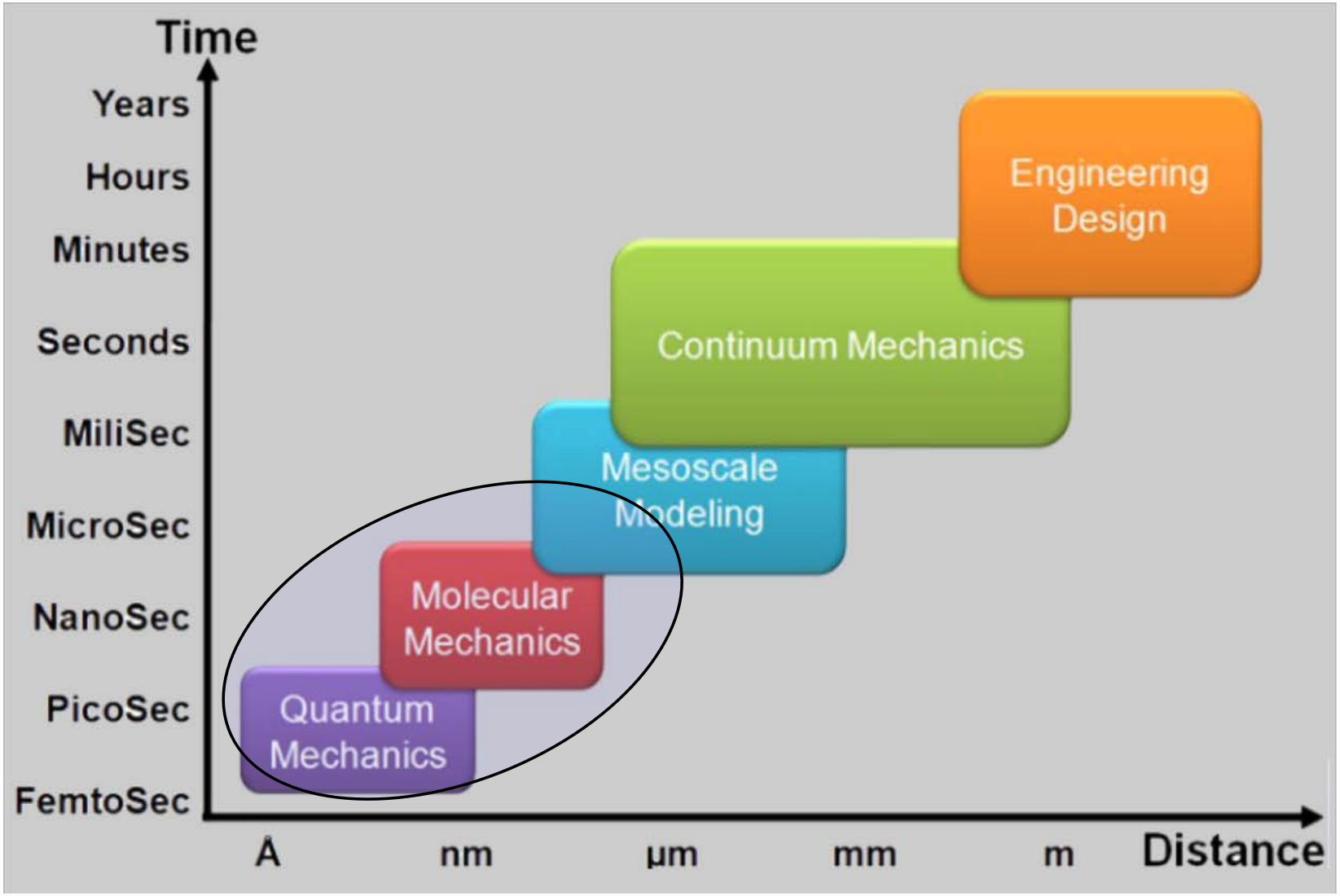
CBE 422
Molecular Modeling Methods

- Forces between molecules
- Molecular mechanics
- Classical molecular simulation methods: Monte Carlo + Molecular Dynamics
- Quantum modeling: Hartree-Fock and density functional theory methods

