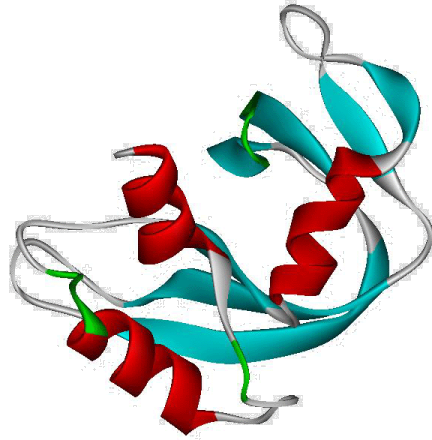




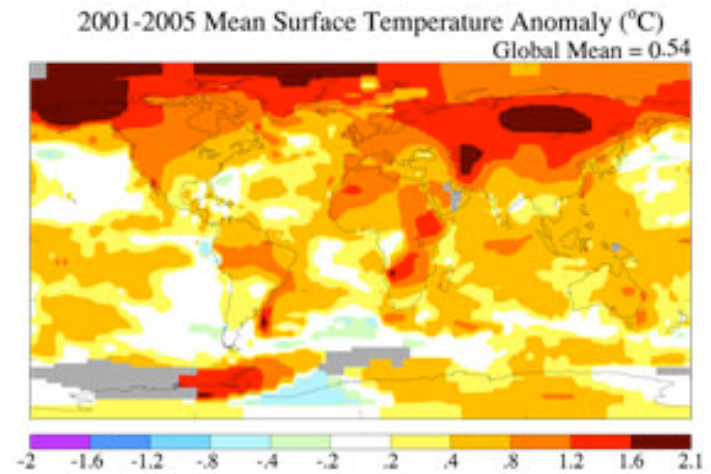
Focus of ChE 520

- Classical molecular simulation methods:
Monte Carlo
Molecular Dynamics
- Hands-on, computational assignments
- Emphasis on fluid properties, phase transitions, advanced sampling methods
- Beginning graduate / advanced undergraduate level

Scientific Computing Applications

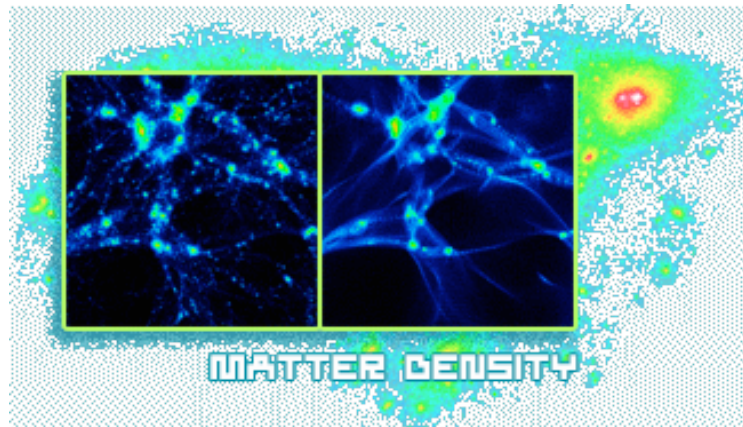


Protein
Folding
(AZP
group)



