Class 2

All about Computers and
High Performance Computing

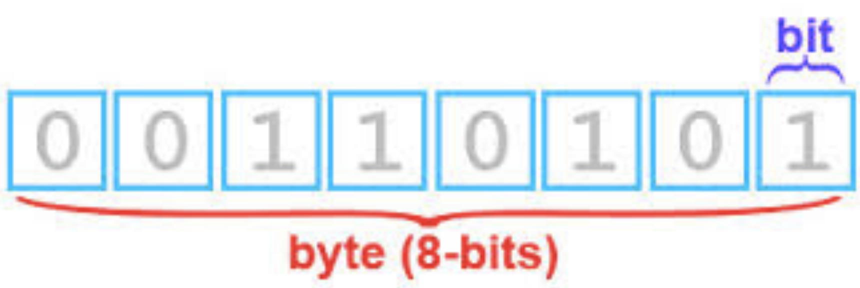
Goals

- Understand high performance computational resources
- ACF – the UTK cluster
- Set up and manage a project directory

Start at the beginning

- The basics of a personal computer
- Computers use a language of 0s and 1s

- Bit = a single stored unit that is either 0 or 1
- Byte = a set of 8 bits



Processor

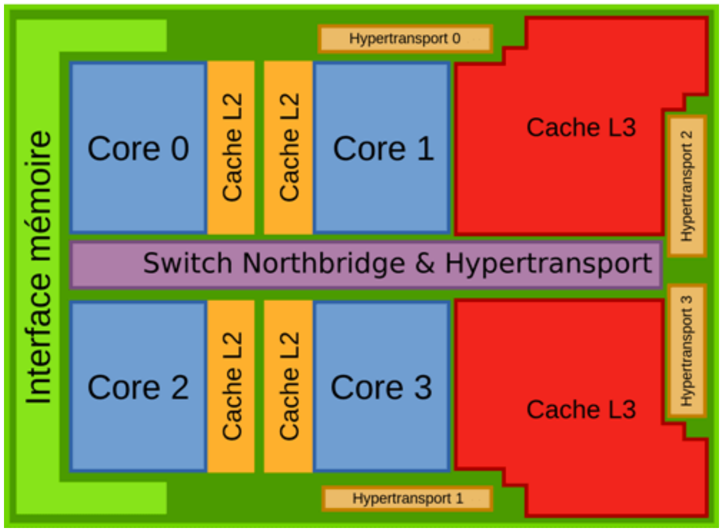
Processor

- The “brain”
- Executes instructions with electronic circuits
- “Clock Speed” is measured in gigahertz (GHz)
- Billions of operations per second (sort of)
- Manufacturers include Intel and AMD
- Also known as: **Central Processing Unit (CPU)**

CPUs are usually 64-bit now (used to be 32-bit, this refers to the amount of data that can be operated on at one time)

Cores

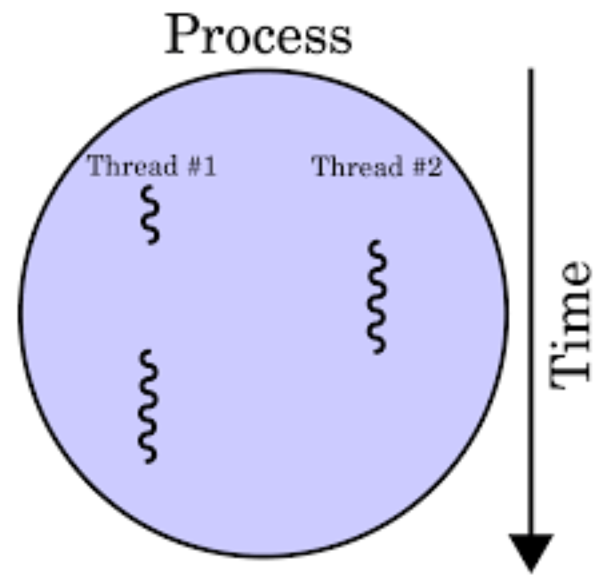
- A processor used to contain only one set of circuits.
- Now processors can contain many “cores”
- Dual core/ Quad core



