Introduction to HPC

CSCI-4850/5850 High-Performance Computing

Spring 2021

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SAINT LOUIS
UNIVERSITY
EST. 1818

Welcome

- Welcome to **High-Performance Computing**

- Tell me about you (to memorize your name/face) quickly!
  - What is your name, major, and year?

Survey (to understand your background)

- Open Canvas, go to Week 1, and complete the “Activity Assignment 1” survey in the class time.

Let us go over the syllabus

- The syllabus could be updated again, so up-to-date syllabus is on Canvas.

Topical Outline

Main topics include basic HPC hardware architectures, parallel programming languages, new trends of HPC, and more. The contents of the course provide a balance of theoretical and practical aspects in parallel computing. A student of this course is expected to develop the right skills to design parallel applications and to effectively use modern HPC platforms.

- Introduction to HPC and parallel programming
- Serial code optimization
- Shared-memory parallel programming with OpenMP
- Distributed-memory parallel programming with MPI
- Python and HPC
- GPU programming with CUDA and OpenACC
- Cloud Computing and HPC

Student Learning Outcomes

At the completion of this course, students will be able to:

- Understand fundamental concepts and new trends in HPC
- Optimize software to take advantage of a processor feature
- Design, implement, and analyze parallel algorithms using OpenMP for shared-memory system
- Design, implement, and analyze parallel algorithms using MPI for distributed-memory system
- Understand the concept and implement GPU programming with CUDA and OpenACC
- Initiate cloud computing project for HPC and parallel programming

Course Textbook and Resources

- No textbook is required, but recommend to have a book
  - Introduction to High Performance Computing for Scientists and Engineers by Georg Hager and Gerhard Wellein, 1st Edition (Chapman & Hall/CRC Computational Science , ISBN-13: 978-1439811924)
- Course website:
  - Canvas will be used to announce schedules, assignments, and lectures.
- Git: How many of you are familiar to Git or GitHub?
  - For further documentation of the use of this system will be announced.

Get into hopper.slu.edu

- Check whether you can log-in our main system, hopper.slu.edu using ssh.
- In Person:
  - Log-in Linux Machine
  - $ ssh YourID@hopper.slu.edu
- Online:
  - Mac user
    - Open a terminal and access by
    - $ ssh YourID@hopper.slu.edu
  - Windows user
    - I recommend you to use a SSH client application such as Bitvise (https://www.bitvise.com/) to log-in the system.

Terminal, Linux, and Shell

- After I hear your background by survey, I will decide what resources will be provided.

Jupyter Notebook

- I strongly recommend you to install Jupyter Lab in your laptop or your desktop.
- https://jupyter.org/
- If you cannot get started, watch the YouTube video “Jupyter Notebook Tutorial: Introduction, Setup, and Walkthrough” (https://www.youtube.com/watch?v=HW29067qVWk)

1. What is the Jupyter Notebook?

In this page briefly introduce the main components of the *Jupyter Notebook* environment. For a more complete overview see References.

Contents

1.1. Notebook document

Notebook documents (or “notebooks”, all lower case) are documents produced by the Jupyter Notebook App, which contain both computer code (e.g. python) and rich text elements (paragraph, equations, figures, links, etc...). Notebook documents are both human-readable documents containing the analysis description and the results (figures, tables, etc..) as well as executable documents which can be run to perform data analysis.

References: Notebook documents in the project homepage and in the official docs.

1.2. Jupyter Notebook App

The *Jupyter Notebook App* is a server-client application that allows editing and running notebook documents via a web browser. The *Jupyter Notebook App* can be executed on a local desktop requiring no internet access (as described in this document) or can be installed on a remote server and accessed through the internet.

Jupyter Lab

jupyterlab.readthedocs.io/en/stable/

JupyterLab

stable

Search docs

GETTING STARTED

- Overview
- Installation
- Starting JupyterLab
- Reporting an issue
- Frequently Asked Questions (FAQ)
- JupyterLab Changelog

USER GUIDE

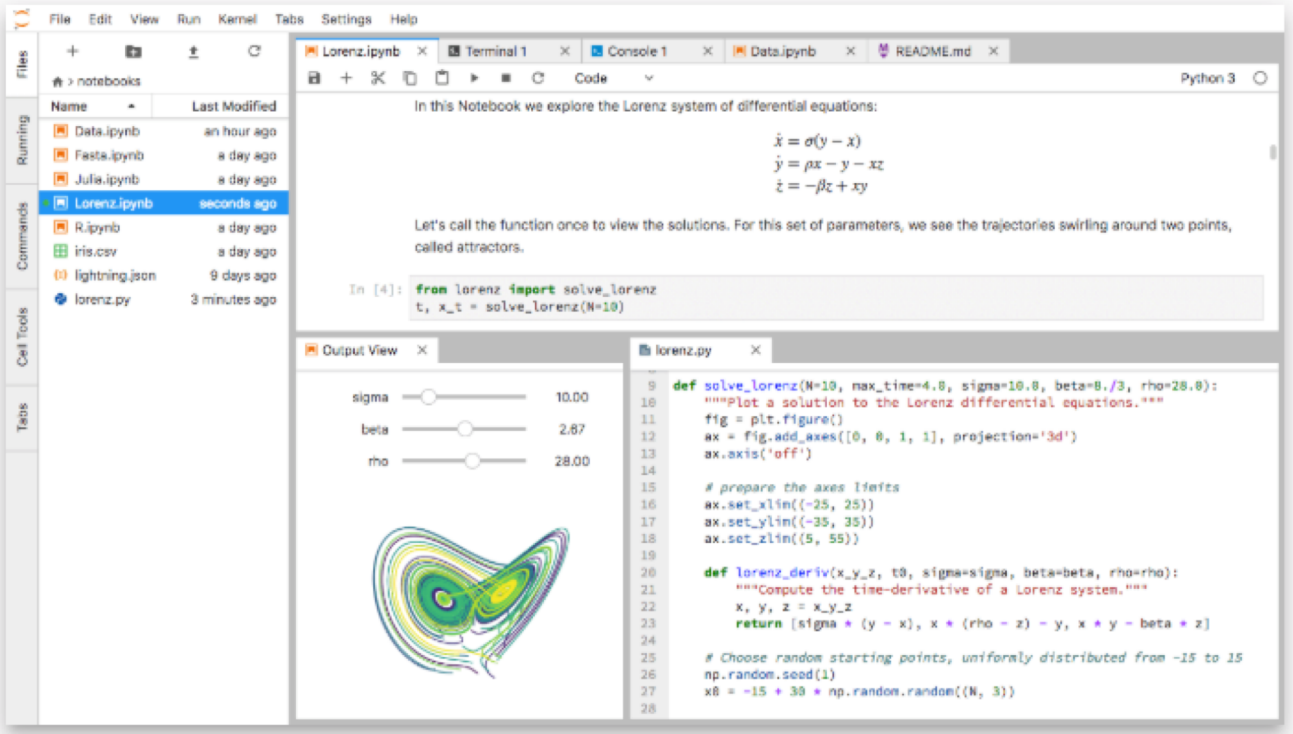
- The JupyterLab Interface
- JupyterLab URLs
- Working with Files
- Text Editor
- Notebooks
- Code Consoles
- Terminals
- Managing Kernels and Terminals
- Command Palette

Docs » JupyterLab Documentation

Jupyter | Edit on GitHub

JupyterLab Documentation

JupyterLab is the next-generation web-based user interface for Project Jupyter. Try it on Binder. JupyterLab follows the Jupyter Community Guides.



