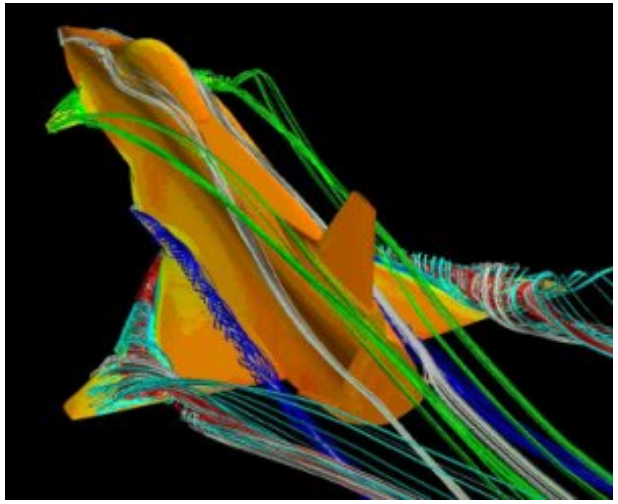
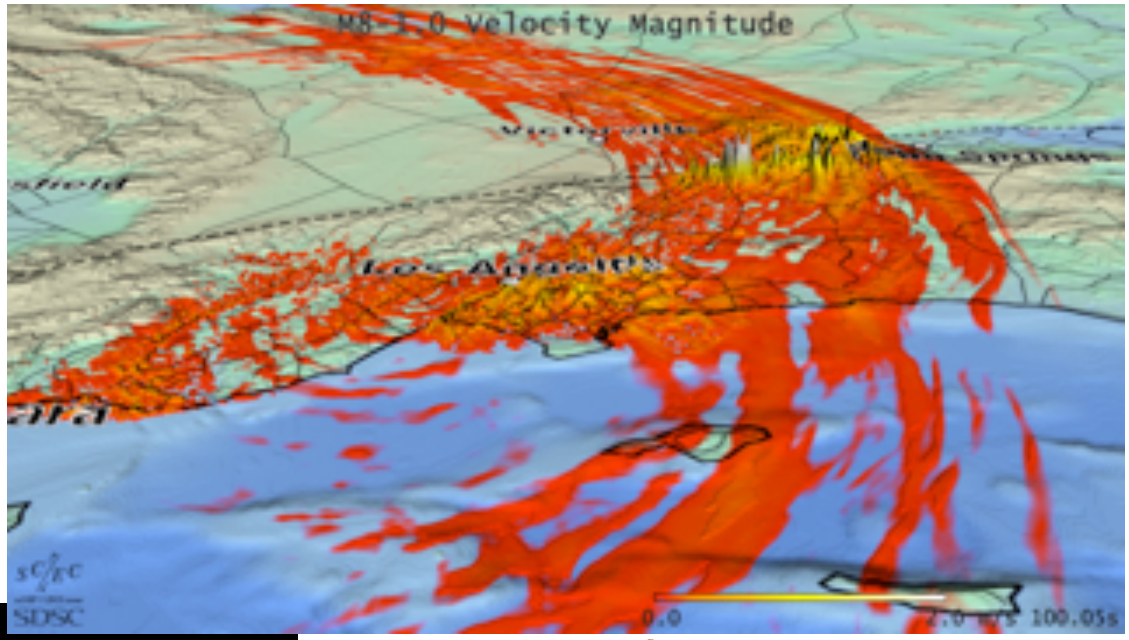
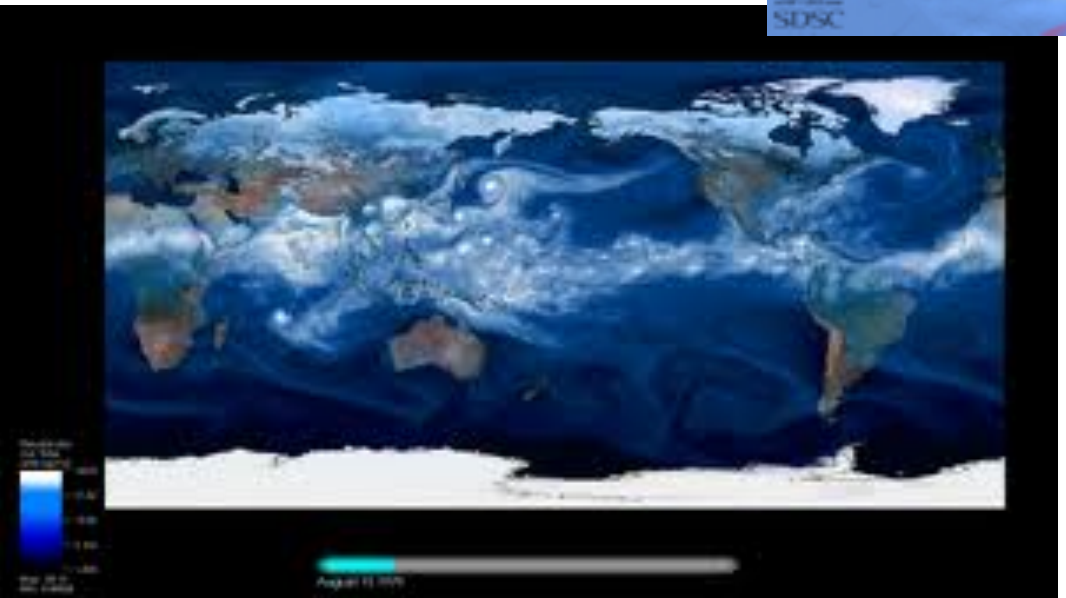
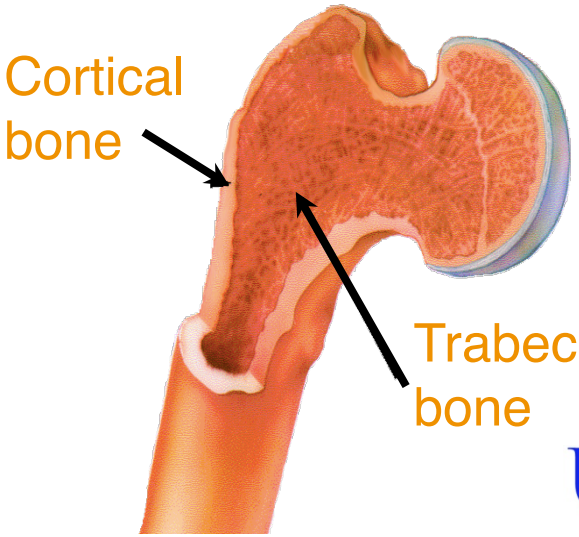
Computational models of the physical world



