Components of a Research Computing Resource

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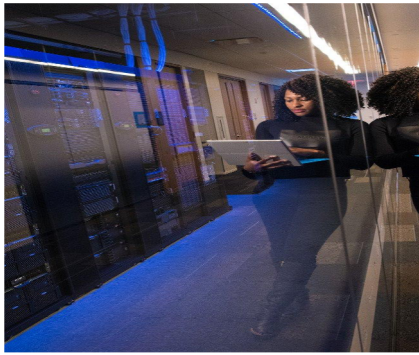
CENTER FOR ADVANCED RESEARCH COMPUTING

- First public HPC Center in the State of New Mexico
- In 2000, UNM, in collaboration with IBM, built the first-ever Linux beowulf cluster in production
- Main research fields:
  - Nuclear
  - Materials science
  - Astrophysics
  - Genome sequencing



What is HPC?

What is a Cluster?

It Depends!

--Henry Neeman

http://www.oscer.ou.edu/acirefvirtres2016_talk_brunson_clusterdesign_20160811.pdf

What is a Cluster!

"... [W]hat a ship is ... It's not just a keel and hull and a deck and sails. That's what a ship needs. But what a ship is ... is freedom."

– Captain Jack Sparrow

"Pirates of the Caribbean"

Credit: Henry Neeman & Dana Brunson

http://www.oscer.ou.edu/acirefvirtres2016_talk_brunson_clusterdesign_20160811.pdf

“High-performance computing (***HPC***) is the use of ***parallel processing*** for running ***advanced application*** programs efficiently, reliably, and quickly.”

http://searchdatacenter.techtarget.com/definition/high-performance-computing-HPC

A cluster **needs** of a collection of small computers, called ***nodes***, hooked together by an ***interconnection network*** (or ***interconnect*** for short).

It also **needs** software that allows the nodes to communicate over the interconnect.

But what a cluster **is** … is all of these components working together as if they’re one big computer ... a **super** computer.

Credit: Henry Neeman & Dana Brunson

http://www.oscer.ou.edu/acirefvirtres2016_talk_brunson_clusterdesign_20160811.pdf

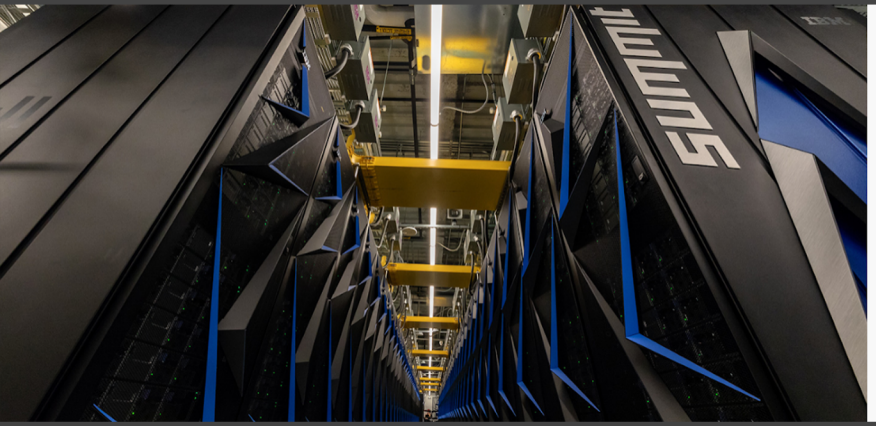
image courtesy of medium.com

Computer Simulation

A computer simulation is a program that attempts to reproduce an **abstract model** of a particular system in the **virtual space** before building it in **reality**.

Parallelism

Performing computations in **parallel** by carrying out many calculations **simultaneously**. Utilizing thousands of general-purpose computers all working together to solve the same **problem** at the **same time**. This in fact is an excellent case for how **modern** supercomputers work.



Summit in its natural habitat - America's Fastest and Smartest HPC Cluster

image courtesy of Oak Ridge National Laboratory website

But, Why?