There are 4 cores in this tiny chip

Multi-threaded

- A single core can run more than one job
- When you run one job on a core, sometimes the core is waiting
- Instead of waiting, work on a different job
- Switch back and forth between jobs, thus getting two things done in the same amount of time



Random Access Memory (RAM)

- This is short term memory
- Fast memory
- CPUs can only load from RAM really fast
- Lots of RAM lets your computer do more things at once or access more data at once
- Stored information is lost if power is lost

8Gb of RAM is currently common for personal computers; 16Gb is also available

Hard Drive

internal

external

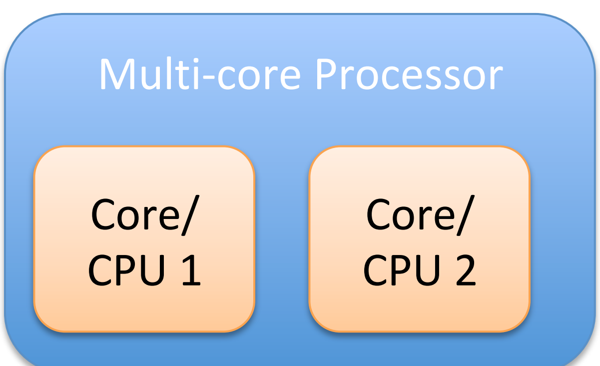
- Long term storage
- Slow memory
- Data is not lost if power is lost
- When you “open” software or a file, the information is loaded from the hard drive to RAM
- The processor can access the information from RAM much faster
- Saving the file writes the new information back to the hard drive

Memory Review

<u>RAM</u>

"Memory"

- Fast
- Expensive
- Volatile

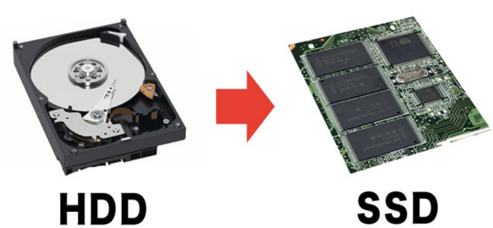


<u>Hard drive</u>

"Filesystem"

"Storage"

- Slow
- Cheap
- Not Volatile



<u>Solid state</u> drives are 5-10X faster than hard drives, but more expensive.

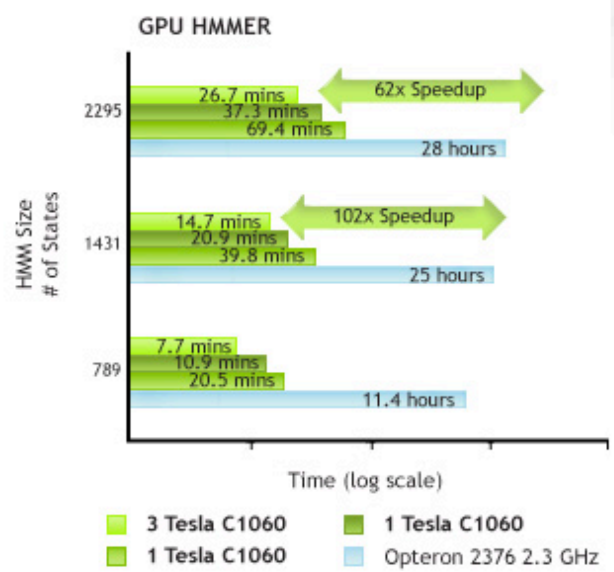
Graphical Processing Unit (GPU)

- Video card
- Specialized CPUs for image processing and computer graphics (monitor, phone screen)
- Highly parallel
- Most processing involves matrix and coordinate systems – this leads to…
- GPUs being co-opted for use in bioinformatics algorithms

Graphical Processing Unit (GPU)