Tentative Class Environments

- Terminal, Linux, and Shell Programming
- C++, Python
- https://git.cs.slu.edu/
- https://jupyter.cs.slu.edu/
- Canvas
- Hopper SLU CS machine (hopper.slu.edu)
- APEX SLU cluster (apex.slu.edu)

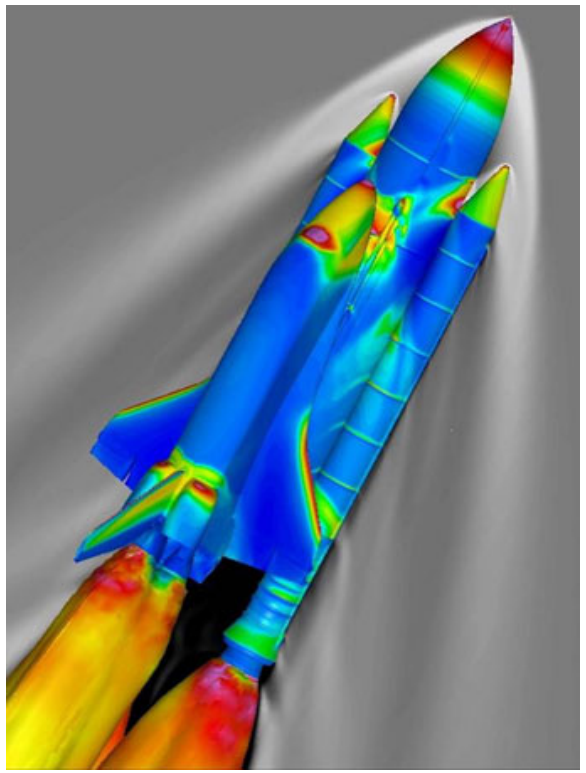
Grading

- **Exam** (45%)
  - Take-home Midterm Exam (20%), Mon, Mar 15 - Fri, Mar 19 (tentative)
  - Take-home Final Exam (25%), Wed, May 12 - Sun, May 16 (tentative)
- **Homework Assignments** (40%)
  - Check the Canvas for the assignments' due dates.
  - There will be reading, written, and programming assignments in a variety of format assignments during the course. Maximum points of the assignments could be different.
  - I usually give you a week time frame to submit the homework. Check the due in the online system.
  - Please read the academic integrity section of this document carefully, since I expect students to work on their own material and hold to high standards of behavior on all assignments.
- **Quiz** (10%)
  - We will have two quizzes (5% each). The quizzes will be true/false, multiple-choice, and some short answer.
  - Tentative schedule: Quiz 1: Tue, March 16, 2021, Quiz 2: Thu, May 6, 2021
- **Attendance and Class Activities** (5%)
  - Including class attendance and participating in discussions and answering questions.

Welcome to HPC course!

- Welcome again!!!
- I will try to provide lots of materials/opportunities to you!!!

What is HPC?

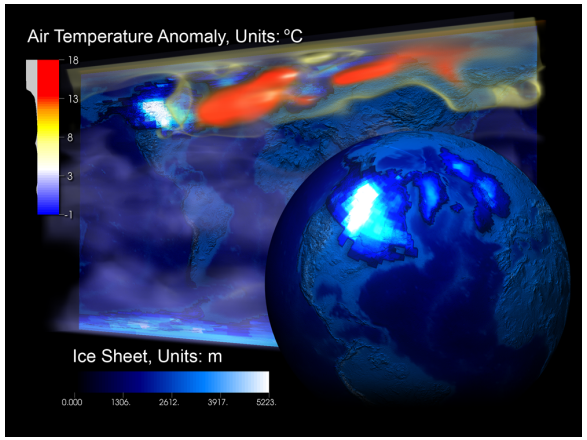


- High-performance computing (HPC) is the use of parallel processing for running advanced application programs efficiently, reliably and quickly.
- "High-Performance Computing most generally refers to the practice of aggregating computing power in a way that delivers much higher performance than one could get out of a typical desktop computer or workstation in order to solve large problems in science, engineering, or business" – insideHPC .

What is HPC?

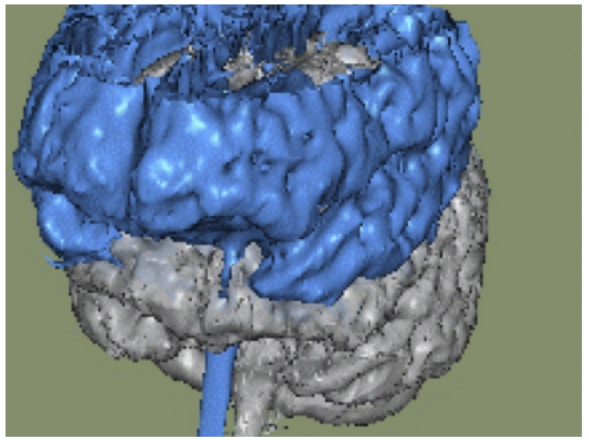
- Definition depends on individual person
  - HPC is when I care how fast I get an answer
- Thus HPC can happen on:
  - A workstation, desktop, laptop, smartphone!
  - A supercomputer
  - A Linux/MacOS/Windows/... cluster
  - A grid or a cloud
  - Cyberinfrastructure = any combination of the above
- HPC also means High-Productivity Computing

Welcome to HPC World!

