

Introduction to Computational Thinking and Python Programming

Instructor: Sarom Leang, PhD (Teacher/Professor)

Assistant: Romin Katre

Innovation Hall 203



Pronouns

- Instructor: Sarom Leang, Ph.D. (Teacher/Professor/Instructor)
- Assistant: Romin Katre

Schedule

- 10:00 AM – 10:15 AM (Homeroom)
- **10:15 AM – 11:35 AM (G1)**
- 11:40 AM – 12:35 PM (Lunch)
- **12:40 PM – 02:00 PM (G2)**



Student Expectations

- **NO FOOD**
- **NO DRINKS** (on the table)
- Be respectful to individuals and property
- Be open to learning
- Be open to not understanding
- Be patient with yourself
- Ask questions
- Explore
- **Embrace failure**

G1

- If we start class 5 minutes early (e.g., at 10:10 AM), then the class will be dismissed to lunch 5 minutes early at 11:30 AM.

G2

- If you arrive in your seat by 12:40 PM then you have the option to finish your lunch in the hallway – if needed.



Course Overview

- This course introduces the fundamental building blocks of computational thinking and computer programming using the Python language.
- Upon successful completion of this course, students will be able to:
 - Improve their problem-solving skills
 - Write, read, and execute Python code using basic data types and operators



Course Overview (cont.)

Exploratory Topics

- Session #1 – October 23, 2023
 - Entrance Survey
 - How Computers Work
- Session #2 – December 2, 2023
 - Parallel Computing
- Session #3 – February 10, 2024
 - Generative Artificial Intelligence
- Session #4 – March 23, 2024
 - Quantum Computing
- Session #5 – April 20, 2024
 - Future of Computing
 - Exit survey

Topics

- Algorithms and Problem Solving
- Debugging and Troubleshooting
- Loops
- Algorithms and Syntax
- Variables and Conditionals
- Variable Arithmetic
- Conditionals (If/Else)
- Compound Conditionals



Entrance Survey (Results)

Question	G1	G2
Computer access at home?	100% Yes	96% Yes
Computer access at school?	100% Yes	100% Yes
Taken this course before?	3 - Yes	2 - Yes
Previous computer programming experience?	7 - Yes	13 - Yes
Grade level	100% - 9th	96% - 9th
Keyboard is an input device	92%	52%
CPU is known as the brain of a computer	78%	64%
A speaker is an example of an output device.	74%	56%
Hard disk, floppy disk, USB disk are examples of storage devices.	92%	68%
Storage device can hold data and programs even if the power is off.	91%	84%
Internet , a worldwide collection of networks that connect institutions and people.	74%	72%
A supercomputer is the fastest, most powerful computer.	70%	60%
Data is raw, unprocessed facts including text, numbers, images, and sounds.	70%	72%
Computer can execute code in machine language .	17%	24%