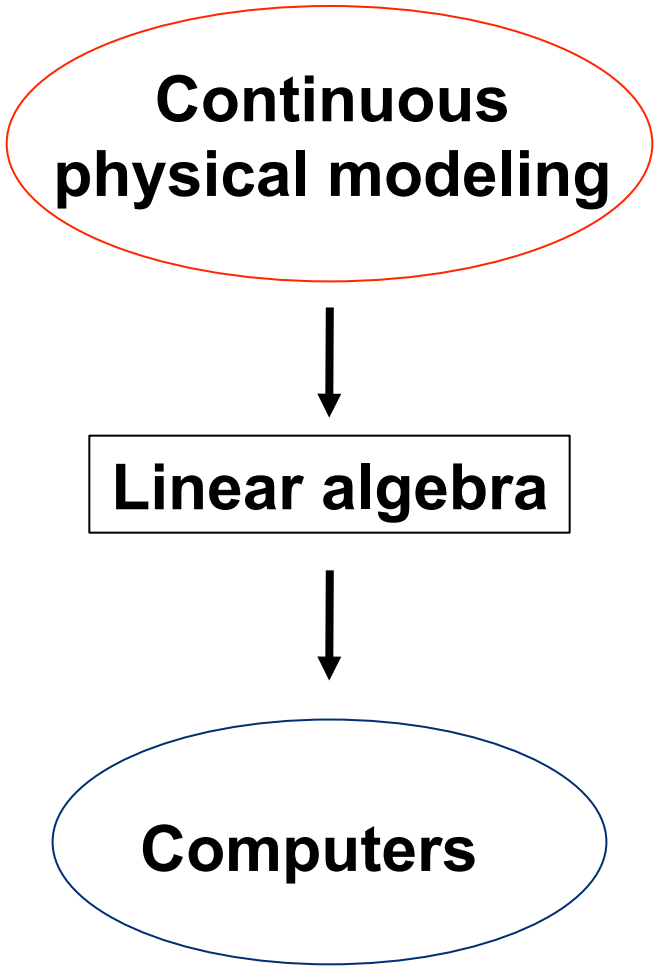






UCSB

"The unreasonable effectiveness of mathematics"



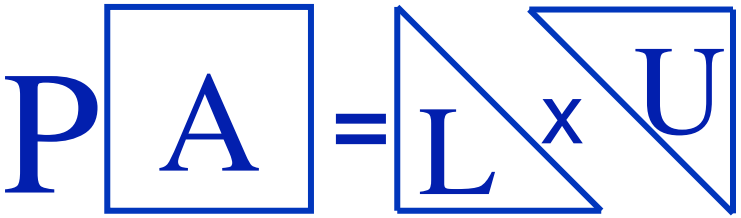
As the "middleware" of scientific computing, linear algebra has supplied or enabled:

- Mathematical tools
- "Impedance match" to computer operations
- High-level primitives
- High-quality software libraries
- Ways to extract performance from computer architecture
- Interactive environments

Top 500 List (November 2014)