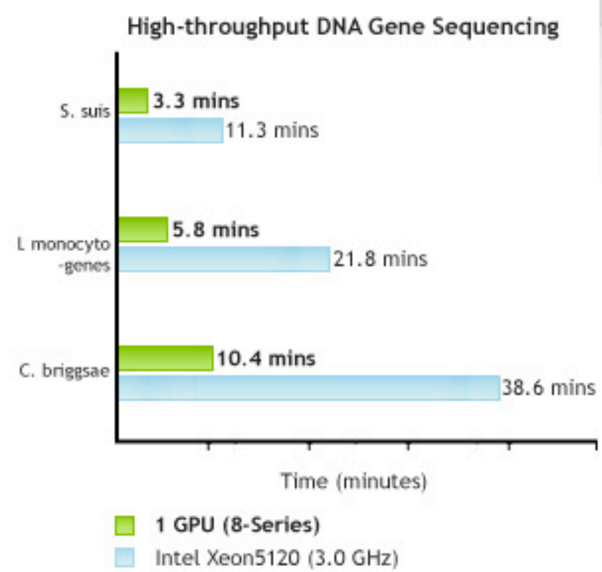
BIOINFORMATICS AND LIFE SCIENCES

Sequencing and protein docking are very compute-intensive tasks that see a large performance benefit by using a CUDA-enabled GPU. There is quite a bit of ongoing work on using GPUs for a range of Bioinformatics and life sciences codes.



Accelerating HMMER using GPUs

Scalable Informatics



MUMmerGPU: High-through DNA sequence alignment using GPUs

Schatz, et al

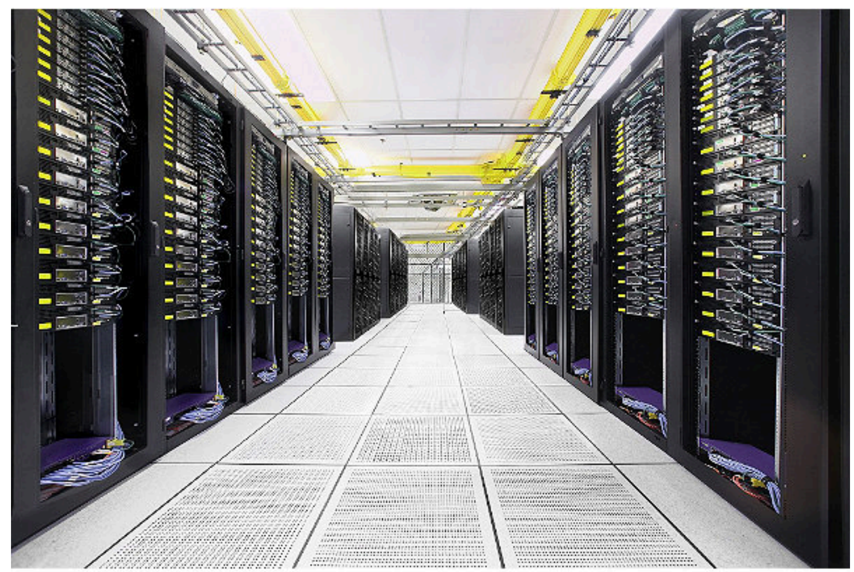
http://www.nvidia.com/object/bio_info_life_sciences.html

High performance computing (HPC)

- Large data is often too much for your small laptop or desktop to handle
- Move to a large computer or clusters of computers – ie “remote” computers
- called **<u>servers</u>**
- HPCs are also called supercomputers

Type the commands

Actual work being done here



Scaling up inside one computer

My “workhorse” computer

- 4 processors
- 10 cores per processor
- = 40 jobs at once
- 512 Gb of RAM
- ~ $14k
- Lives in the UTK server room with other computers