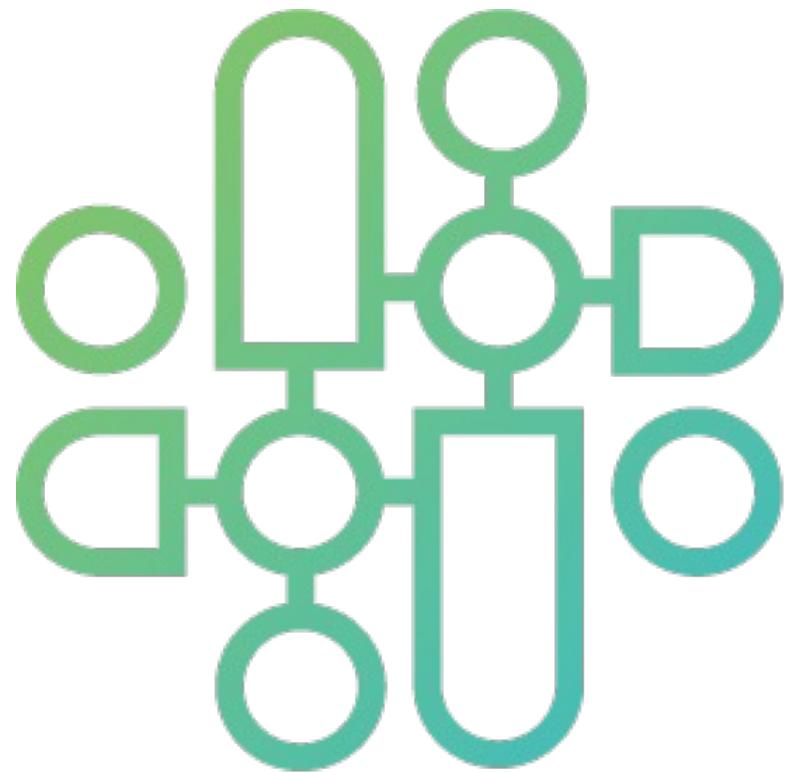


Use of Class Time

- Course is capped at 60 seats
- Each seat costs \$50
- EIP has invested \$3000 to offer this course
- Bring in schoolwork to occupy yourself



Supercomputing Conference



SC23

Denver, CO | i am hpc.

HPC = high performance computing



High Performance

Example	General	High	Metrics
Cars	Consumer e.g., Ford Fusion	Performance e.g., Formula-1, Koenigsegg Agera	<ul style="list-style-type: none">• Speed• Torque (force)• Horse-power (force x distance)
Computers	Consumer e.g., Alienware Area 51	Performance e.g., HPE Cray Frontier	<ul style="list-style-type: none">• Operations per second• Number of CPUs• Aggregate memory



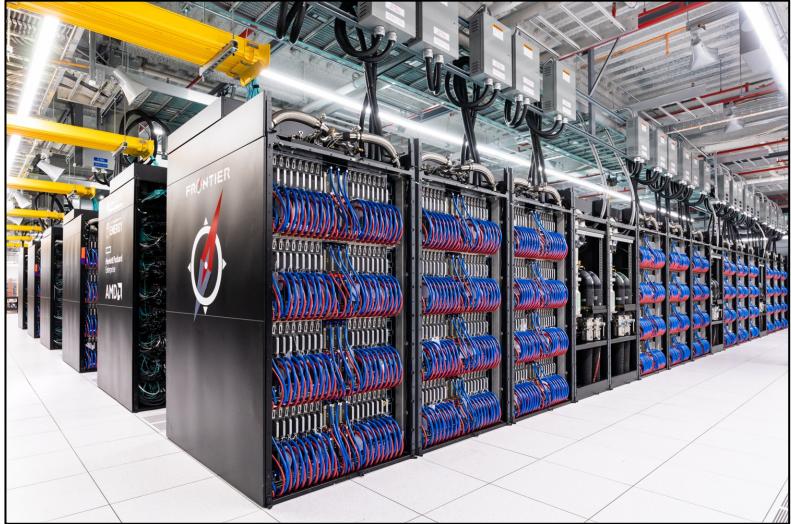
High Performance Computing

Specs	Alienware Area 51	IBM Summit (4,608 nodes) #7
CPU	1x AMD Ryzen 2950X 16-core/32-threads 4.4 GHz	2x IBM Power9 22-core/96-threads 3.07 GHz
GPU	2x NVIDIA RTX 2080 Ti	6x NVIDIA Volta V100
Memory	64 GB	512 GB
Floating point operations per second (FLOPS)	700 GFLOPS	42000 GFLOPS (per node) 42 TFLOPS (per node) 60x 200000000 GFLOPS (total) 200 PFLOPS (total) 285,714x

Top 5 Supercomputers

Rank	Country / System	Rpeak (PFlops/s)
1	USA / Frontier AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE	1,685
2	USA / Aurora Intel Xeon CPU Max 9470 52C 2.4 GHz, Intel Data Center GPU, Slingshot-11, Intel	1,059
3	USA / Eagle NVIDIA H100, NVIDIA Infiniband NDR, Microsoft	846
4	Japan / Fugaku A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu	537
5	Finland / LUMI AMD Optimized 3 rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE	531

Top 5 Supercomputers





FIRST TO BREAK THE
EXASCALE BARRIER AND
FASTEST COMPUTER
IN THE WORLD

1.1
EXAFLOPS

FRONTIER CAN DO MORE
THAN 1 QUINTILLION
CALCULATIONS PER SECOND.