- Hands-on, computational assignments
- Final project on mutually agreed-upon topic

Time and Length Scales

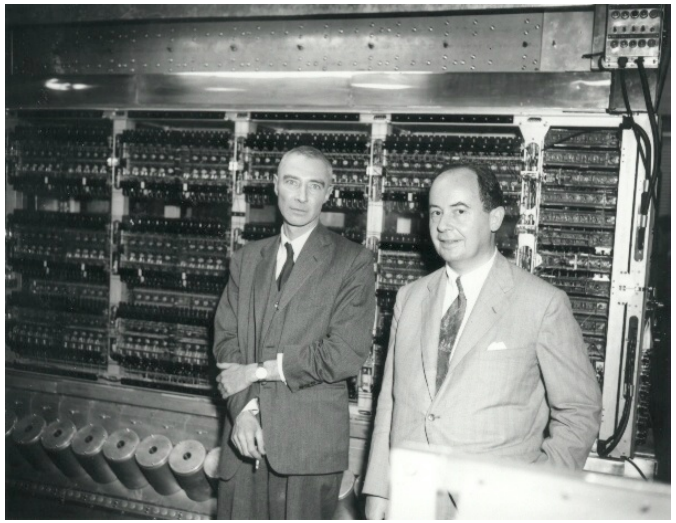


source: http://eeoren.etu.edu.tr/iwpmeo/

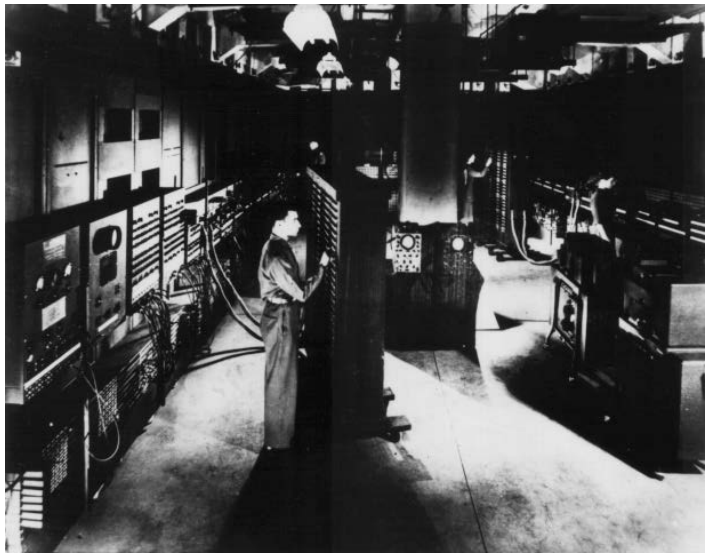
Early History of Computers

- John von Neumann (1903-1957), among first four faculty of IAS: Princeton "stored program+data" versus Harvard architecture
- ENIAC (1946) – U. Penn
- UNIVAC (1951) – U.S. Census Bureau
- IBM 650 (1954) – 1st mass-produced
- DEC PDP 8 (1965) – 1st minicomputer
- CRAY I (1976) – vector "supercomputer"
- Today: "commodity" clusters

www.computerhistory.org/timeline/
en.wikipedia.org/wiki/Harvard_architecture
en.wikipedia.org/wiki/John_von_Neumann
This NY Times article