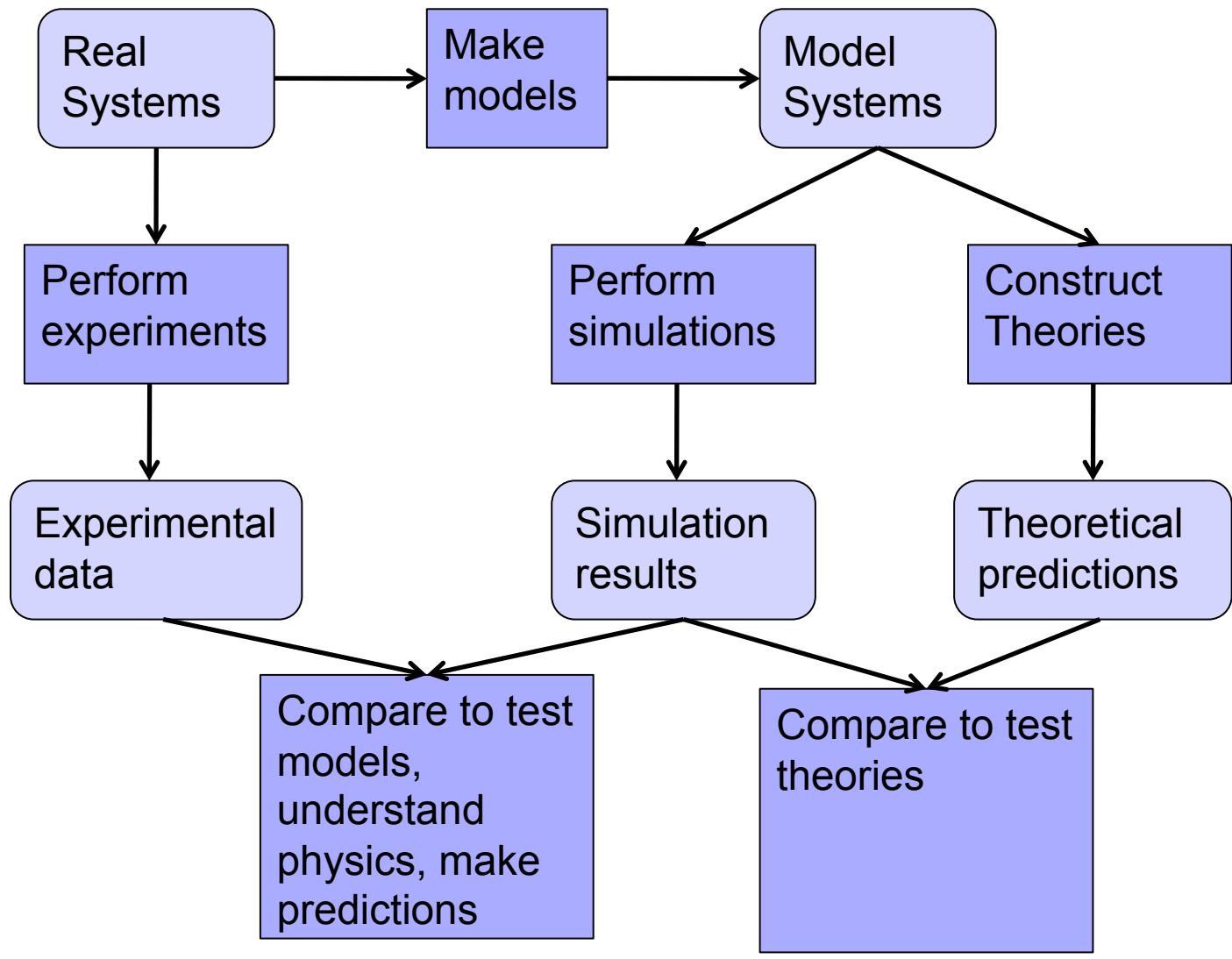
Climate / weather modeling

<http://www.giss.nasa.gov/research/news/20060925/>



Astrophysics

J.P. Ostriker, Princeton



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



Practical issues

- Instructor: Thanos Panagiotopoulos (azp@princeton.edu), A-317 E-Quad.
- Course web site: <http://paros/che520>
- Book: D. Frenkel & B. Smit, "Understanding Molecular Simulation," 2nd Ed., Academic Press, 2002; see http://molsim.chem.uva.nl/frenkel_smit/
- Lectures: Tu+Th 9-10:20, A224
make-up: Mo 3:30-4:50, A224



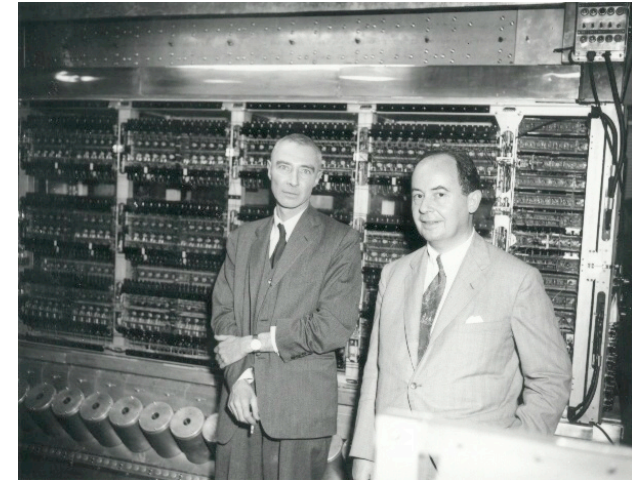
Practical issues - Grading

- 50% 4-5 Assignments
- 40% Final project (of your choice, after consultation with me)
- 10% Class participation

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](#)