1
SECOND

IF EACH PERSON ON EARTH
COMPLETED **ONE CALCULATION**
PER SECOND, IT WOULD TAKE MORE
THAN **4 YEARS** TO DO WHAT AN EXASCALE
COMPUTER CAN DO IN **1 SECOND**.

700
PETABYTES

FRONTIER'S ORION STORAGE
SYSTEM HOLDS **33 TIMES** THE
AMOUNT OF DATA HOUSED IN
THE LIBRARY OF CONGRESS.

8,000
POUNDS

EACH CABINET WEIGHS
THE EQUIVALENT OF
2 FULL-SIZE
PICKUP TRUCKS.

6,000
GALLONS

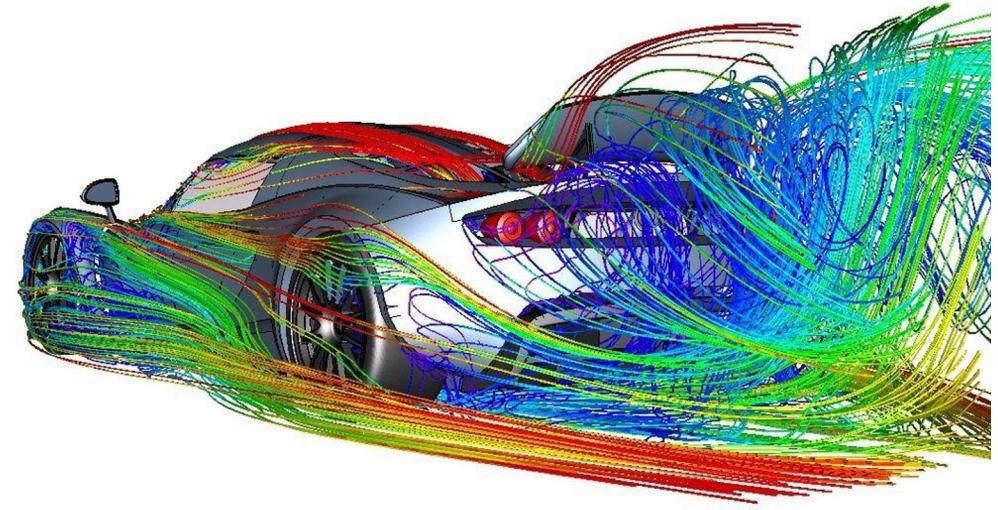
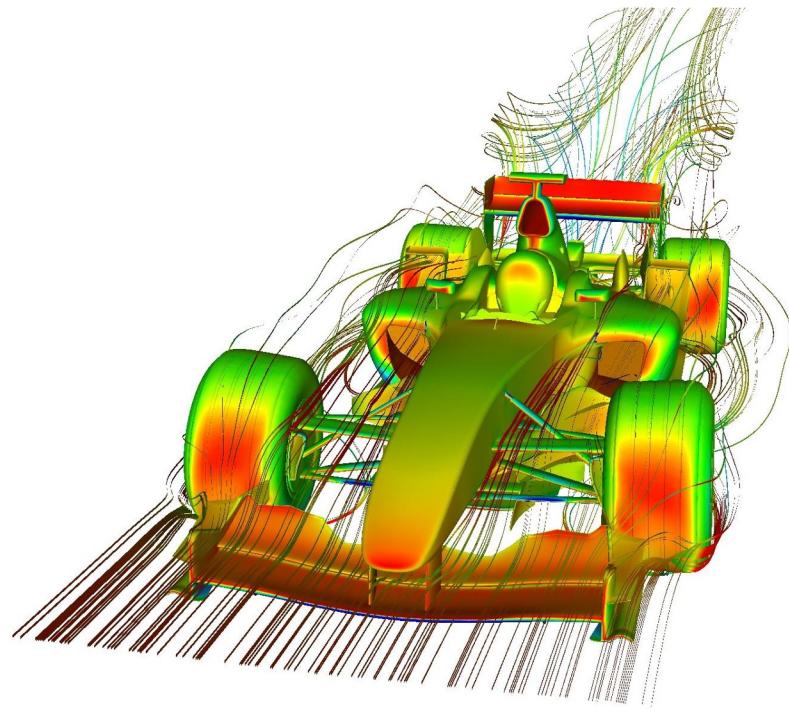
OF **WATER** IS MOVED THROUGH
THE SYSTEM **PER MINUTE** BY
FOUR **350-HORSEPOWER PUMPS**.
THESE POWERFUL PUMPS COULD FILL AN
OLYMPIC-SIZED SWIMMING POOL
IN ABOUT **30 MINUTES**.

