

Why Do HPC?

What is a high-performance computing system and why would anyone use it?

Geoffrey Lentner, Rosen Center for Advanced Computing John K. Holmen, Oak Ridge Leadership Computing Facility

What is a supercomputer?

SC23
Denver, CO | i am hpc.

- Built from many servers
- Interconnected over fast networks
- Data storage systems (similar)
- Typically running UNIX-like OS
- Managed by batch scheduler
- Running special software



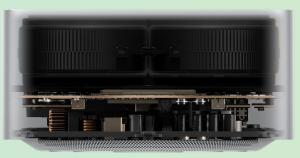
HPE Cray EX2500 and Cray XD2000 https://www.hpe.com/us/en/compute/hpc.html

Personal computing is getting pretty super...



- Personal and lab workstations are orders of magnitude more capable and affordable than in previous decades
- ARM-based platforms with >30 teraflops
- Many terabytes of solid-state storage
- Familiar



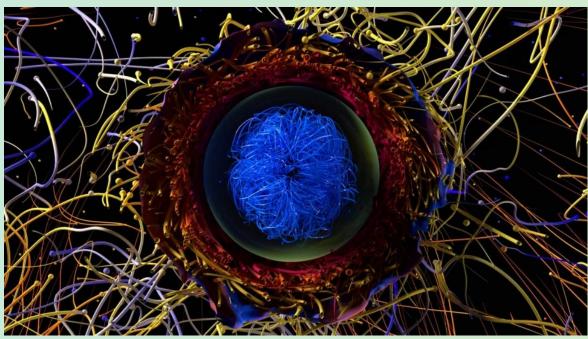


Apple Mac Studio with M2 Ultra https://www.apple.com/mac-studio/

When would you use a supercomputer?

- Applications can be ...
 - too slow,
 - too many,
 - too big,
 - too complex,
 - too expensive,
 - too data intensive, or even
 - too dangerous





ALCF Visualization and Data Analytics Team;
Adam Burrows and the Princeton Supernova Theory Group, Princeton University
https://www.alcf.anl.gov/news/simulating-supernova-explosions-3d

Video: https://www.youtube.com/watch?v=0DSk1wPc_cE
SC22: Visualizing the Supernova Explosion of a 25-Solar-Mass Star and the Simultaneous Birth of ...

It's either Capacity or Capability

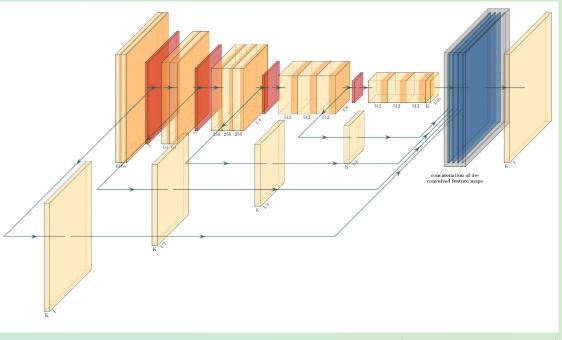


- Even things possible on a personal computer can require HPC because of limitations on capacity; e.g.,
 - too many tasks make the problem too slow to complete (months vs hours)
- For some applications, a personal computer is not capable; e.g.,
 - too big to simulate on a single machine, or
 - too complex to do on normal hardware, or
 - too expensive or too dangerous to allow study in the real-world

Too many and too slow ...



- Deep learning is possible, but
 - train faster on specialized hardware, and
 - exploring many, many models can take months on a single machine
- Data processing is possible, but
 - there might be too much data for your local hard drive, or
 - processing in serial can be too slow

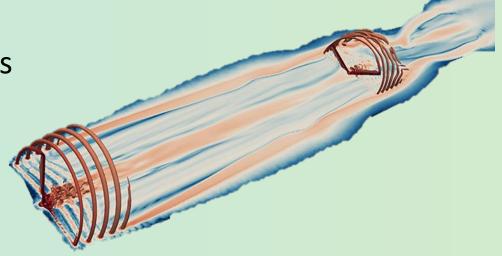


FCN-32 (plotted using *PlotNeuralNet*) https://github.com/Harislqbal88/PlotNeuralNet

Too big and too complex ...



- Scheduling for airlines routing thousands of flights and millions of passengers;
 - too complex to complete in a timely fashion with so many variables and permutations
- Trajectory planning for space-flight missions
 - too complex, involving incredible fidelity over long time spans,
- Model simulations for turbine efficiency
 - too big to simulate on one machine

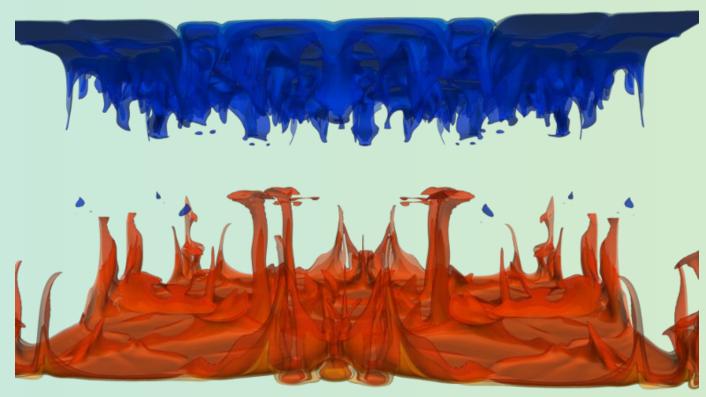


Wind Turbine Modeling and Validation, National Renewable Energy Lab (NREL) https://www.nrel.gov/wind/modeling-validation.html

Too expensive and too dangerous ...