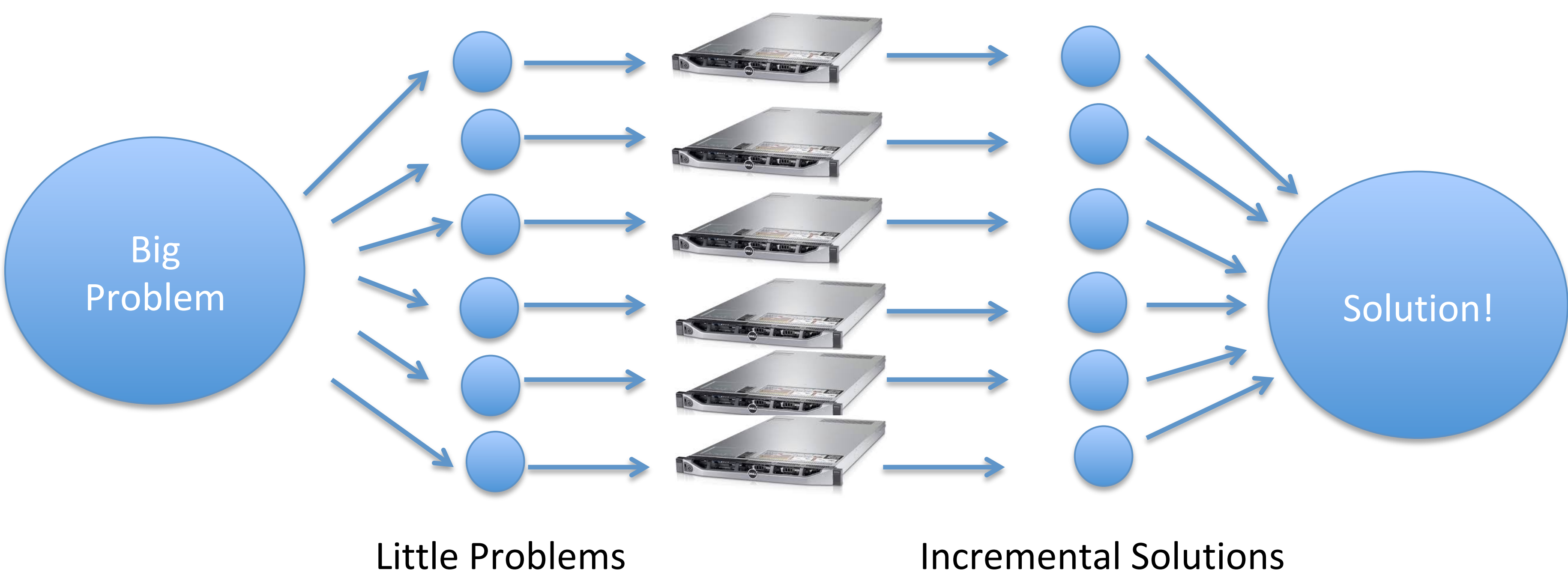
This is by no means a particularly large supercomputer by research standards.

Scaling up to many computers

- Massively parallel
- Tens of thousands of processors across thousands of machines
- Need controller software to coordinate activities
- Individual computers do not share RAM

Parallelism

- dividing a single job among multiple processors
- Objective is to run a program in less time
- Some activities are more easy to divide than others
- There are different ways to have parallel processing



Single Server

- Many CPUs in a single computer
- All can access the same RAM

- Many people are all in the same room
- Puzzle pieces are all on a table in the middle

- People = CPUs
- Puzzle pieces = Data
- Table = RAM

Parallel (Multi-computer, or “distributed memory”)

- Split the job across different computers
- RAM is not shared

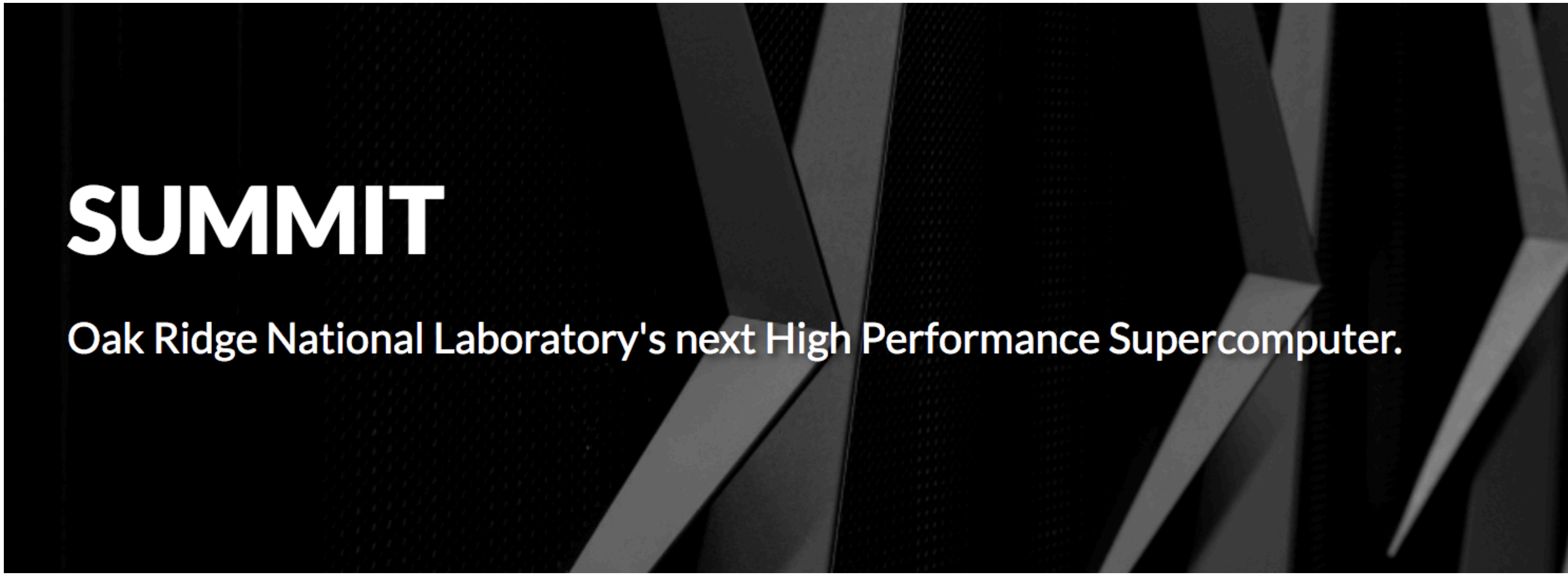
- People are in different rooms
- Puzzle pieces must be divided up between each person
- Some things are easier to divide up than others

