Introduction to High Performance Computing in Bio Sciences

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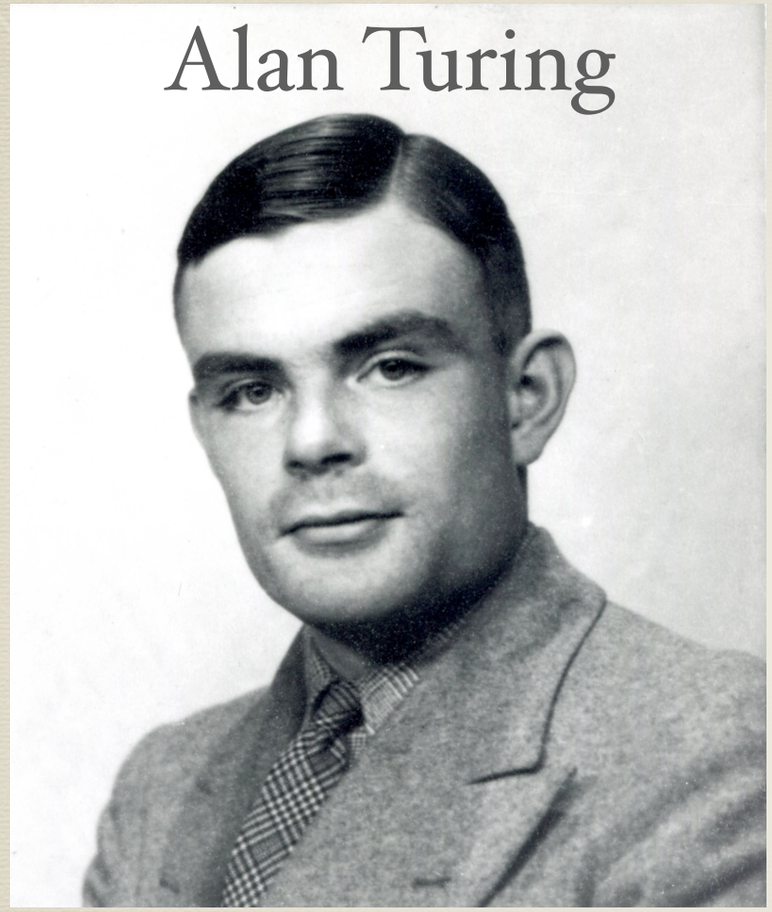
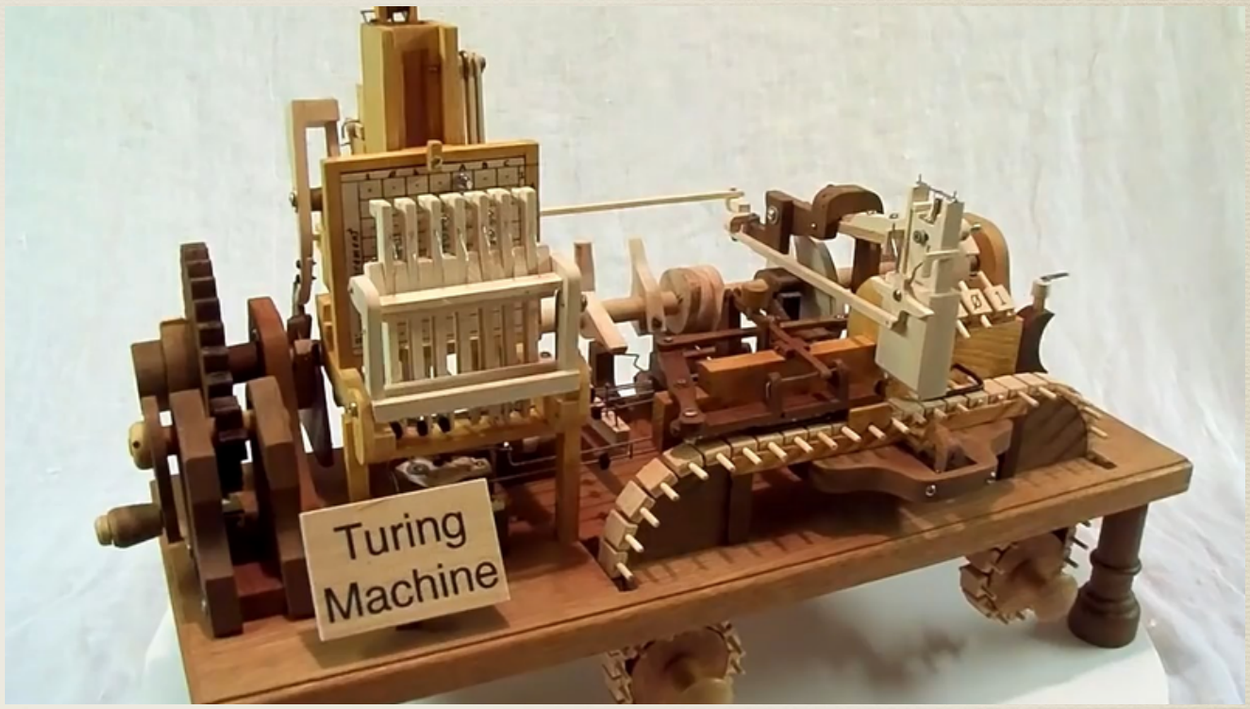
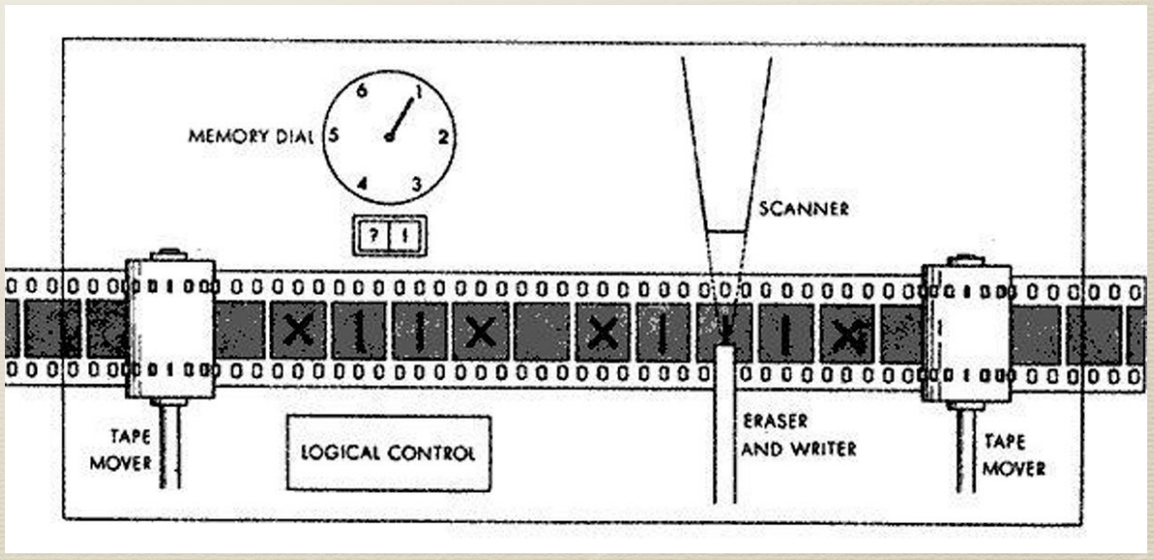
What is a Computer?

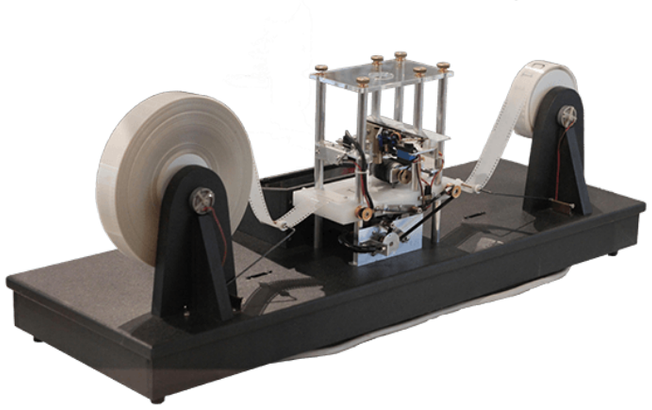




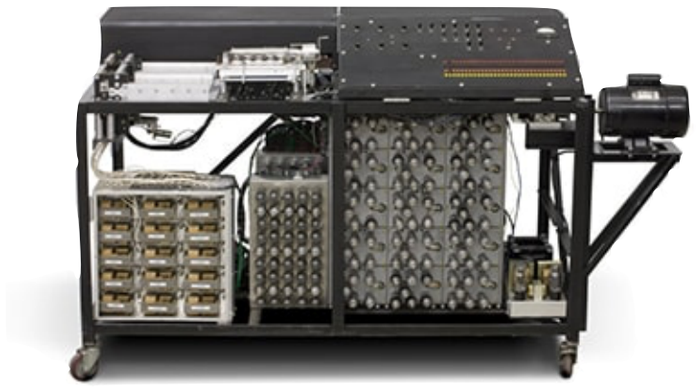
In 1936 he proposed an abstract machine that manipulates symbols on a strip of tape according to a table of rules.



