The Physics of Quantum Computing – The Next Paradigm in High-Performance Computing?

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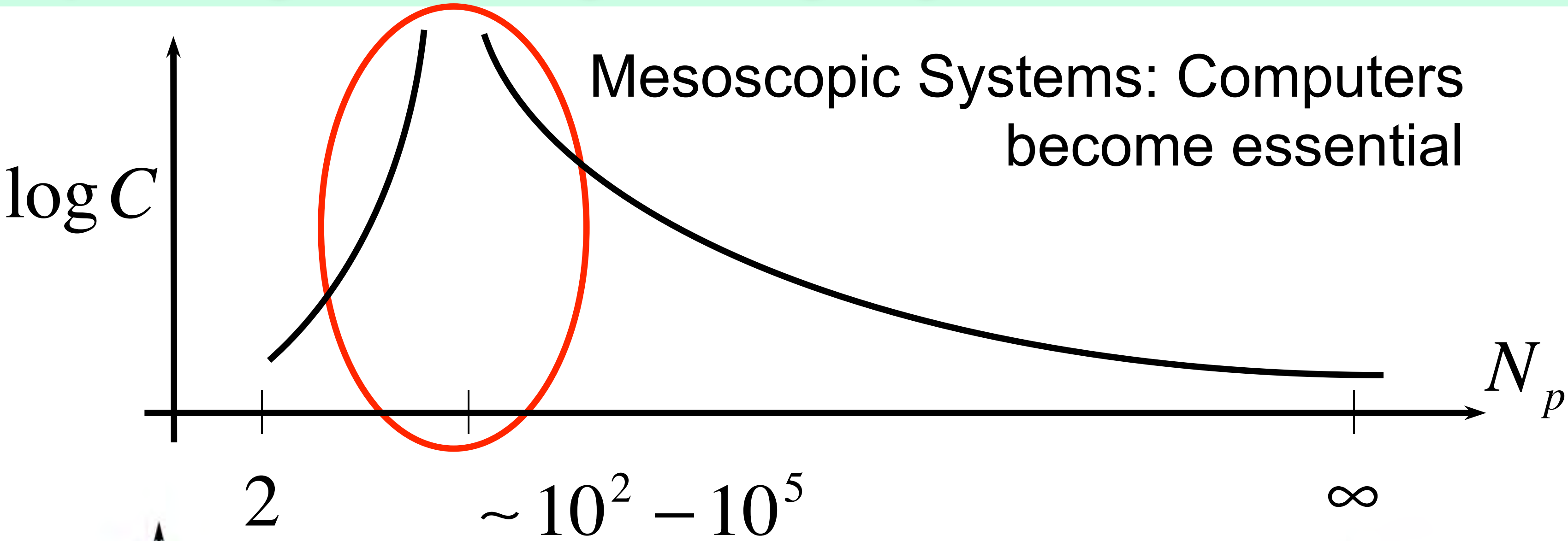
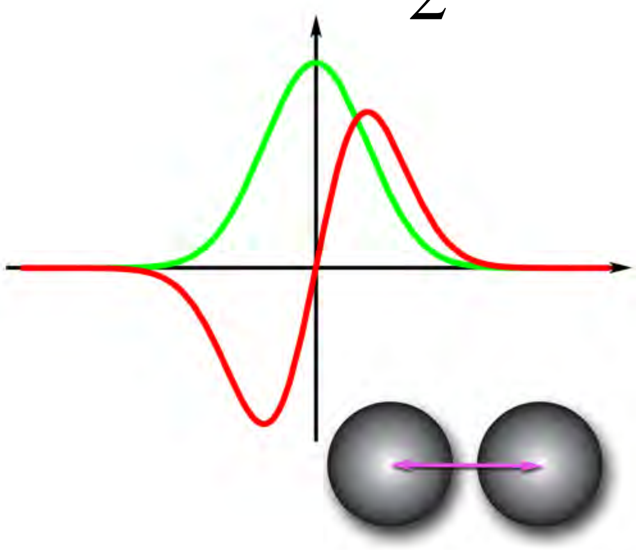
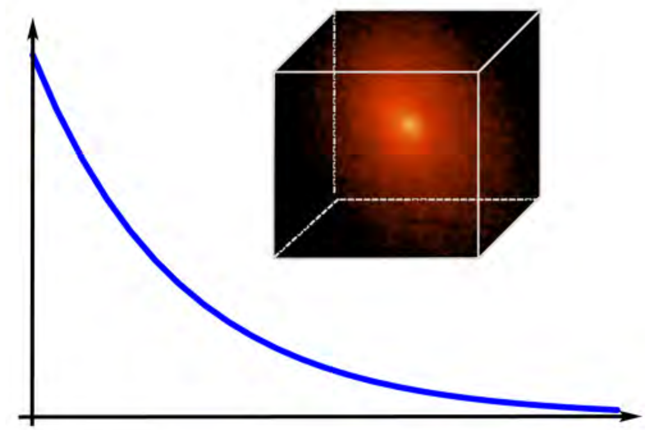
ICER

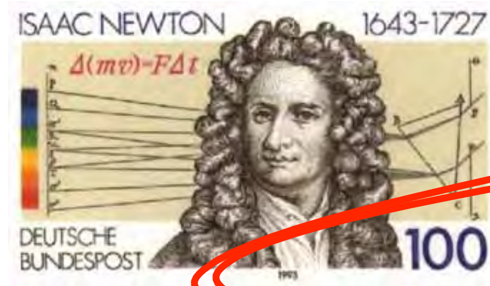
Complexity in Many-Body Systems







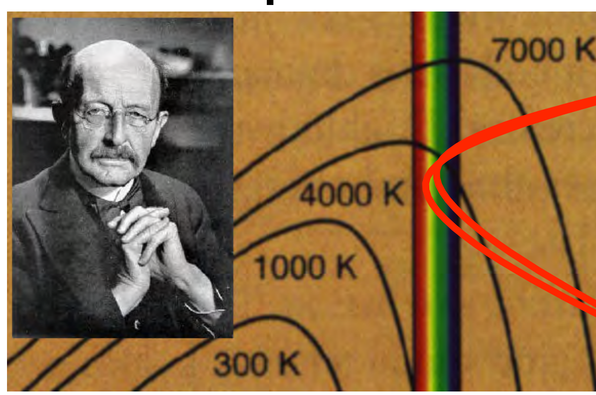
(very abbreviated) History of Physics



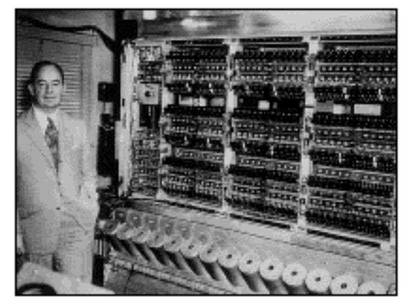
time

1700s: Newton invents calculus to describe mechanics

1800s: Faraday et al. study electricity&magnetism in experiments



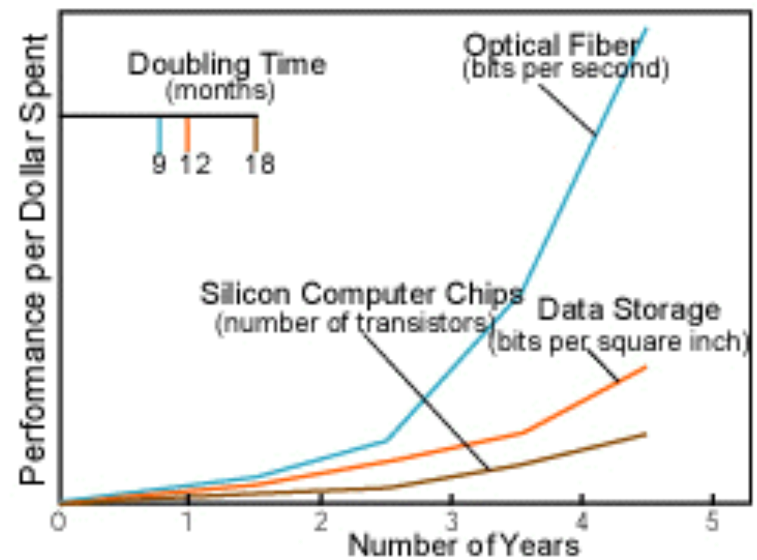
1900s: Theoretical physics (Planck, Einstein) explores the quantum world



2000s: Computational physics emerges as third branch of physics (von Neumann)

History of Computers (Moore's Law)

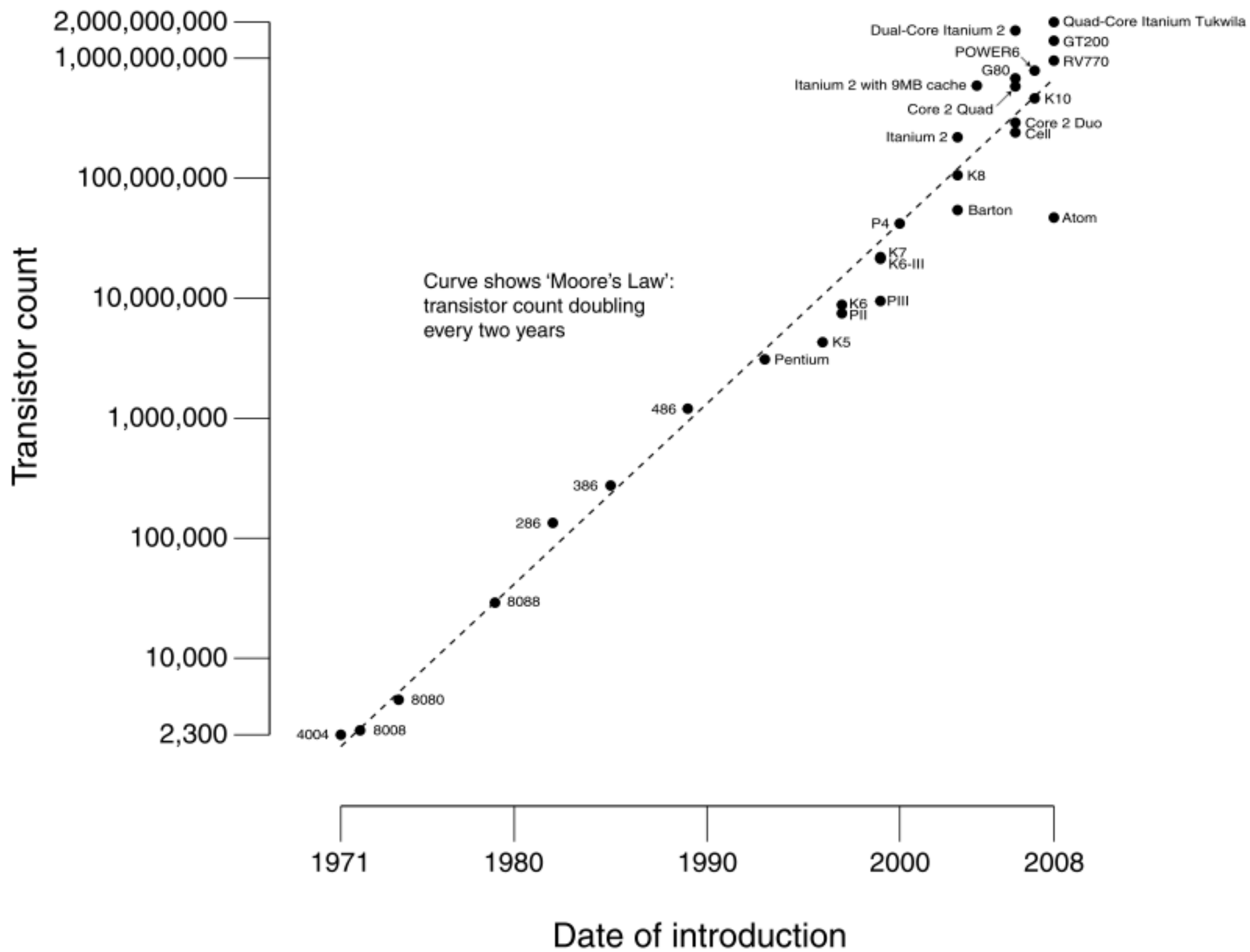
- Computer speed doubles every 2 years (Moore's Law)
- Data storage density doubles every 12 months
- Network speed doubles every 9 months
- Physics limits not to be reached for another decade or more



Moore's Law vs. storage improvements vs. optical improvements. Graph from Scientific American (Jan-2001) by Cleo Vilett, source Vined, Khoslan, Kleiner, Caufield and Perkins.

History of Computers (Moore's Law)

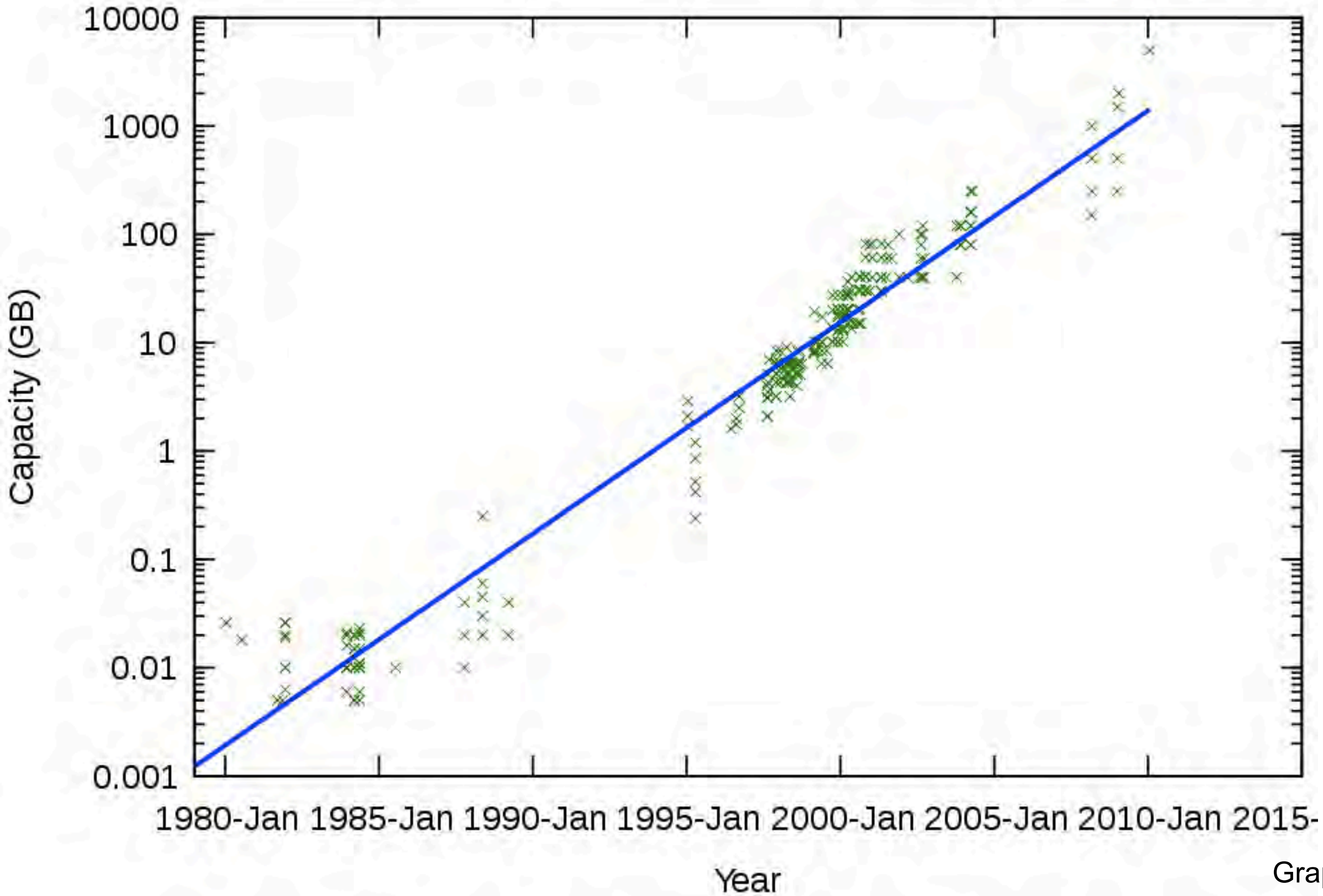
CPU Transistor Counts 1971-2008 & Moore's Law