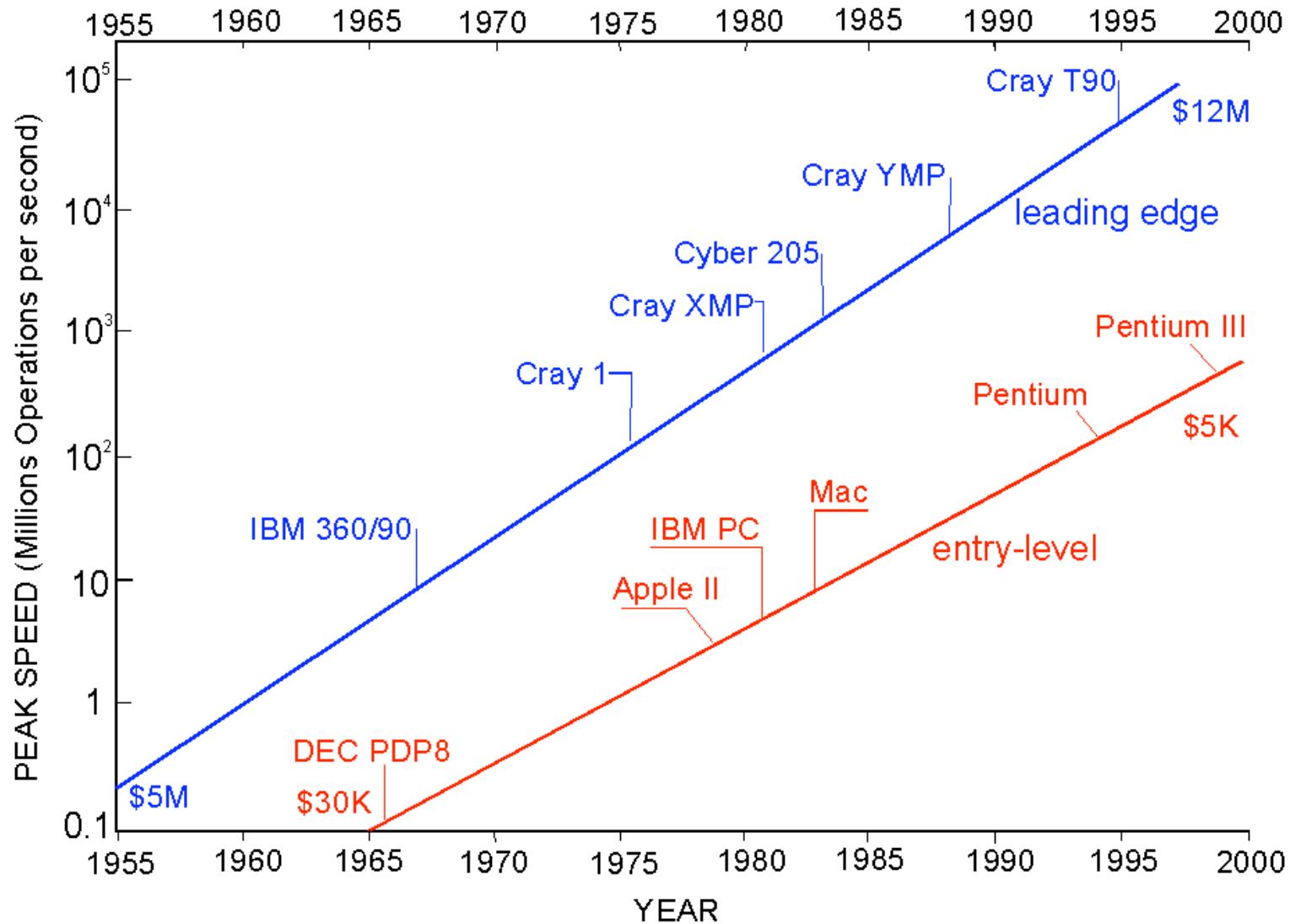


J. Robert Oppenheimer and John von Neumann in front of the Institute computer (IAS Archives photo)



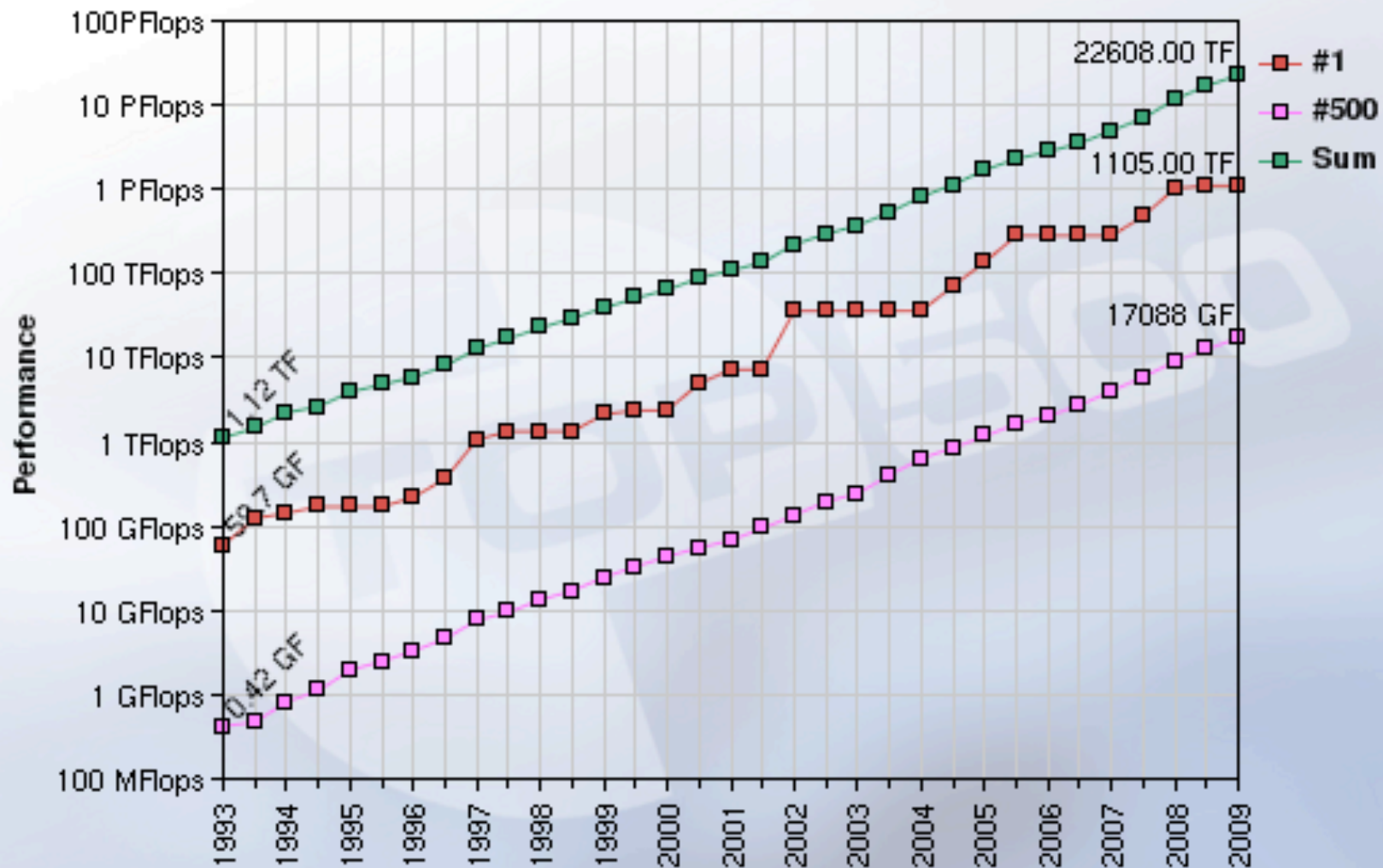
ENIAC - U. S. Army Photo

Moore's "Law" (see <http://c2.com/cgi/wiki?MooresLaw>)



Adapted from AE Brenner, Physics Today, Oct. 1996

Performance Development



Princeton University High Performance Computing Systems

	Processor Speed	Memory per Core	Interconnect	Total Cores	Total RAM	Local Disk	Total Flops (LINPACK)
Hecate SGI Altix	1.5 GHz Itanium	4 GB (min)	NUMALink	192	1 TB	10 TB	1.1 Tflops
Orangena IBM Blue Gene	700 MHz PPC	256 MB	2.8 GB/s Proprietary	2048	512 GB	8 TB	4.7 Tflops
Della Dell Linux Cluster	3.2 GHz Xeon /3.0 GHz Woodcrest	4 GB	Gig-E / Infiniband	1024	4 TB	3 TB	3.8 Tflops (est.)
Woodhen Dell Linux Cluster	2.66 GHz Woodcrest	2 GB	Infiniband	768	1.5 TB	15 TB	5.8 Tflops
Artemis SGI Linux Cluster	2.83 GHz Harpertown	4 GB	Infiniband	1536	6 TB	47 TB	15 Tflops (est.)
Sesame Dell Linux Cluster	2.66 GHz Nehalem	3 GB	Infiniband	3584	11 TB	20 TB	38 Tflops (est.)

Last Updated (Tuesday, 05 May 2009 08:45)



Computer Software

- Operating System (MAC OS, Windows, Linux)
- Applications (e.g. Word, Excel, Matlab)
- Open-source packages (e.g. Towhee, 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".

Photo # NH 96566-KN First Computer "Bug", 1945