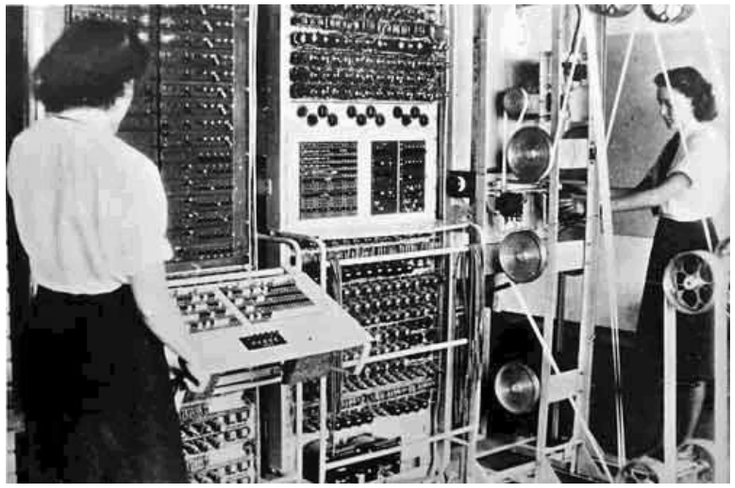
Evolution



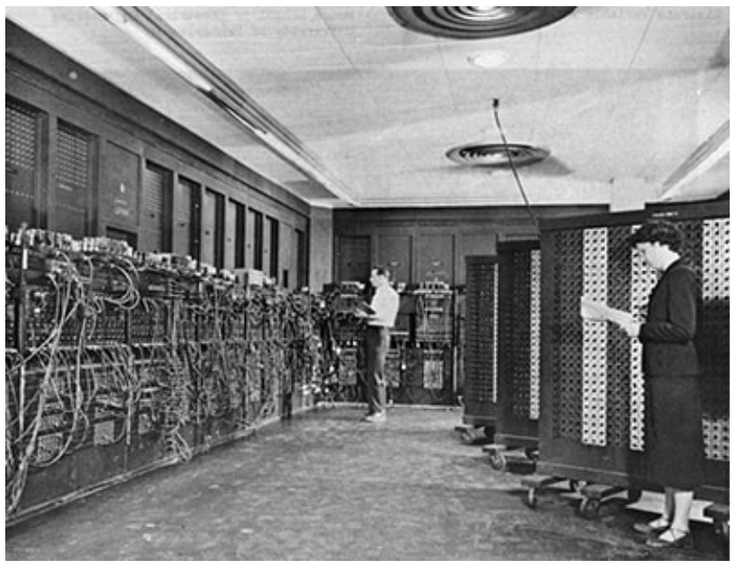
1936 Turing (the concept)



1942
Atanasoff-Berry
Computer (ABC)



1943 Colossus



1946 ENIAC

1975
IBM 5100

1981
Osborne 1

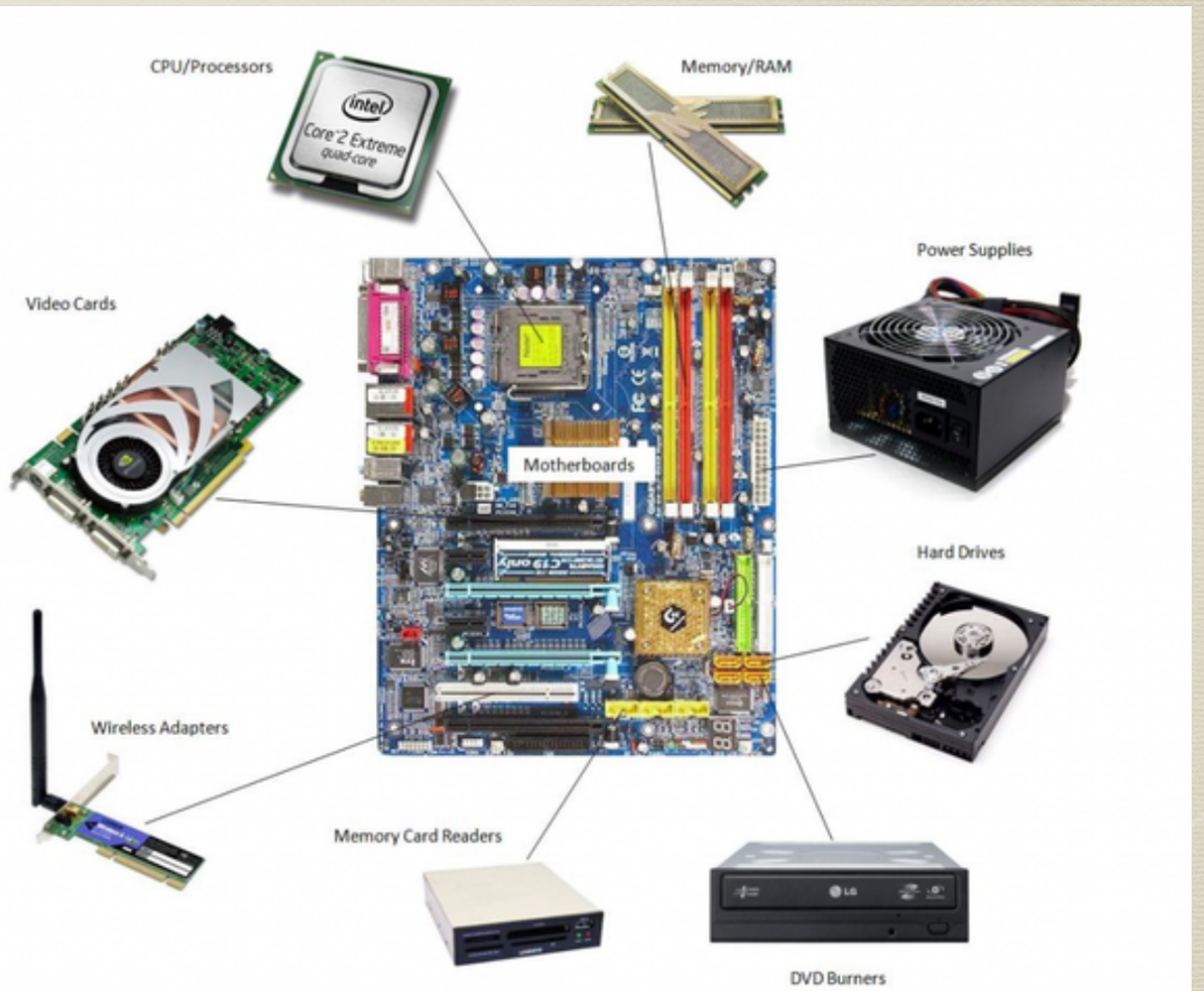
1965 Programma 101

1976 Apple 1

1981
IBM 5150

Images from the Blog "History of Modern Computer"

Parts of a Computer



Genomics: How big are genomes?