1. To resolve tomorrow’s problems, which can’t be studied using today’s infrastructure, by using computer simulations
2. Cluster HPC helps bypassing the limitations of Moore's law
3. Increase the research outcomes by an order of magnitude by manipulating excessive data points and machine learning
4. Solve expensive and dangerous problems in simulations

HPC Challenges..

Staffing

$$$

Power, Space, Cooling

Return on Investment (ROI)

“The Purpose of Research Computing is the Research, not the Computing”

Jonathan Dursi - https://www.dursi.ca/post/purpose-of-research-computing

Hats HPC staff “geeks” wear

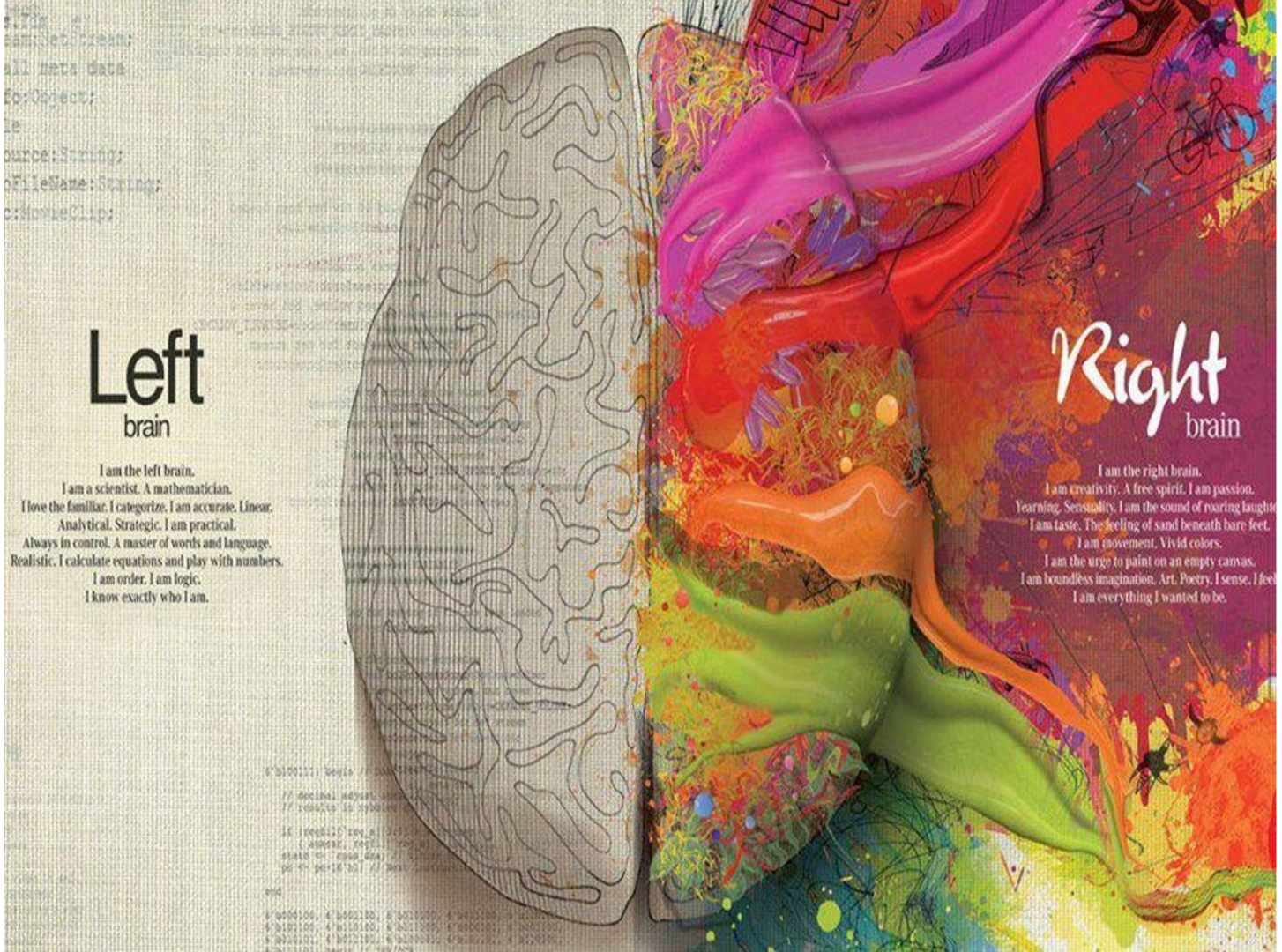
- HPC Engineer
- Security/Network/Storage
- Research and Development
- CI Facilitator/Applications Scientist
- Negotiator and translator (Enterprise <-> Research)
- Heating, ventilation, and air conditioning (HVAC)