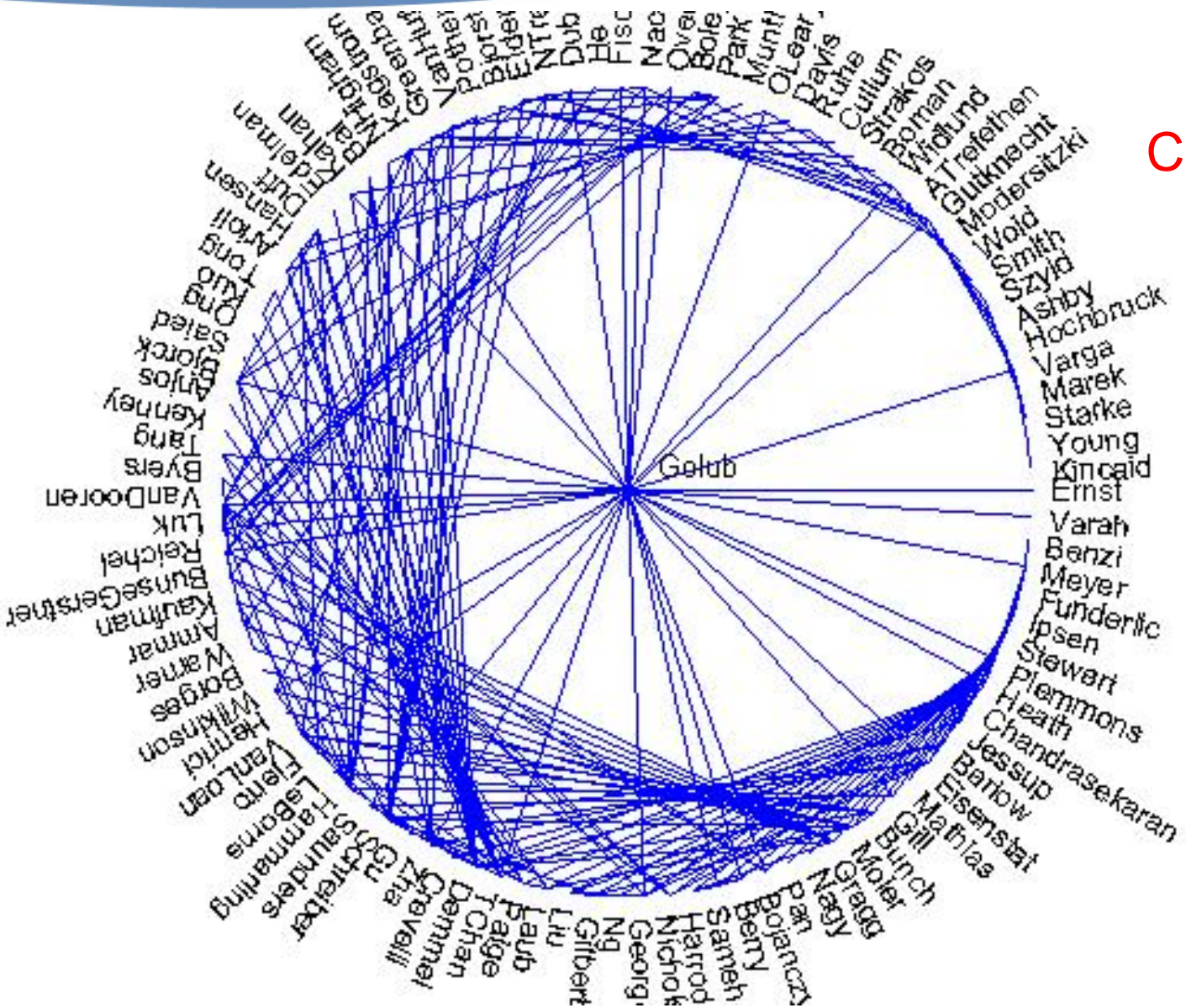
Top500 Benchmark:

Solve a large system of linear equations by Gaussian elimination



RANK	SITE	SYSTEM	CORES	RMAX (TFLOP/S)
1	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7
2	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0
5	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786,432	8,586.6
6	Swiss National Supercomputing Centre (CSCS) Switzerland	**Piz Daint** - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Cray Inc.	115,984	6,271.0
7	Texas Advanced Computing Center/Univ. of Texas United States	**Stampede** - PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi SE10P Dell	462,462	5,168.1
8	Forschungszentrum Juelich (FZJ) Germany	**JUQUEEN** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	458,752	5,008.9
9	DOE/NNSA/LLNL United States	**Vulcan** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	393,216	4,293.3
10	Government United States	Cray CS-Storm, Intel Xeon E5-2660v2 10C 2.2GHz, Infiniband FDR, Nvidia K40 Cray Inc.	72,800	3,577.0