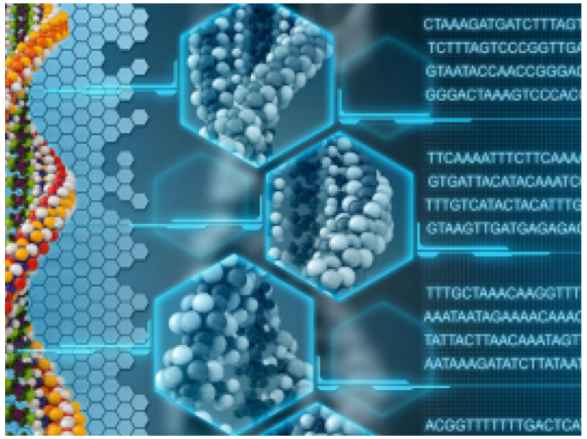


Climate

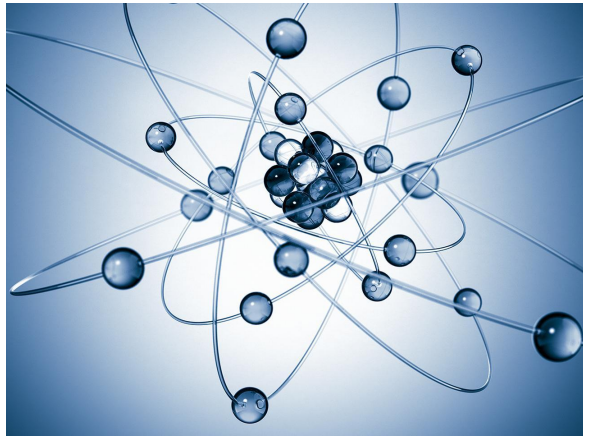
Finance



Medical



Bioinformatics

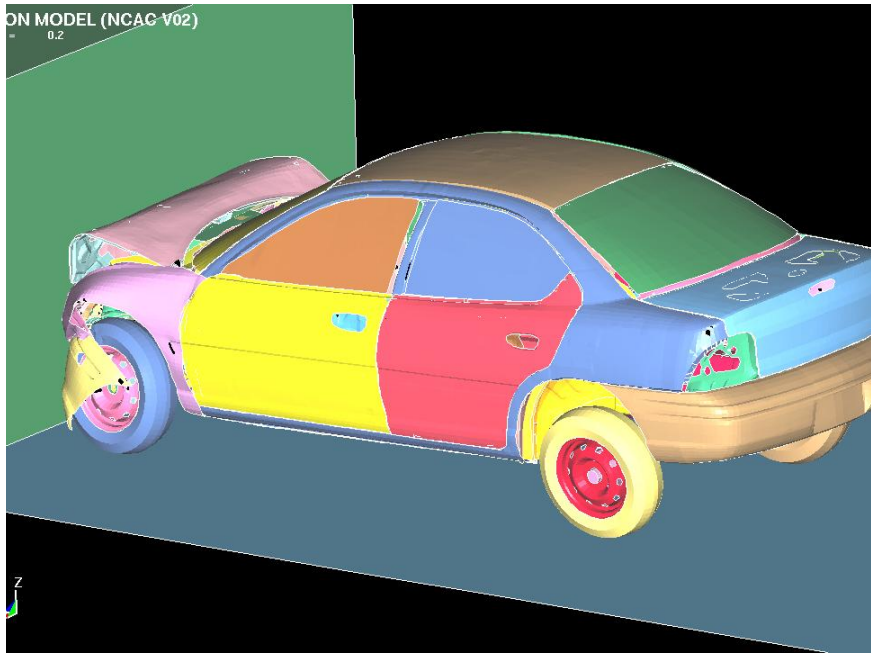


Physics

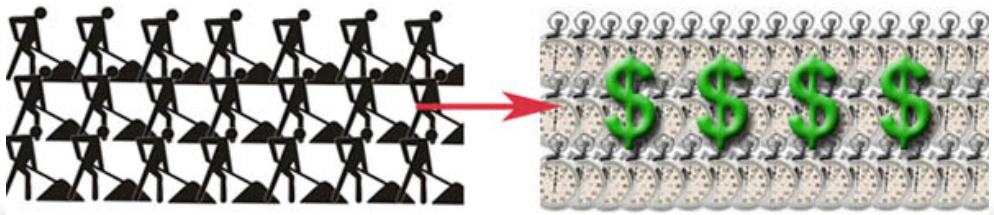
Entertainment

Why do we need HPC?

Save Time and Money

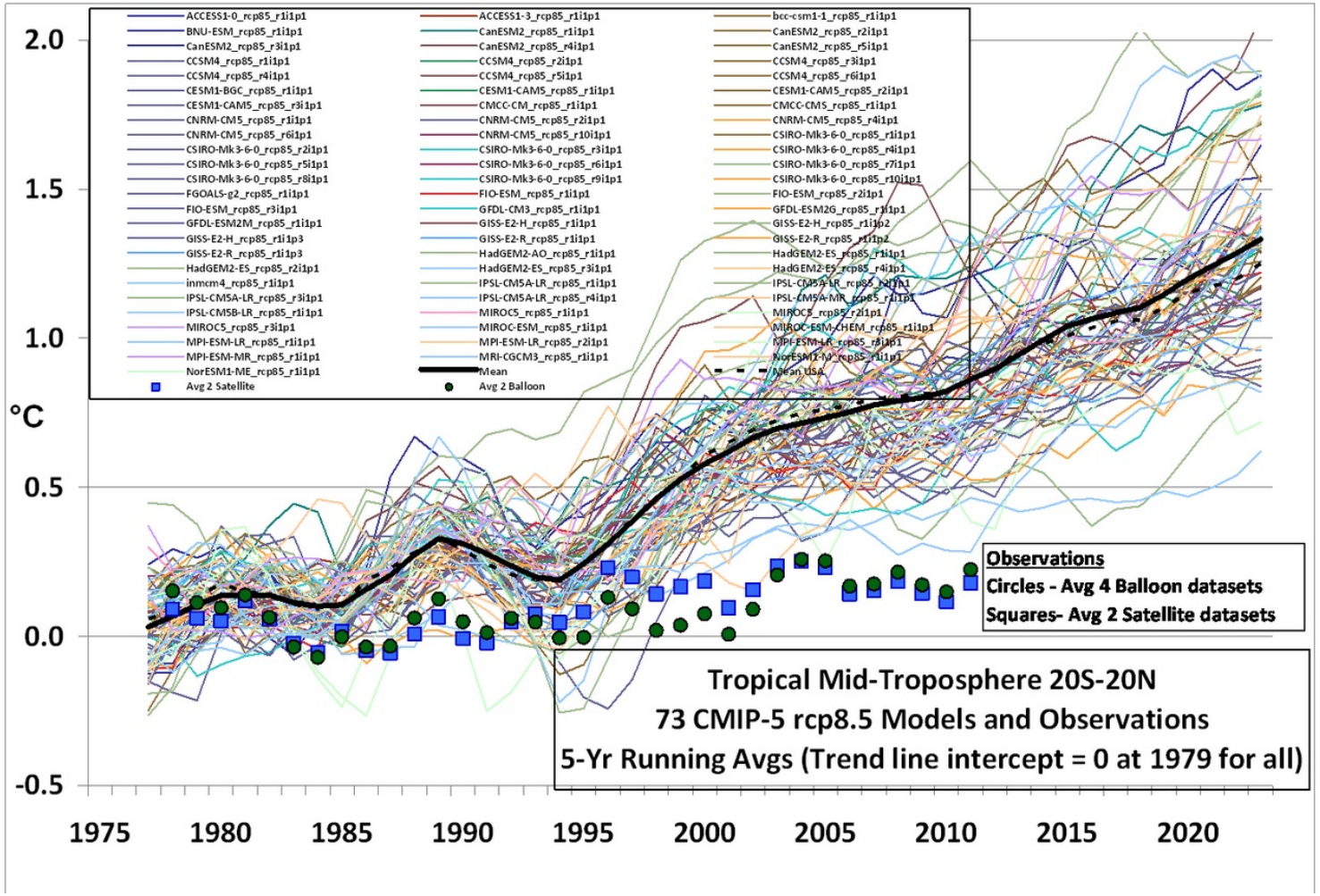


$500,000 vs $10



Why do we need HPC?

Human cannot calculate, but computer can!