“Mile wide and half inch deep”

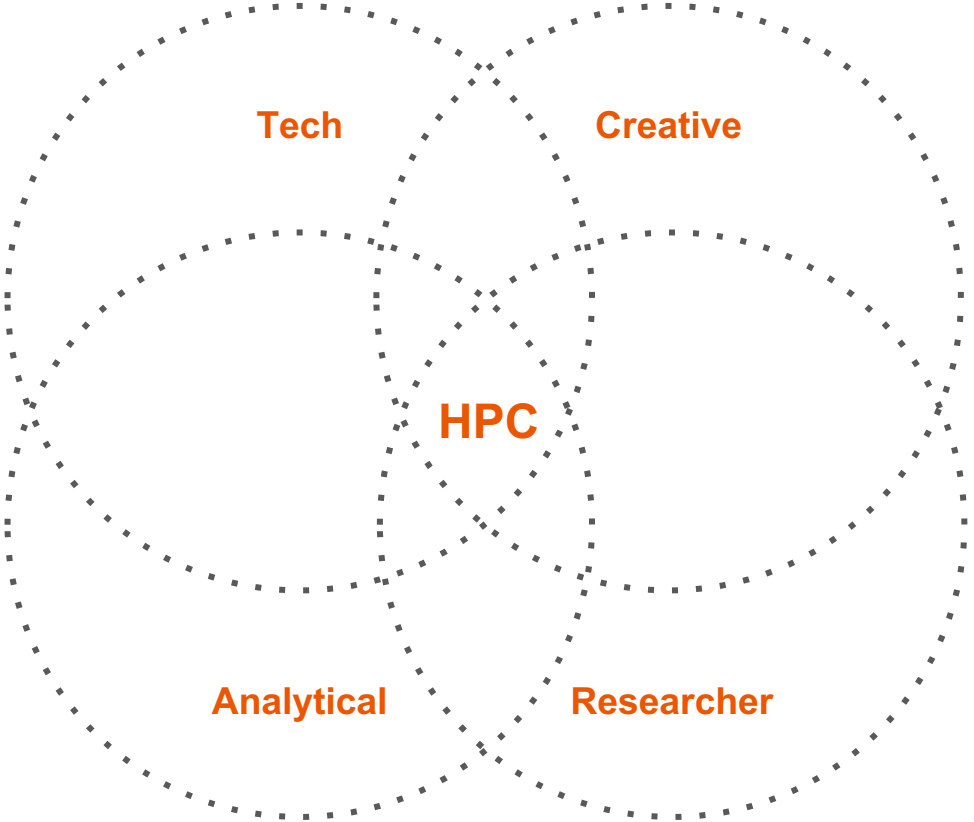
"It couldn’t be a grad student; we had to hire a real person."

--Anonymous ;)

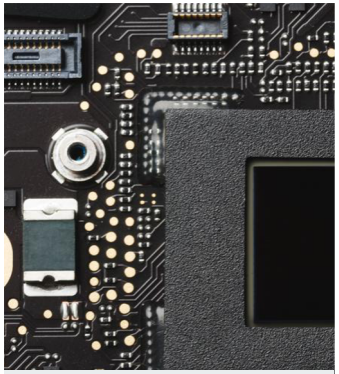
Understanding the Design


Left
brain
I am the left brain.
I am a scientist. A mathematician.
I love the familiar. I categorize. I am accurate. Linear.
Analytical. Strategic. I am practical.
Always in control. A master of words and language.
Realistic. I calculate equations and play with numbers.
I am order. I am logic.
I know exactly who I am.
Right
brain
I am the right brain.
I am creativity. A free spirit. I am passion.
I am taste. The feeling of sand beneath bare feet.
I am movement. Vivid colors.
I am the urge to paint on an empty canvas.
I am everything I wanted to be.