- Weapons research
 - Cannot detonate weapons
- Nuclear reactor safety
 - Cannot intentionally melt
 down a nuclear reactor



Lentner 2023, in prep

What is a Leadership Computing Facility (LCF)?



- LCF centers partner with users to enable science and engineering breakthroughs
- Mission: Deploy and operate the computational and data resources required for such breakthroughs
- LCF centers provide resources to investigate otherwise inaccessible systems at every scale
 - Galaxy Formation and Supernovae to Automobiles and Nanomaterials



https://www.flickr.com/photos/olcf/52117623798

Oak Ridge Leadership Computing Facility (OLCF)



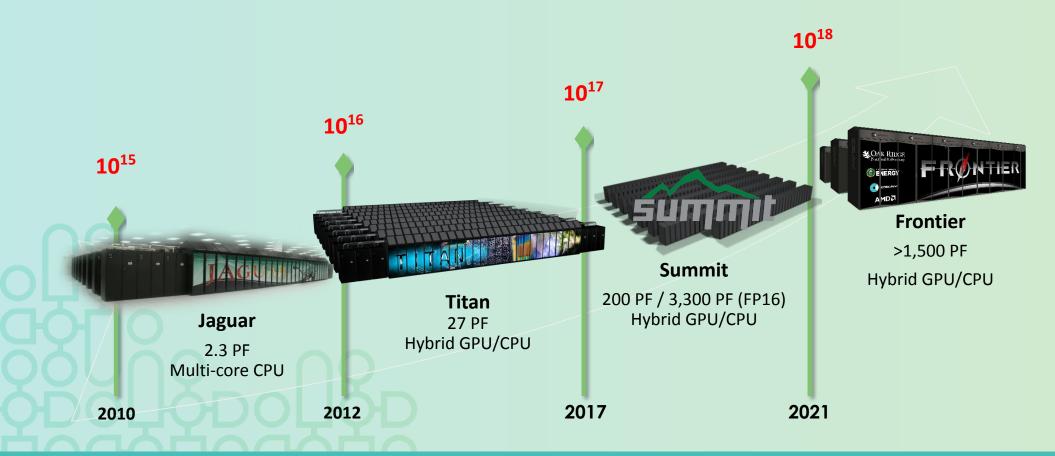
- One of two Department of Energy LCF's
- Based in Oak Ridge, TN at the Oak Ridge National Laboratory (ORNL)
- Department of Energy-funded research
 - Neutron Science, High-Performance Computing, Advanced Materials, Biology and Environmental Science, Nuclear Science and Engineering, Isotopes, and National Security
- Largest, most modern center for unclassified computing in the US



https://www.ornl.gov/sites/default/files/styles/basic_page_hero/public/20 08-P01679.jpg

ORNL has had a Top 10 supercomputer in every year since the OLCF was founded in 2005





Frontier Fun Facts



- 1 Exaflop => 10¹⁸ Calculations per Second
 - Frontier can do in 1 second what would take over 4
 years if everyone on Earth did 1 calculation per second
- Theoretical peak of 2 Exaflop
 - Compute similar to 194,544 PS5s
- Achieved peak of 1.194 Exaflop
 - First exascale system on Top500
- System consists of 9,408 nodes
 - 9,408 CPUs and 75,264 logical GPUs



https://www.flickr.com/photos/olcf/52117588486/

Frontier Fun Facts



- 74 cabinets weighing 8,000 pounds each
 - Total weight similar to a Boeing 747
- 90 miles of cables
 - Denver, CO to Wyoming Border
- 6,000 gallons of water moved per minute
 - Pumps can fill an Olympic pool in 30 minutes
- 700 PB of storage
 - 25 Mt. Everests of DVDs

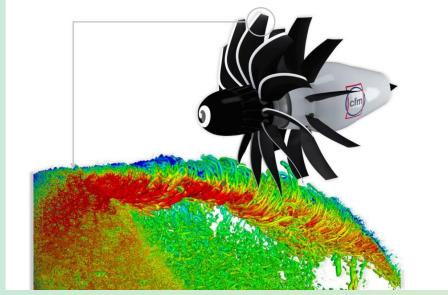


https://www.flickr.com/photos/olcf/52117839159/

Example Use Case



- GE Aerospace is designing next-gen commercial aircraft engines
- Frontier enables better evaluation of engine technologies at flight scale
- Software designed to model engine performance and noise levels
- Resulting runs simulated air movement for a full-scale open fan engine design with incredible detail

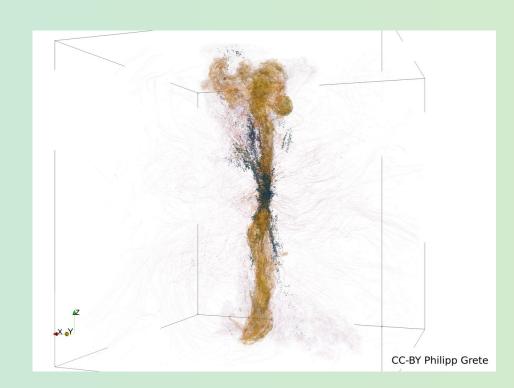


Credit: CFM, GE Research https://www.ornl.gov/sites/default/files/styles/main_image_style/public/202 3-08/GEAerospaceEngine.jpg

Example Use Case



- An INCITE team is simulating a more detailed universe
- Frontier enables higher levels of resolution
- Software designed to model turbulence and feedback from active galactic nuclei jets in galaxy groups and clusters
- Resulting runs simulated the jet and surrounding diffuse plasma with incredible detail





Questions?

This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.