40
MEGAWATTS

FRONTIER'S MECHANICAL
PLANT CAN COOL THE
EQUIVALENT POWER DEMAND OF
ABOUT **30,000 U.S. HOMES**.

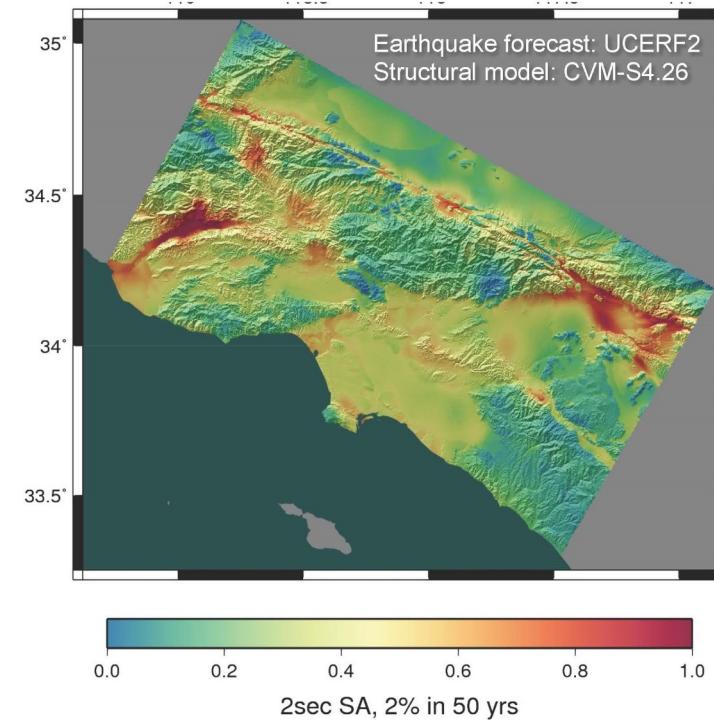
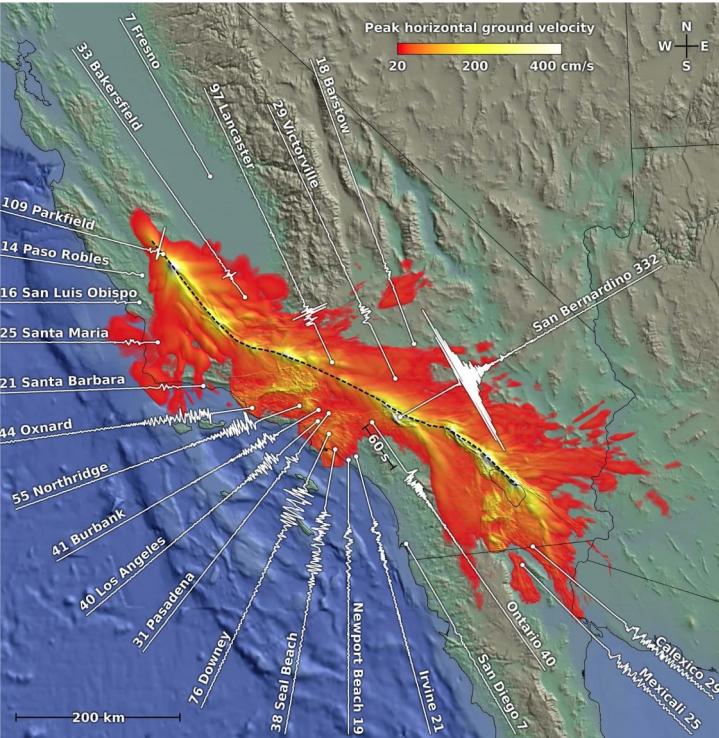