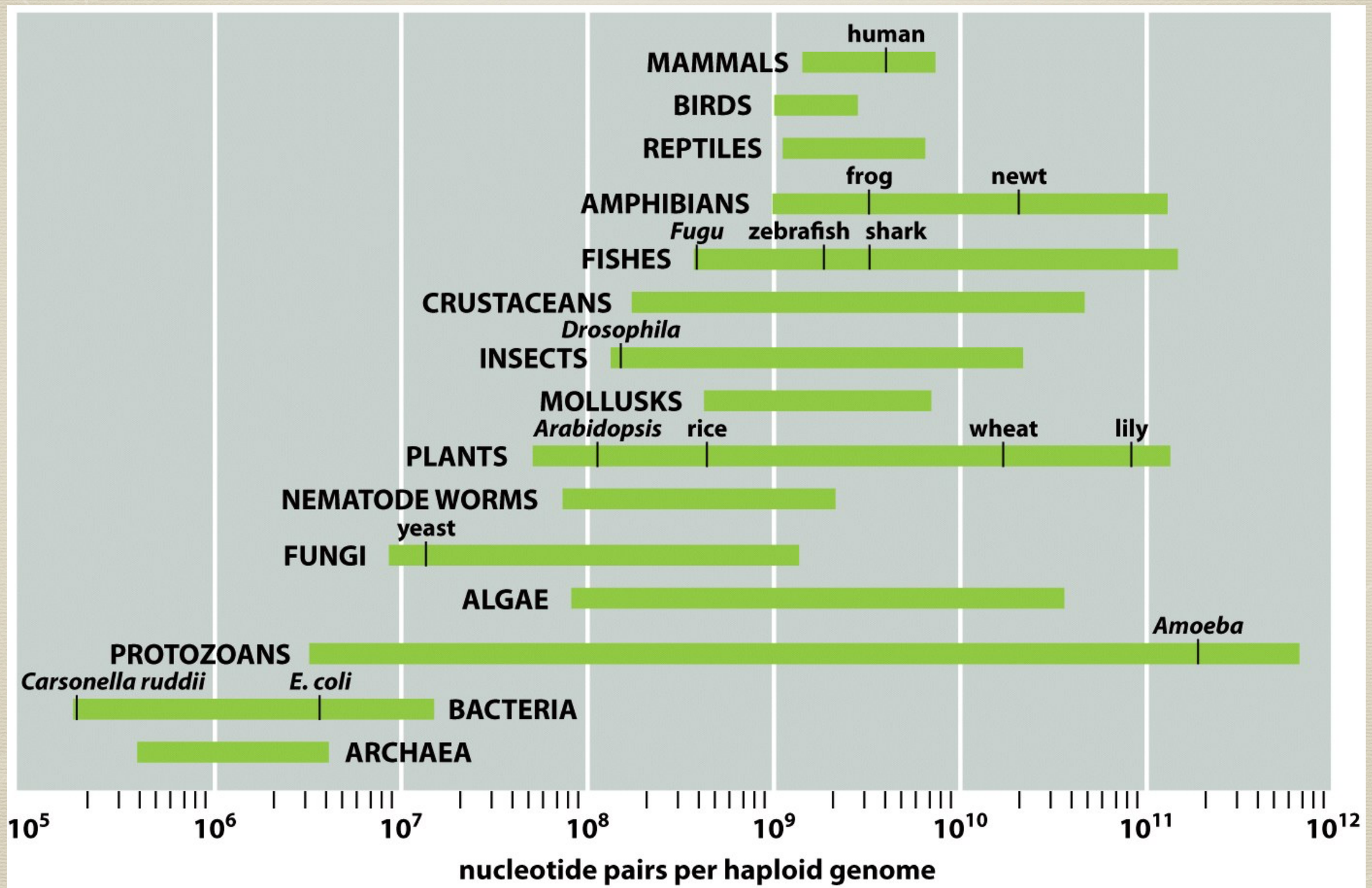


Figure 1-41 Essential Cell Biology 3/e (© Garland Science 2010)

The Future of Genomic Data

Scott D. Kahn

Science 11 Feb 2011
Vol. 331, Issue 6018,
pp. 728-729

DOI:
10.1126/science.1197891

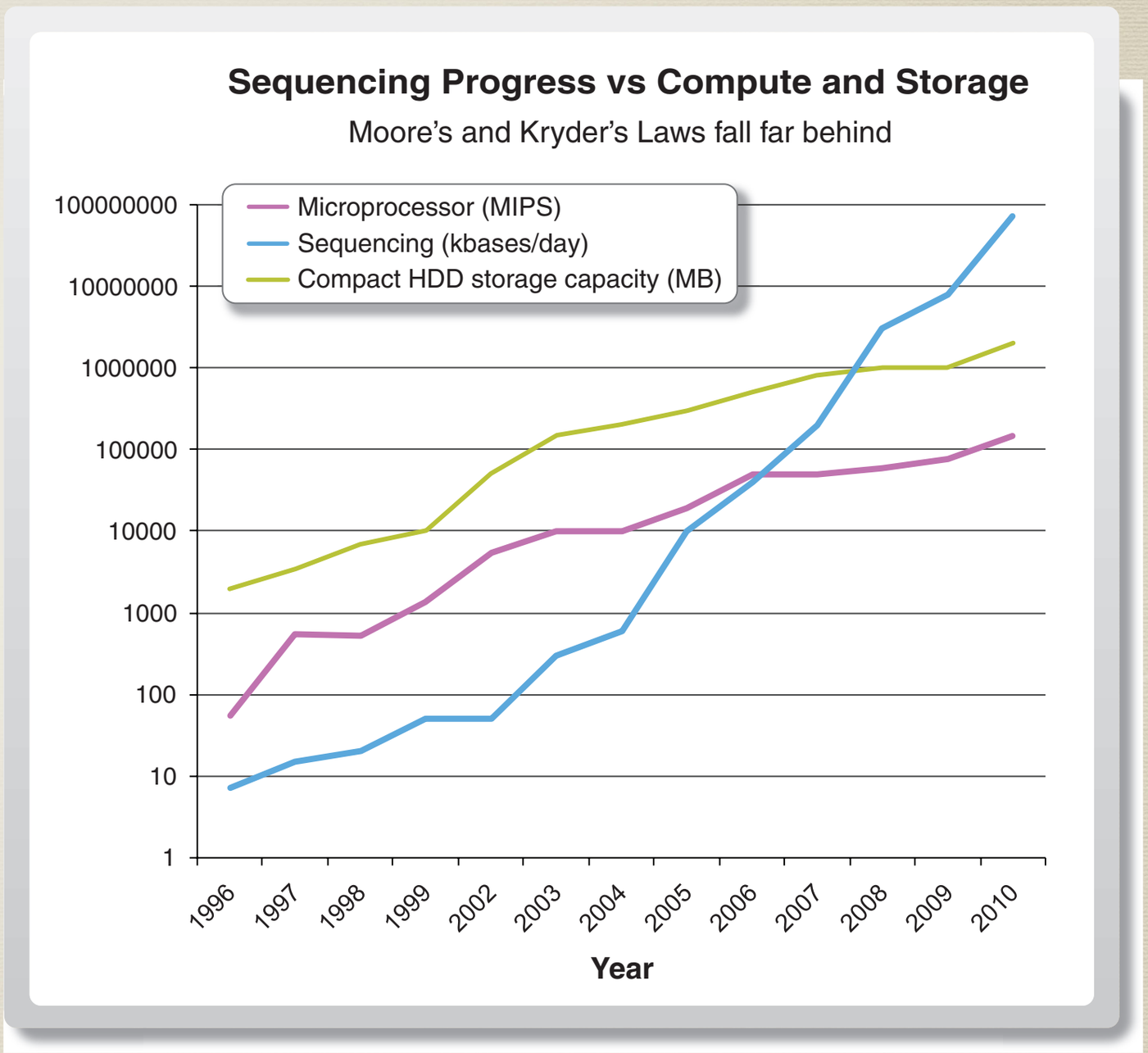
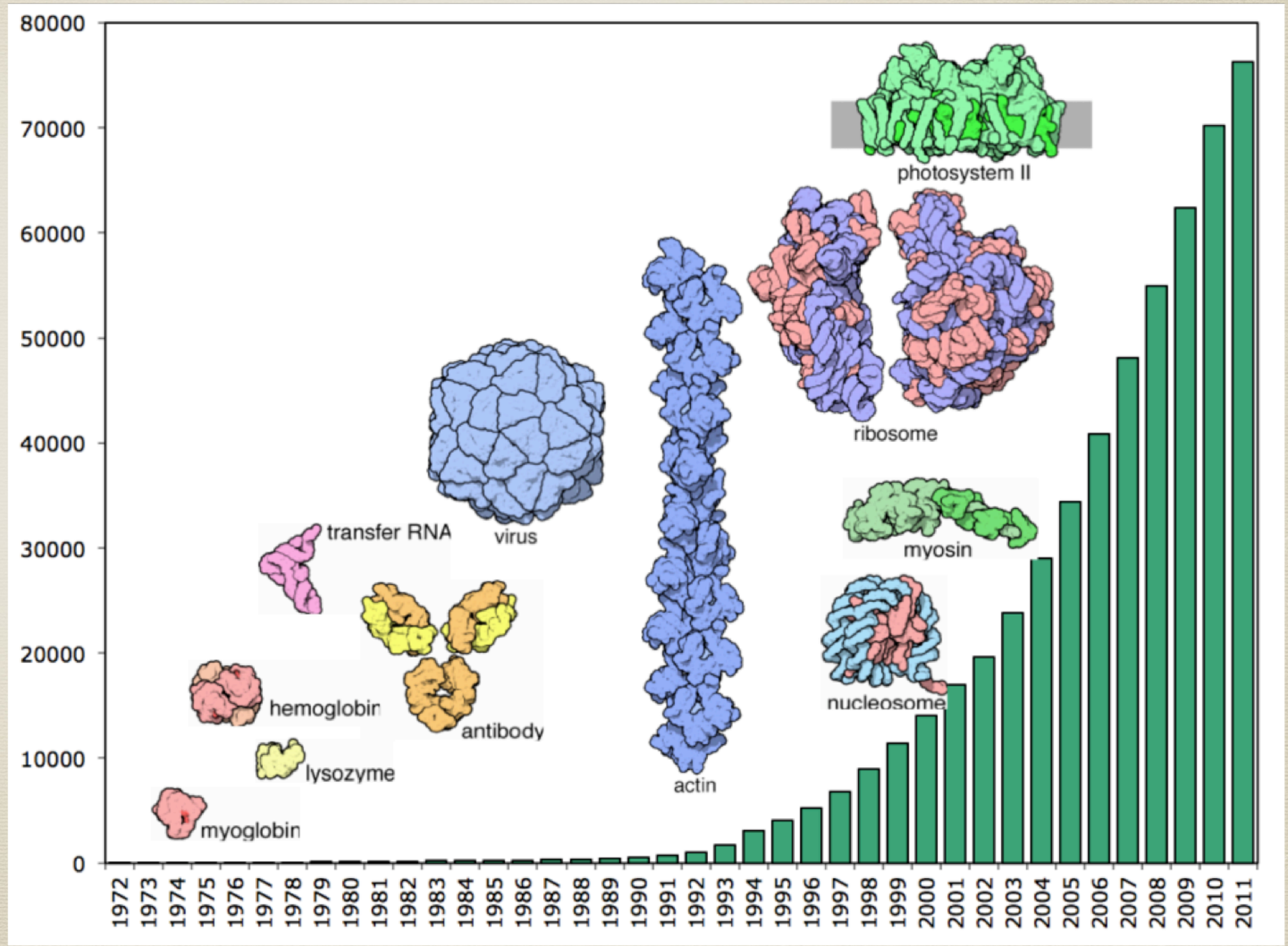


Fig. 1. A doubling of sequencing output every 9 months has outpaced and overtaken performance improvements within the disk storage and high-performance computation fields.