Graph: Wikipedia 2009

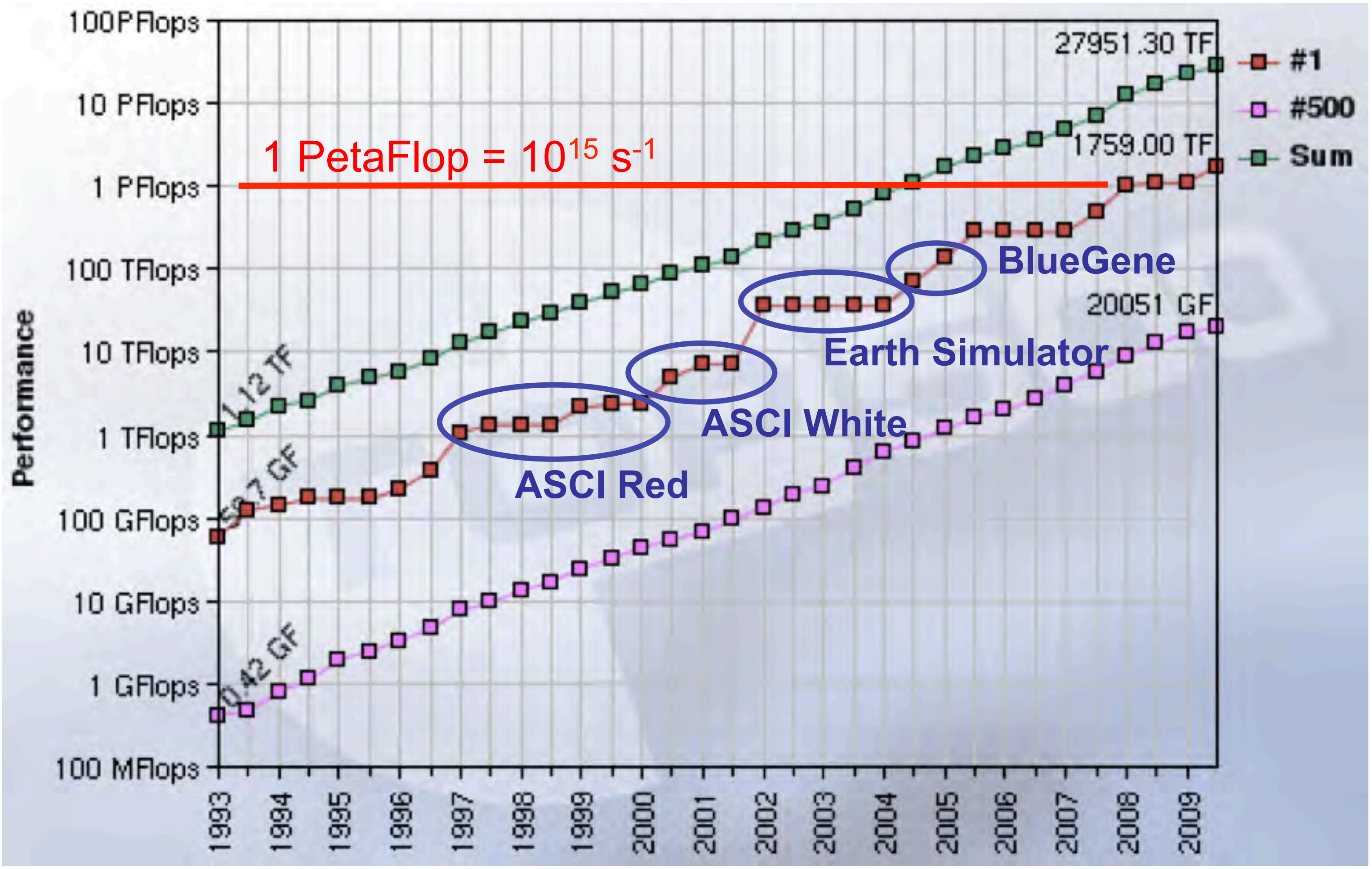
History of Computers (Moore's Law)

- PC storage capacity doubles every 2 years, too



Graph: Wikipedia 2009

History of Computers (Speed Record)



Source: http://www.top500.org

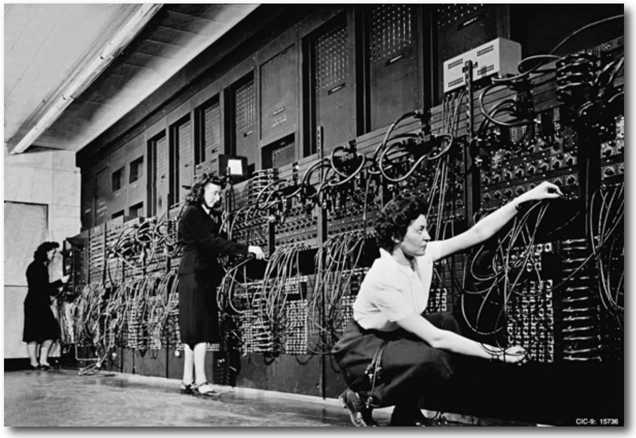
Top 10 Computers in the World

Rank	Site	Computer
1	Oak Ridge National Laboratory United States	Jaguar - Cray XT5-HE Opteron Six Core 2.6 GHz Cray Inc.
2	DOE/NNSA/LANL United States	Roadrunner - BladeCenter QS22/LS21 Cluster, PowerXCell 8i 3.2 Ghz / Opteron DC 1.8 GHz, Voltaire Infiniband IBM
3	National Institute for Computational Sciences/University of Tennessee United States	Kraken XT5 - Cray XT5-HE Opteron Six Core 2.6 GHz Cray Inc.
4	Forschungszentrum Juelich (FZJ) Germany	JUGENE - Blue Gene/P Solution IBM
5	National SuperComputer Center in Tianjin/NUDT China	Tianhe-1 - NUDT TH-1 Cluster, Xeon E5540/E5450, ATI Radeon HD 4870 2, Infiniband NUDT
6	NASA/Ames Research Center/NAS United States	Pleiades - SGI Altix ICE 8200EX, Xeon QC 3.0 GHz/Nehalem EP 2.93 Ghz SGI
7	DOE/NNSA/LLNL United States	BlueGene/L - eServer Blue Gene Solution IBM
8	Argonne National Laboratory United States	Blue Gene/P Solution IBM
9	Texas Advanced Computing Center/Univ. of Texas United States	Ranger - SunBlade x6420, Opteron QC 2.3 Ghz, Infiniband Sun Microsystems
10	Sandia National Laboratories / National Renewable Energy Laboratory United States	Red Sky - Sun Blade x6275, Xeon X55xx 2.93 Ghz, Infiniband Sun Microsystems

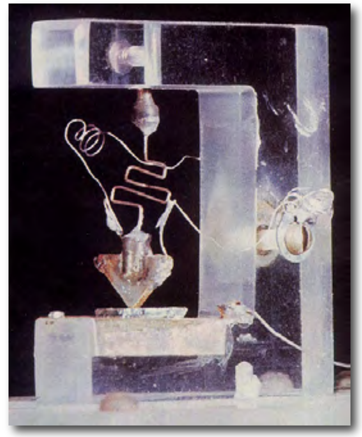
Source: http://www.top500.org

History of Computers

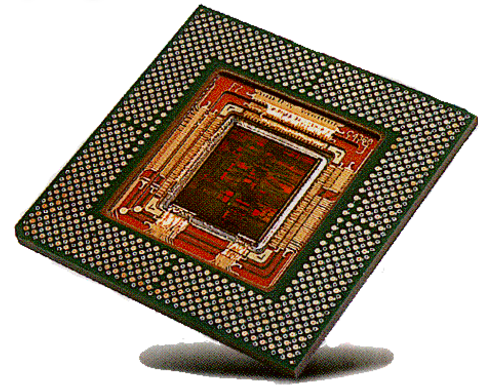
Driven by demand from and inventions by physical scientists!



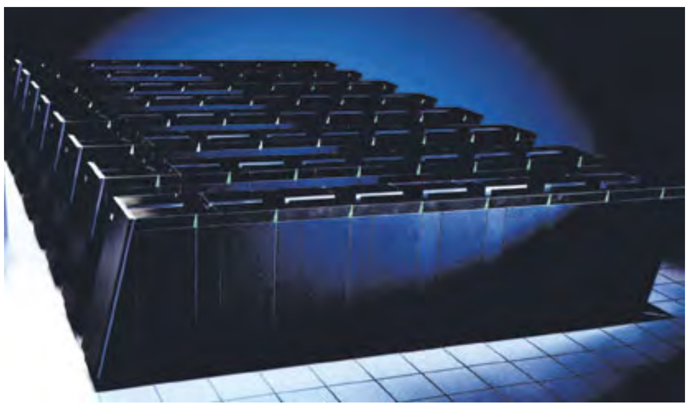
1946: ENIAC



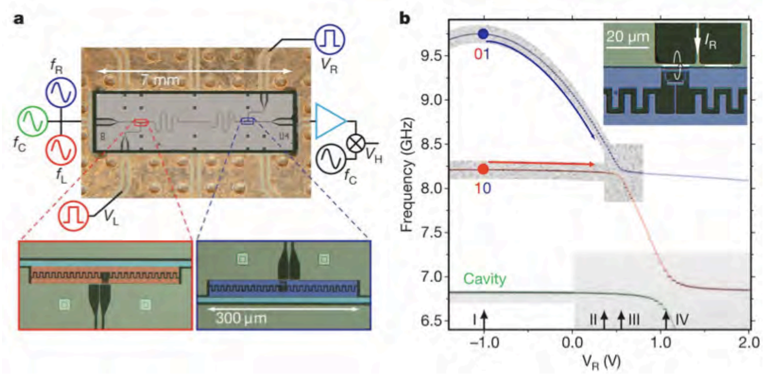
1947: Transistor (Bardeen, Brattain, Shockley)



2000: 100 million transistors in each PC chip



2004: BlueGene

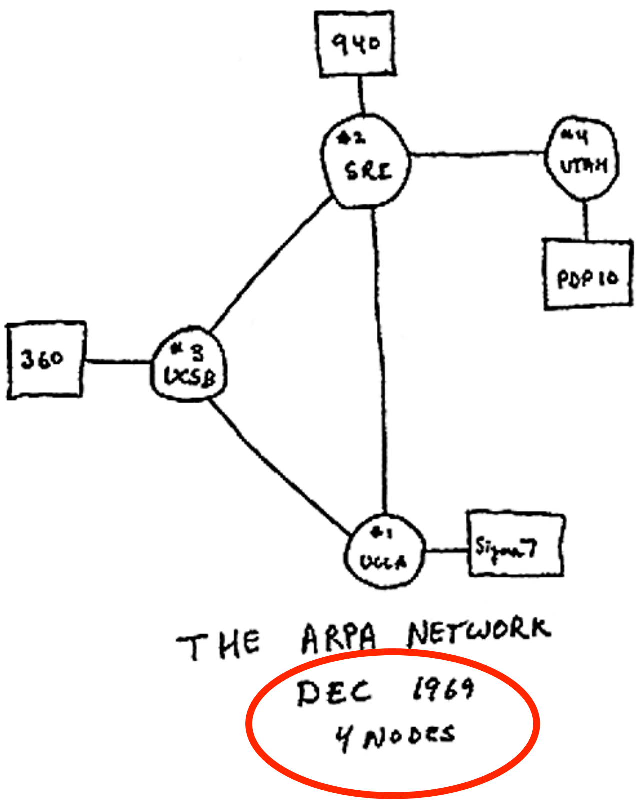


2009+: Quantum Computer

Will history repeat itself?

History of the Network

More important than the CPU!