- People = CPUs
- Puzzle pieces = Data
- Table = RAM

Parallel processing

- Parallel across computers is much more difficult to implement for complex problems
  - Assembly
- Fortunately we have many problems in bioinformatics that are modular and scale gracefully to many computers ("embarrassingly parallel") – little to know work is involved in splitting the problem into small pieces
  - BLAST
  - Sequencing alignments
- If software can be automatically run across many computers, documentation will usually mention MPI (message passing interface)

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY



Processor: IBM POWER9™

GPUs: NVIDIA Volta

Nodes: 4,608

Node Performance: 42TF

Memory/node: 512GB DDR4 + 96GB HBM2

NV Memory/node: 1600GB

Total System Memory: >10PB DDR4 + HBM + Non-volatile

Interconnect Topology: Mellanox EDR 100G InfiniBand, Non-blocking Fat Tree

Peak Power Consumption: 13MW

Advanced Computing Facility (ACF)

- Scientific Linux
- Any UTK affiliated researcher (student, faculty or staff) can get access
- Higher priority access for those who buy in
- Monster Node! 1Tb of RAM shared across 48 cores

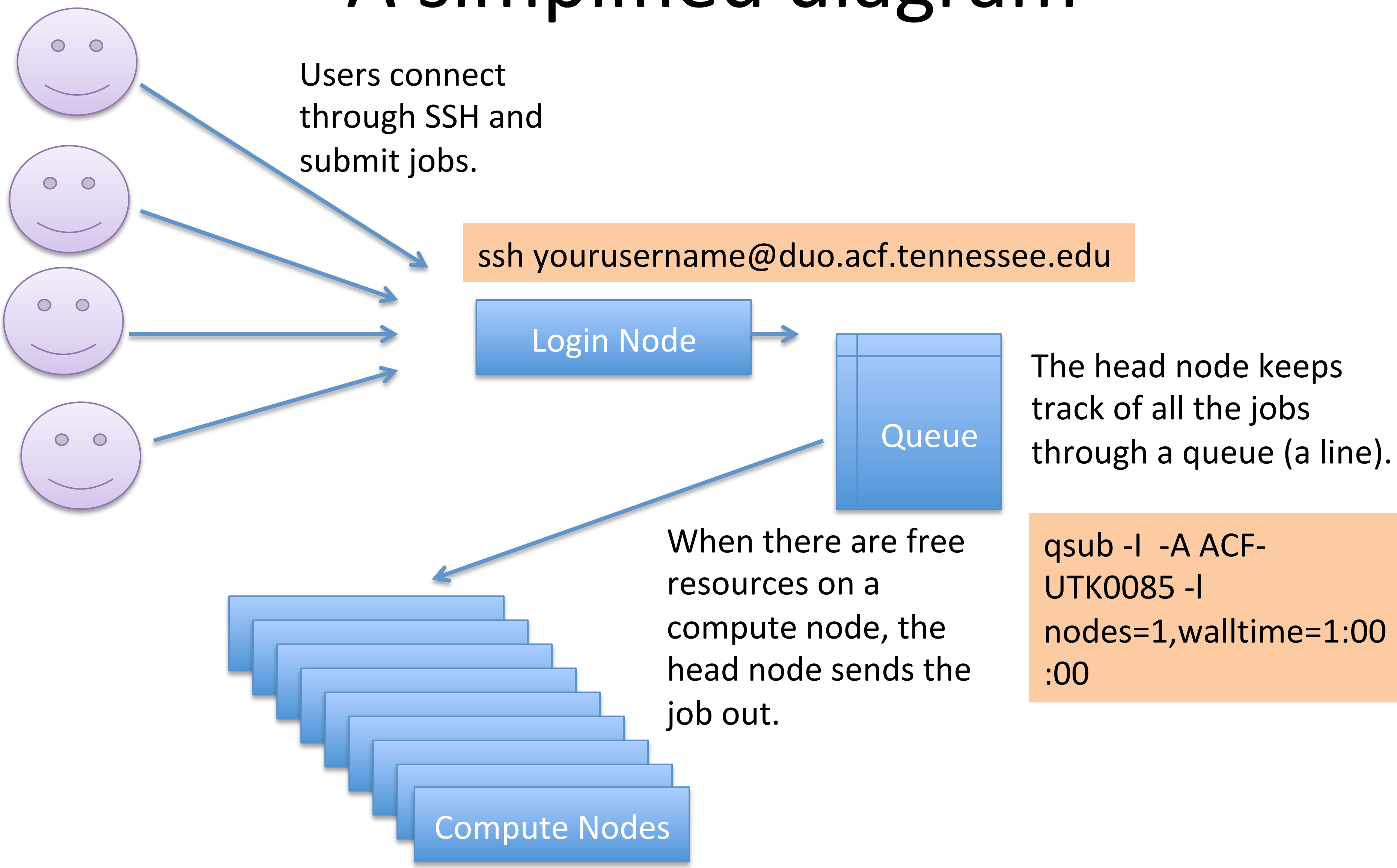
https://www.nics.tennessee.edu/computing-resources/acf

Submit via

Mixed architectures

Node Set	Intel® Xeon® CPU	Nodes	Cores/Node	GB Mem/Node	Total Cores	Interconnect
beacon	E5-2670	43	16	256	688	FDR
rho	E5-2670	48	16	32	768	QDR
sigma	E5-2680	108	24	128	2,592	FDR
sigma_bigcore	E5-2680	10	28	128	280	FDR