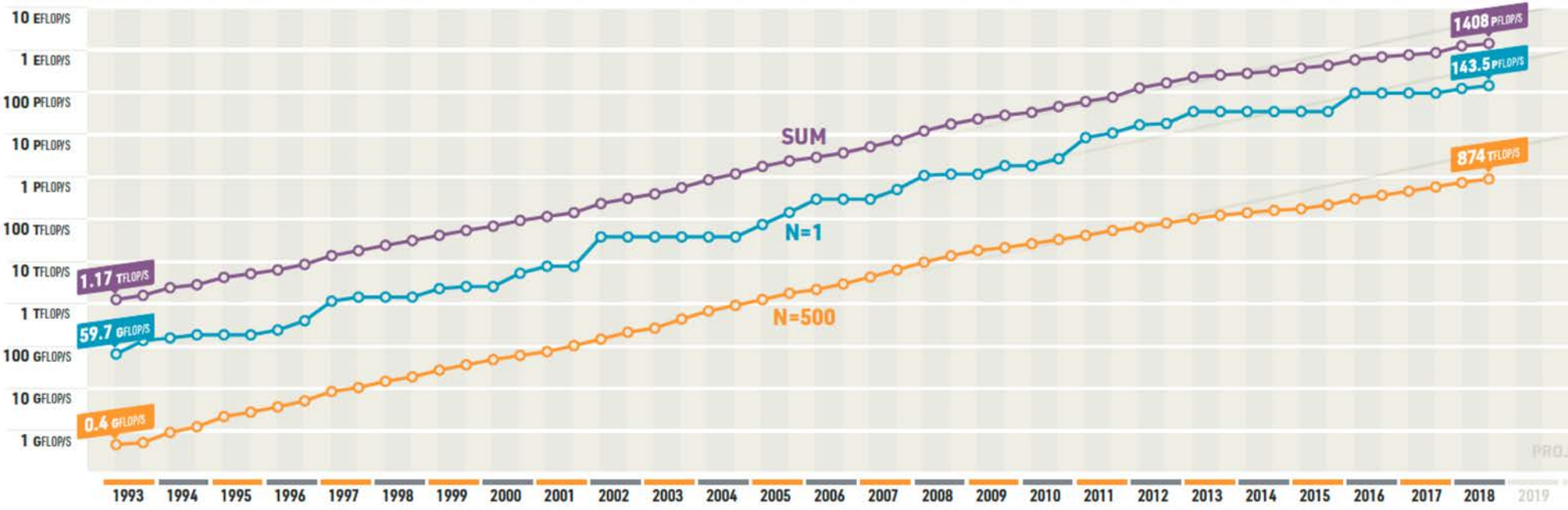


J. Robert Oppenheimer and John von Neumann in front of the Institute computer (IAS Archives photo)



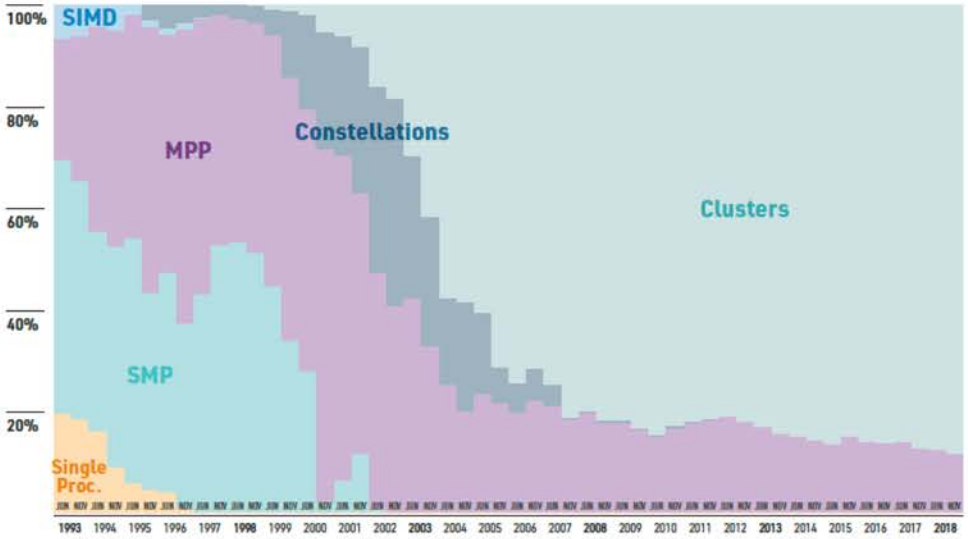
ENIAC - U. S. Army Photo

PERFORMANCE DEVELOPMENT

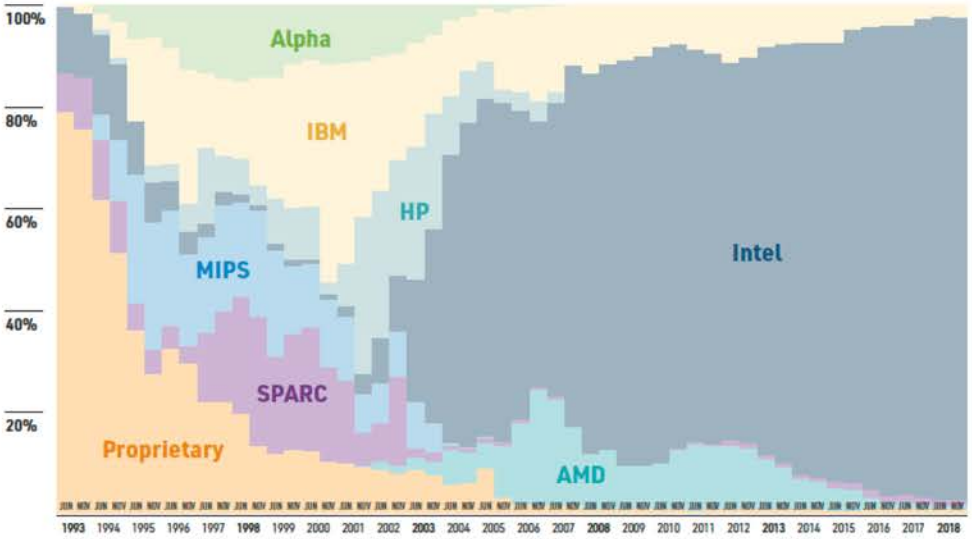


http://top500.org