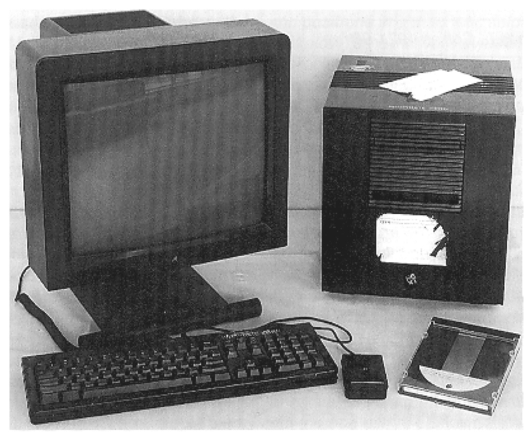


Netscape

1994: Andreessen

Google

1998: Page, Brin



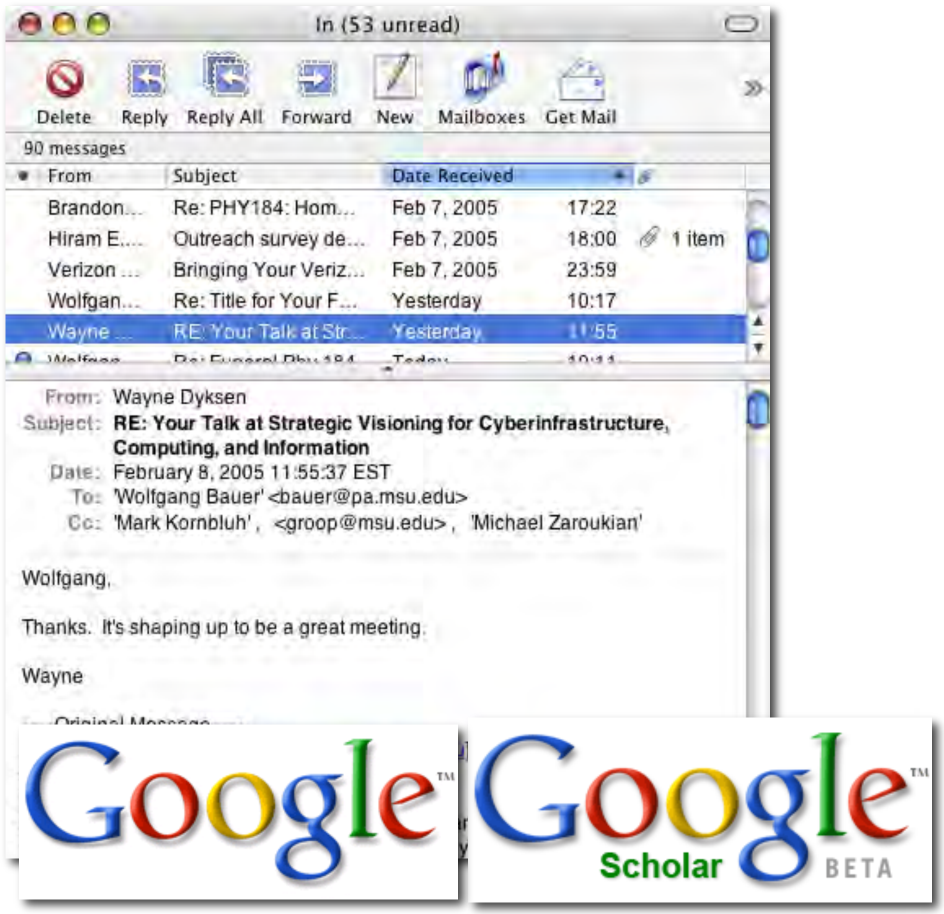
1989: WWW, Berners-Lee

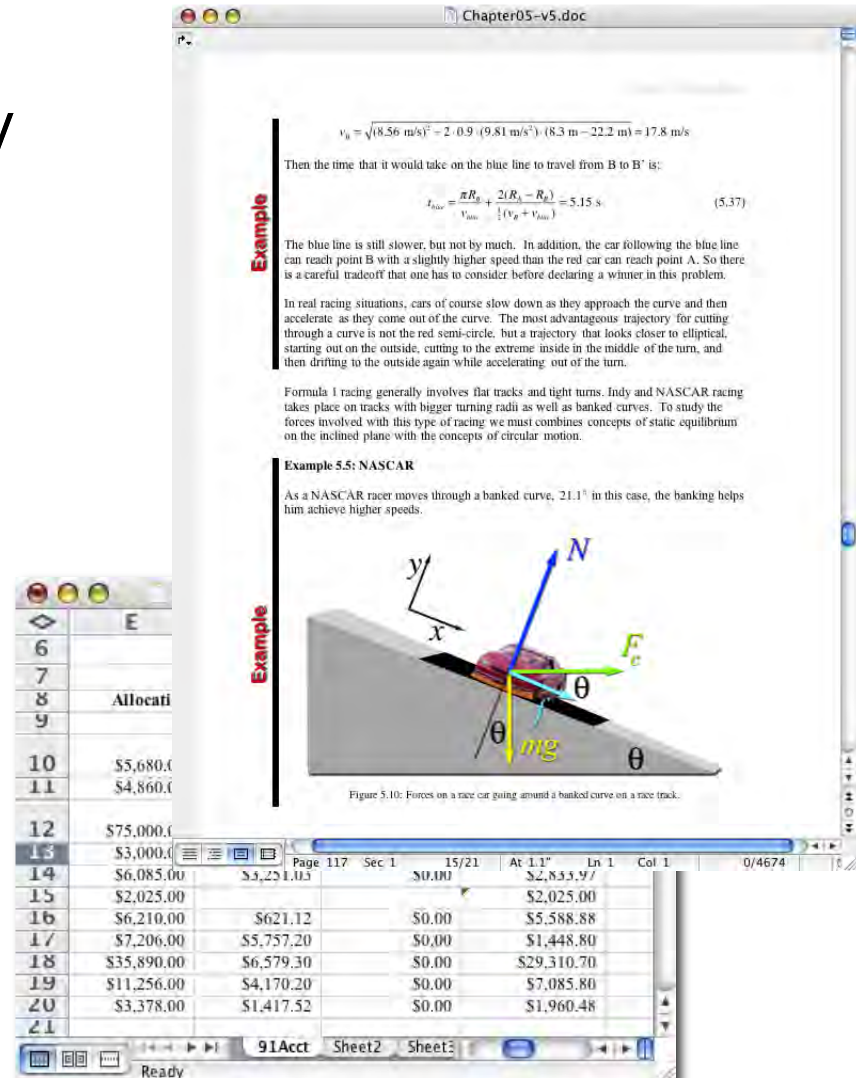
2007: iPhone (Apple)

Use of Computers: Email & Office Software

For all of us:

- significant fraction of our workday





Use of Computers: Programming

Languages:

- FORTRAN
- C(++)
- Java

E_field.java

E_field.java:235 drawEquiLine()

```java
    }

    public void drawEquiLine(double V, double x0, double y0, Graphics g) {
            int i=0;
            while ( i<10000 ){  // maximum number of line segments
                    i++;
                    double x=0, y=0;
                    int ix0 = (int)x0;
                    int iy0 = (int)y0;
                    double x01 = x0-x1;
                    double x02 = x0-x2;
                    double y01 = y0-y1;
                    double y02 = y0-y2;
                    double q1r = q1 / Math.pow(x01*x01 + y01*y01, 1.5);
                    double q2r = q2 / Math.pow(x02*x02 + y02*y02, 1.5);
                    double Ex = x01 * q1r + x02 * q2r;
                    double Ey = y01 * q1r + y02 * q2r;
                    double E = Math.sqrt(Ex*Ex + Ey*Ey);
                    // now find vector perpendicular to this one and move along it
                            x = x0 - 0.2 * Ey/E;
                            y = y0 + 0.2 * Ex/E;
                            x0 = x;
                            y0 = y;
                            if (x<724 && x>11 && y<558 && y>68) {
                                    g.drawLine(ix0,iy0,(int)x,(int)y);
                                    g.drawLine(ix0,2*y1-iy0,(int)x,(int)(2*y1-y));
                            }
                    // exit conditions: line crosses the connection line between 2 charges
                    if ((y1-iy0)*(y1-y) < 0) return;


            }
    }

    public void drawFieldLine(int thecase,  int nsteps, double x0, double y0, double thesign, Graphics g) {
            int i=0;
            while ( i<3000 ){  // maximum number of line segments
```

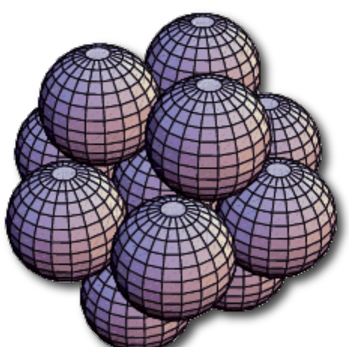
Use of Computers: Symbolic Manipulation

Programs:

- Mathematica
- Maple
- MathLab

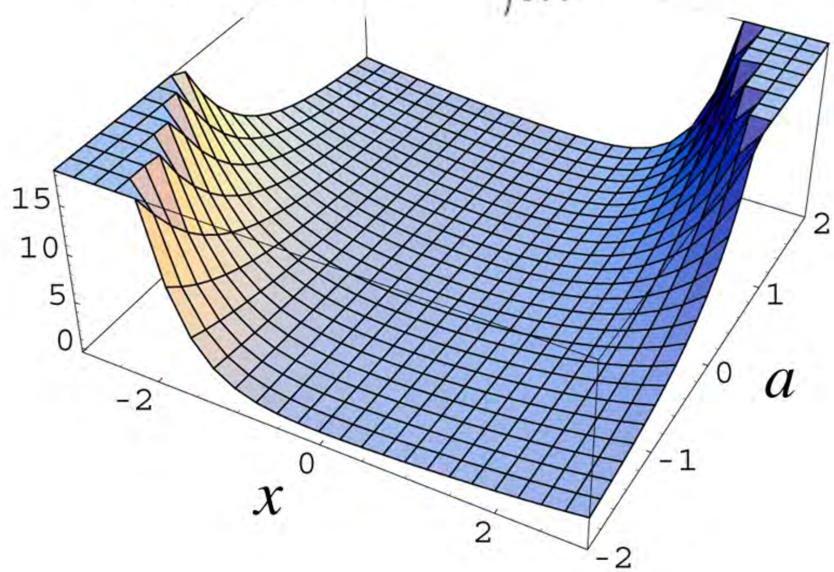
Real Mathematics Research:

e.g. Kepler Conjecture



```
In[1]:= DSolve[{y''[x] == a y'[x] + y[x], y[0] == 1,
          y'[0] == 0}, y, x]
```

Out[1]= $\{\{y \to \text{Function}\left[\{x\}, \frac{1}{2\sqrt{4+a^2}}\left(a\, e^{\frac{1}{2}\left(a-\sqrt{4+a^2}\right)x} + \sqrt{4+a^2}\, e^{\frac{1}{2}\left(a-\sqrt{4+a^2}\right)x} - a\, e^{\frac{1}{2}\left(a+\sqrt{4+a^2}\right)x} + \sqrt{4+a^2}\, e^{\frac{1}{2}\left(a+\sqrt{4+a^2}\right)x}\right)\right]\}\}$



Use of Computers: Data Collection

Use of Computers: Enabling Science

Three high-tech buzzwords:

Progress in

BIO

relies on advances in

NANO

And both are dependent on

INFO

High Performance Computing Center @ MSU

- **Green, SGI Altix 3700 Bx2,** originally purchased with 64 1.6GHz Itanium2 processors, 256GB of memory, and 6.4TB of scratch disk, has since been expanded to 128 processors and 576GB RAM. Its companion user node, white, is a four-processor system, suitable for compiling and short tests.
- **Wilson is a 512-core cluster from Western Scientific**. Each of the 128 nodes contains 2 dual-core AMD Opterons running at 2.2GHz, 8GB of memory, and 100GB of local disk. The cluster is tied together with 1Gb Ethernet and Infiniband. A Lustre filesystem provides 8TB of scratch space.
- **Brody is a 1024-core cluster from SGI.** Each of the 128 nodes contains 2 quad-core Xeons at 2.3GHz, 8GB of memory, and 250GB of local disk. Brody shares the same Ethernet and Infiniband networks as Wilson along with the Lustre filesystem.

High Performance Computing Center @ MSU

- **Starting in 2010/11**

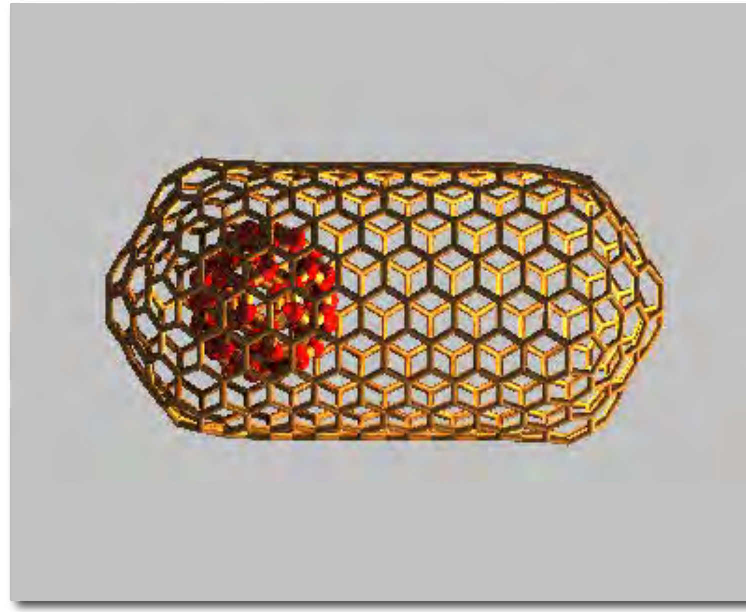
Member Institutions

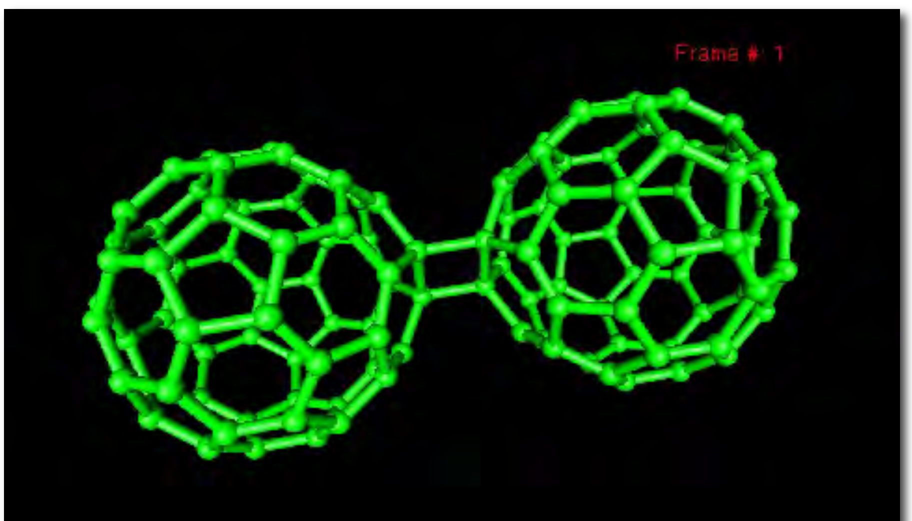
Charter members of the Great Lakes Consortium for Petascale Computation include:

- Argonne National Laboratory
- Chicago State University
- Fermi National Accelerator Laboratory
- Illinois Math and Science Academy
- Illinois Wesleyan University
- Indiana University
- Iowa State University
- Krell Institute, Inc.
- Los Alamos National Laboratory
- Louisiana State University / Center for Computation & Technology
- Michigan State University
- Northwestern University
- The Ohio State University
- Parkland College (Illinois)
- Pennsylvania State University / Institute for CyberScience
- Purdue University
- Shiloh Community Unit School District #1 (Illinois)
- Shodor Education Foundation, Inc.
- SURA (Association of more than 60 universities in the southeastern United States)
- University of Chicago
- University of Illinois at Chicago
- University of Illinois at Urbana-Champaign
- The University of Iowa
- University of Michigan
- University of Minnesota / Minnesota Supercomputing Institute
- University of North Carolina, Chapel Hill / Renaissance Computing Institute
- University of Wisconsin, Madison
- Wayne City High School (Illinois)

Computational Nano-Science

- Prediction of materials' structures and properties
- *Ab initio* calculations of quantum forces between atoms
- Density functional theory

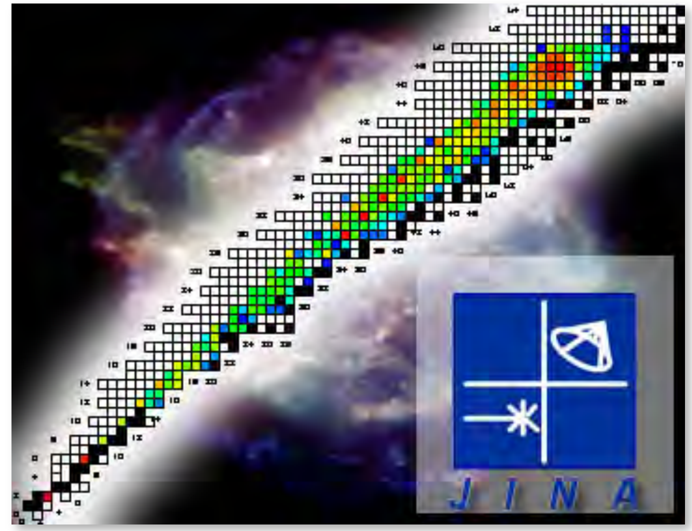




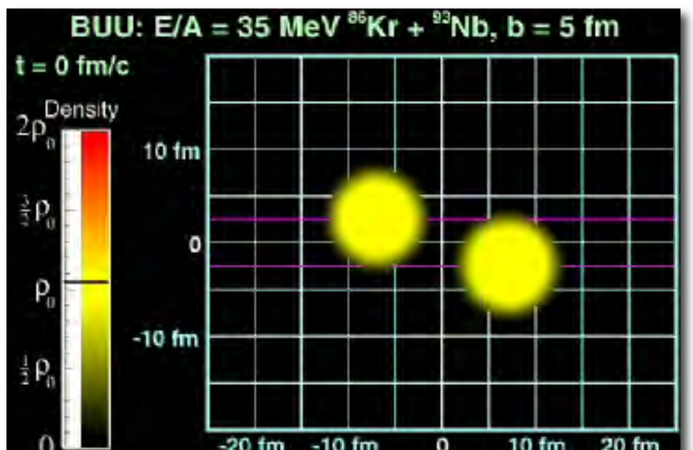
- Example 1: Carbon pea-pod memory
  - U.S. Patent 6,473,351
- Example 2: Time dependence of buckyball fusion
- Calculations done with Earth Simulator