Proteomics

Size and Complexity

Image: RCSB.org



What is a Supercomputer?

A supercomputer is a computer that is much faster than computers of the same generation.

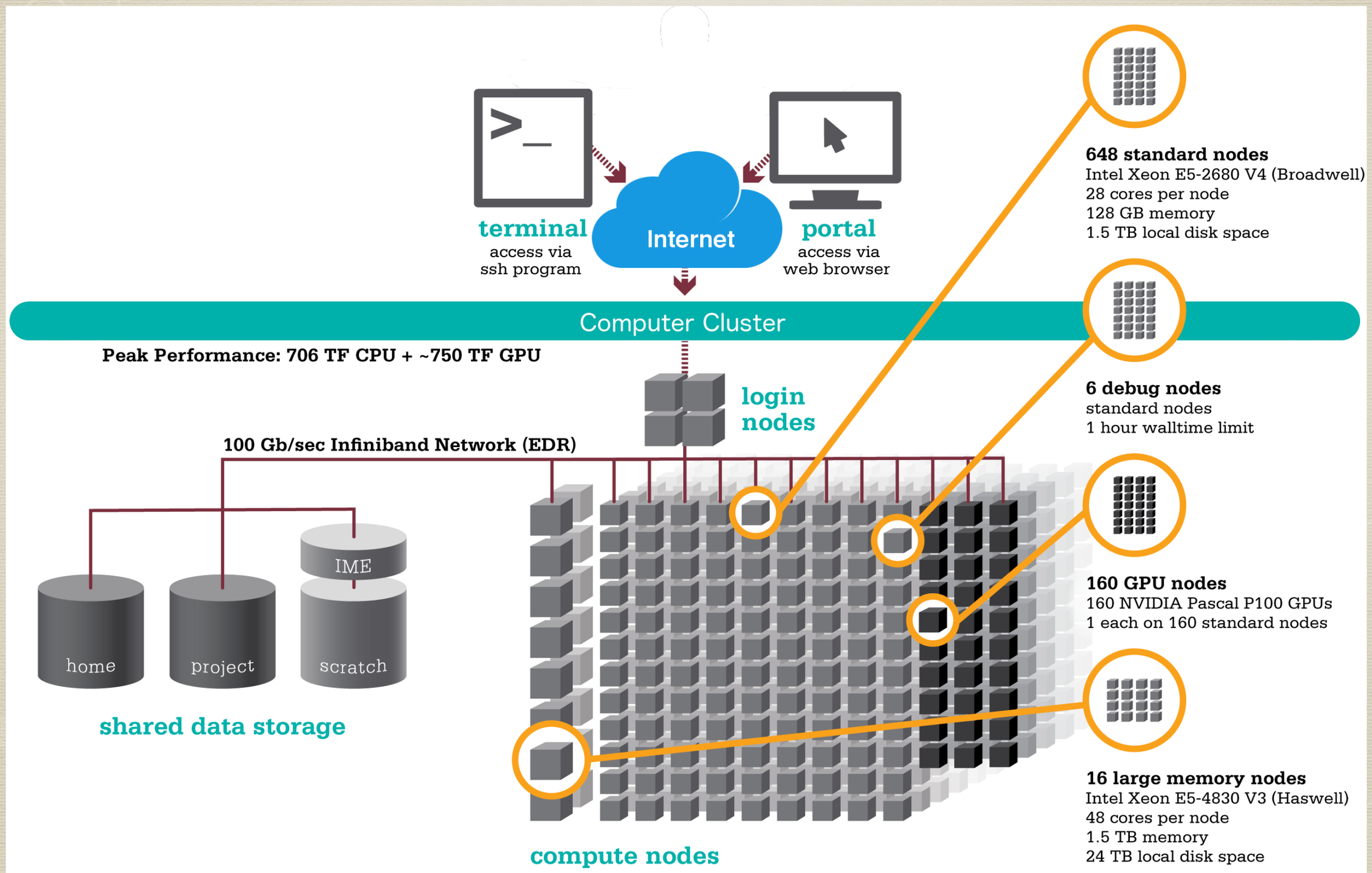
What is a SuperComputer

Summit can calculate 200 PetaFLOPS.
That's 200,000 trillion calculations per second,

What is a Computer Cluster

* Computer Clusters are the most common form of Supercomputer nowadays.
* A computer cluster is built from “relatively normal” computers stacked in a rack and connected with a network.

Anatomy of a Computer Cluster

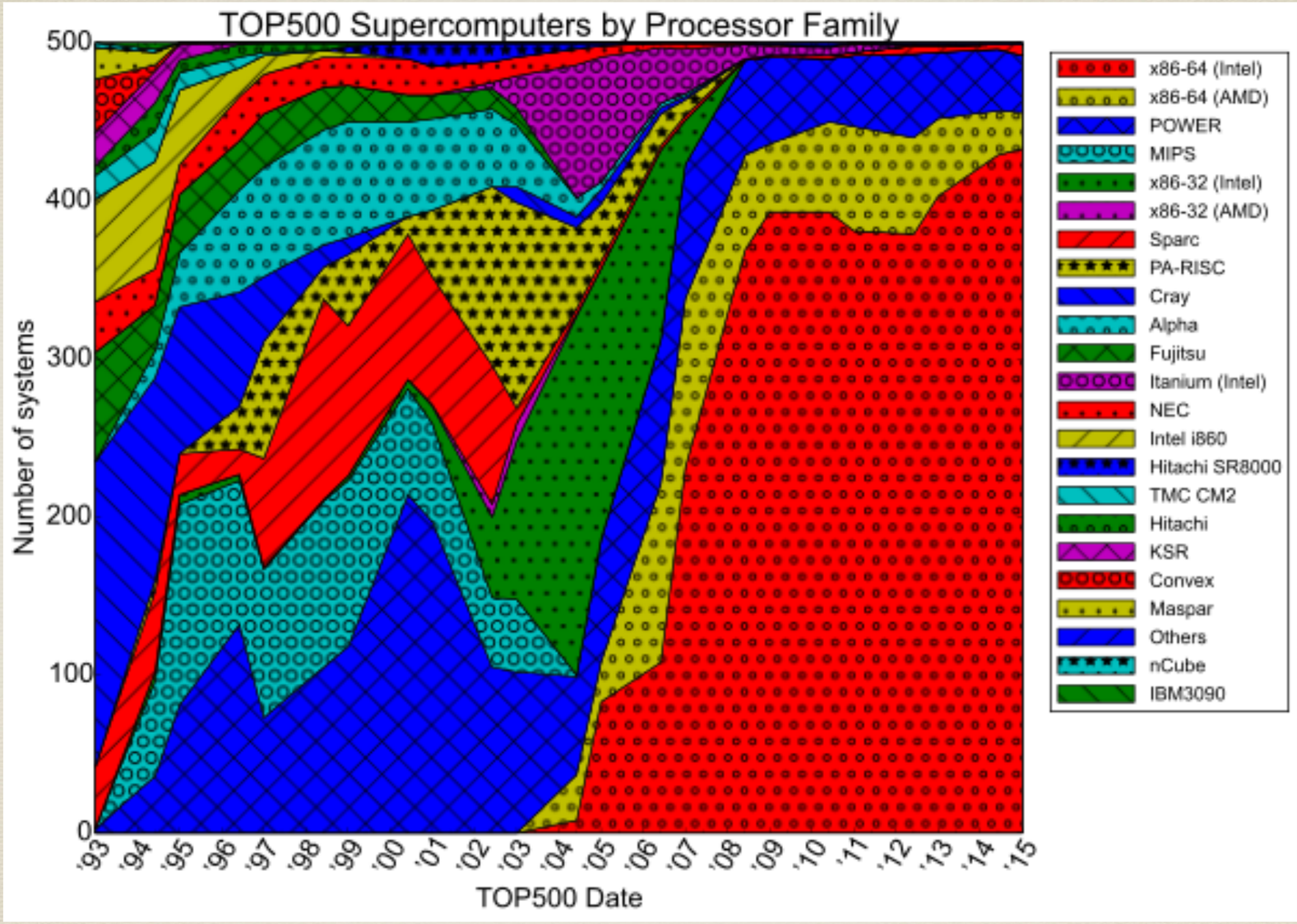


One Example: PSC Bridges

Regular Shared Memory (RSM) Nodes
Number of Nodes: 752
Number of Sockets per Node: 2
CPU: Intel Haswell (E5-2695 v3)
CPUs; 14 cores/CPU; 2.3 - 3.3 GHz