Grand Challenge Problems

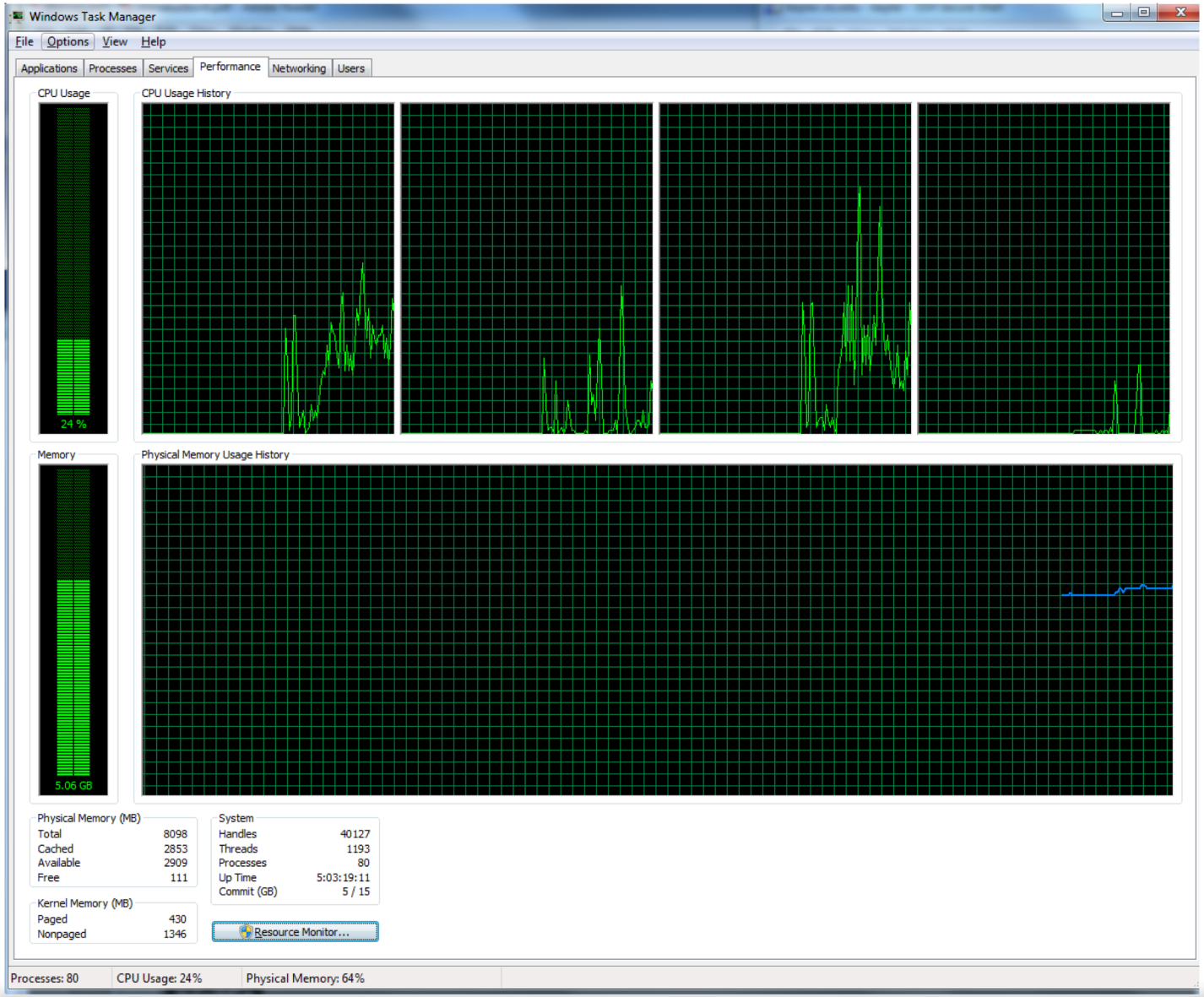
Big problems

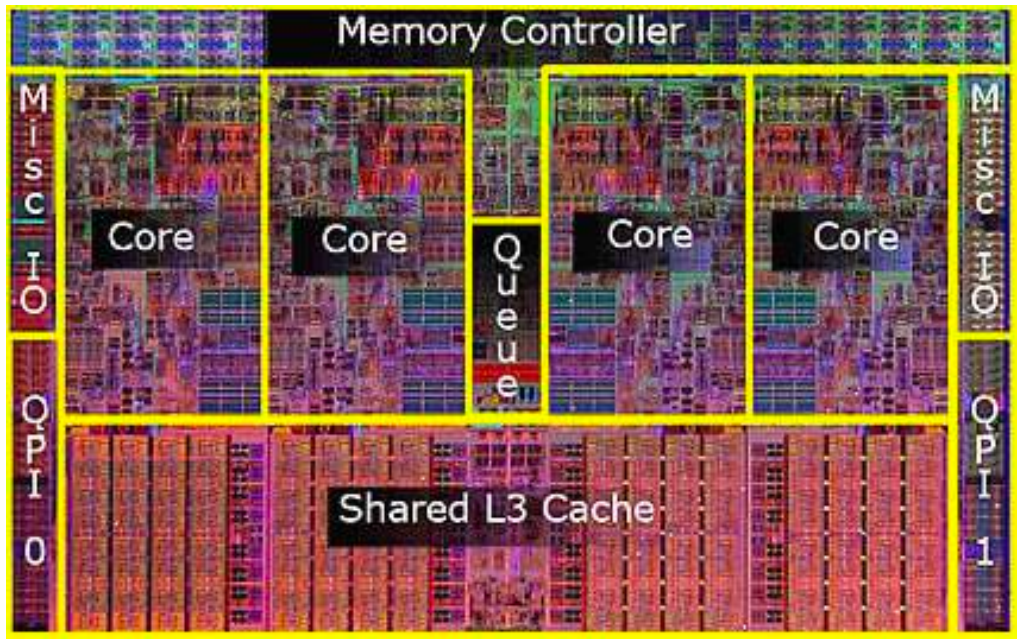
- A "Grand Challenge" problem is a problem that cannot be solved in a reasonable amount of time with today's computers
- Examples of Grand Challenge problems:
  - Human health and disease
  - Applied Fluid Dynamics
  - Meso- to Macro-Scale Environmental Modeling
  - Ecosystem Simulations
  - Biomedical Imaging and Biomechanics
  - Molecular Design and Process Optimization
  - Fundamental Computational Sciences
  - Nuclear power and weapons simulations

Why would HPC matter to you?

- Scientific computing is becoming more important in many research disciplines
- Problems become more complex, need teams of researchers with diverse expertise
- Scientific (HPC) application development often limited by lack of training
- More knowledge about HPC leads to more effective use of HPC resources and better interactions with (computational) colleagues