Supercomputing Applications



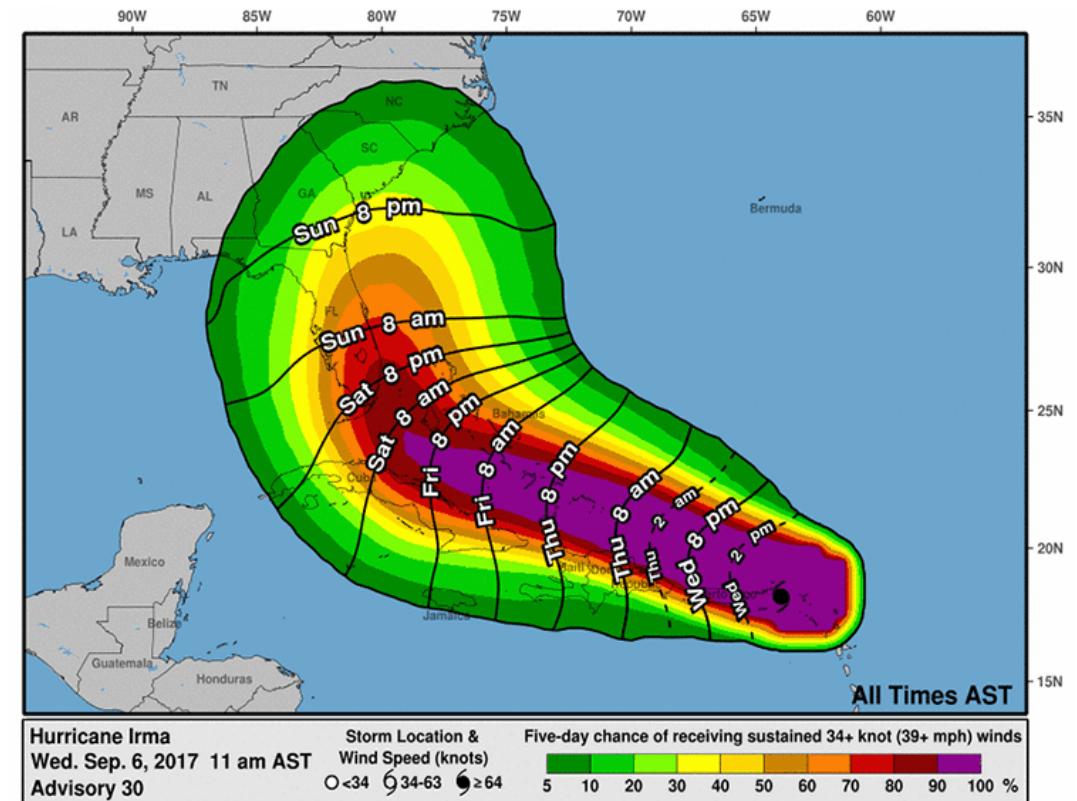
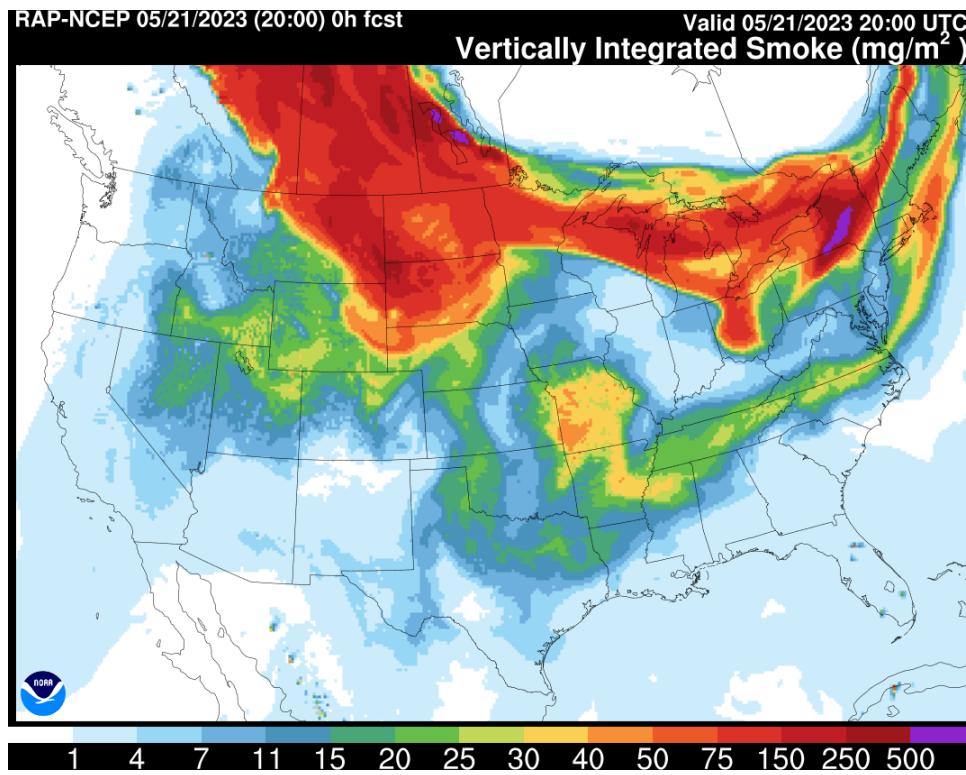
Computational Fluid Dynamics (CFD)