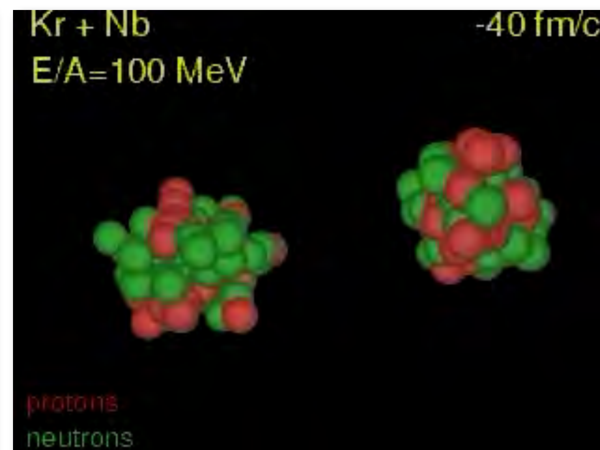
David Tomanek, MSU-PA

Computational Nuclear Physics



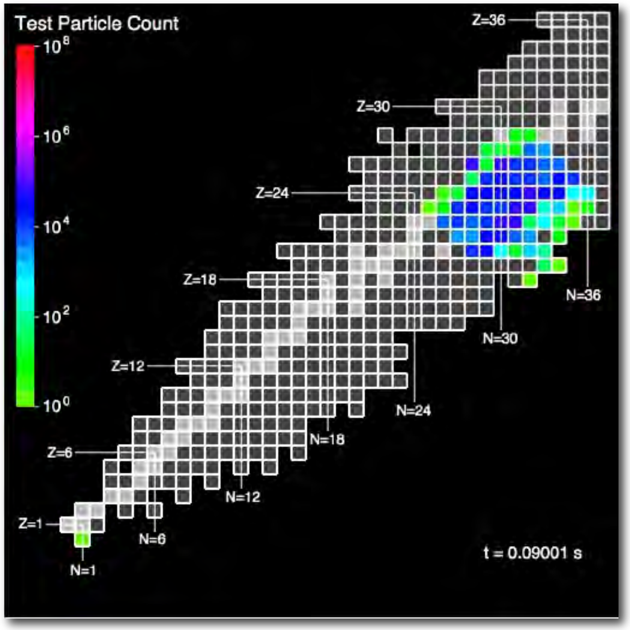
- Big questions:
  - How are the heaviest elements made in the universe?
  - What is the equation of state of nuclear matter?
- Experimental Facilities
  - NSCL, FRIB
- Computational Tools
  - Transport Theory
  - Reaction Networks



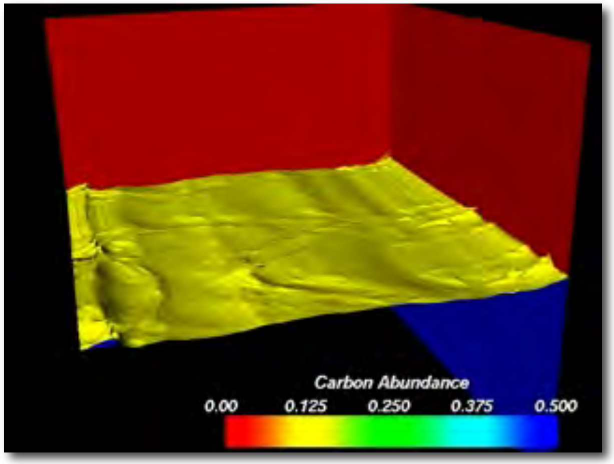


Computational Astrophysics

- Astrophysics has to answer questions without any chance of doing experiments
- Running computer simulations and comparing their output to static observations is only path to progress



Terrance Strother

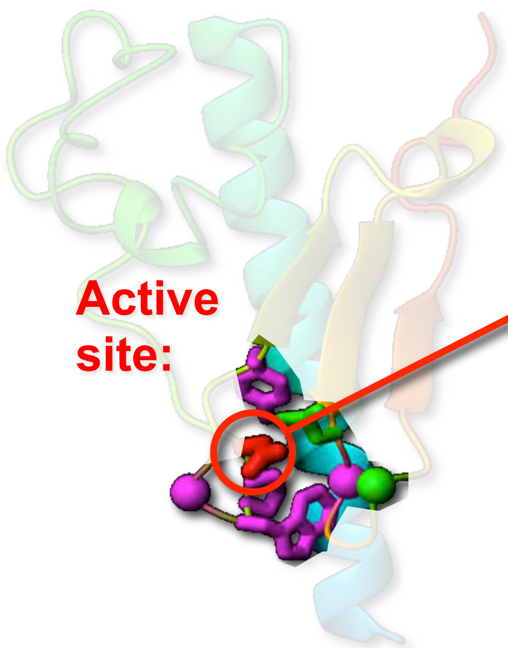


Ed Brown, with Flash Center, Chicago

Computational Biochemistry

- Protein folding
  - 3d structure from genetic code sequence
  - Constrained molecular dynamics calculations

Example: Cholera protein
- *Vibrio cholerae*
- acts like a piston to push out cholera toxin
- calculations predict structure



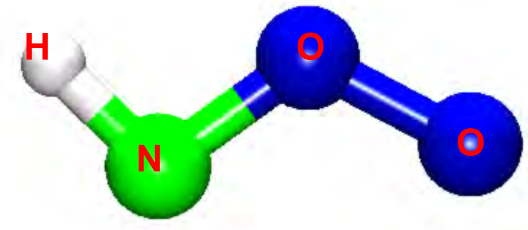
Calculation prediction: knock out this residue and neutralize poison

88 (3 GHz) processors
200 Gflop/s
Wedemeyer, Feig

Computational Quantum Chemistry

- Coupled Cluster Methods
  - Inclusion of many-particle correlation effects
  - Highly successful in quantum chemistry
  - Now also ported to nuclear physics
  - Extremely predictive
    - Example: HNOO controversy - CC methods determined which experiment was right (!!!)

Imine Peroxide



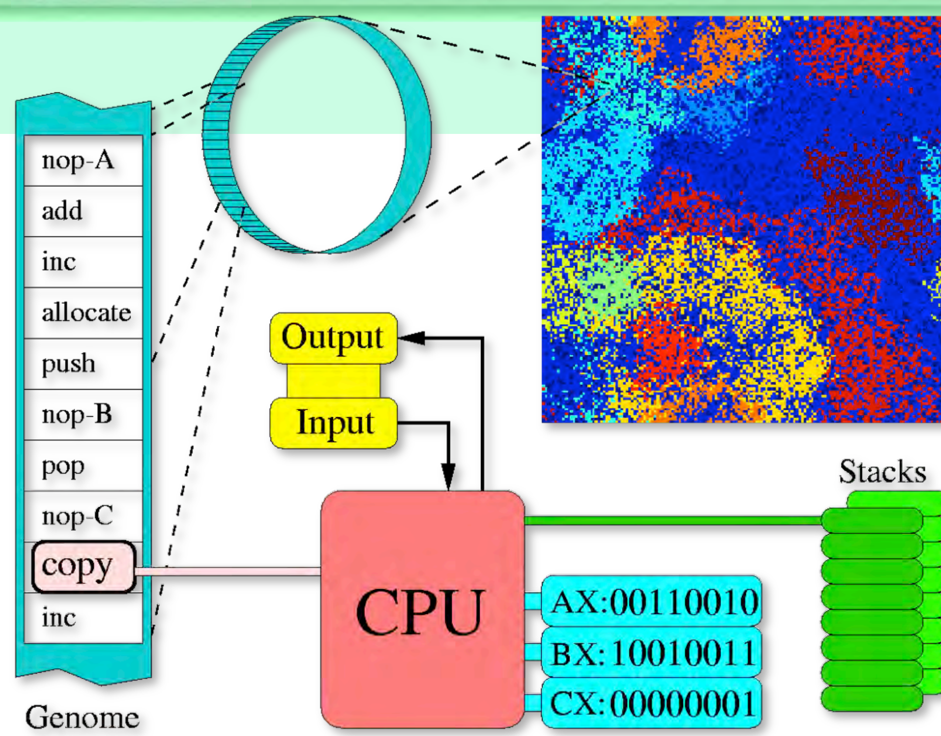
P. Piecuch et al.

Fundamental Frequency	Exp: LBSW	Exp.:LGDS	CCSD(T)	CR-CCSD(T)	CCSD(TQ$_f$)	CCSDT-3(Q$_f$)
f_1 (NH stretch)	3287.7	3165.5	3189	3198	3188	3188
f_2 (HNO bend)	not observed	1485.5	1492	1509	1494	1499
f_3 (NO stretch)	1381.6	1092.3	1147	1116	1123	1126
f_4 (OO stretch)	843.2	✔ 1054.5	1042	1078	1047	1071
f_5 (NOO bend)	670.1	not observed	650	653	650	650
f_6 (torsion)	790.7	764.0	764	777	757	757

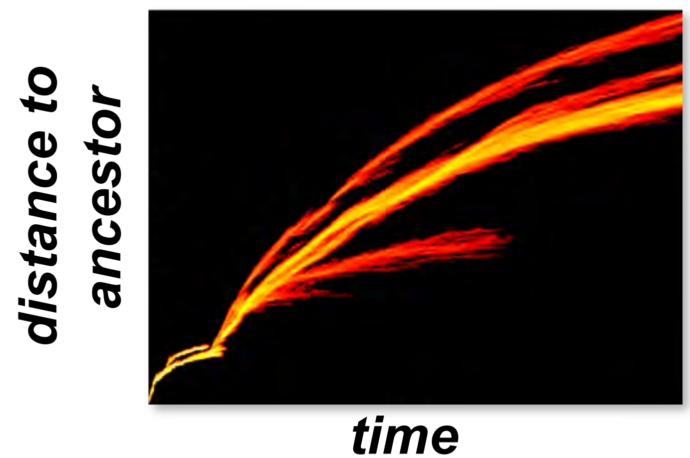
•**LBSW:** P. Ling, A.I. Boldyrev, J. Simons, and C.A. Wight, *J. Am. Chem. Soc.* 120, 12327 (1998).
•**LGDS:** S.L. Laursen, J.E. Grace Jr., R.L. DeKock, and S.A. Spronk, *J. Am. Chem. Soc.* 120, 12327 (1998).

Digital Evolution

- “Computer Viruses”
- Self-replicating pieces of code
- Random mutation
- Competition for space on hard drive according to fitness criteria
- Many orders of magnitude faster than watching E-coli bacteria grow and divide



- Digital organisms ***SOLVE*** computational problems.



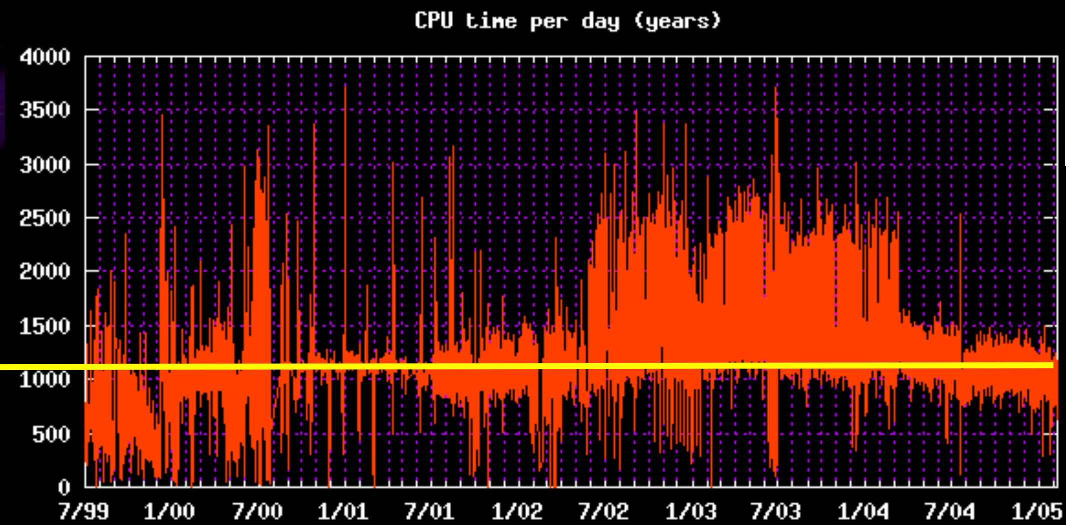
- 2010: BEACON NSF STC (Goodman et al.)

Richard Lenski, Charles Ofria, et al.

Computing with the Internet: SETI

SETI@home
The Search for Extraterrestrial Intelligence

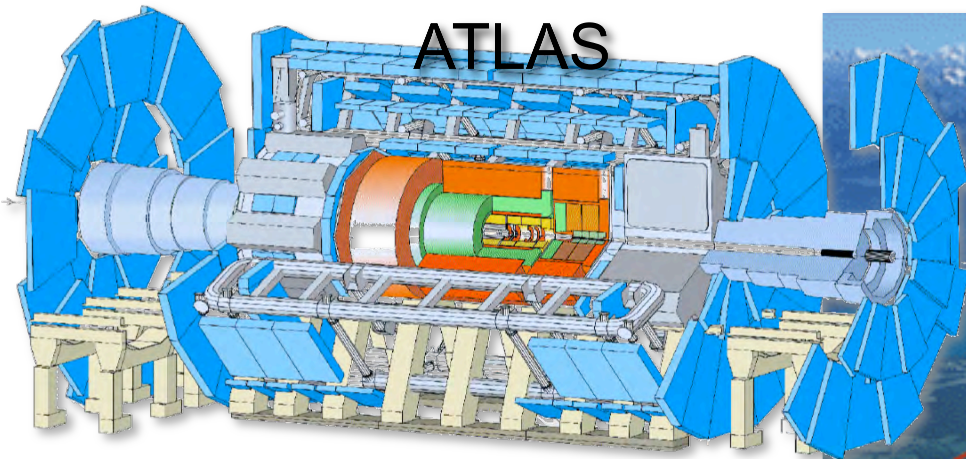
> 1000 CPU years/day !