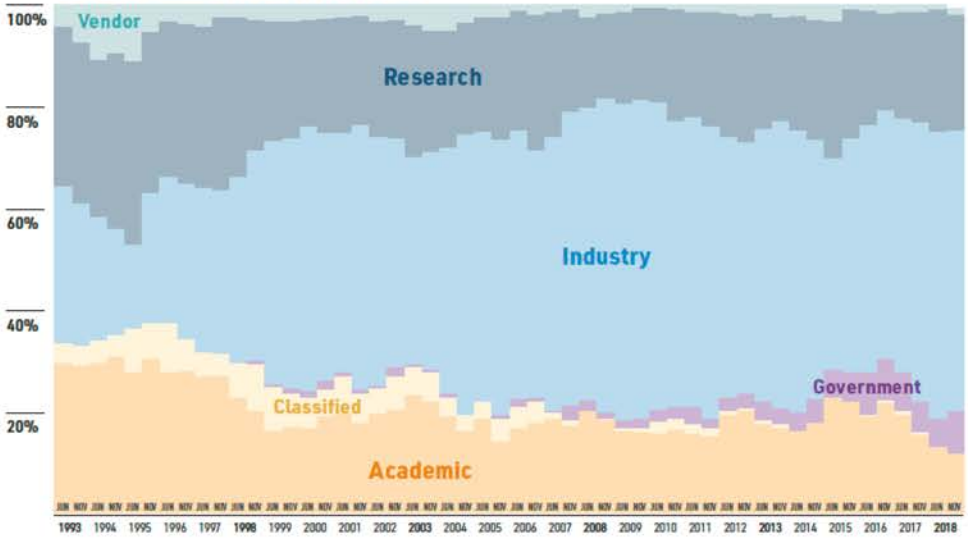
ARCHITECTURES



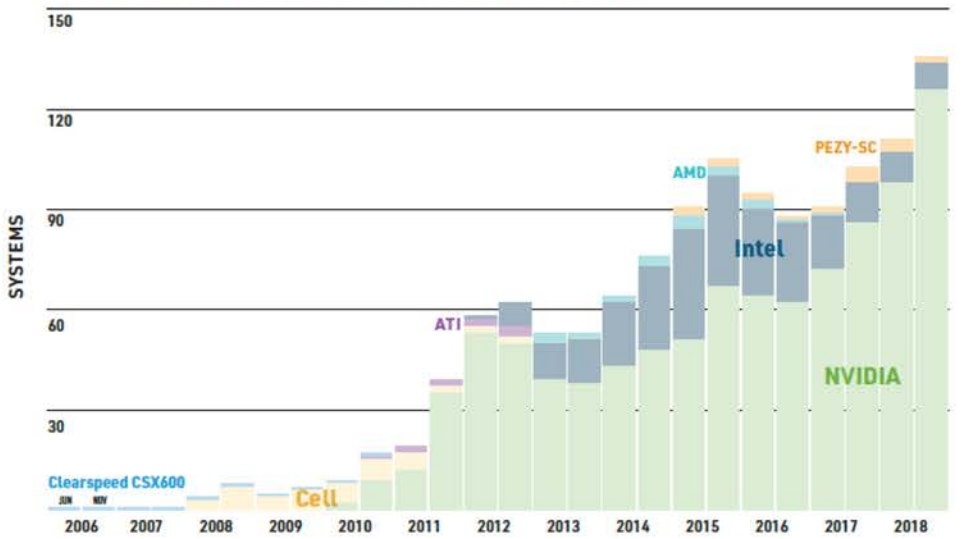
CHIP TECHNOLOGY



INSTALLATION TYPE



ACCELERATORS/CO-PROCESSORS

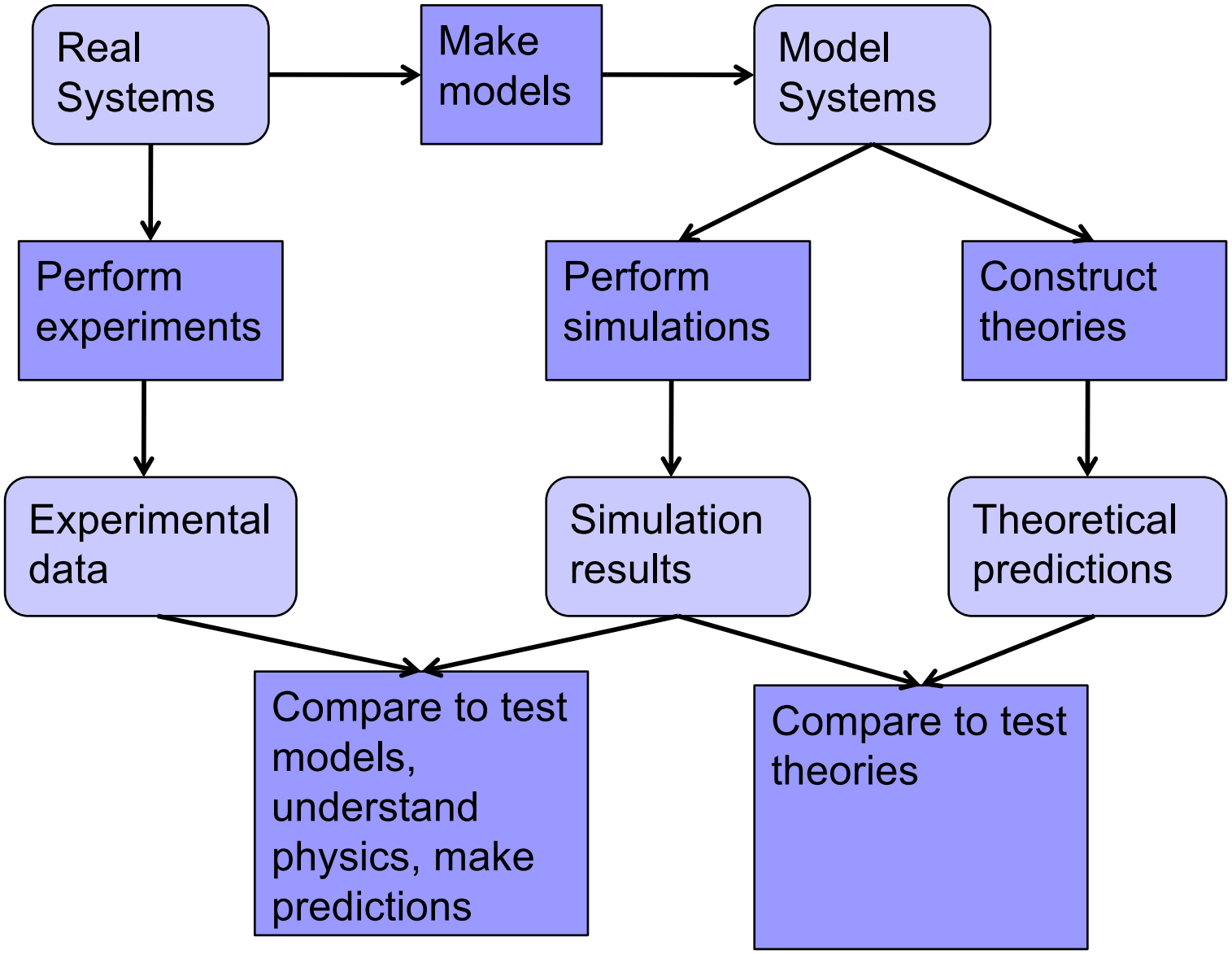


http://top500.org

Princeton Research Computing

Large Clusters	Processor Speed	Nodes	Cores per Node	Memory per Node	Total Cores	Inter-connect	Performance: Theoretical
TigerGPU **Dell Linux Cluster**	2.4 GHz Xeon Broadwell E5-2680 v4	80	28	256 GB	2240	Omnipath	86 TFLOPS
	1328 MHz P100 GPU		4 GPU/node	16 GB/GPU	320 GPUs		1504 TFLOPS
TigerCPU **HPE Linux Cluster**	2.4 GHz Skylake.	408	40	192 GB (40 w/768 GB)	16320	Omnipath	>1103 TFLOPS
Della **Dell Linux Cluster**	2.5 GHz_Ivybridge 2.6 GHz_Haswell 2.4 GHz_Broadwell 2.4 GHz_Skylake	80 32 48 64	20 20 28 32	128 GB 128 GB 128 GB 192 GB	5632	QDR Infiniband	267+ TFLOPS
Perseus **Dell Linux Cluster**	2.4 GHz Xeon	320	28	128 GB	8960	FDR Infiniband	344 TFLOPS