Memory: RAM 128GB, DDR4-2133
Cache 35MB LLC
Node-local storage: 2 HDDs, 4TB each

Supercomputers by Architecture



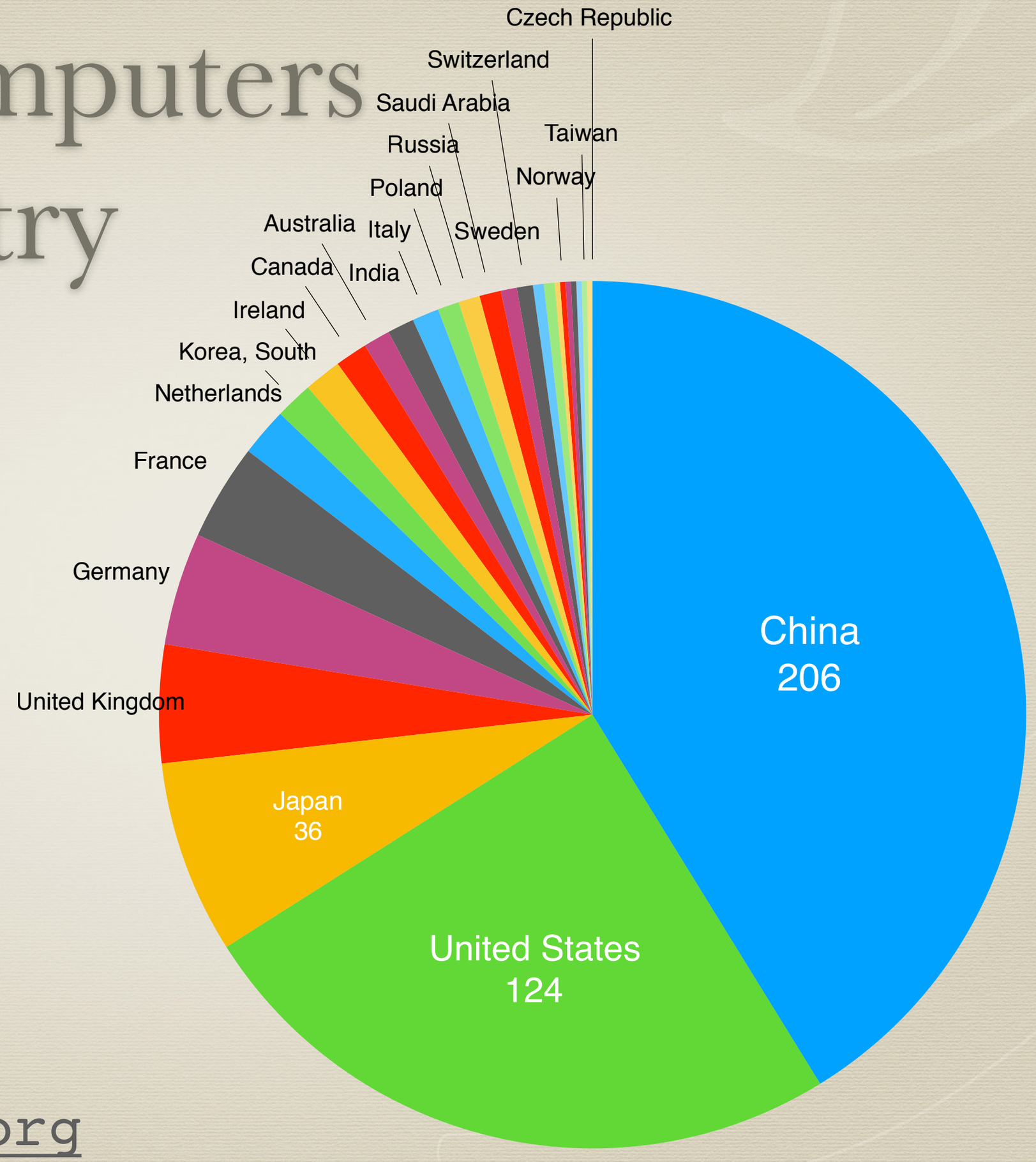
As of June 2018, TOP500 supercomputers are now all 64-bit, mostly based on x86-64 CPUs (Intel EMT64 and AMD AMD64 instruction set architecture)