monster	E5-2687W	1	24	1,024	24	Ethernet
knl	Phi® 7210	4	64	256	256	EDR
skylake	Gold 6148	16	40	192	640	EDR
skylake_volta	Gold 6148 NVIDIA V100 GPU	1	40	40	40	EDR
Totals		**231**		**32,768**	**5,288**	

A simplified diagram



SSH

- Secure shell
- Network protocol – secure channel of communication between a client and a server
- This is the most common way to connect to a remote computer
- Its encrypted and its available on all UNIX/Linux systems
- To log into ACF, you should ssh into the login node:

ssh yourusername@duo.acf.tennessee.edu

Text editors

- Programming must be done with a text editor
  - Plain text, not Word
  - Nano is okay but not very feature-rich
- Python needs text to be well formatted. Whitespace matters.
- Recommended (and free):
  - vim (for the brave)
  - emacs (for the brave who want to argue with vim'mers)
  - gedit (for the time constrained who want to move fast)

Grid Engine

- The software for distributed resource management (ie computational cluster)
- Determines when and where to execute jobs
- Manages resources (keeps jobs from trying to use the same resources)
- Determines user priority and job priority
- Optimizes – like a puzzle, tries to figure out how to get the most jobs executed in the fastest amount of time

No computation on the head node.

Anything that will run for longer than a minute or take more than 1Gb of RAM should be submitted to the scheduler

The grid engine is like an air traffic controller.

A simplified diagram