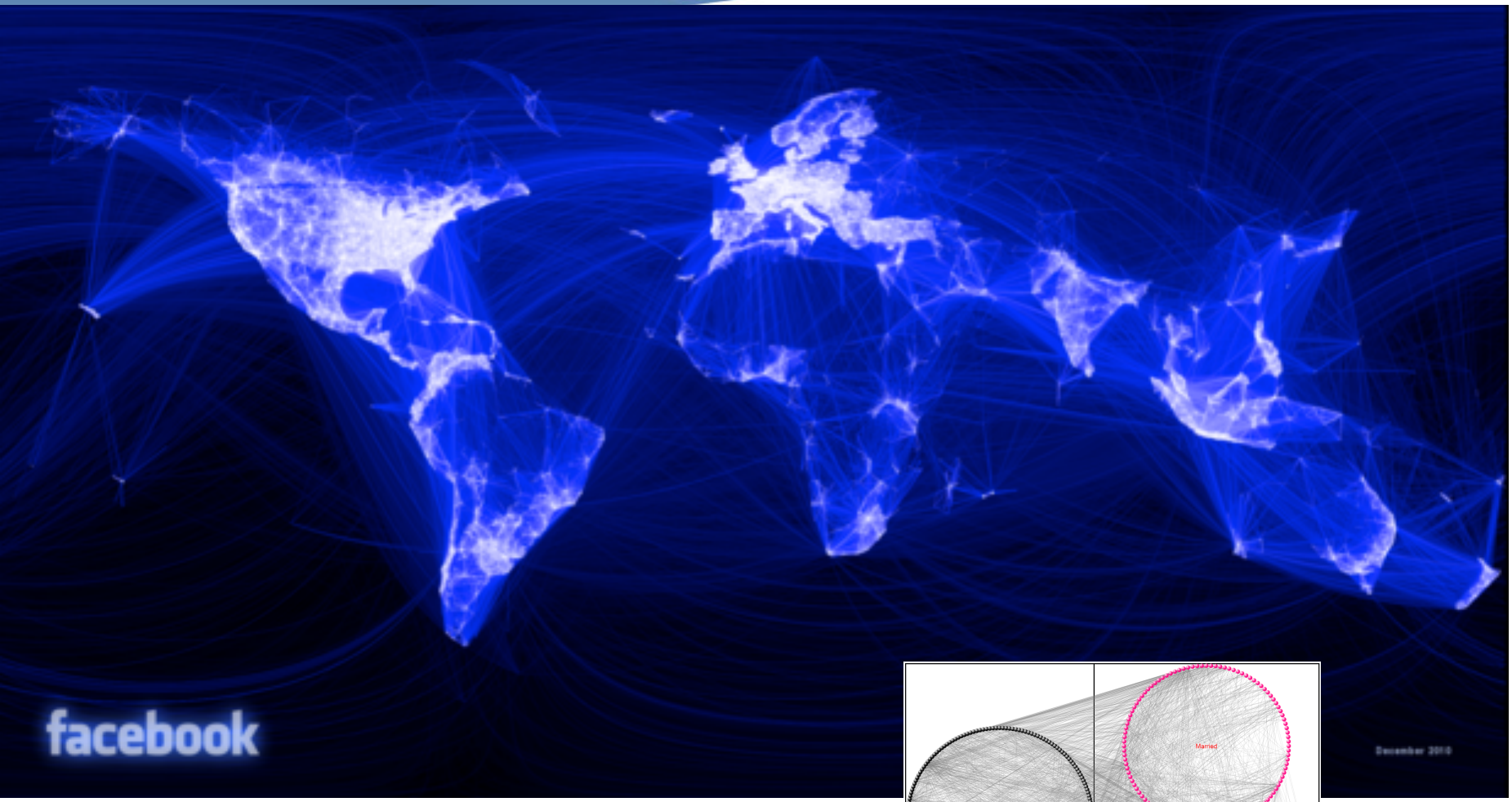
Social network analysis (1993)

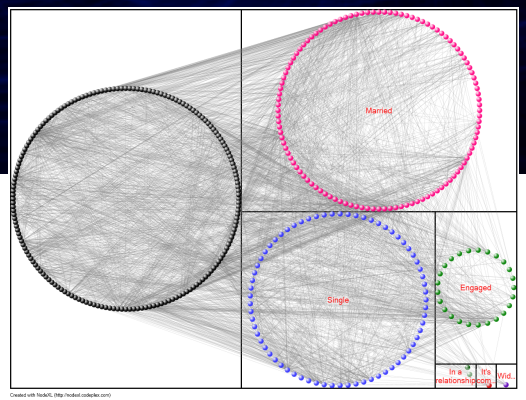


Co-author graph from 1993 Householder symposium

UCSB

Social network analysis (2015)