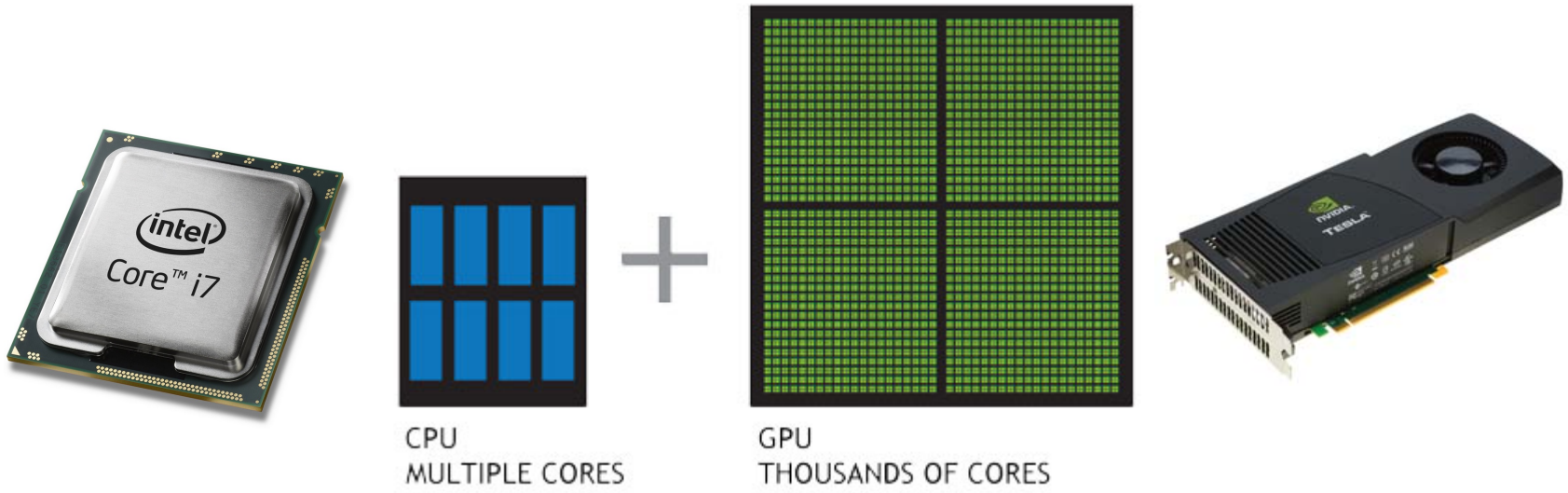
Your Laptop is HPC?





New Trend of Desktops/Laptops

- Two major trends:
  - Through the application of multicore computing. Processor architects focus on throughput, not clock speed, to improve performance.
  - Access to widely available graphic processing units (GPUs) for general processing.

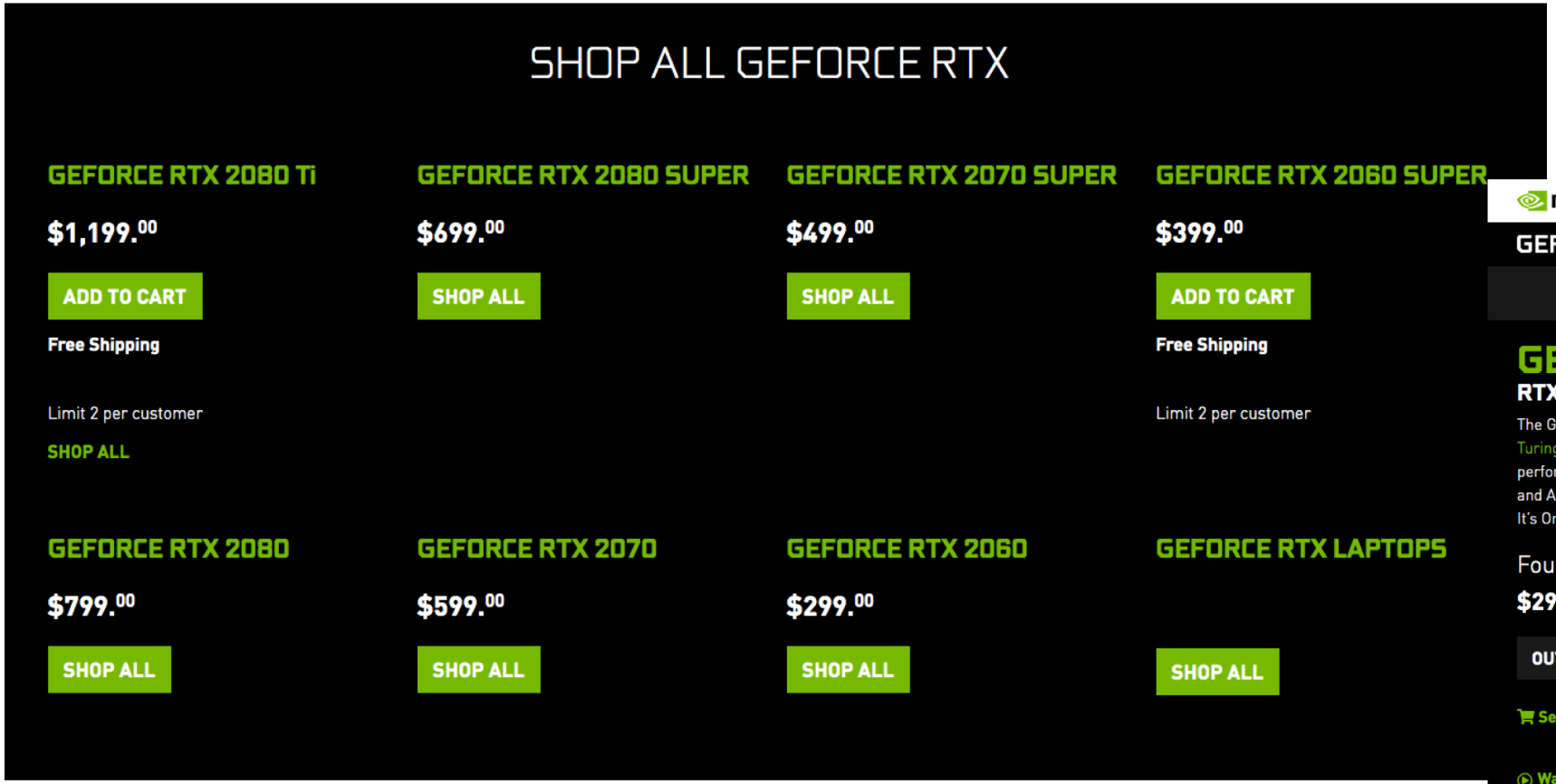


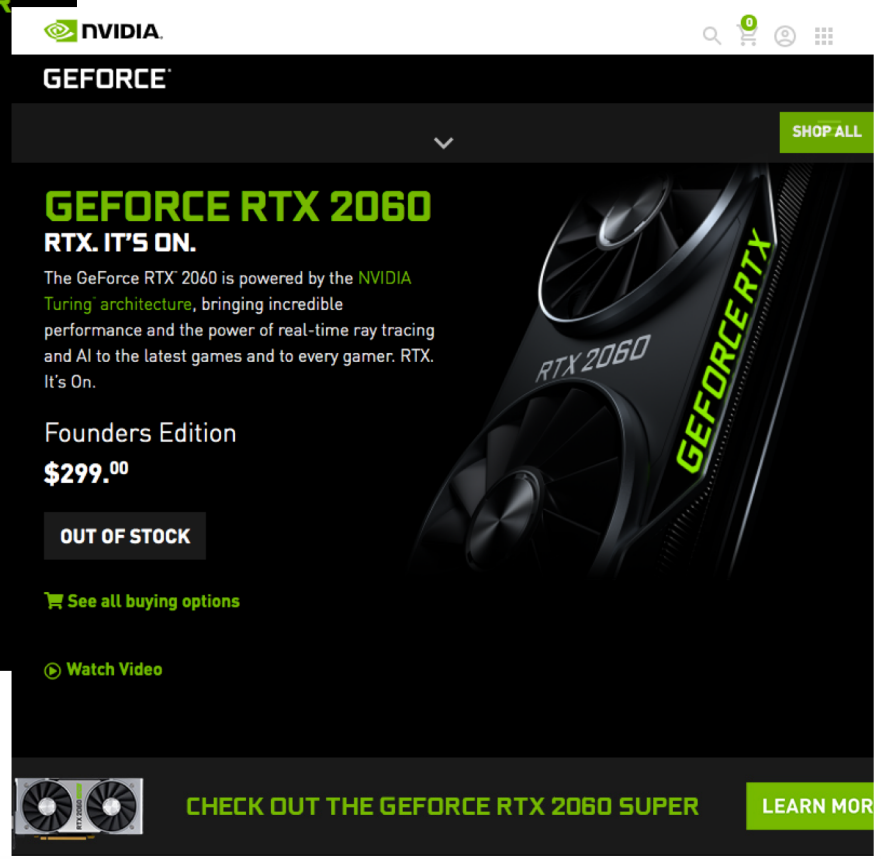
GPU

- GPU: Graphics Processing Unit
  - Designed for real-time graphics
  - Present in almost every PC
  - Increasing realism and complexity