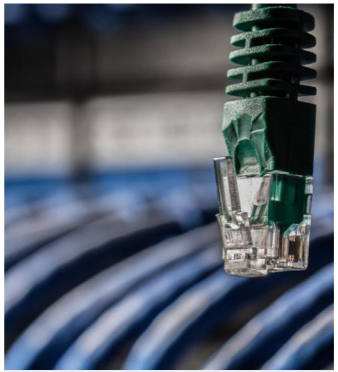
Point of View



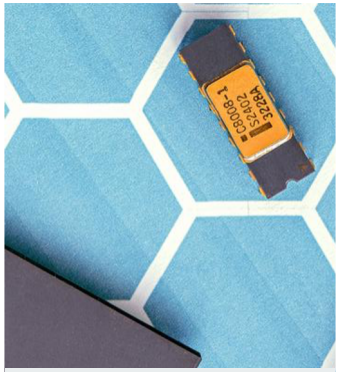
Cluster Components



Compute

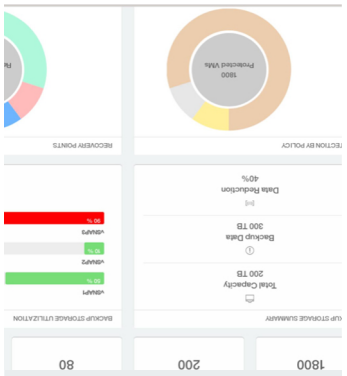


Network



Storage

Batch Scheduler



HPC SW

Compute

- CPU
- GPU
- Memory
- Interconnects
- Diskful/Diskless

Network Interconnects

Main factors:

- Latency
- Bandwidth

Types

- InfiniBand
- Ethernet

image courtesy of Mellanox Store website

Storage

Storage Usage

- Home directories
- Scratch space
- Project space

Storage Types

- Traditional file systems
- Parallel file systems

Resource Manager/ Scheduler

Resource Manager oversees the available resources of the cluster

- Warewulf, xCAT..

Scheduler determines what runs where..

- Slurm, Torque, Moab..