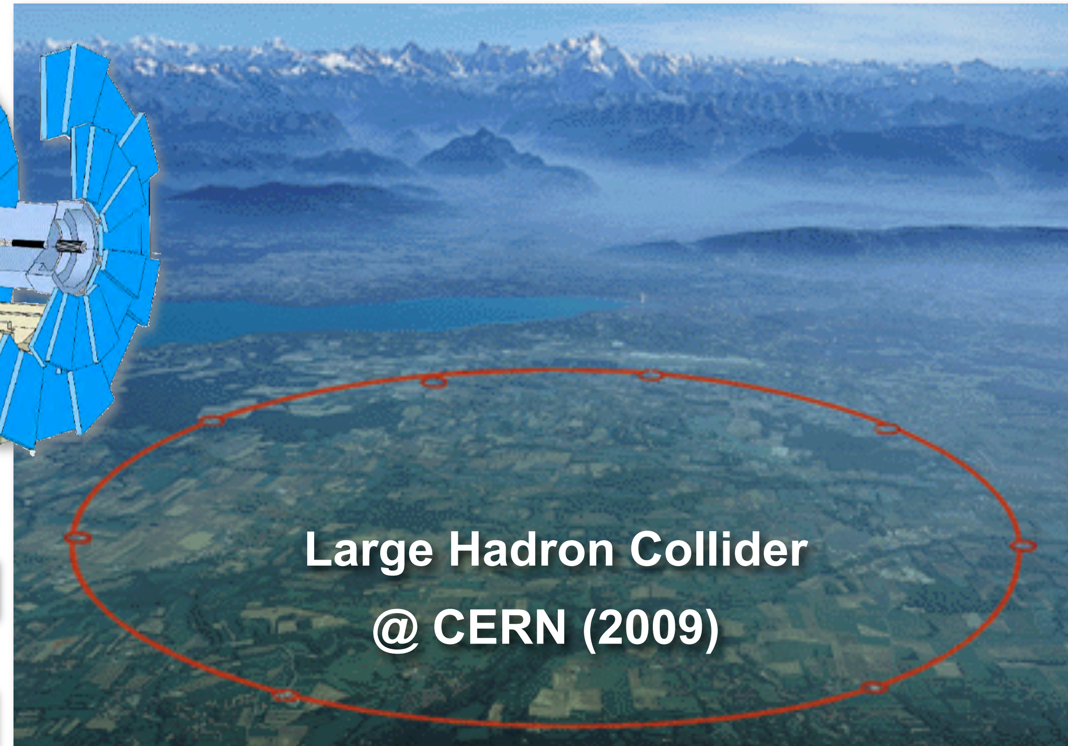


	Total	Last 24 Hours
Users	5343984	1049
Results received	1758329525	1320508
Total CPU time	2213000.413 years	963.120 years
Floating Point Operations	6.441670e+21	5.149981e+18 (59.61 TeraFLOPs/sec)
Average CPU time per work unit	11 hr 01 min 30.6 sec	6 hr 23 min 20.9 sec

~60 TeraFLOP/s

Computing for Data Reduction





Data rate: 40 MHz, 40 TB/s

Level 1 - Special hardware

75 kHz, 75 GB/s

Level 2 - embedded processors

5 kHz, 5 GB/s

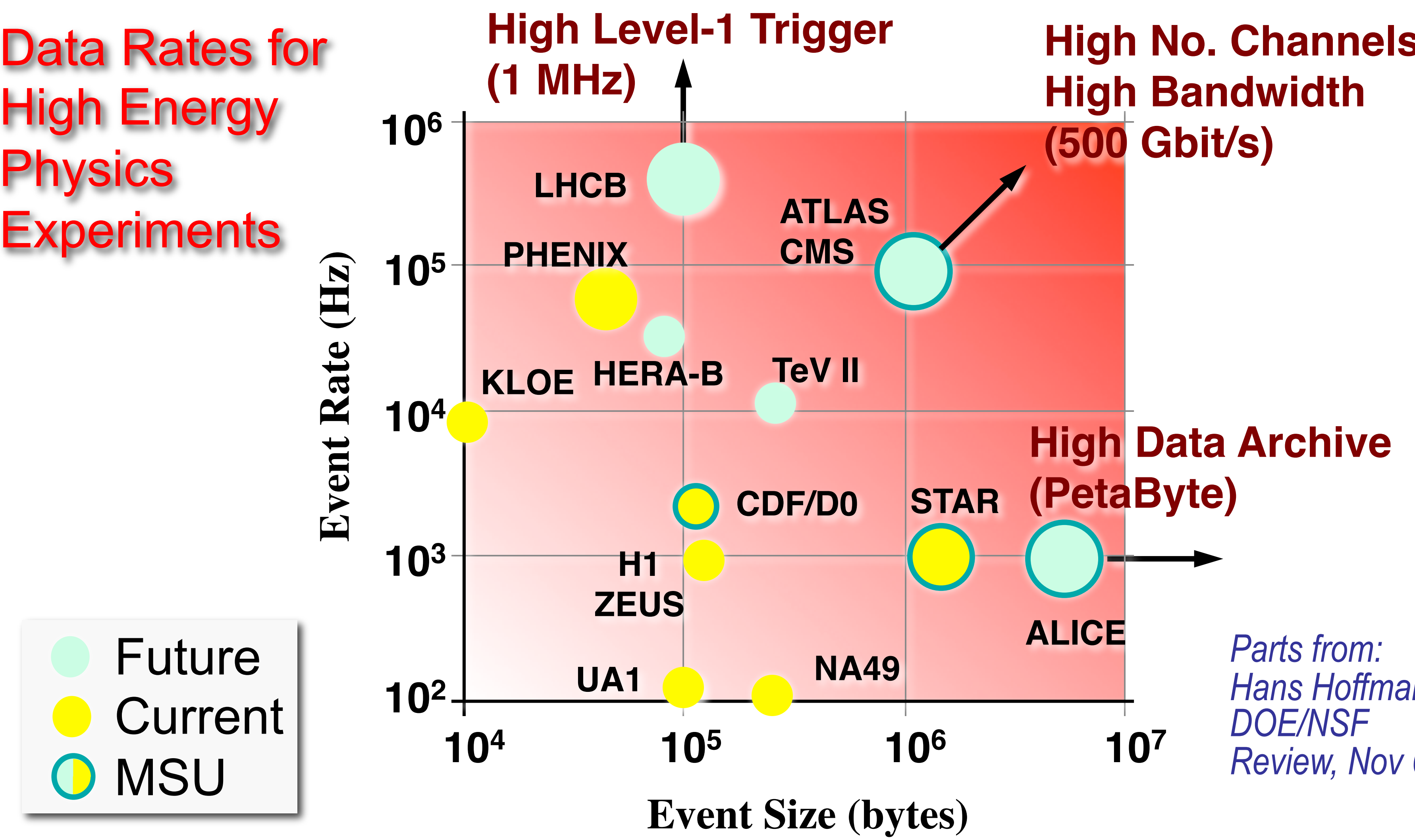
Level 3 - dedicated PCs

100 Hz, 100 MB/s

Data storage and offline analysis
ATLAS: **~10 PetaByte/year**
(~10,000 PC hard drives of 1 TB)