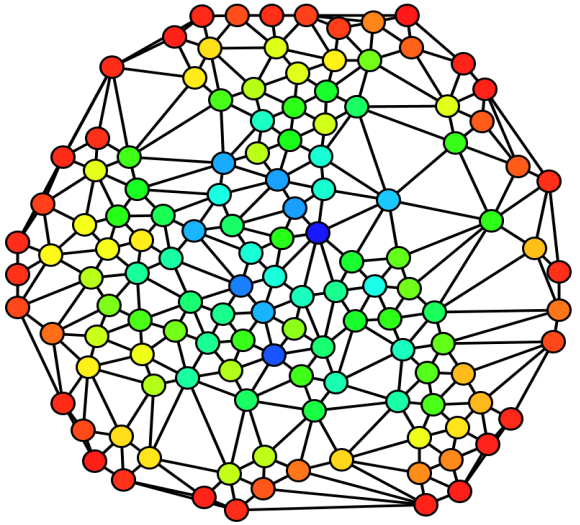


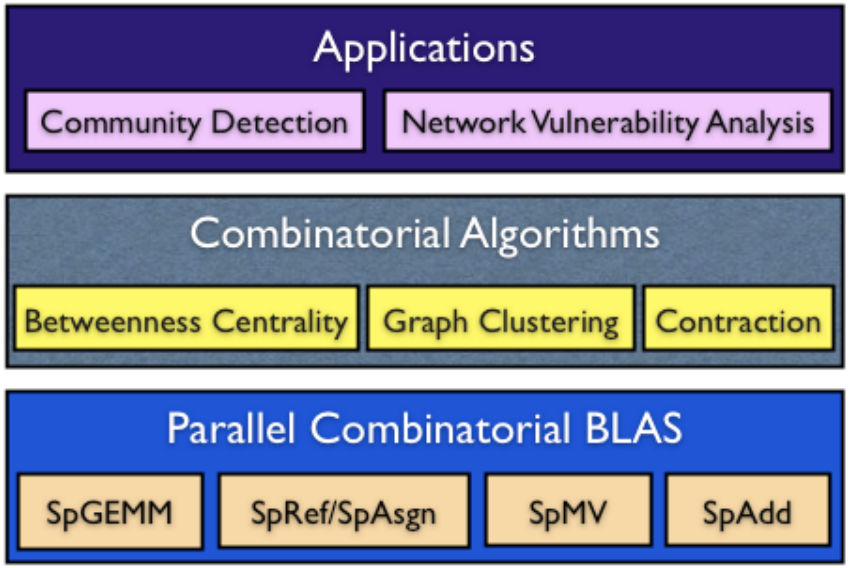


Facebook graph:
> 1,000,000,000 vertices

UCSB

Social network analysis





A typical software stack for an application enabled with the Combinatorial BLAS

Betweenness Centrality (BC)

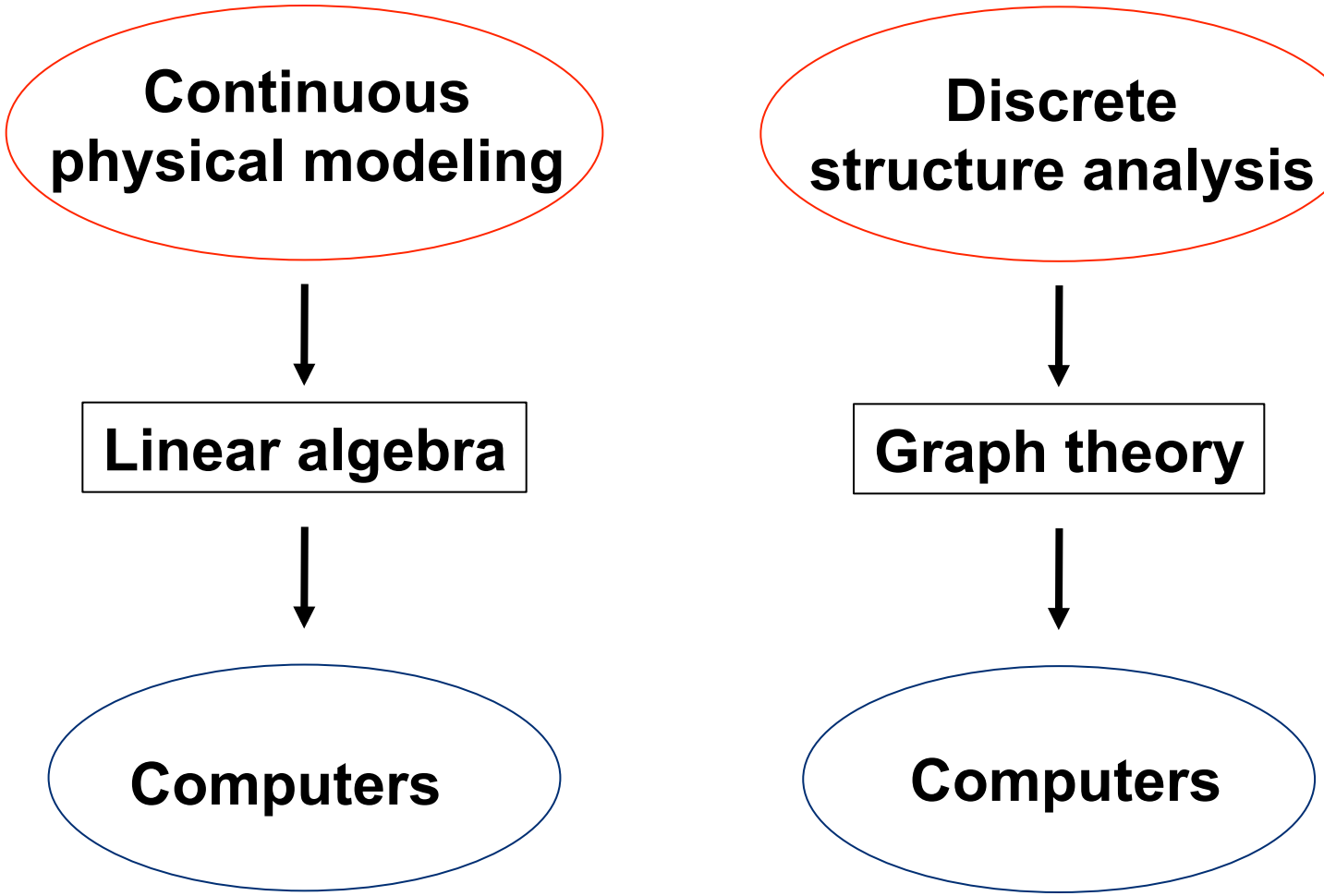
$C_B(v)$: Among all the shortest paths, what fraction of them pass through the node of interest?

$$C_B(v) = \sum_{\substack{s \neq v \neq t \in V \\ s \neq t}} \frac{\sigma_{st}(v)}{\sigma_{st}}$$

Brandes' algorithm

UCSB

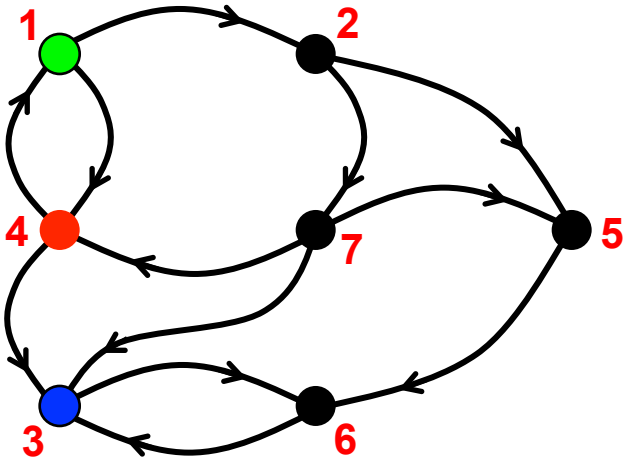
An analogy?