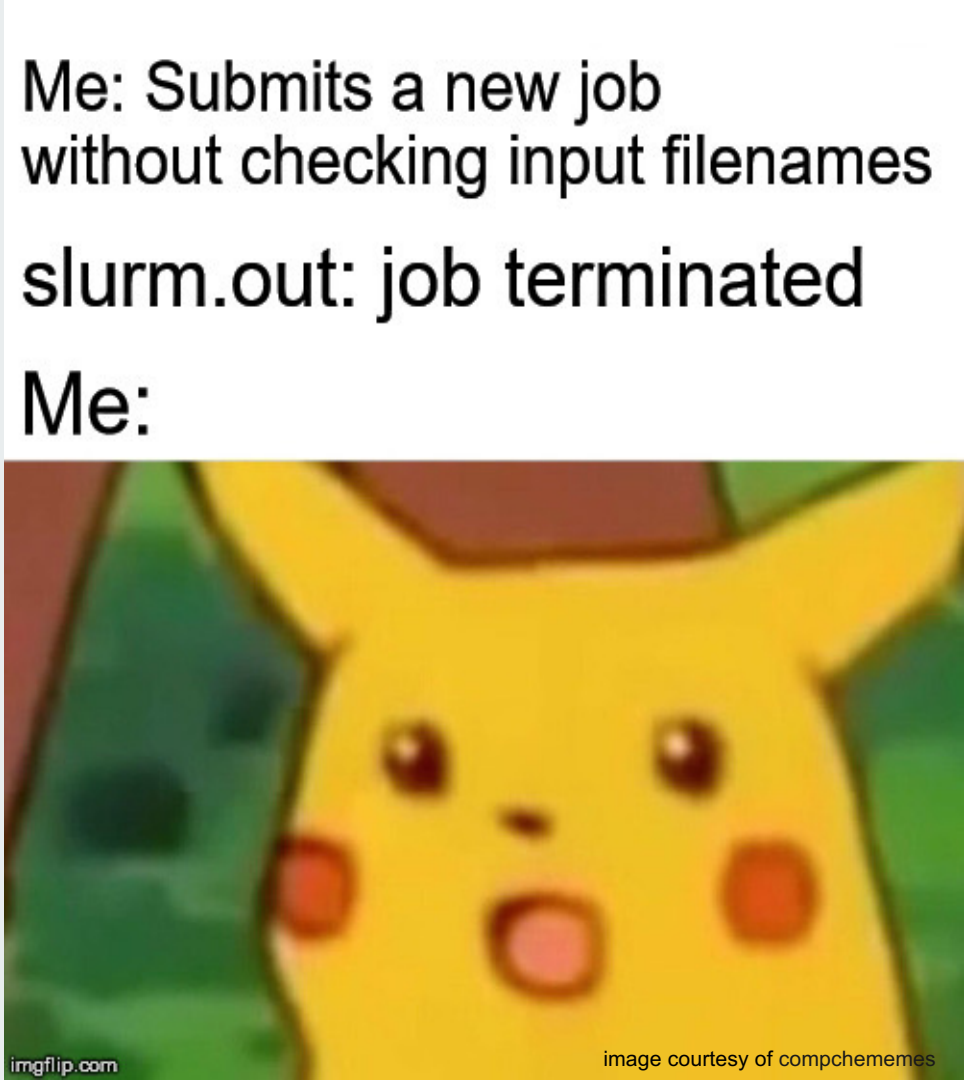


image courtesy of compchememes

HPC Software

- General usage
- Field dependant

Other Components

- Management/Head nodes
- Login nodes
- Benchmarks
- Security and logs
- Monitoring utilities
- Backup systems
- Cooling systems
- Backup power
- Licensing
- Web interfaces/science gateways
- Data Transfer Nodes (DTN)
- Science DMZ

http://www.oscer.ou.edu/acirefvirtres2016_talk_brunson_clusterdesign_20160811.pdf