Supercomputers by Country

Top500

List of June 2018

Number of Computers



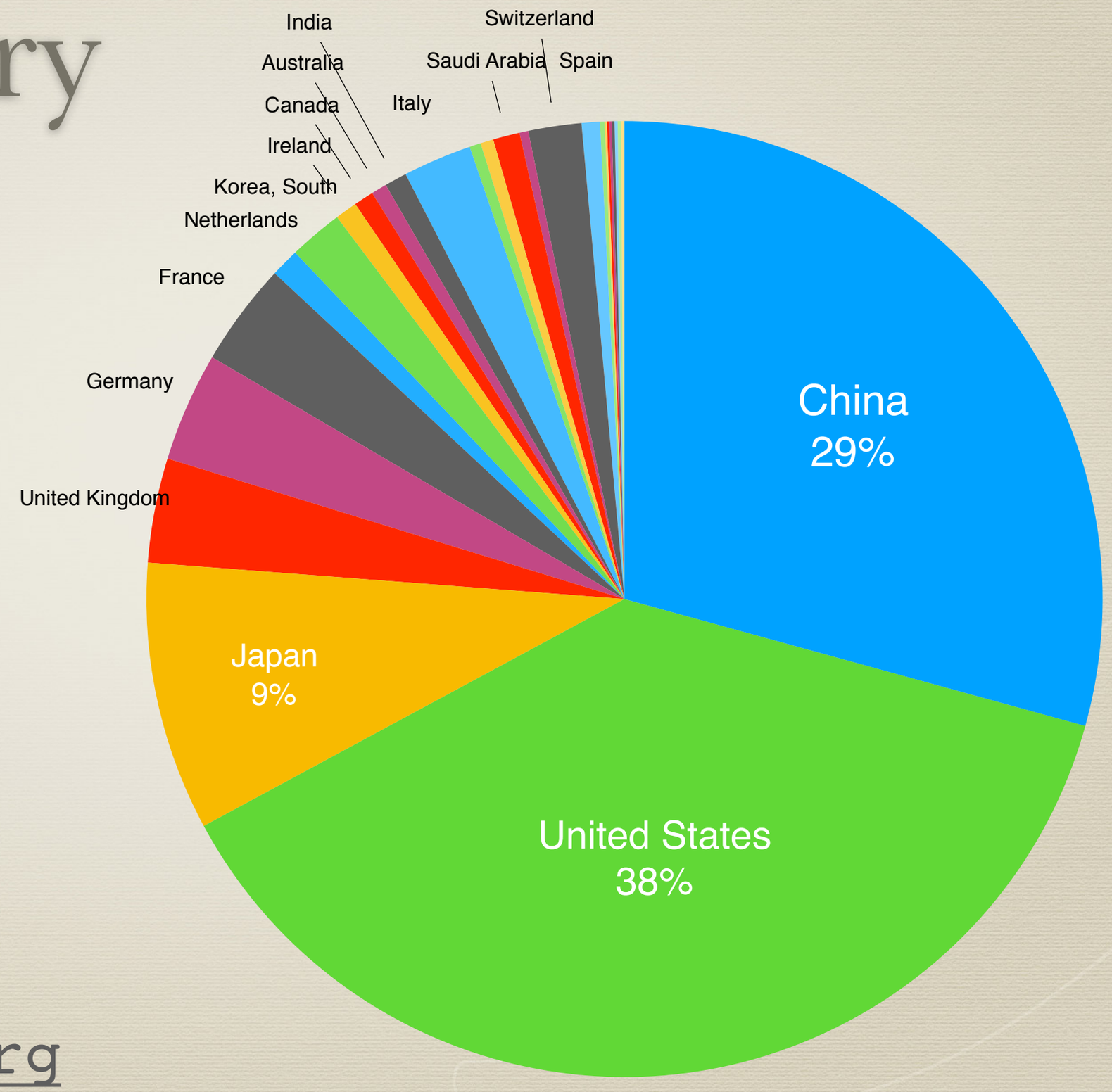
http://top500.org

Supercomputers by Country

Top500

List of June 2018

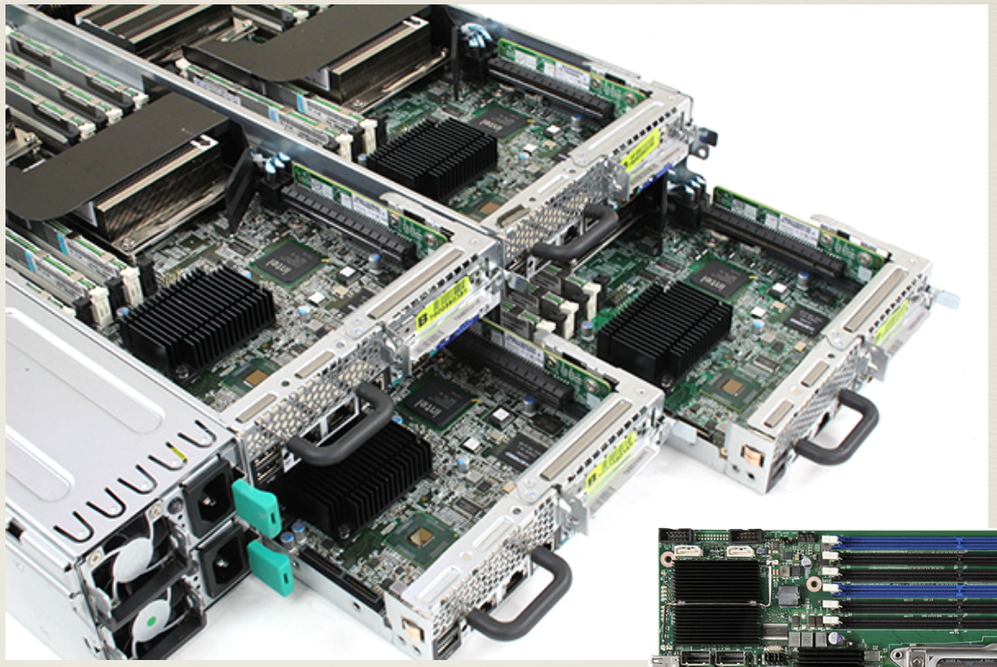
Performance: Rmax (GFLOPS) LINPACK



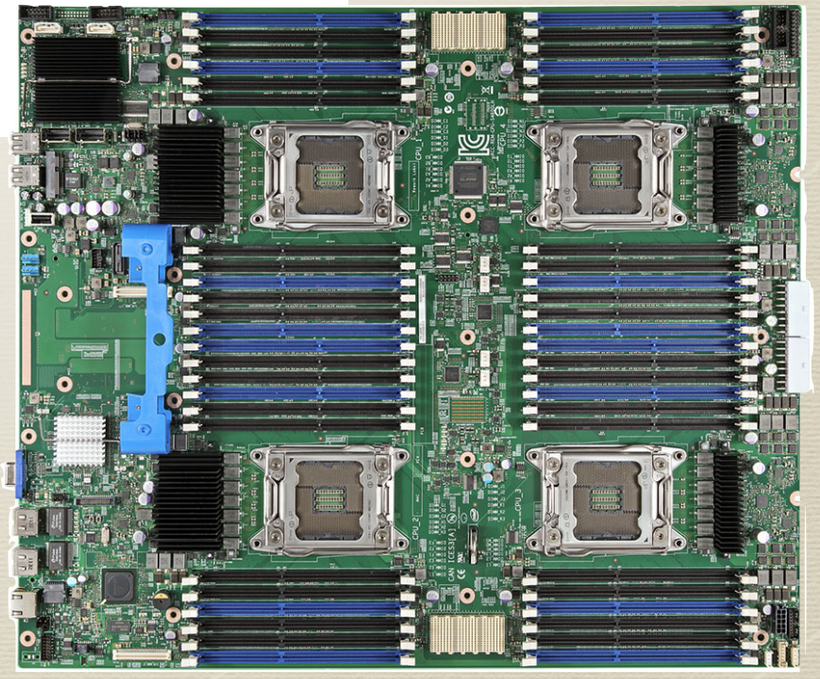
http://top500.org

Compute nodes, processors, sockets, cores and pipelines.

Rack with Compute Nodes

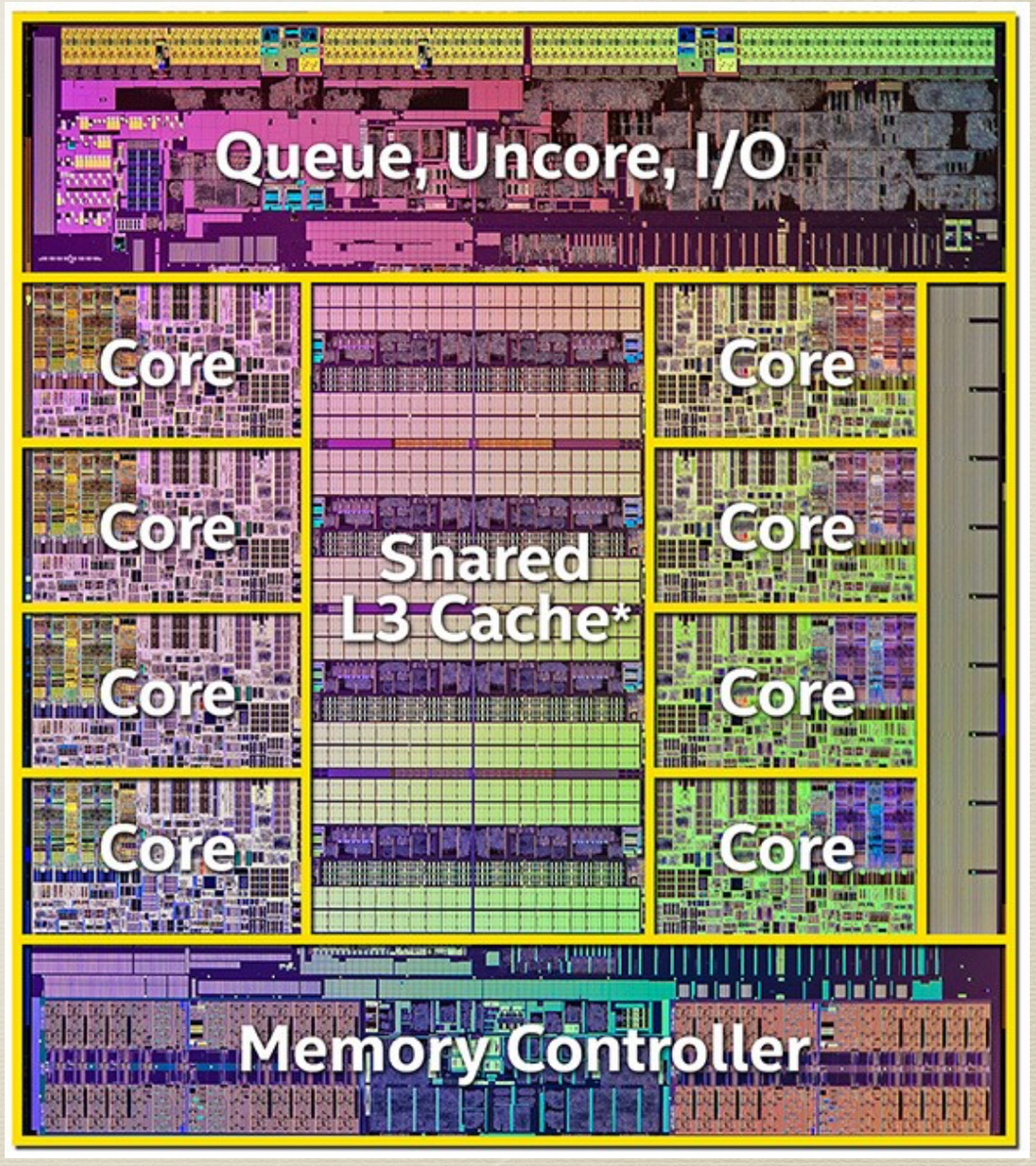


Blade Server



4-Socket Mainboard

Compute nodes, processors, sockets, cores and pipelines.