Continuous physical modeling
Linear algebra
Computers
Discrete structure analysis
Graph theory
Computers

Graph 500 List (November 2014)

Graph500 Benchmark:

Breadth-first search in a large power-law graph



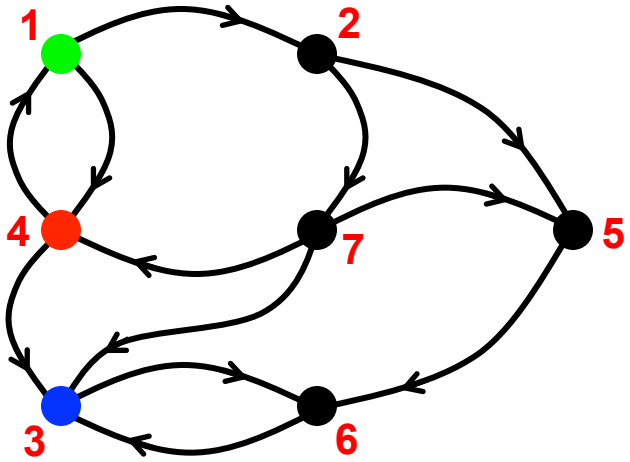
No.	Rank	Machine	Installation Site	Number of nodes	Number of cores	Problem scale	GTEPS
1	1	DOE/NNSA/LLNL Sequoia (IBM - BlueGene/Q, Power BQC 16C 1.60 GHz)	Lawrence Livermore National Laboratory	98304	1572864	41	23751
2	2	K computer (Fujitsu - Custom supercomputer)	RIKEN Advanced Institute for Computational Science (AICS)	82944	663552	40	19585.2
3	3	DOE/SC/Argonne National Laboratory Mira (IBM - BlueGene/Q, Power BQC 16C 1.60 GHz)	Argonne National Laboratory	49152	786432	40	14982
4	4	JUQUEEN (IBM - BlueGene/Q, Power BQC 16C 1.60 GHz)	Forschungszentrum Juelich (FZJ)	16384	262144	38	5848
5	5	Fermi (IBM - BlueGene/Q, Power BQC 16C 1.60 GHz)	CINECA	8192	131072	37	2567
6	6	Tianhe-2 (MilkyWay-2) (National University of Defense Technology - MPP)	Changsha, China	8192	196608	36	2061.48
7	7	Turing (IBM - BlueGene/Q, Power BQC 16C 1.60GHz)	CNRS/IDRIS-GENCI	4096	65536	36	1427
8	7	Blue Joule (IBM - BlueGene/Q, Power BQC 16C 1.60 GHz)	Science and Technology Facilities Council - Daresbury Laboratory	4096	65536	36	1427