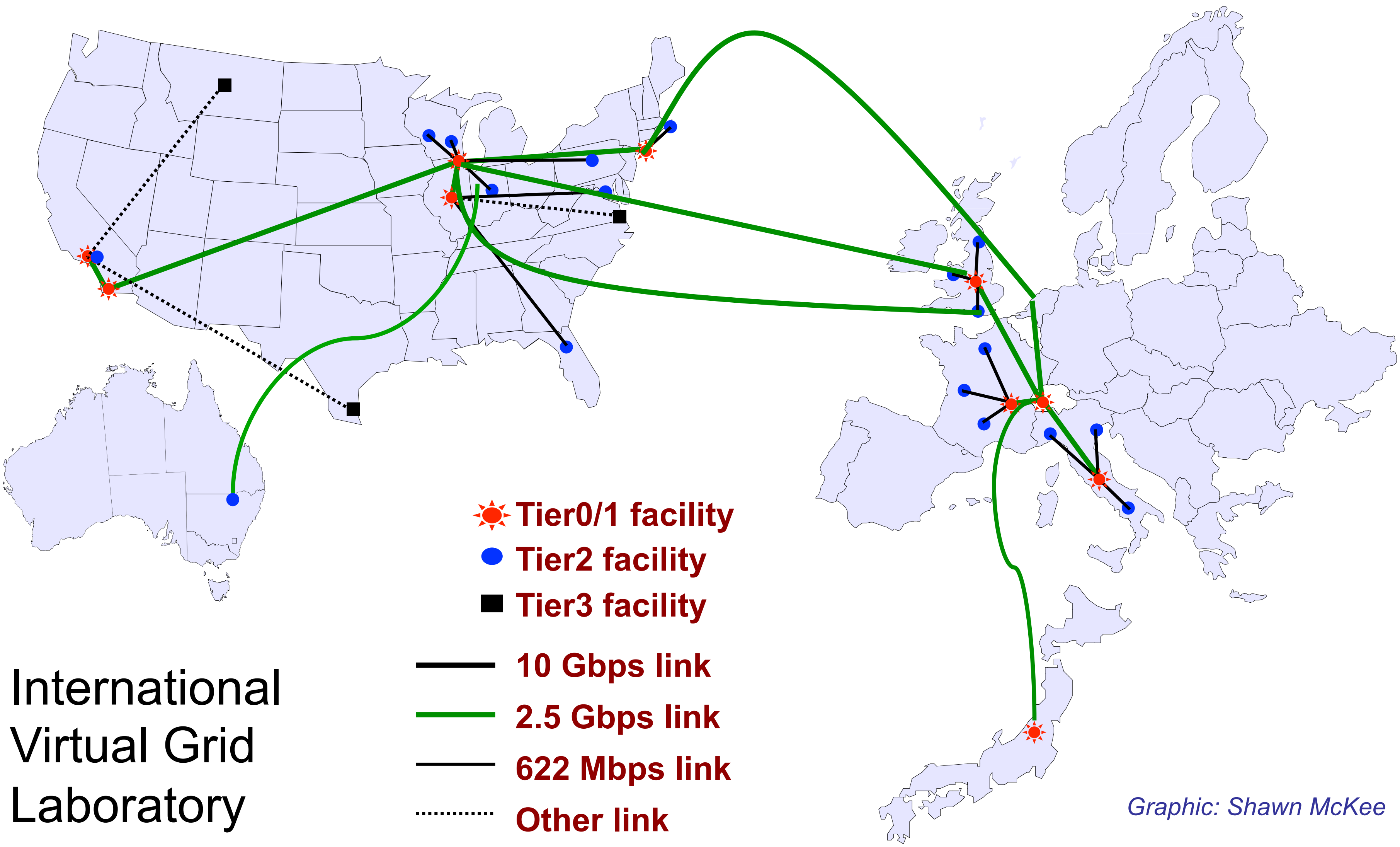
Data Streams for Different Experiments

Data Rates for High Energy Physics Experiments



Parts from: Hans Hoffman DOE/NSF Review, Nov 00

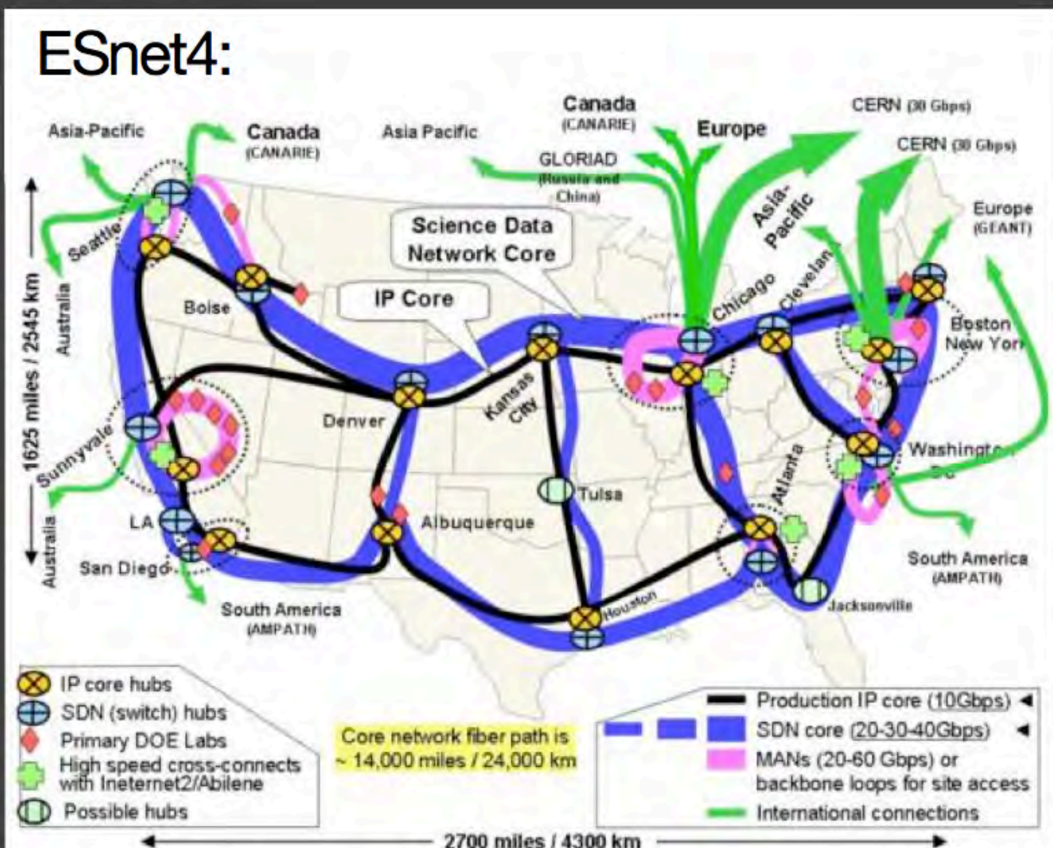
Computing with the Internet: Grid



International Virtual Grid Laboratory

Graphic: Shawn McKee

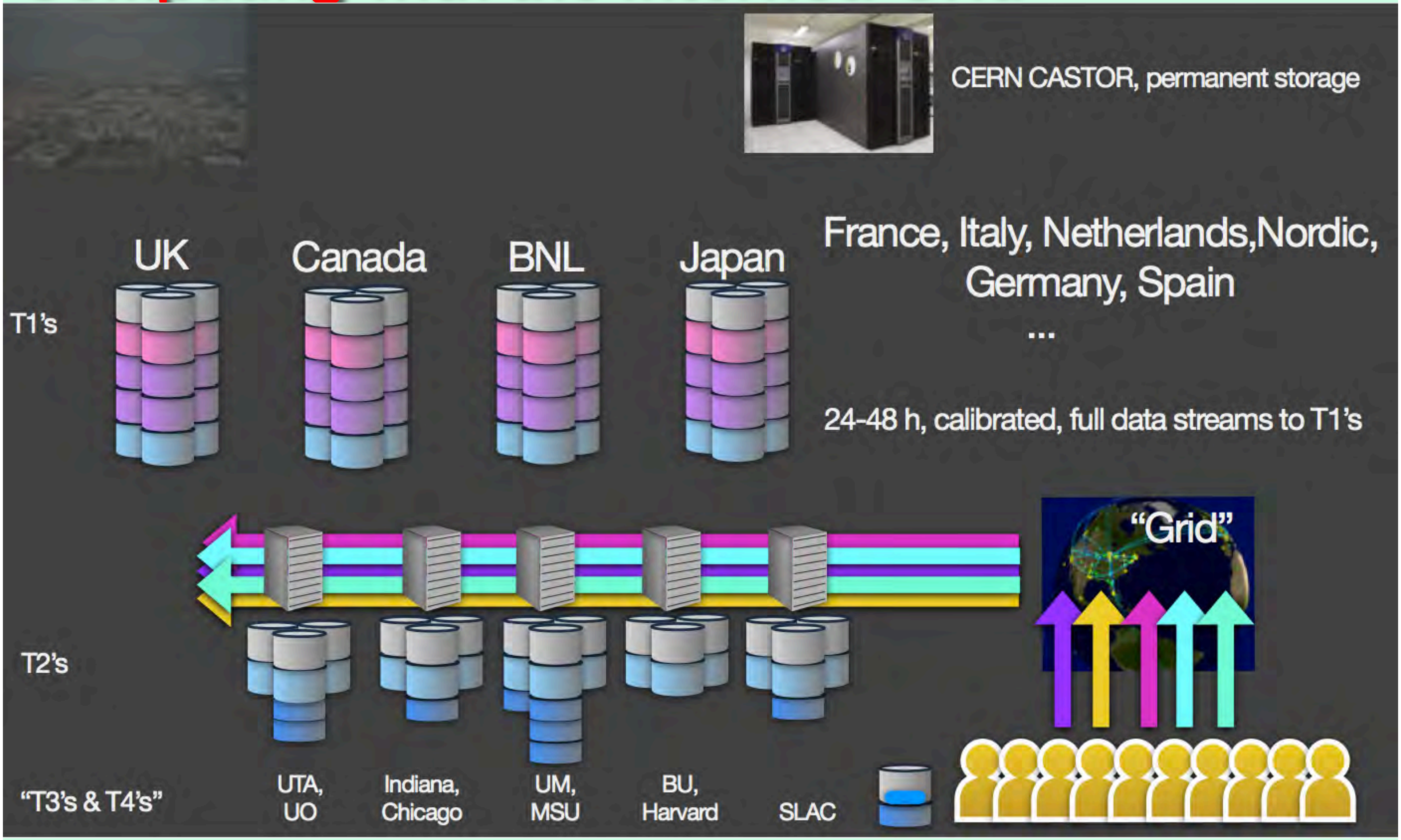
Computing with the Internet: Grid



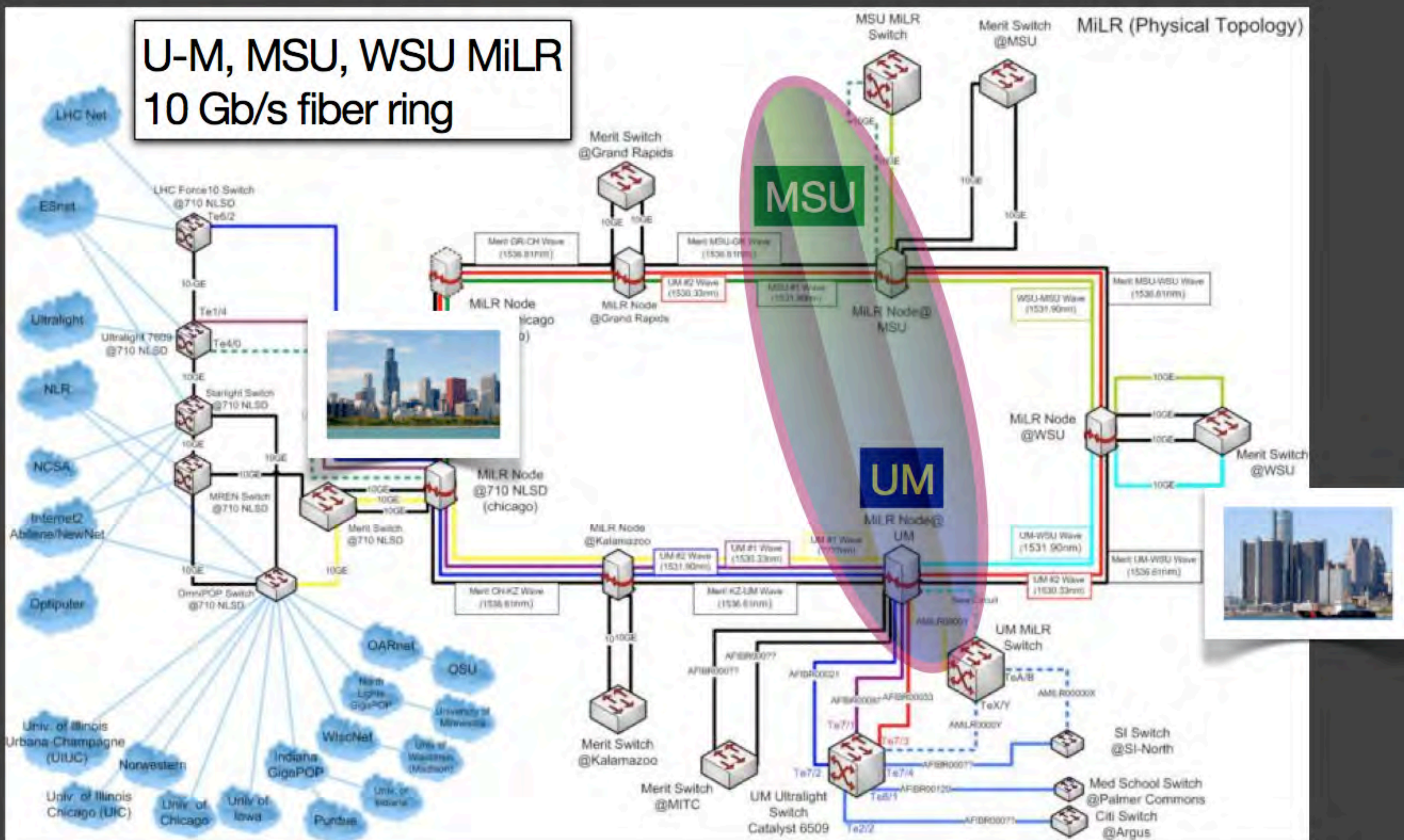
the infrastructure:

"Energy Science Network" (ESnet)

Computing with the Internet: Grid



Computing with the Internet: Grid



Computing with the Internet: Grid

5 Racks running since December

Hardware:

computing:

Dell Poweredge 1950

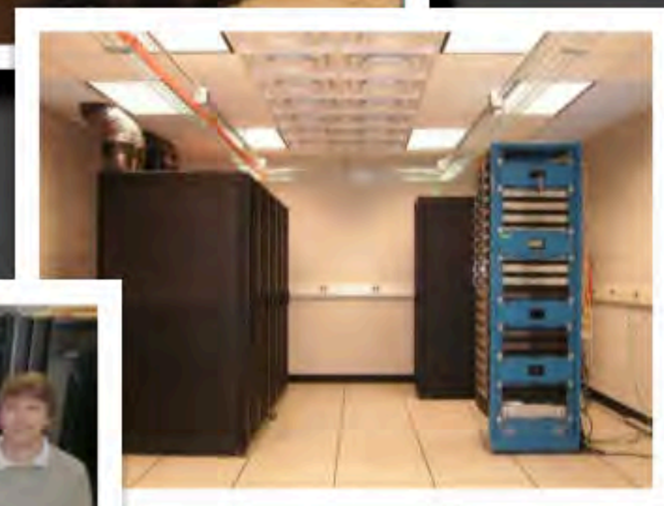
54 nodes Intel Xeon 5355, 2.67 GHz dual, quad core

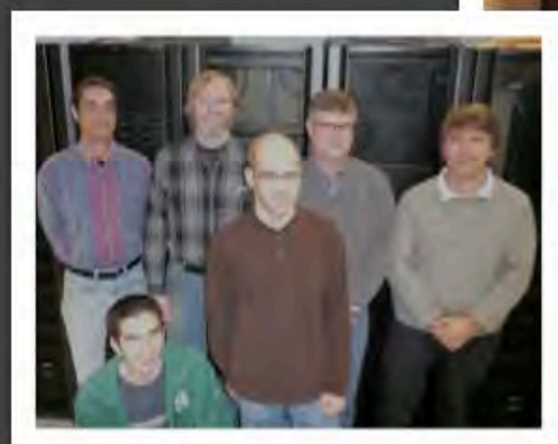
(SPECint_2000: ~2178/cpu => ~17,424/node => 940k SPECint2000)

storage:

PowerVault MD1000

225,000GB storage in 5 shelves





Computers in Teaching

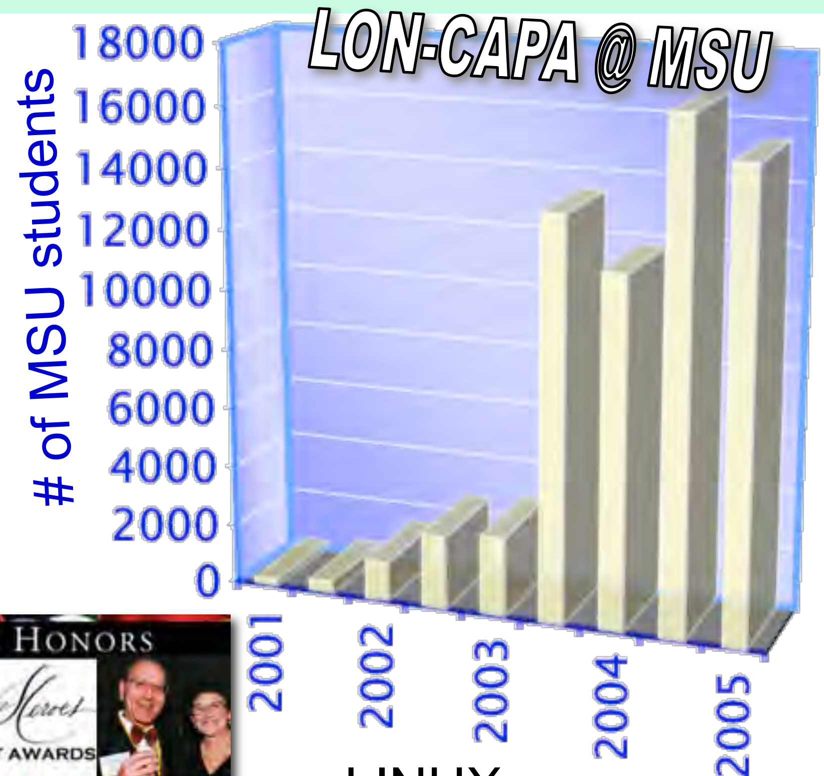
- ***Core Business of Any University:***

  Creation, Application, and
  Dissemination of Knowledge Information

- Information Technology has changed the way that knowledge/ information is created in the physical sciences
- Information Technology is changing the way that knowledge/ information is delivered in the 21st century
  - Current virtual university delivery models have not even begun to scratch the surface of what is possible with the availability of essentially infinite bandwidth!
  - Adaptive, immersive, customized learning environments!
  - Brick&Mortar advantages will go away!
- ***We cannot afford to outsource the management of Information Technology to commercial entities!***

Computers in Teaching: LON-CAPA

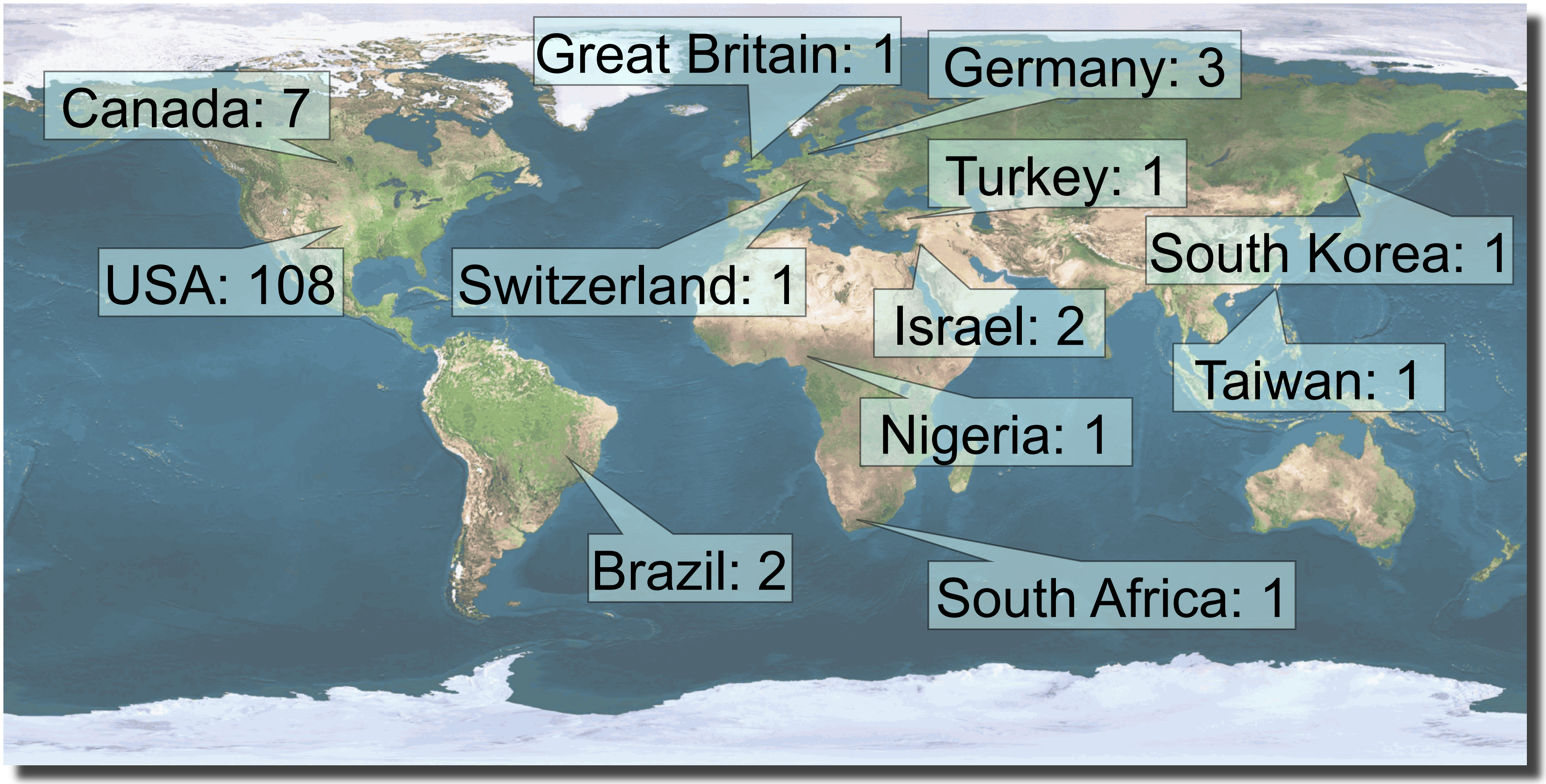
- ***Research***: artificial intelligence, databases, expert systems, genetic algorithms, self-organization
- Content sharing across the net
- Customized content delivery for individual students
- Seamless internationalization
- ~70 US universities in collaboration
- MSU leadership (NSF ITR)



- LINUX, Apache, GNU public license
- Library of >10^5 reusable resources (web page, movie, applet, graphic, …)

G. Kortemeyer et al.

Computers in Teaching: LON-CAPA



Predictions

- Predictions are hard …
  - *"Prediction is very difficult, especially about the future"*
    (Niels Bohr, Nobel 1922)
  - *"I think there is a world market for maybe five computers"*
    (Thomas Watson Sr., IBM president, in 1943)
- But still useful …
  - *Predictions are like Austrian train schedules. Austrian trains are always late. So why do the Austrians bother to print train schedules? How else would they know by how much their trains are late?*
    (Viktor Weisskopf, paraphrased)
- So here we go …
  - Moore's Law will continue for at least another 2 decades
  - Network bandwidth will become infinitesimally cheap and eventually (~2 decades) saturate the human input bandwidth
  - Caution 1: *"Software is a gas" (Nathan Myrvold)*
  - Caution 2: Growth in content will only be linear, not exponential

Feynman's Thoughts

"Simulating Physics with Computers"
International Journal of Theoretical Physics, **21** (6/7), p 467 (1982)

Feynman's Thoughts: Topics

1. Introduction
2. Simulating Time
3. Simulating Probability
4. Quantum Computers - Universal Quantum Simulators
5. Can Quantum Systems be Probabilistically Simulated by Classical Computers
6. Negative Probabilities
7. Polarization of Photons - Two States Systems
8. Two-Photon Correlation Experiment

$$a = \text{ANNIHILATE} = \begin{array}{c|cc} & \text{OCC} & \text{UN} \\ \hline \text{OCC} & 0 & 0 \\ \text{UN} & 1 & 0 \end{array} = \tfrac{1}{2}(\sigma_x - i\sigma_y)$$

$$a^* = \text{CREATE} = \begin{array}{|cc} \hline 0 & 1 \\ 0 & 0 \end{array} = \tfrac{1}{2}(\sigma_x + i\sigma_y)$$

$$n = \text{NUMBER} = \begin{array}{|cc} \hline 1 & 0 \\ 0 & 0 \end{array} = a^*a = \tfrac{1}{2}(1 + \sigma_z)$$

$$\mathbb{1} = \text{IDENTITY} = \begin{array}{|cc} \hline 1 & 0 \\ 0 & 1 \end{array}$$

- Fundamental problem of classical computers: cannot simulate negative probabilities.