Supercomputing Applications



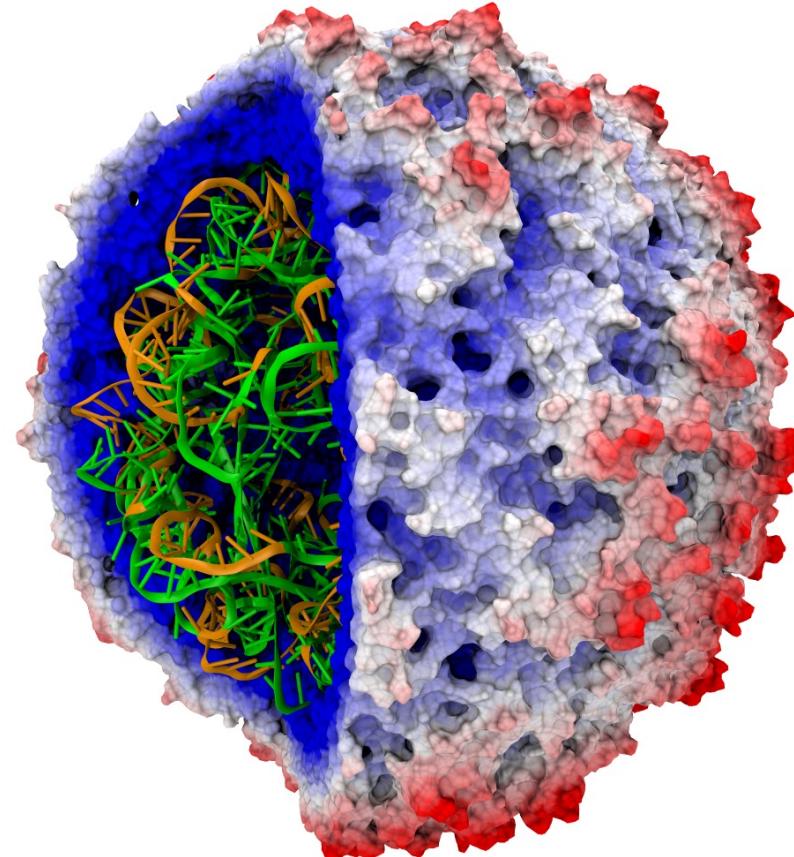
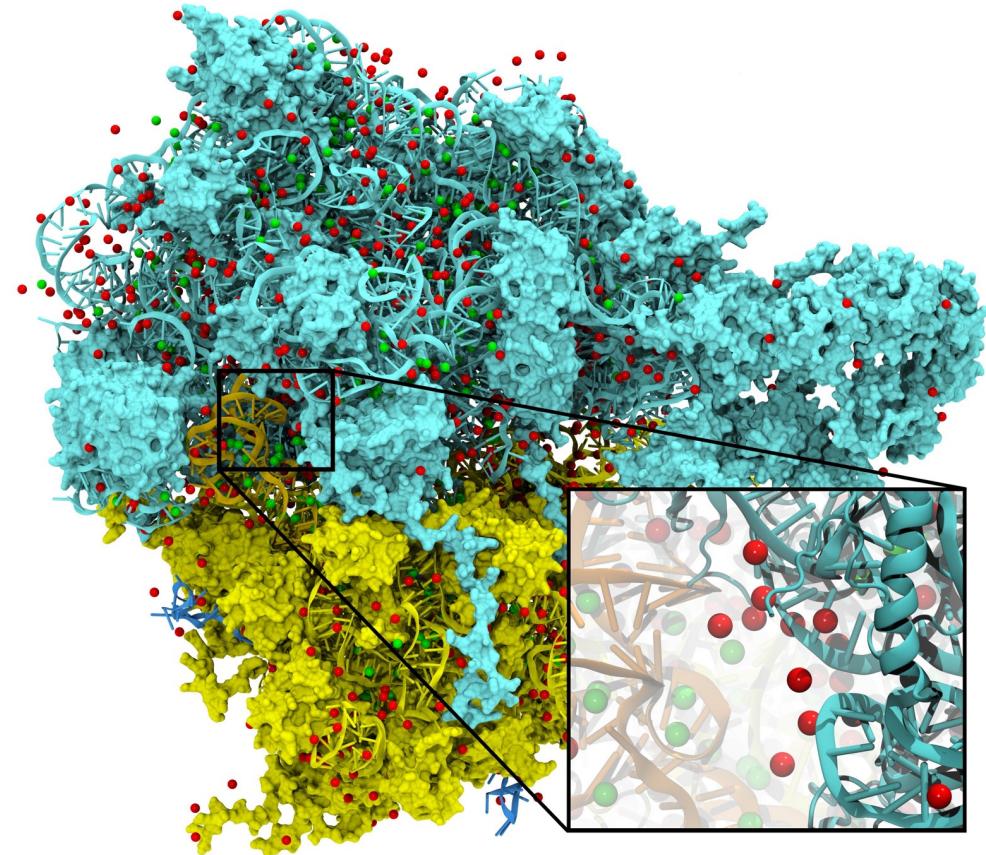
Seismic Modeling