Traditional HPC Cluster

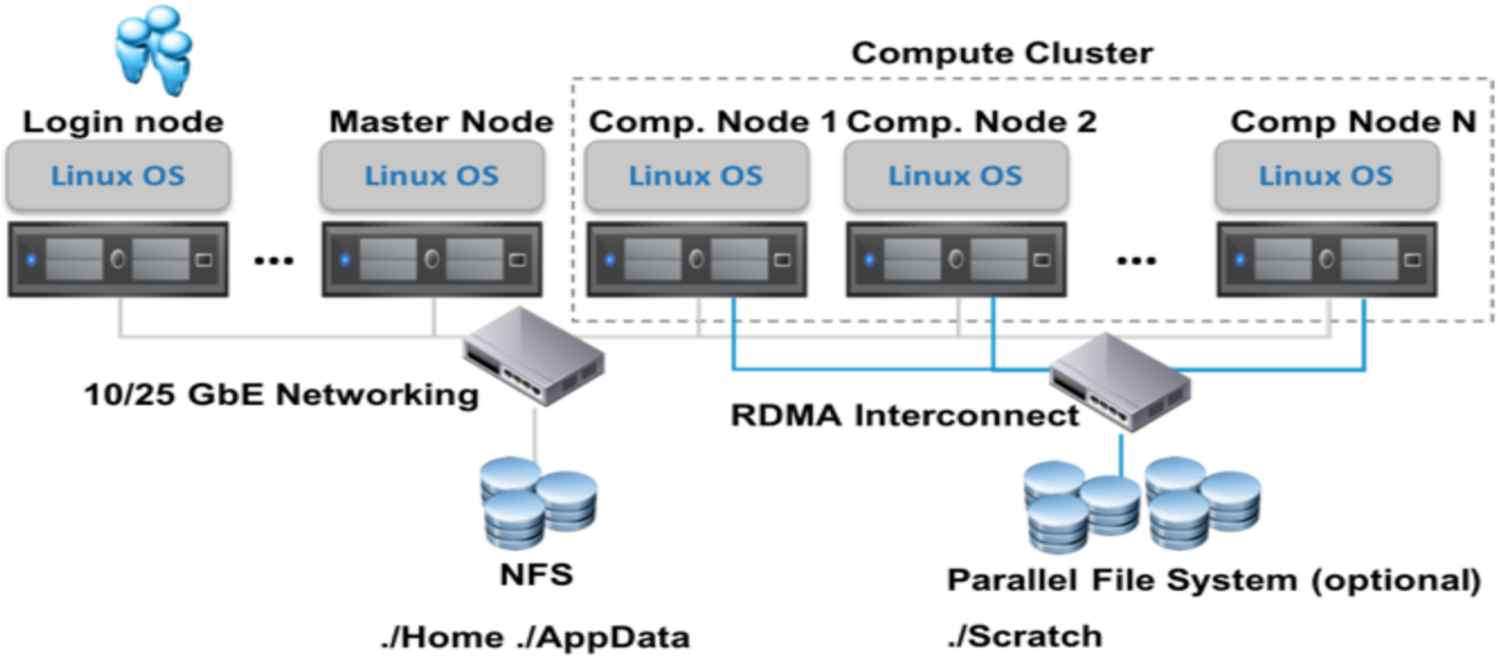


image courtesy of VMware Blogs website

Acquisition start to finish

- Get Money
- Spec system based on what's needed
- Get bids (informally or formally)
- Buy
- Don't sign acceptance before you test everything with at least some of your workloads

Be warned: No matter what you do, the minute you send out the PO you'll think of something you should've done differently.

And it's okay, we all feel that way.

http://www.oscer.ou.edu/acirefvirtres2016_talk_brunson_clusterdesign_20160811.pdf

HPC in the Cloud

Pros

- Cost
- Easy to build
- Cloud bursting
- Huge business investments

Cons

- Cost
- Compliance
- Vendor specific
- Harder to track on the institutional level

