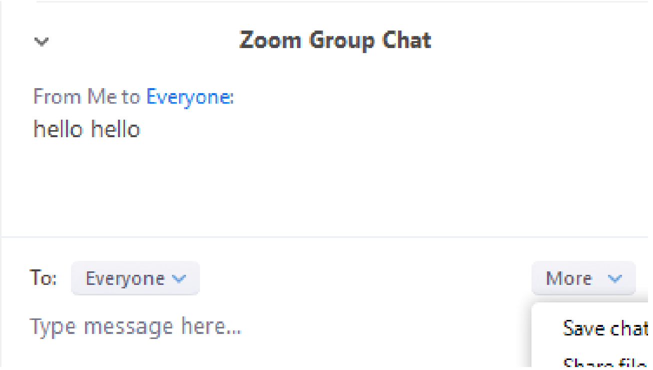


- **Copy and paste the github link from the browser URL box (https://github.com/lsuhpchelp/loniscworkshop2025/blob/main/day1/Python101.ipynb) into the below the location to have it rendered: https://nbviewer.jupyter.org/**



Questions?

- ✓ Type your question in the Zoom chat window. (Preferred)



- ✓ Raise your hand if you do want to ask a question with your microphone, we can unmute you.