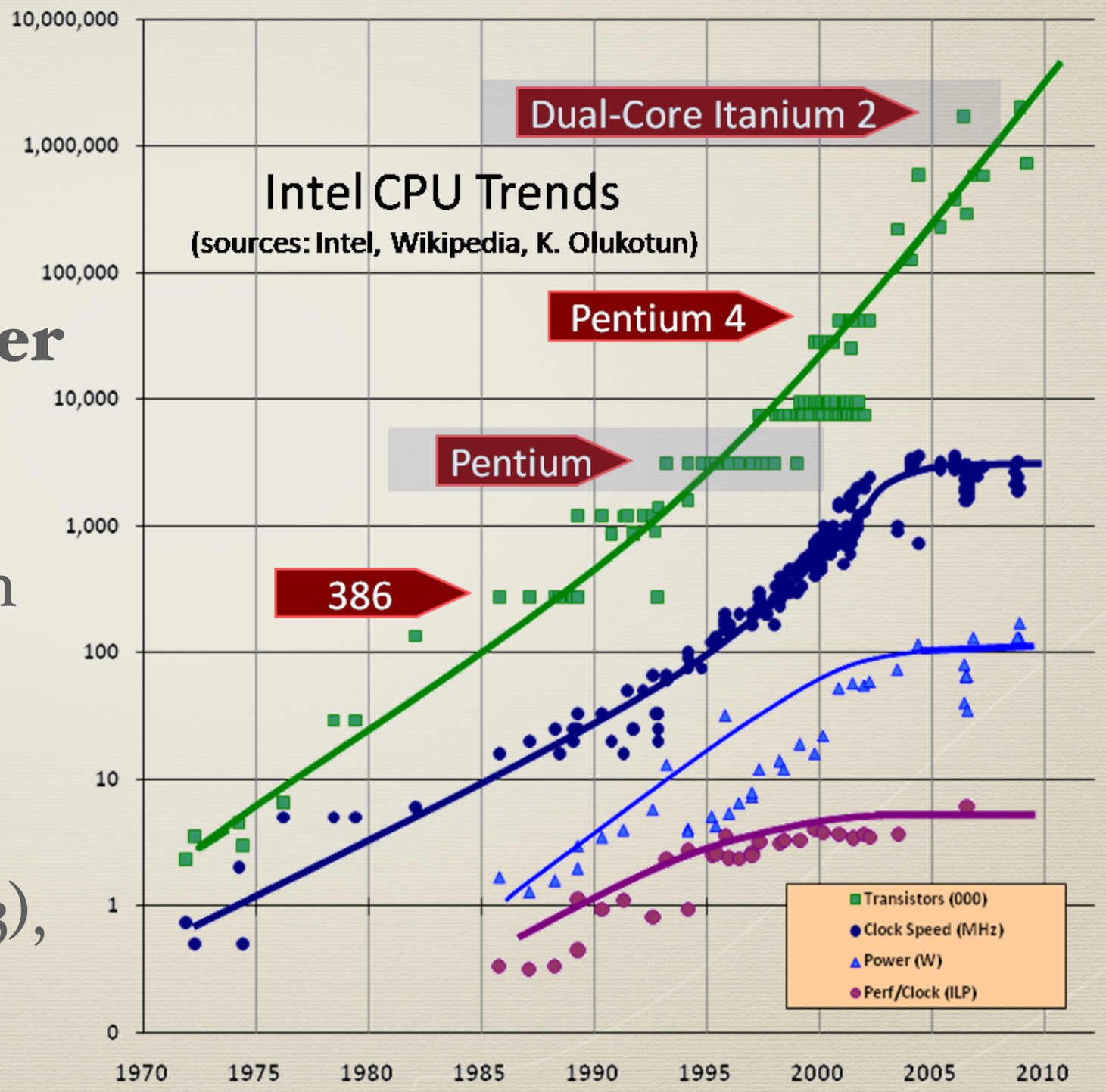


Parallel Computing

The Free Lunch Is Over

A Fundamental Turn Toward Concurrency in Software

Herb Sutter
(Dr. Dobb's Journal, 30(3), March 2005)



Storage Hierarchy

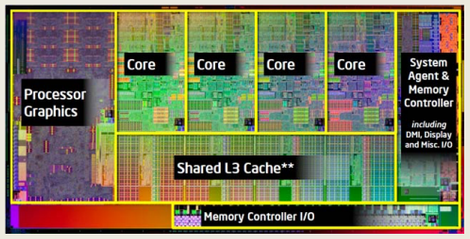
Speed

Cost

600GB/s

Processor Registers

Cache Levels



46GB/s

1,2,3

$20/MB

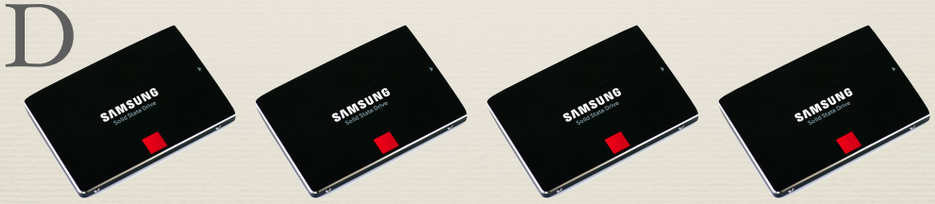
15GB/s

RAM

$15/GB

SSD

200-550MB/s



$0.20/GB

50-120MB/s

HDD

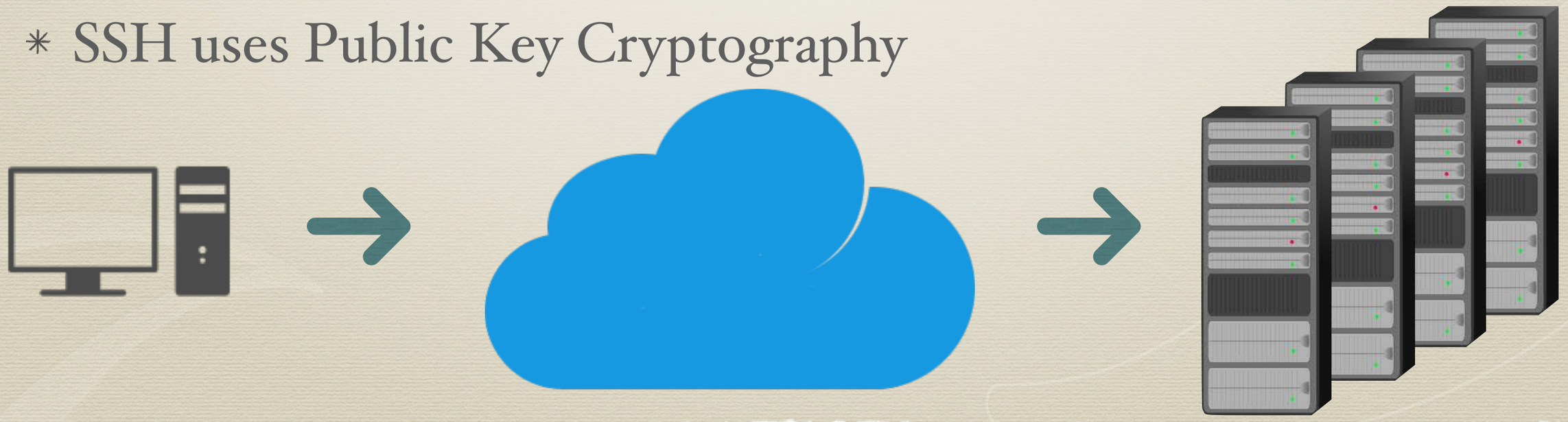
$0.04/GB

Secure Shell (SSH)

* Secure Shell (SSH) is a cryptographic network protocol for operating network services securely over an unsecured network.

* SSH provides a secure channel over an unsecured network in a client-server architecture, connecting an SSH client application with an SSH server.

* SSH uses Public Key Cryptography



Public Key Cryptography

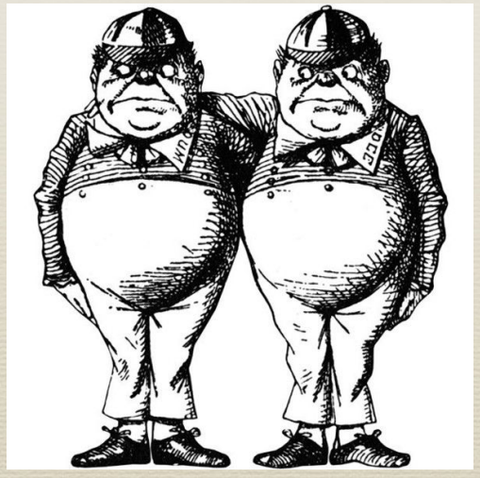
The problem with unencrypted communications

Alice

Hello, I am Alice

prove it!

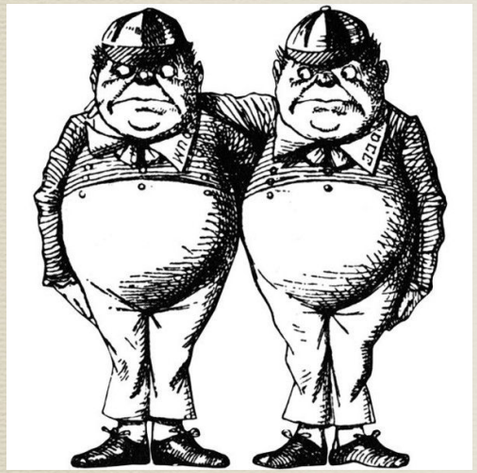
The password is “wonderland”



Bob

Public Key Cryptography

The problem with unencrypted communications



fake-Alice

Hello, I am Alice

prove it!

The password is “wonderland”

Bob

Public Key Cryptography

Negotiating Encryption for the Session

Symmetrical Encryption

Private

Public

Simplified Diffie-Hellman Procedure

Hello, lets choose a big prime number

10334794858749038232287

This is my public

This is my public

Alice

25724021

Now, we can talk... Hello, I am Alice

prove it!