Cloud/Virtualized HPC Cluster

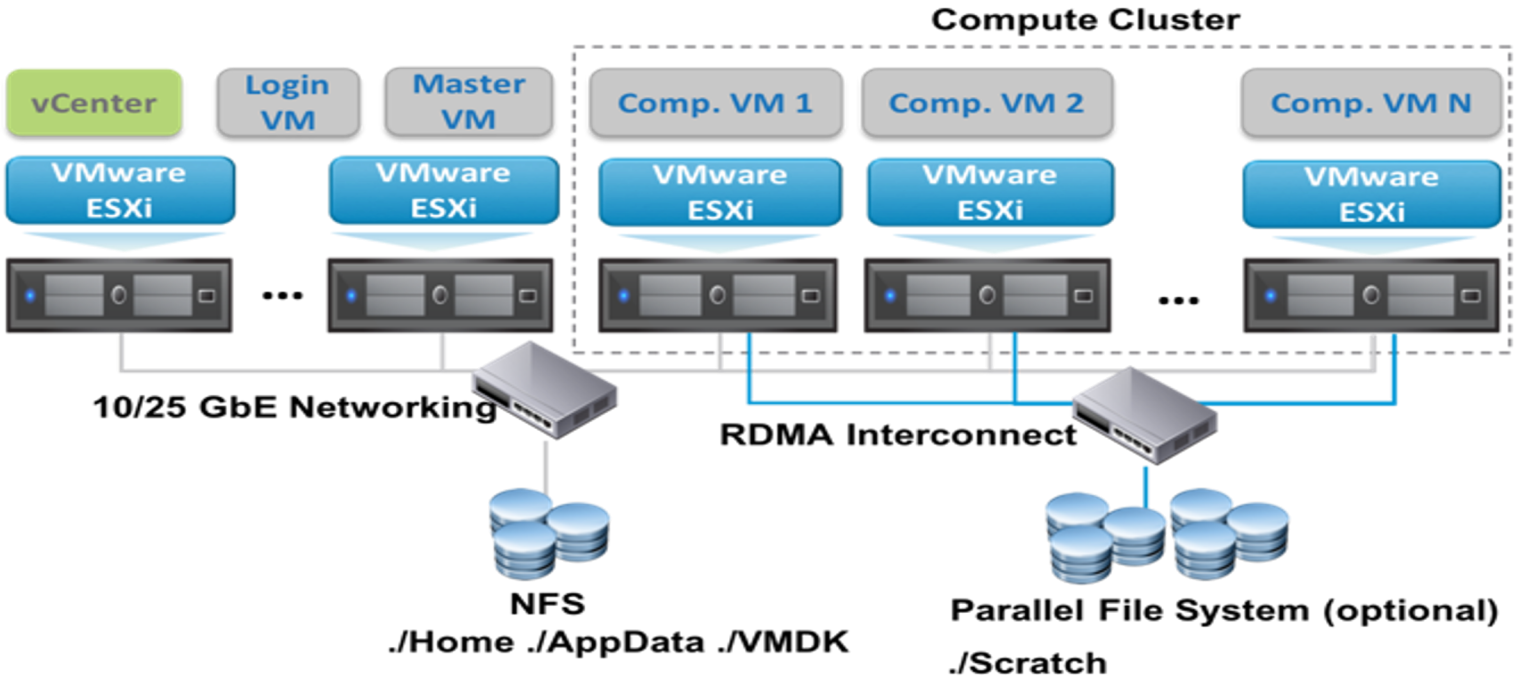


image courtesy of VMware Blogs website

Computational Science vs Computer Science

How long is a trillion seconds?

~32,000 years

Computers store numbers in floating-point format, so they are called floating-point numbers.

A single instruction like addition or multiplication is called an operation,

HPC speed is measured in terms of floating-point operations per second or Flop/s (Flops)

Rmax - Maximal LINPACK performance achieved

Rpeak - Theoretical peak performance

Ops per second	Scientific Notation	Metric Prefix	Unit
1 000	10^3	Kilo	Kflops
1 000 000	10^6	Mega	Mflops
1 000 000 000	10^9	Giga	Gflops
1 000 000 000 000	10^{12}	Tera	Tflops
1 000 000 000 000 000	10^{15}	Peta	Pflops
1 000 000 000 000 000 000	10^{18}	Exa	Eflops

Performance

CPU clock frequency in GHz
Clock speed in cycles per second (Hertz)
# of floating-point operations per cycle

Example:
2.6 GHz processor
2.6 billion cycles per second
16 floating-point operations per cycle
16 x 2.6 billion = 41.6 Billion Flops
41.6 GFlops

Top 500 History - Peak Speed (Rmax)

1993
Loremujitsu Numerical Wind Tunnel
124.50 GFLOPS
National Aerospace Laboratory, Tokyo, Japan

1997
Intel ASCI Red/9152 1.338 TFLOPS
DoE-Sandia National Laboratories, New Mexico, USA

2008
IBM Roadrunner 1.026 PFLOPS
DoE-Los Alamos National Laboratories, New Mexico, USA

2018
IBM Summit 122.3 PFLOPS
DoE-Oak Ridge National Laboratory, Tennessee, USA

2021
Leonardo 250 PFLOPS,
10 ExaFLOPS of FP16 AI performance
EuroHPC Italy "pre-exascale"

20XX
TBD - First EFLOPS?