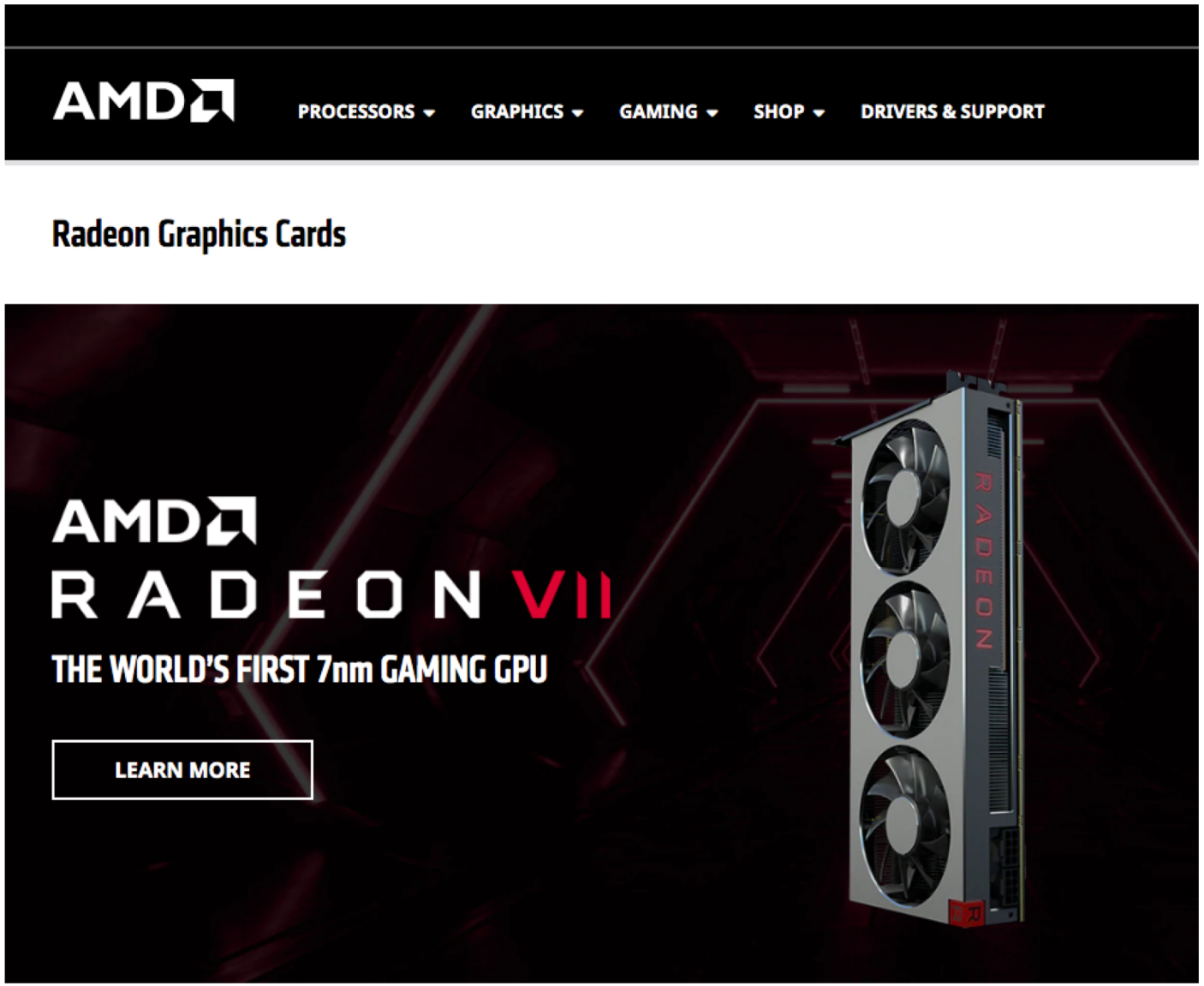
NVIDIA GPU

The Best Budget Graphics Cards in 2020 (by my quick and inaccurate search, I am not playing game anymore)





AMD Radeon



- My MacBook Pro has Radeon Pro 560

lambdalabs.com

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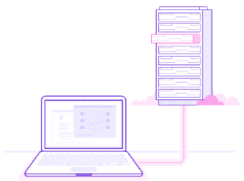
GPU compute built for deep learning

GPU cloud, workstations, servers, and laptops built for deep learning. Speed up PyTorch, TensorFlow, Keras, and save up to 90%.

Talk to an engineer

Deep Learning Laptop

GPU Workstation



GPU Cloud

GPU Cluster

Quadro GPU Server

Tesla GPU Server

New! Quadro RTX A6000, RTX 3090, RTX 3080, RTX 3070 pre-order >

Deep learning workstation with up to 4 GPUs

NVIDIA RTX 3090, RTX 3080, RTX 3070, Titan RTX, Quadro RTX 5000, RTX 6000, RTX 8000, and RTX A6000 options. Pre-installed with Ubuntu, TensorFlow, PyTorch, Keras, CUDA, and cuDNN.

Customize now

Technical specifications

GPU	Up to 4x NVIDIA GPUs Choose from RTX 30 series (Ampere), Titan RTX, Quadro RTX 8000, and RTX 6000
Processor	AMD Ryzen or Intel Core i9 Configurable up to 64 cores, 128 threads, and 256 MB cache
Memory	Up to 256 GB Fits up to eight 32 GB DIMMs at 3200 MHz

From $5,486.00

Free 30-day returns

Processor

AMD Threadripper 3960X
24 cores, 3.80 GHz, 128 MB cache

GPUs

2x RTX 3070 (pre-order)

Memory

64 GB

Operating System Drive

1 TB SSD (NVMe) - $336

2 TB SSD (NVMe)

$5,486.00

Apply for a discount

Workstation, Cluster, Supercomputer?