Supercomputing Applications



Weather Modeling

Supercomputing Applications

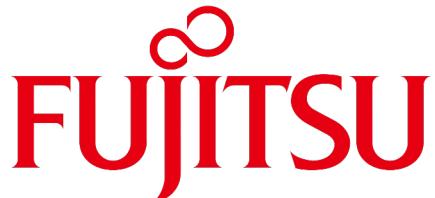
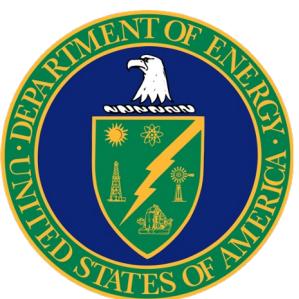
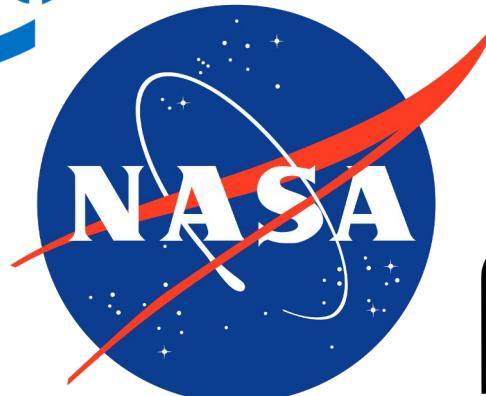
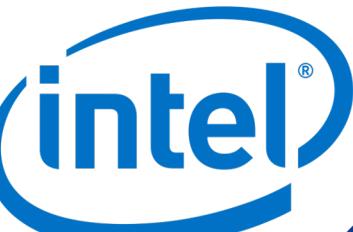


Molecular Simulations

Who is Interested in HPC?