https://www.top500.org/

https://www.cineca.it/en/hot-topics/Leonardo-announce

Quantum Computers

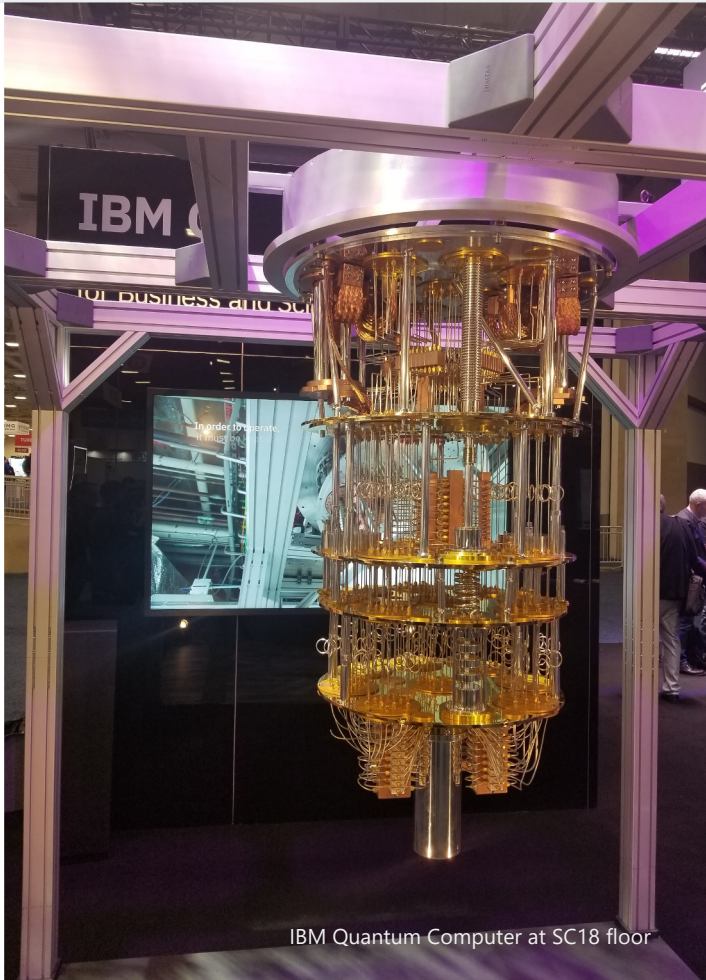
Transistors are already at the atom size,, what's next!

The use of quantum-mechanical phenomena such as superposition and entanglement to perform computations.

Qubits vs Binary bits

- 1 or 0 quantum state
- 1 and 0 superposition states

Using quantum algorithms to solve specific complex problems beyond the capabilities of a classical HPC



IBM Quantum Computer at SC18 floor

Great article by Scott Aaronson

“What Makes Quantum Computing So Hard to Explain?”

“

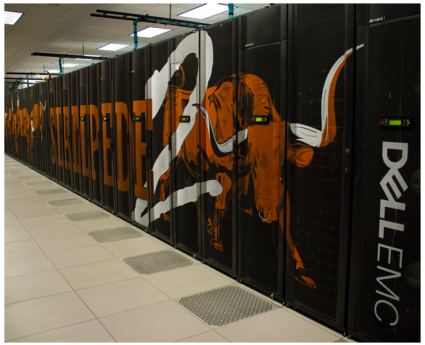
- What superposition really means is “complex linear combination.”
- “complex” in the sense of a real plus an imaginary number, while “linear combination” means we add together different multiples of states.
- So a qubit is a bit that has a complex number called an amplitude attached to the possibility that it’s 0, and a different amplitude attached to the possibility that it’s 1.
- These amplitudes are closely related to probabilities, in that the further some outcome’s amplitude is from zero, the larger the chance of seeing that outcome; more precisely, the probability equals the distance squared.

”

https://www.quantamagazine.org/why-is-quantum-computing-so-hard-to-explain-20210608/

XSEDE HPC Systems

01 | Stampede2 | TACC
02 | Comet | SDSC
03 | Bridges-2 | PSC
04 | Jetstream | IU
05 | Open Science Grid | OSG
06 | Ranch | TACC



XSEDE

Extreme Science and Engineering Discovery Environment

image courtesy of XSEDE website

https://www.xsede.org/ecosystem/resources

Thank You!

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