- Most workstation computers today are parallel workstations

  multi-core processors

- Running Linux OS (or MacOS X) allows programming like traditional Unix workstation

- Software to use multi-cores/threads
  - Pthreds, OpenMP, Multiprocessing

- All processors have access to all memory
  - Uniform memory access (UMA):

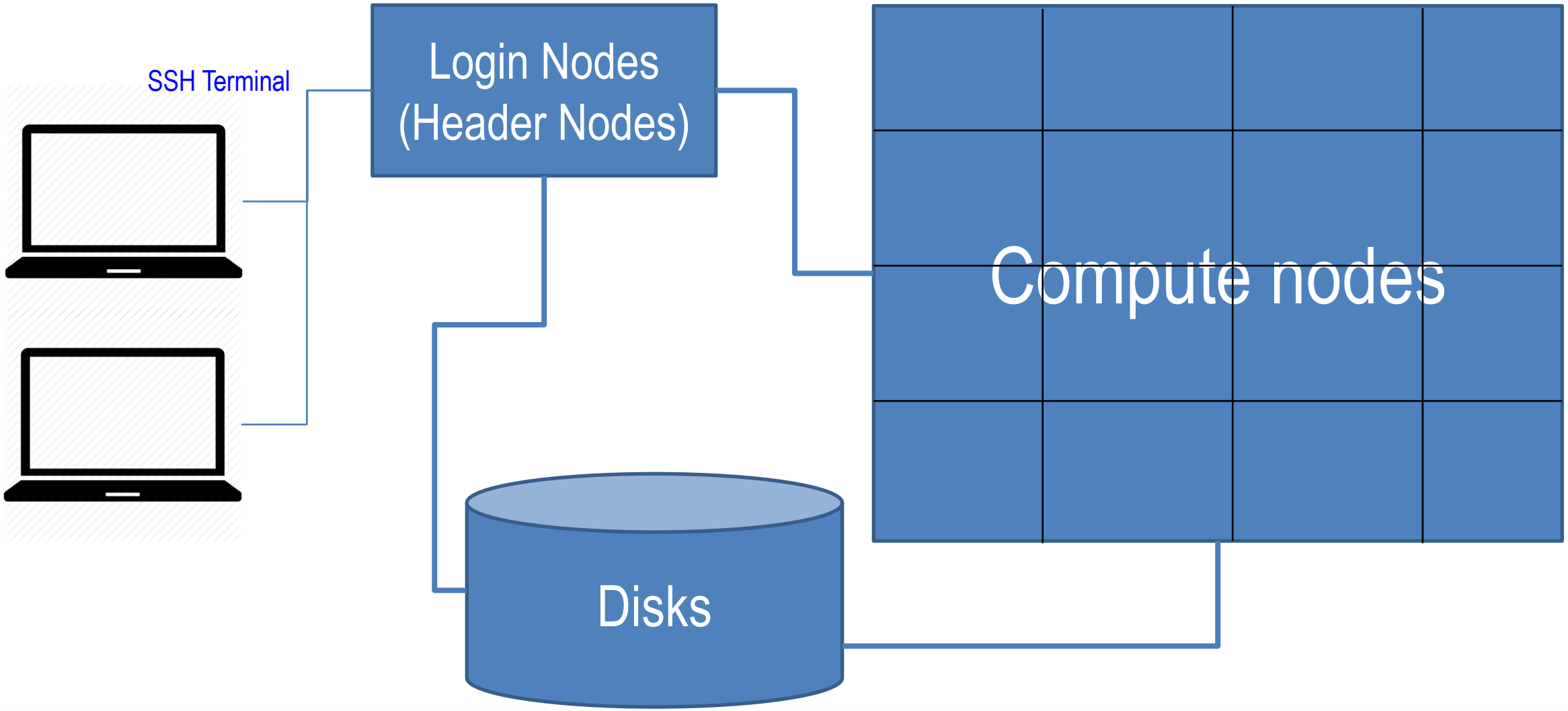
    1 memory pool for all, same speed for all
  - Non-uniform memory access (NUMA):

    multiple pools, speed depends on “distance”

Workstation, Cluster, Supercomputer?

- A cluster needs:
  - Several computers, nodes, often in special cases for easy mounting in a rack
  - One or more networks (interconnects) to hook the nodes together
  - Software that allows the nodes to communicate with each other (e.g. MPI)
  - Software that reserves resources to individual users
- A cluster is: all of those components working together to form one big computer

Typical HPC (Cluster/Server) System Layout

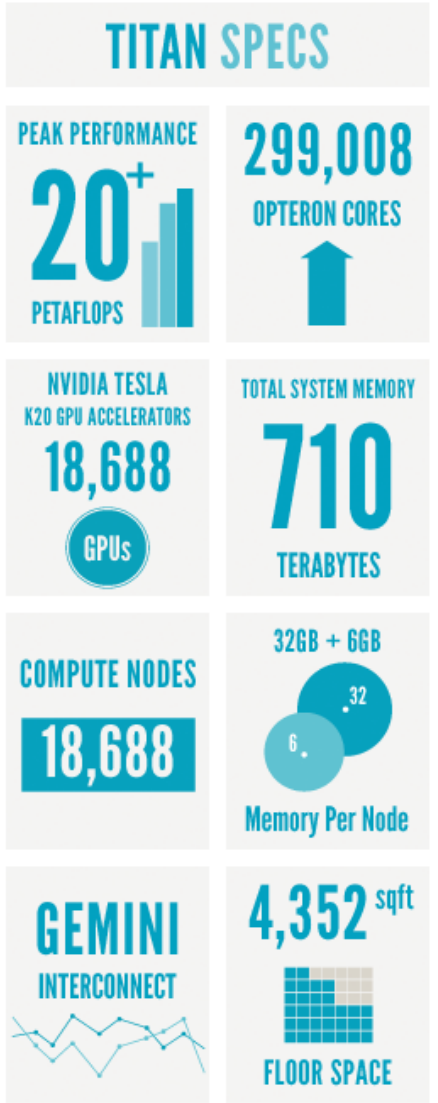


Workstation, Cluster, Supercomputer?

- A supercomputer is a computer with a high-level computational capacity compared to a general-purpose computer.
  - The most visible manifestation of HPC
  - Programs run on the fastest and largest computers in the world (Top500 List, https://www.top500.org/)
  - Performance of a supercomputer is measured in tera scale floating-point operations per second (Tflops)

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	537,212.0	29,899
2	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	200,794.9	10,096
3	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438
4	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371

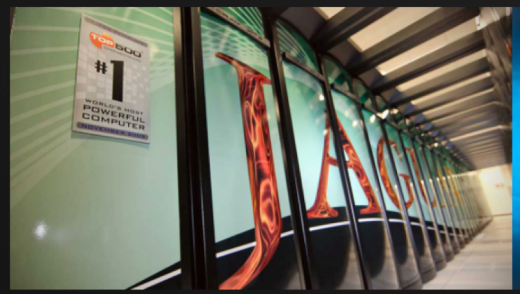
Oak Ridge National Lab Supercomputing Center (2012-2015)



Oak Ridge National Lab Supercomputing Center

WORLD LEADING SYSTEMS

Oak Ridge National Laboratory has decades of experience in delivering, operating, and conducting research on world-leading supercomputers. Since 2005, Oak Ridge National Laboratory has deployed Jaguar, Titan, and Summit, each the world's fastest computer in its time. Frontier will leverage ORNL's extensive experience and expertise in GPU-accelerated computing to become the US Department of Energy's next record-breaking supercomputer when it debuts in 2021.



JAGUAR

No. 1 in 2009, 2010

TITAN

No. 1 in 2012

SUMMIT

No. 1 in 2018

FRONTIER

Coming in 2021

Cloud Computing

- "Cloud Computing", by definition, refers to the on-demand delivery of IT resources and applications via the Internet with pay-as-you-go pricing.
- Cloud Computing provides a simple way to access servers, storage, databases and a broad set of application services over the Internet.
- Cloud Computing providers such as Amazon Web Services own and maintain the network-connected hardware required for these application services, while you provision and use what you need via a web application.