- Classical computers get two-photon correlation experiment wrong
- => Quantum cryptography

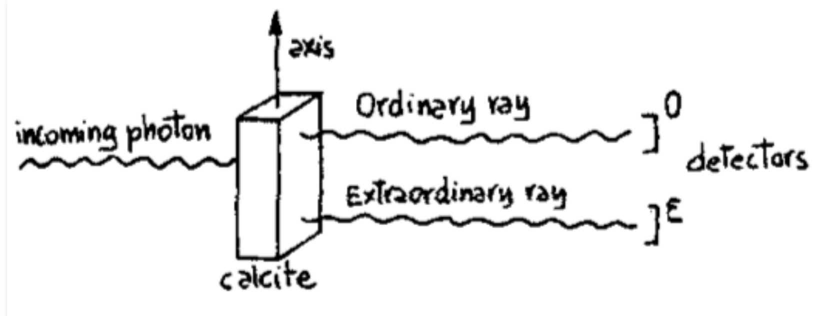


Fig. 2.

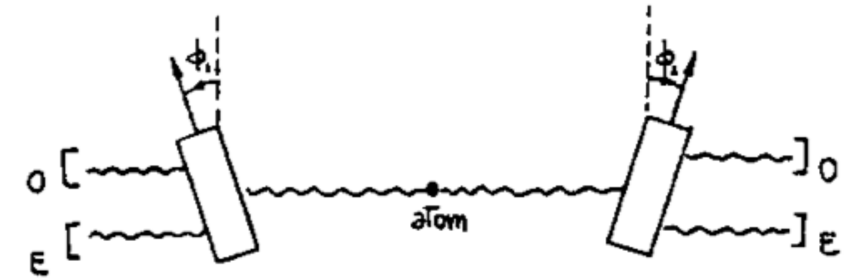


Fig. 4.

Why Quantum Computer?

- Need a quantum computer to really simulate a quantum system!

And I'm not happy with all the analyses
that go with just the classical theory,
because nature isn't classical, dammit, and
if you want to make a simulation of nature,
you'd better make it quantum mechanical,
and by golly it's a wonderful problem,
because it doesn't look so easy.

Richard P. Feynman, 1981

Future of Computing: Quantum Computer

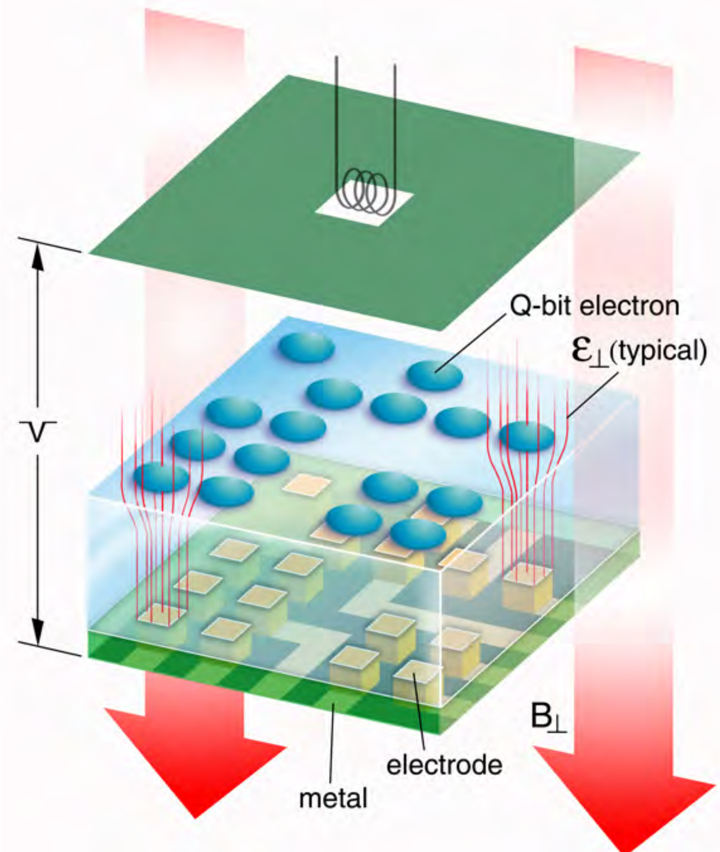
- Quantum two-state system
  - States denoted as $|0\rangle$ and $|1\rangle$
  - Transitions between states can be induced externally
  - System can be in *superposition* of two states:

  qubit, $|\psi\rangle = c_1|1\rangle + c_0|0\rangle$ with $|c_1|^2 + |c_0|^2 = 1$
- 2 qubit system: $|\psi\rangle = c_{11}|11\rangle + c_{10}|10\rangle + c_{01}|01\rangle + c_{00}|00\rangle$
- 3 qubit system:

$$|\psi\rangle = c_{111}|111\rangle + c_{110}|110\rangle + c_{101}|101\rangle + c_{100}|100\rangle$$
$$+ c_{011}|011\rangle + c_{010}|010\rangle + c_{001}|001\rangle + c_{000}|000\rangle$$

- Number of coefficients grows as 2^n.

Future of Computing: Quantum Computer



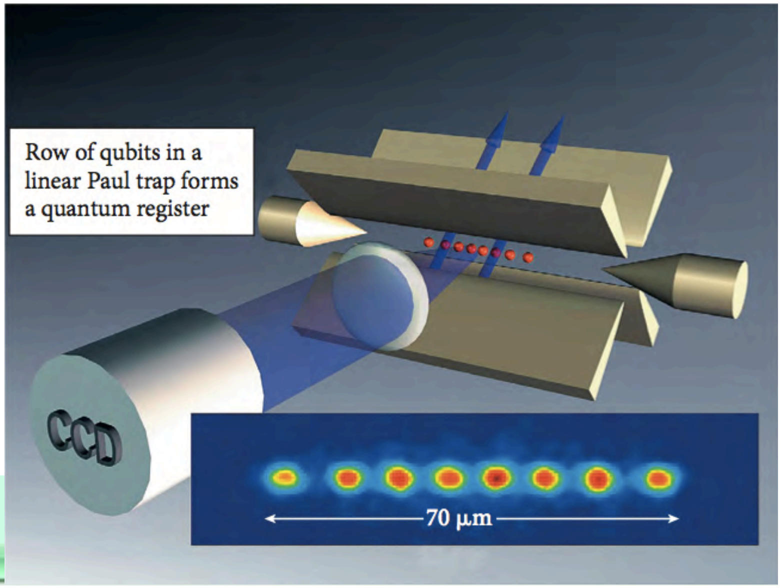
Proposed 16-bit quantum computer design: electrons on liquid helium (M. Dykman et al.)

- Conventional computer:
  - *N* processors can process *N* instructions simultaneously
- Quantum computer:
  - *N* processors can process 2^N instructions simultaneously
- Example:
  - $N = 16$: $2^{16} = 65{,}536$
  - $N = 32$: $2^{32} = 4{,}294{,}967{,}296$

Future of Computing: Quantum Computer

- Beautiful mathematics
  - Lots of concepts already developed in the early days of quantum mechanics
  - Key ingredient: ***Entanglement***
  - Surprising applications in a few algorithms (database sort, integer factorization)
- Candidates:
  - Electrons on liquid helium
  - Trapped ions
  - Superconducting circuits, SQUIDs
  - Optical lattices
  - NMR
  - BEC-based
  - Cavity QED
  - …
- **But:** where is the experimental manifestation for large *N*?

R. Blatt "Quantum Information Processing: Dream and Realization," Entangled World, pp. 235– 270, Wiley-VCH, Weinheim 2006.

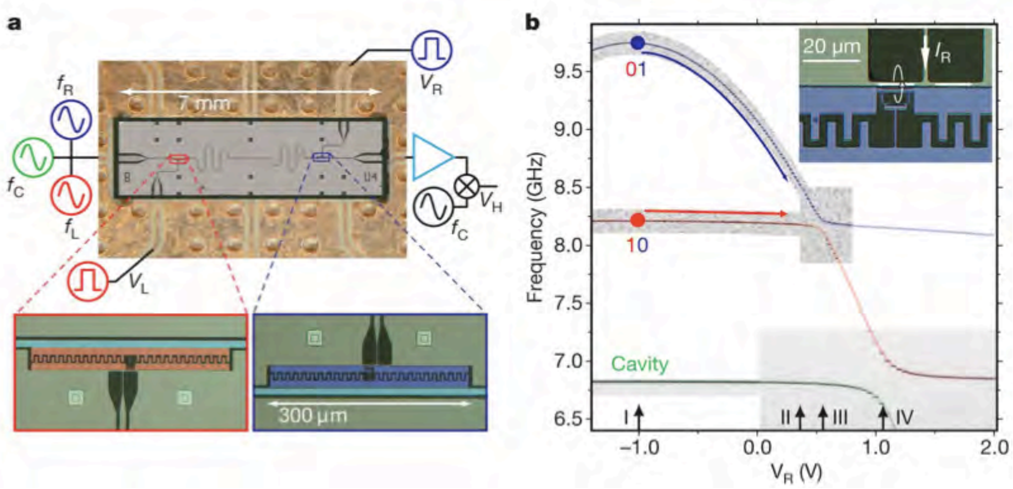


Future of Computing: Quantum Computer

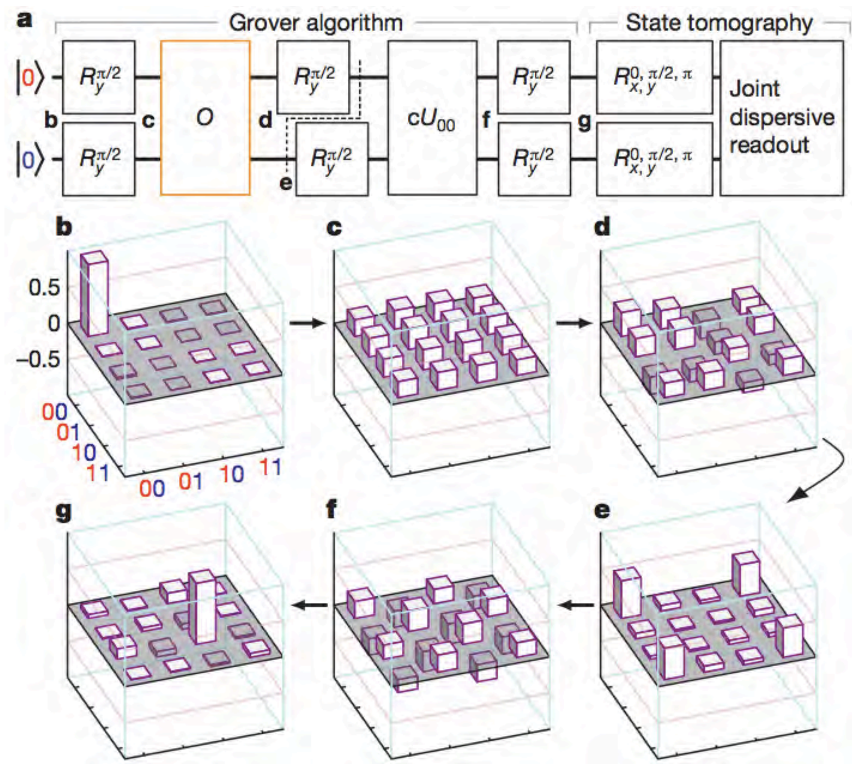
What problem can a quantum computer solve?

- Database search ✔
  - Grover's algorithm
- Factorization of large integers (✔)
  - Polynomial instead of exponential time
  - Very interesting for encryption/decryption
    - Encryption algorithm: Multiply two large prime numbers
    - Decryption: factorization takes prohibitively long (classically, but not with a quantum computer)
- Error correction algorithm ✔

Future of Computing: Quantum Computer



L. DiCarlo et al.
(Yale, Waterloo, Wien),
Nature **460**, 240 (2009)



- Interesting recent example:
  - Superconducting 2-qubit system
  - Microwave cavity
- Entanglement on demand
- Experimental implementation of Grover's search algorithm

Future of Computing: Quantum Computer

- Can general purpose quantum computing really work for large number of qubits?
- Fully entangled state = many-body wave function

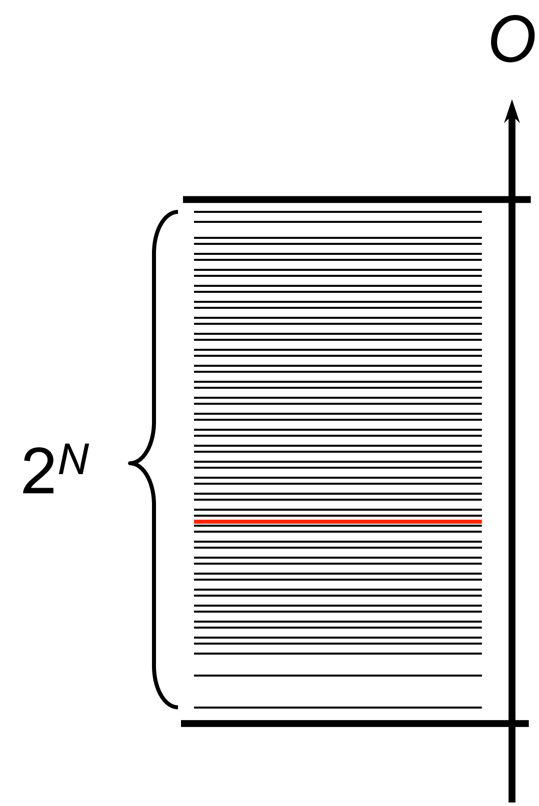
$$|123...N\rangle = |1\rangle \otimes |2\rangle \otimes |3\rangle \otimes ... \otimes |N\rangle$$

- Conduct measurement

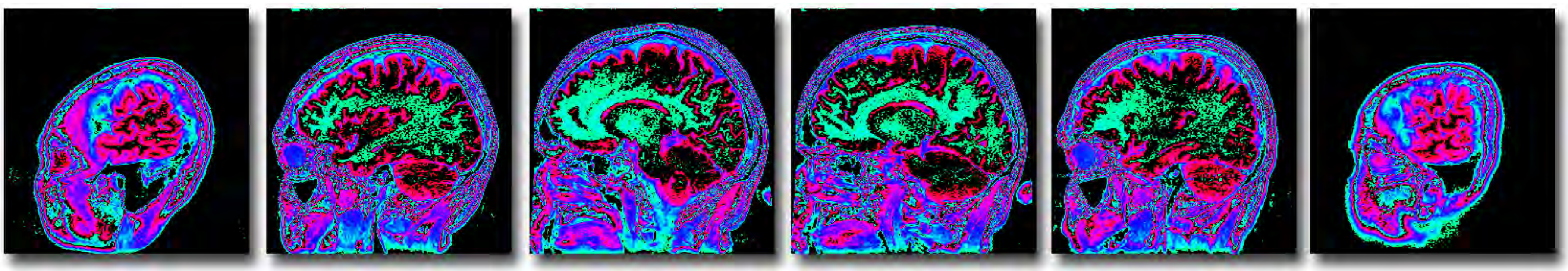
$$O = \langle 123...N|\hat{O}|123...N\rangle$$

- Demand absence of degeneracy to make measurement result single-valued function
- Physical upper and lower boundaries
- Must fit 2^N discrete values in finite band
- Q-factor problem

$$Q = 2\pi \frac{E}{|\Delta E|}$$



Brain Computing



Brain Computing

Neurons

- conducts the necessary currents by electrochemical means, via the movement of ions (mainly Na^+, K^+, and Cl^-).
- receive signals from other neurons through dendrites and send signals to other neurons through an axon.