https://researchcomputing.princeton.edu/systems-and-services/available-systems

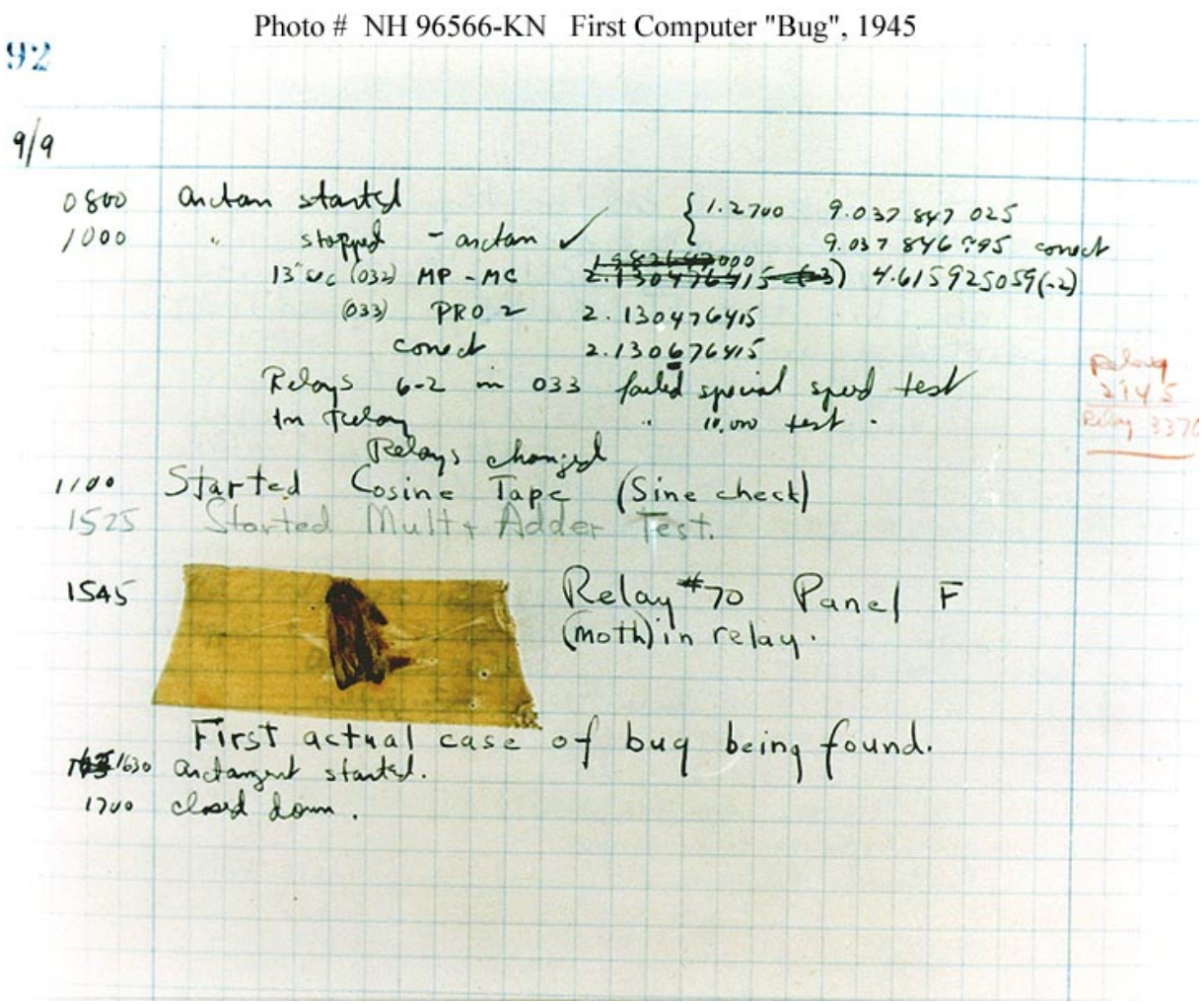


Adapted from Allen and Tildesley, *Computer Simulation of Liquids*, Oxford 1987

Computer Software

- Operating System (Mac OS, Windows, Unix/Linux)
- Applications (e.g. Matlab, Hyperchem)
- Open-source packages (e.g. Towhee, LAMMPS, Gromacs)
- User Code
  - Compiled programs (Fortran or C)
  - High-level scripting (e.g. Python)

Moth found trapped between points at Relay # 70, Panel F, of the Mark II Aiken Relay Calculator while it was being tested at Harvard University, 9 September 1945. Lieutenant Grace Murray Hopper affixed the moth to the computer log, with the entry: "First actual case of bug being found". She put out the word that she had "debugged" the machine, thus introducing the term "debugging a computer program".



http://www.history.navy.mil/photos/pers-us/uspers-h/g-hoppr.htm