What is Parallel Computing?

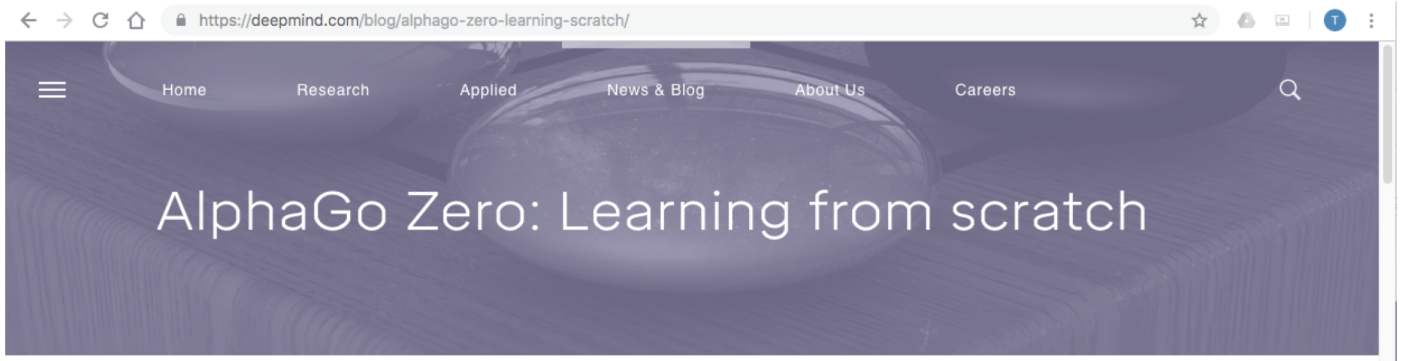
- Parallel computing is the use of multiple processing entities in combination to solve a single problem.
- It is not always obvious that a parallel algorithm has benefits, unless we want to do things …
  - faster: doing the same amount of work in less time
  - bigger: doing more work in the same amount of time
- Both of these reasons can be argued to produce better results, which is the only meaningful outcome of program parallelization

Parallel Processing with Big Data

- Discrepancy between the explosive growth rate in data volumes and the improvement trends in processing and memory access speeds necessitates that parallel processing be applied to the handling of extremely large data sets.

HPC + AI

- Google AlphaGo



Artificial intelligence research has made rapid progress in a wide variety of domains from speech recognition and image classification to genomics and drug discovery. In many cases, these are specialist systems that leverage enormous amounts of human expertise and data.

However, for some problems this human knowledge may be too expensive, too unreliable or simply unavailable. As a result, a long-standing ambition of AI research is to bypass this step, creating algorithms that achieve superhuman performance in the most challenging domains with no human input. In our most recent paper, published in the journal Nature, we demonstrate a significant step towards this goal.

Configuration and strength[63]

Versions	Hardware	Elo rating	Matches
AlphaGo Fan	176 GPUs,[52] distributed	3,144[51]	5:0 against Fan Hui
AlphaGo Lee	48 TPUs,[52] distributed	3,739[51]	4:1 against Lee Sedol
AlphaGo Master	4 TPUs,[52] single machine	4,858[51]	60:0 against professional players; Future of Go Summit
AlphaGo Zero	4 TPUs,[52] single machine	5,185[51]	100:0 against AlphaGo Lee 89:11 against AlphaGo Master
AlphaZero	4 TPUs, single machine	N/A	60:40 against AlphaGo Zero

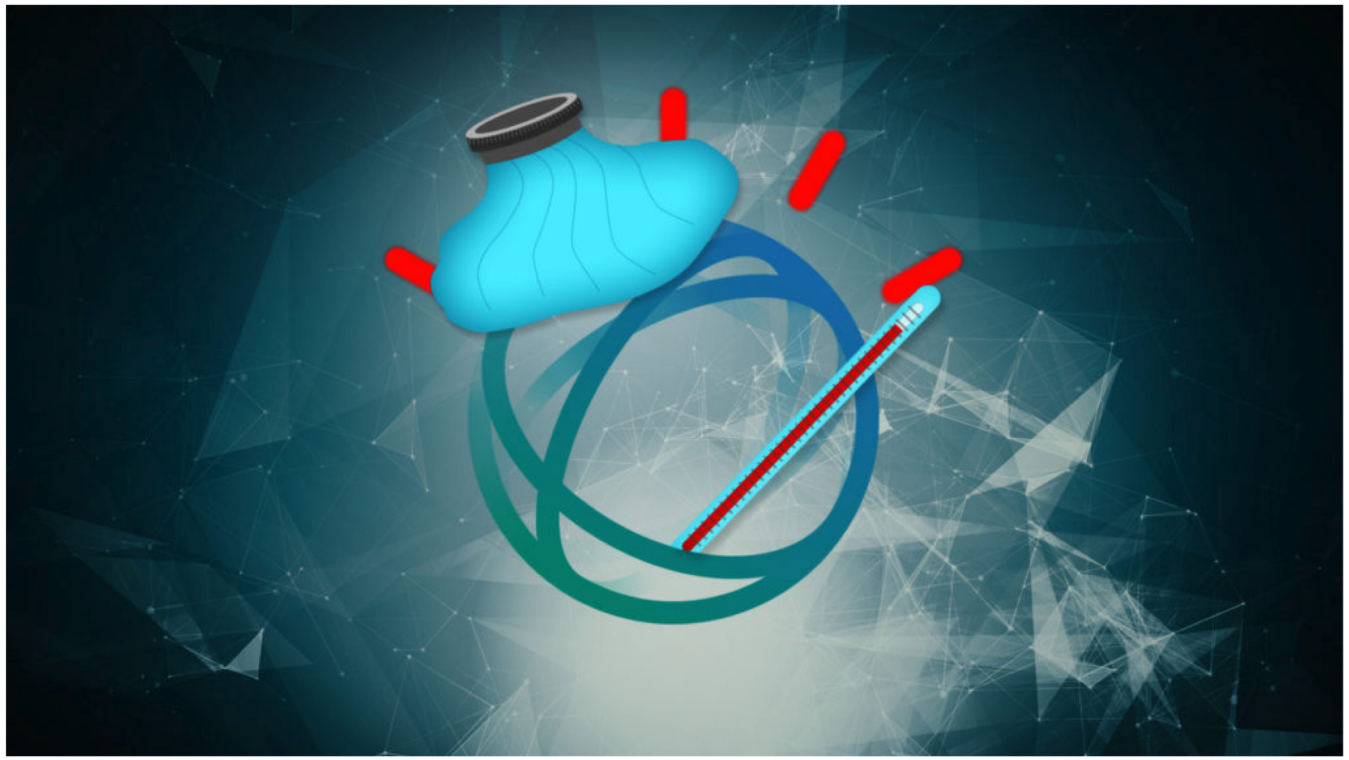
HPC + AI… Not matured yet…

EXCLUSIVE

STAT+

IBM's Watson supercomputer recommended 'unsafe and incorrect' cancer treatments, internal documents show

By CASEY ROSS @caseymross and IKE SWETLITZ @ikeswetlitz / JULY 25, 2018



Welcome to HPC world!

- Welcome!!!
- Lots of opportunities for you!!!