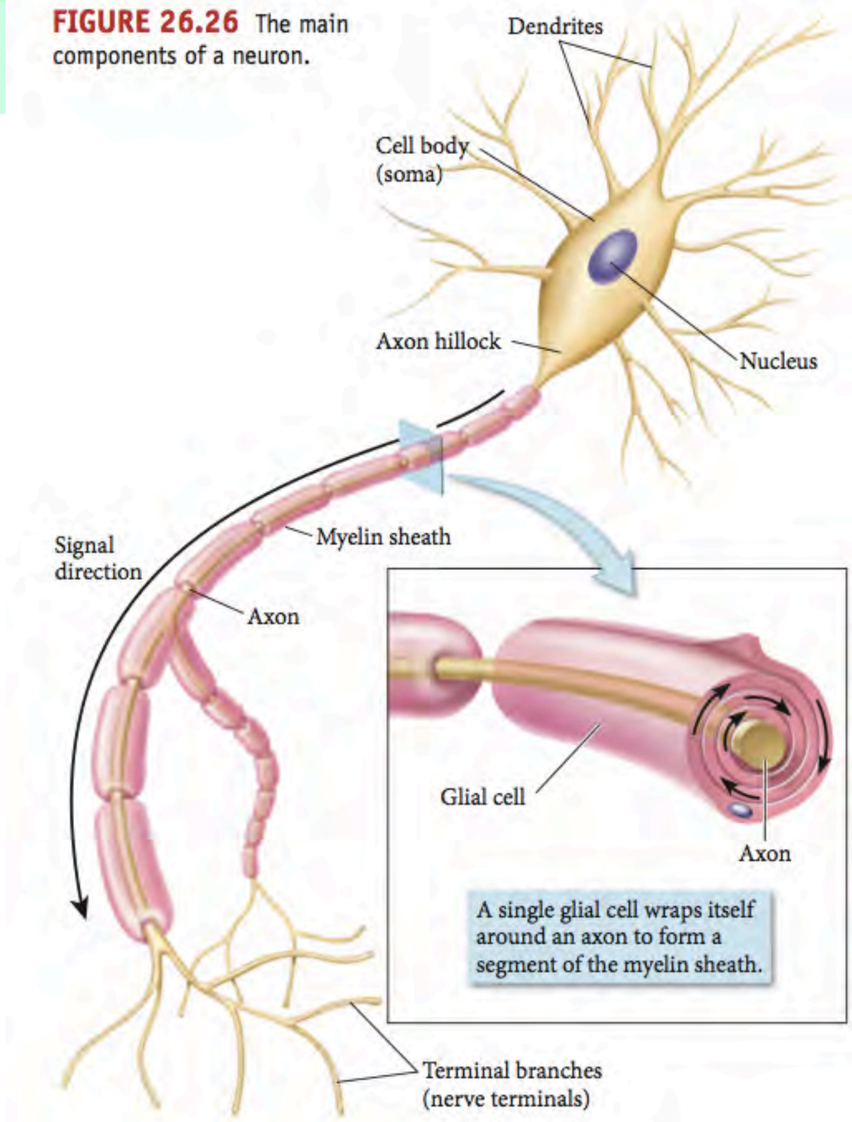
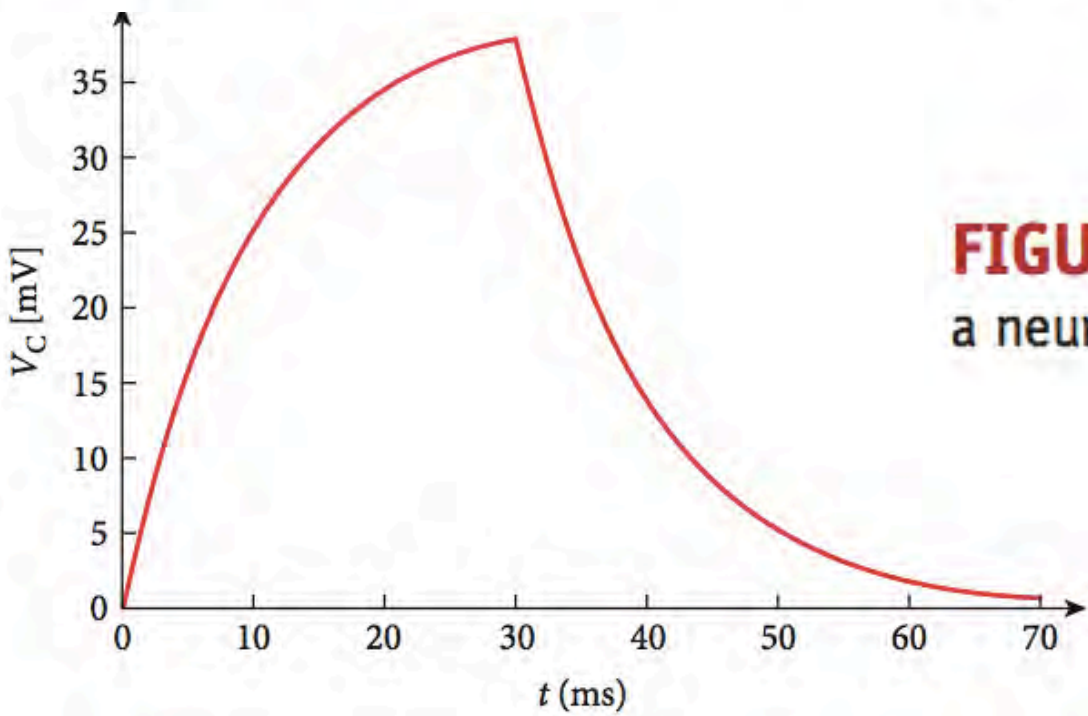


FIGURE 26.26 The main components of a neuron.

FIGURE 26.28 Potential difference on the capacitor in a model neuron.



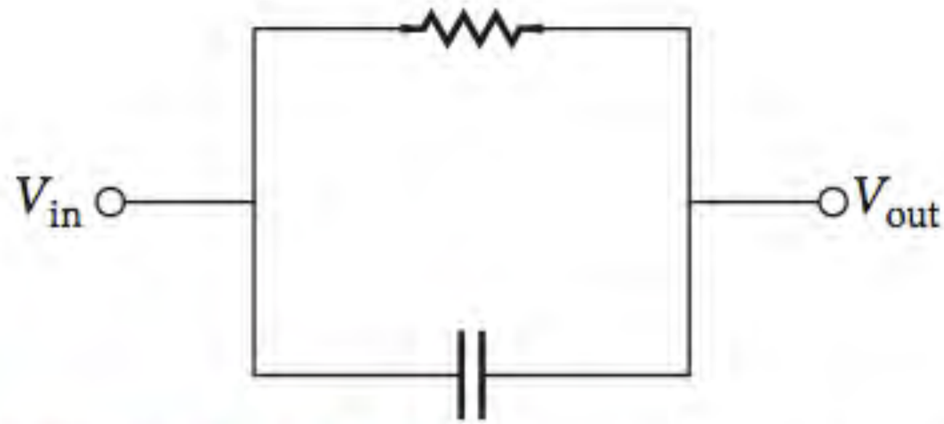


FIGURE 26.27 Simplified model of a neuron as an RC circuit.

Brain Computing: Numbers

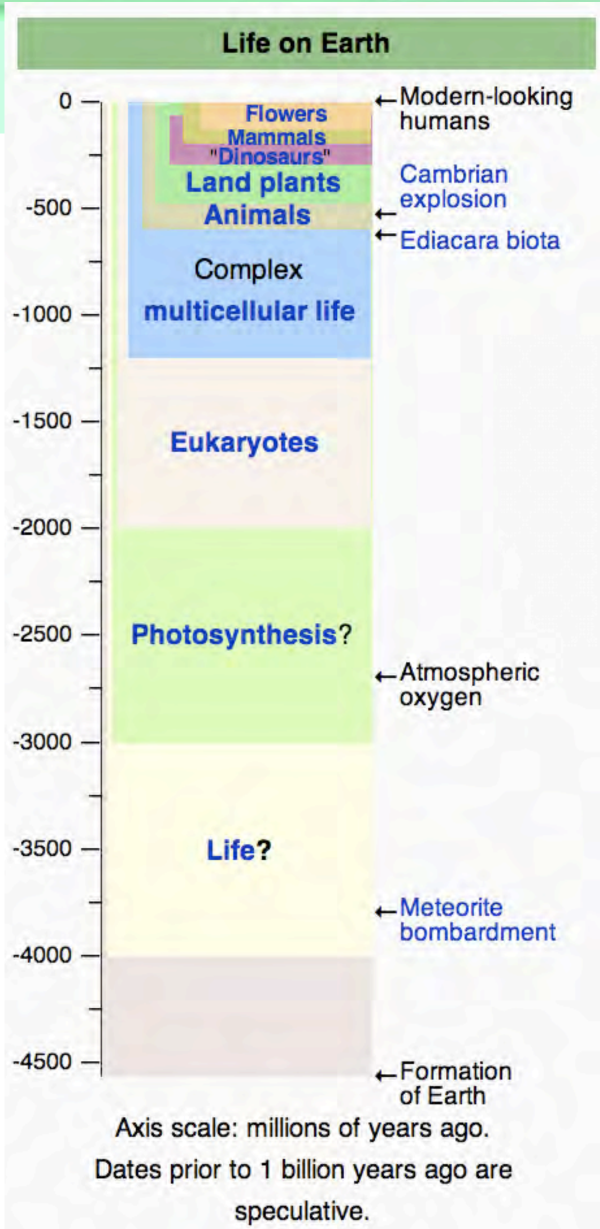
- Neurons: ~ 100 billion
- Synapses/neuron: ~1500
- Number of synaptic firings: 30/s
- Number of calculations per firing = 2 (read current, add to total in neuron)
- Flops: $10^{11} \cdot 1500 \cdot 30 \cdot 2 \sim 10^{16}$ = **10 PetaFlops** (other estimates range up to 300 PetaFlops)

Brain = Quantum Computer?

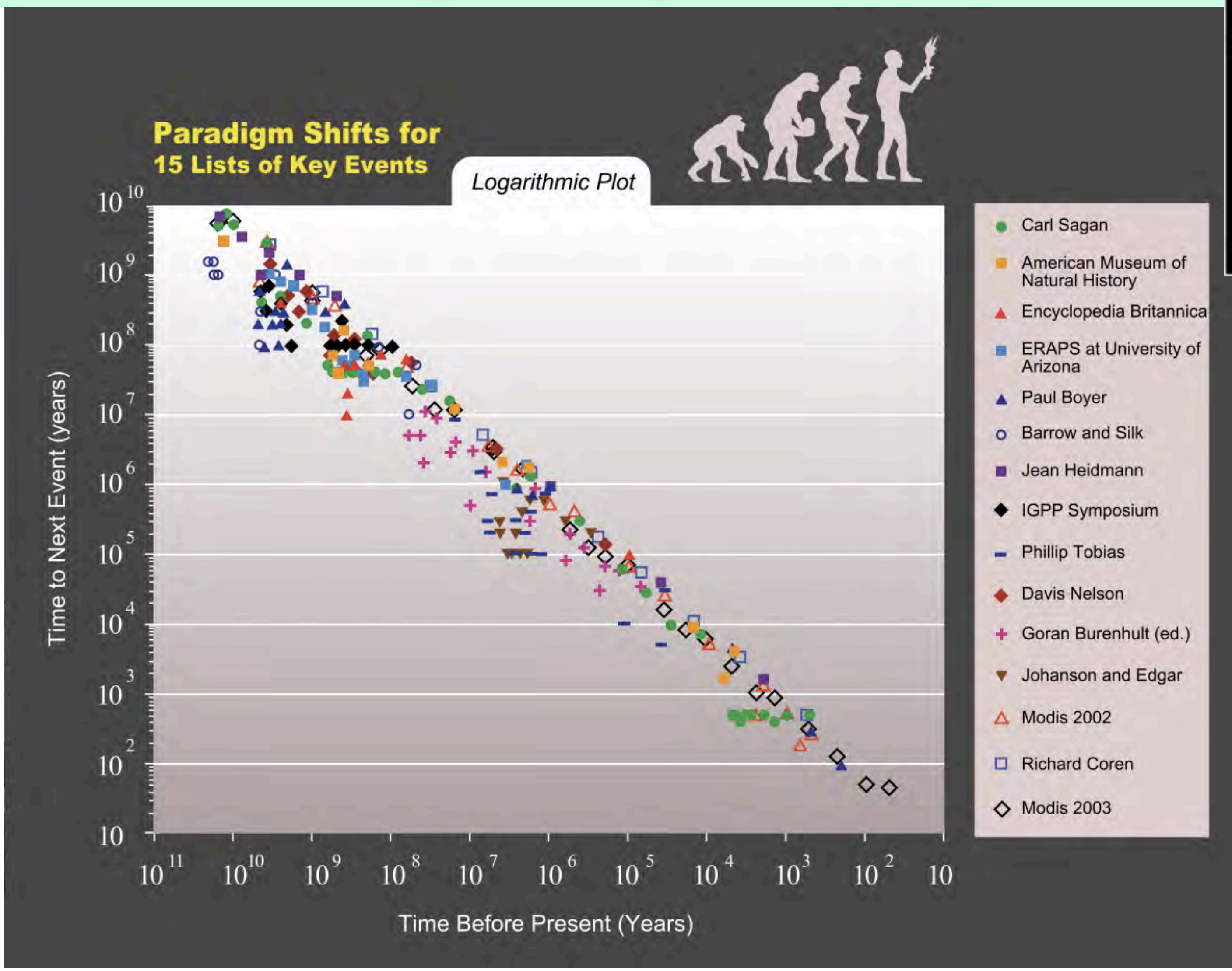
- NO!!!
  - Integration of (large number of) analog signals
  - Not a digital computer
  - But: “analog” does not mean “quantum”
  - No entanglement
- Word of caution:
  - Evolution usually picks the best approach
  - If a universal quantum computer would be possible and superior to a classical computer, our brain would be one
- Quantum Computer impossible?

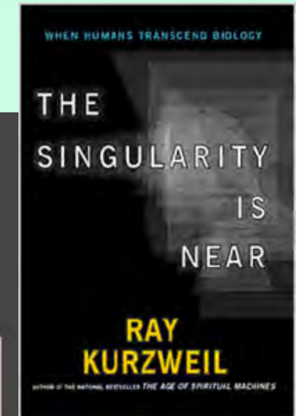
The Kurzweil Singularity

- Plot time difference between significant events in the past vs. time when event occurred
  - Example of such a list
  - Clearly, other list are possible, but the result is universal
- Result: Power law!



The Kurzweil Singularity





Summary: High Performance & Quantum Computing

- High performance computing is still following Moore's Law, now for more than 50 years
- Limits of growth of classical computing due to heat dissipation in processors, limiting the processor density
- Quantum computing promises a viable alternative
- Quantum computing works!
- Quantum computing will *not* be a solution for a general purpose computer in the foreseeable future