Session Key

Bob

728875333451

Job Scheduler and Resource Manager

* An HPC cluster is used by many people at the same time.

* A job scheduler is a computer application for controlling unattended background program execution of jobs.This is commonly called batch scheduling, as execution of non-interactive jobs is often called batch processing.

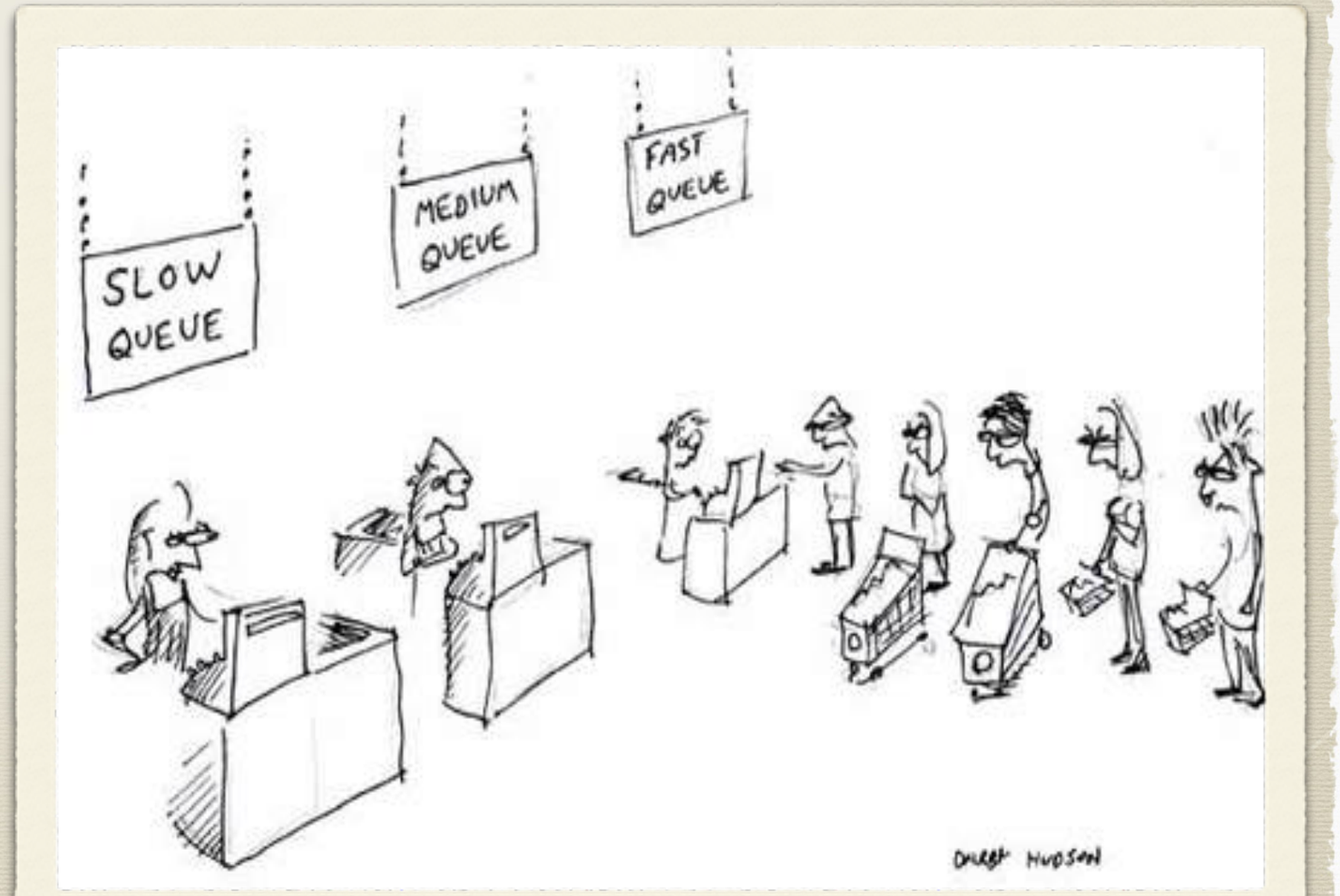
* Jobs are not supposed to run when launched, but when the right match of job and resources available is found. **Asynchronous execution.**

The concept of queues

* Queue is a way of associate resources to demands.
* Which queue to use is a **user** choice
* Which jobs run firsts is a **resource manager** choice.

`qstat -Q`

Queue	Wall Time
`debug`	15 min
`standby`	4 hours
`comm_mmem_day`	24 hours
`comm_mmem_week`	168 hours
`comm_256g_mem`	168 hours



Interactive Jobs

`qsub -I`

More examples:

`qsub -I -q debug` Running on the "debug" queue (15 min walltime)

`qsub -X -I -q comm_mmem_day`
Allows windows to pop up from remote compute node and using one day queue

`qsub -I -l nodes=1:ppn=4`
Using 4 cores on one compute node.

Non-interactive Jobs

`qsub JobScript.sh`

* Use non-interactive jobs for **long**, fully automatic jobs that are able to run to completion **without user** interaction

* The submission script has a double role:
    * Declare the requirements for execution via command line or #PBS comments
    * Contains the commands to be executed on the compute node.

Non-interactive Jobs

`qsub JobScript.sh`

```
#!/bin/bash

#PBS -N MY_JOB
#PBS -q debug
#PBS -j oe
#PBS -l nodes=1:ppn=2

cd $PBS_O_WORKDIR

source /shared/software/miniconda3/etc/profile.d/conda.sh
conda activate tpd0001

bowtie2 -x lambda_virus -U $SCRATCH/reads_1.fq -S eg1.sam

conda deactivate
```

PBS Directives Summary

Option	Description	Example
`-l walltime=hh:mm:ss`	Requests the amount of time needed for the job. Default is one hour.	`#PBS -l walltime=10:00:00`
`-l nodes=n:ppn=p`	Requests number of nodes and processors per node. The range of ppn values depends on the hardware you are running on. Default is one processor on one node.	`#PBS -l nodes=2:ppn=12` `#PBS -l nodes=3:ppn=8`
`-l nodes=n:ppn=p:feature`	Requests a node with a particular feature. Features like *smp, ivy, haswell, broadwell, avx, avx2, adx, f16c*	`#PBS -l nodes=1:ppn=8:haswell`
`-l pvmem=amount`	Maximum amount of virtual memory used by any single process in the job. Can use suffixes like kb, mb, gb	`#PBS -l pvmem=8000mb`
`-N jobname`	Sets the job name, which appears in status listings and is used as the prefix in the job's output and error log files. The job name must not contain spaces.	`#PBS -N Test_job2`

PBS Directives Summary

Option	Description	Example
`-j oe`	By default, PBS returns two log files, one for the standard output stream (stdout), the other for the standard error stream (stderr). This option joins both into a single log file.	`#PBS -j oe`
`-m [a][b][e]` `-m n`	Use any combination of the letters a, b, and e; do not include the brackets. Requests a status email when the job begins (b), ends (e), or aborts (a). The n option requests no email, but you'll still get email if the job aborts.	`#PBS -m abe` for lots of email `#PBS -m n` for minimal email
`-o filename`	Renames the output log file.	`#PBS -o test.out`
`-I`	Requests an interactive batch job.	`qsub -I`
`-X`	Enables X11 forwarding. Useful primarily in interactive batch jobs.	`qsub -I -X`
`-W depend=afterany:jobid`	This job may be scheduled for execution only after job jobid has terminated.	`#PBS -W depend=afterany:123456`

Storage on Spruce

Spruce offers several places for storing data

1. `$HOME (/users/<username>):`
   10GB (with backup)

2. `$SCRATCH (/scratch/<username>):`
   Unlimited storage (be kind), no backup.
   Data could be erased.

3. `Data Depot (/depot/<pi_name>):`
   PIs can by storage in 1 TB increments, with backup

Conda and Bioconda

* **Conda** is an open source package management system and environment management system that runs on Windows, macOS and Linux. Conda quickly installs, runs and updates packages and their dependencies.

* **Bioconda** is a channel for the conda package manager specializing in bioinformatics software.

* **Bioconda** offers more than 4000 packages for bioinformatics.

Bioconda on Spruce

```
source /shared/software/miniconda3/etc/
profile.d/conda.sh

conda activate tpd0001
```

Conclusions (to remember)

* The current problems on science (in particular Bio Sciences) are not only about size but also about complexity.

* High Performance Computing (HPC) infrastructures are tools to tackle the challenges of current research questions. They are to brain like hammers are to arms.

* Understanding command line interface and queue systems are needed to leverage that power to your hands.

HPC @ WVU

* My email: gufranco@mail.wvu.edu
* Helpdesk (Tickets):
  https://helpdesk.hpc.wvu.edu
* Wiki (How to use):
  https://wiki.hpc.wvu.edu
* ITS page (What is):
  https://it.wvu.edu/research/research-computing