NVIDIA
Hewlett Packard Enterprise



Google Cloud



ORACLE®

Microsoft
aws



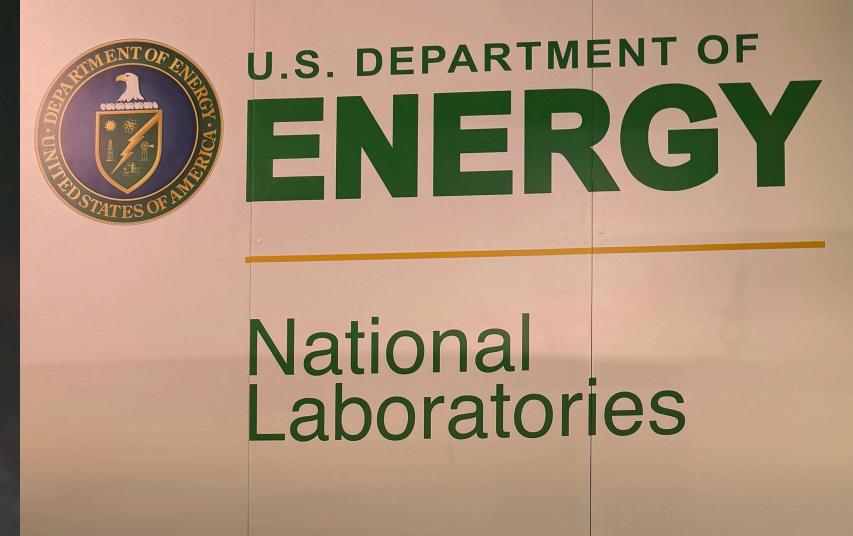
Who is Interested in HPC?



Generative AI



Dr. Hakeem Oluseyi, Astrophysicist



National Laboratories

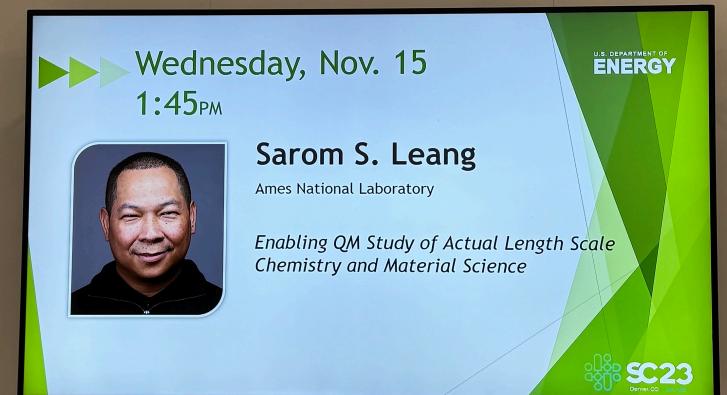
Featured Presentation



Meow Wolf Art Installation



Networking Receptions



Wednesday, Nov. 15
1:45PM

Sarom S. Leang

Ames National Laboratory

Enabling QM Study of Actual Length Scale
Chemistry and Material Science

SC23
Denver CO

Exercise – Human Supercomputer?

- **Challenge:** 500 piece jigsaw puzzle
- **Goal:** Get the most number of correctly connected pieces within the established time frame
- We will assign groups of (or close to):
 - 1
 - 2
 - 4
 - 8
 - 16

Exercise – Human Supercomputer?

- **Challenge:** 500 piece jigsaw puzzle
- **Goal:** Get the most number of correctly connected pieces within the established time frame
- We will assign groups of (or close to):
 - 1
 - 2
 - 4
 - 8
 - 16

# Solvers	G1 (# connected)	G2 (# connected)
1		
2		
4		
8		
16		

Before You Begin

- Spend 5 minutes to strategize your approach.
- Assign 1 person as the leader of your group.
- The group leader will assign tasks the other members of the group.



Discussion – Human Supercomputer

- Expected results?
- Approaches/strategies?
- Benefits of working in your environment?
- Challenges of working in your environment?
- What do you expect to happen to the results if the number of puzzle pieces increased (more puzzle pieces)?
- What do you expect to happen to the results if the number of puzzle pieces decreased (less puzzle pieces)?



Computational Thinking

- Decomposition – breaking up the problem into smaller tasks
 - Sorting
 - Identifying edge pieces
 - Identifying similar colored pieces
 - Connecting
 - Edge pieces
 - Different sections of the puzzle based on color pattern
 - Combining
 - Joining together connected pieces from different sections of the puzzle

Computational Thinking

- Algorithm – your approach to solving a problem or set of problems
 - Consist of a sequence of instructions
 1. Flip all puzzle pieces upwards
 2. Sort edge pieces from non-edge pieces
 3. Sort pieces based on color similarity
 4. Connect edge pieces
 5. Connect pieces based on color similarity
 6. Joining connected pieces
 7. Connect pieces based on shape similarity