Floating-Point vs. Graphs, November 2014

34 Petaflops

$$P\,A = L \times U$$

24 Terateps



34 Peta / 24 Tera is about 1,400

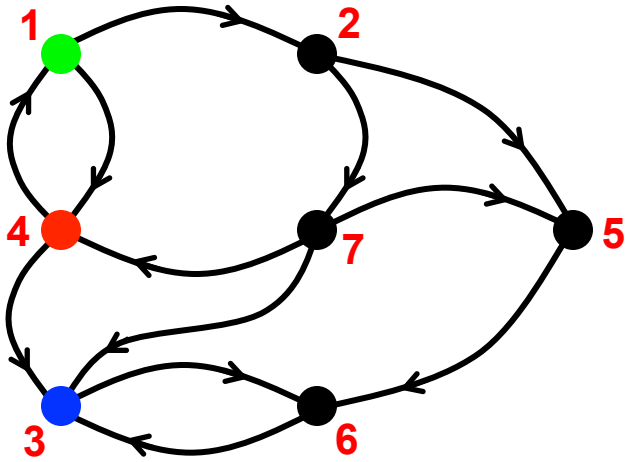
UCSB

Floating-Point vs. Graphs, November 2014

34 Petaflops

$$P\,A = L \times U$$

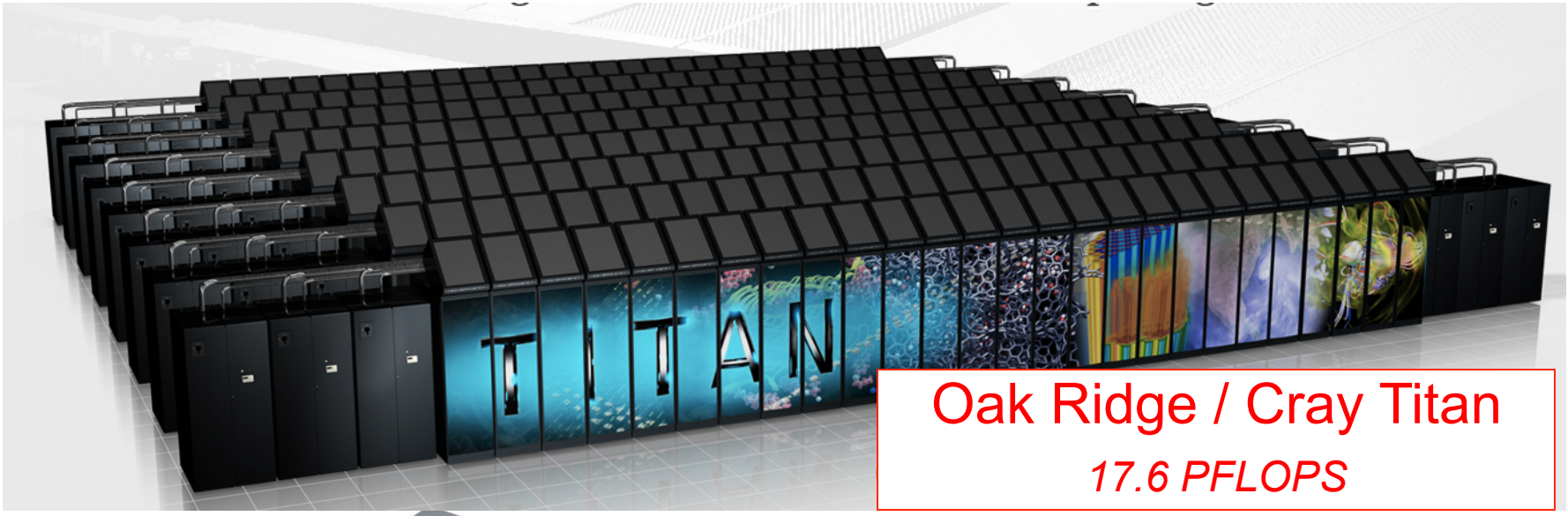
24 Terateps



Nov 2014:	**34 Peta / 24 Tera**	**~ 1,400**
Nov 2010:	**2.5 Peta / 6.6 Giga**	**~ 380,000**

UCSB

Parallel Computers Today



Oak Ridge / Cray Titan

17.6 PFLOPS

Nvidia GK110 GPU:

1.7 TFLOPS

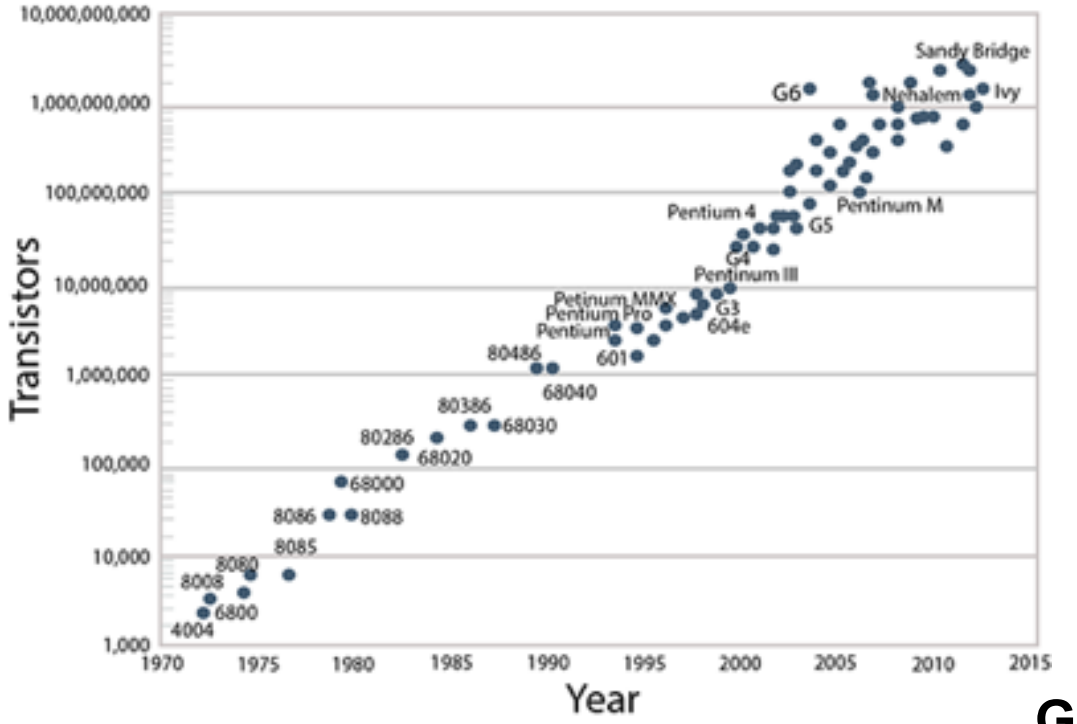
61-processor Intel Xeon Phi:

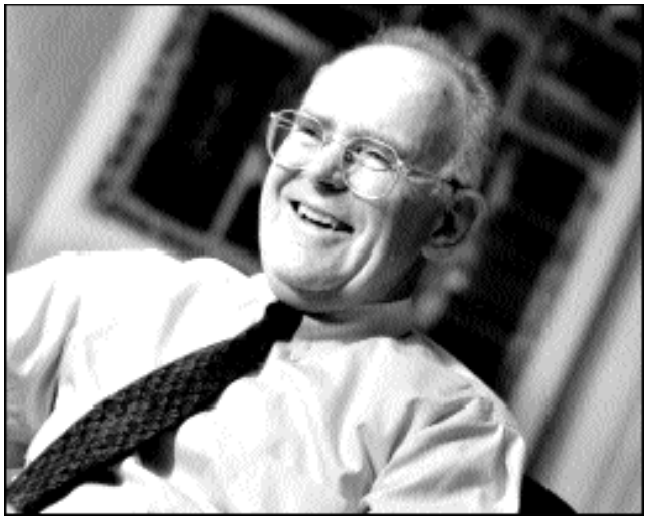
1.0 TFLOPS

- TFLOPS = 10^{12} floating point ops/sec
- PFLOPS = 1,000,000,000,000,000 / sec

Supercomputers 1976: Cray-1, 133 MFLOPS (10^6)

Technology Trends: Microprocessor Capacity



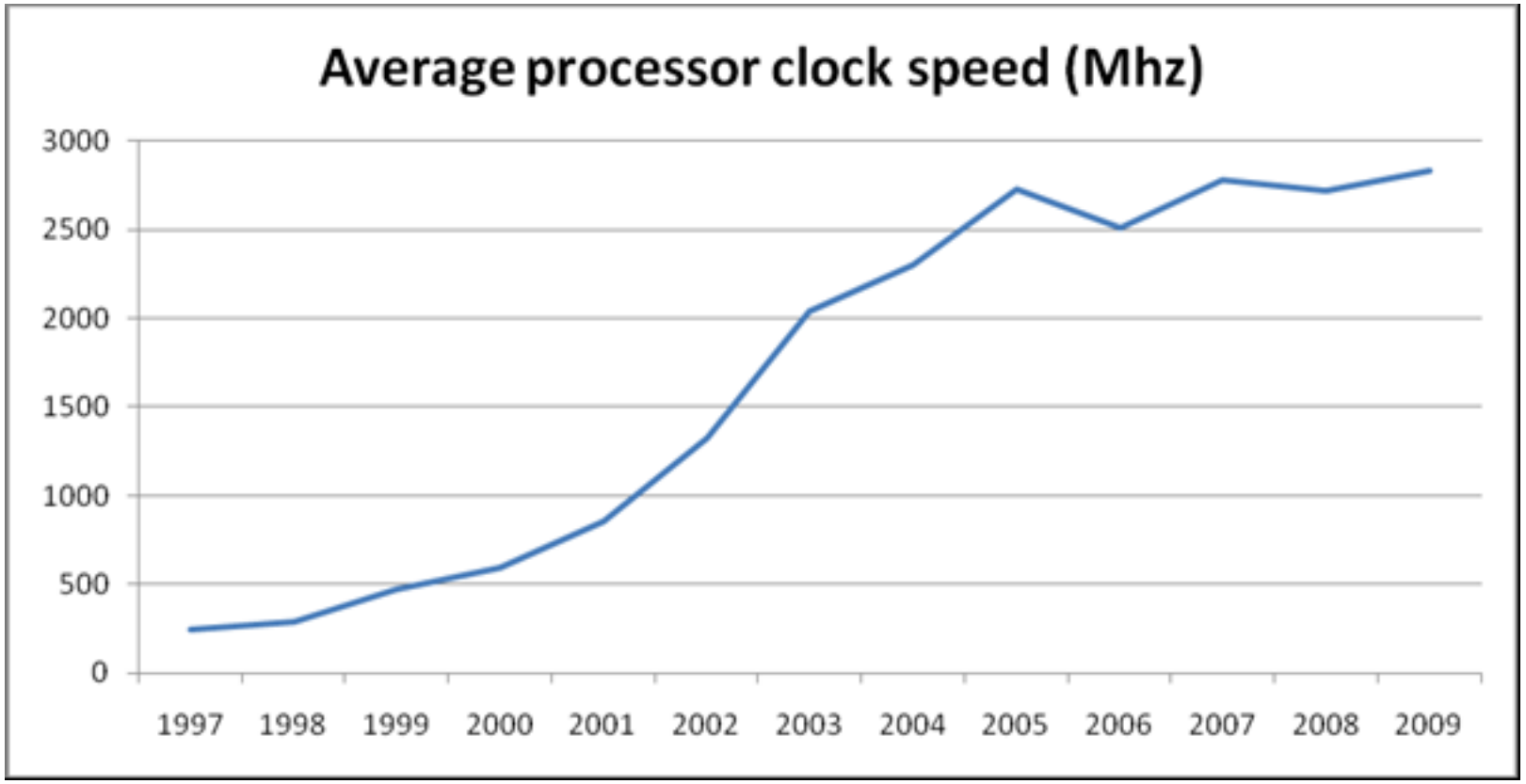


Moore's Law: # transistors / chip doubles every 1.5 years

Gordon Moore (Intel co-founder) predicted in 1965 that the transistor density of semiconductor chips would double roughly every 18 months.

Microprocessors keep getting smaller, denser, and more powerful.

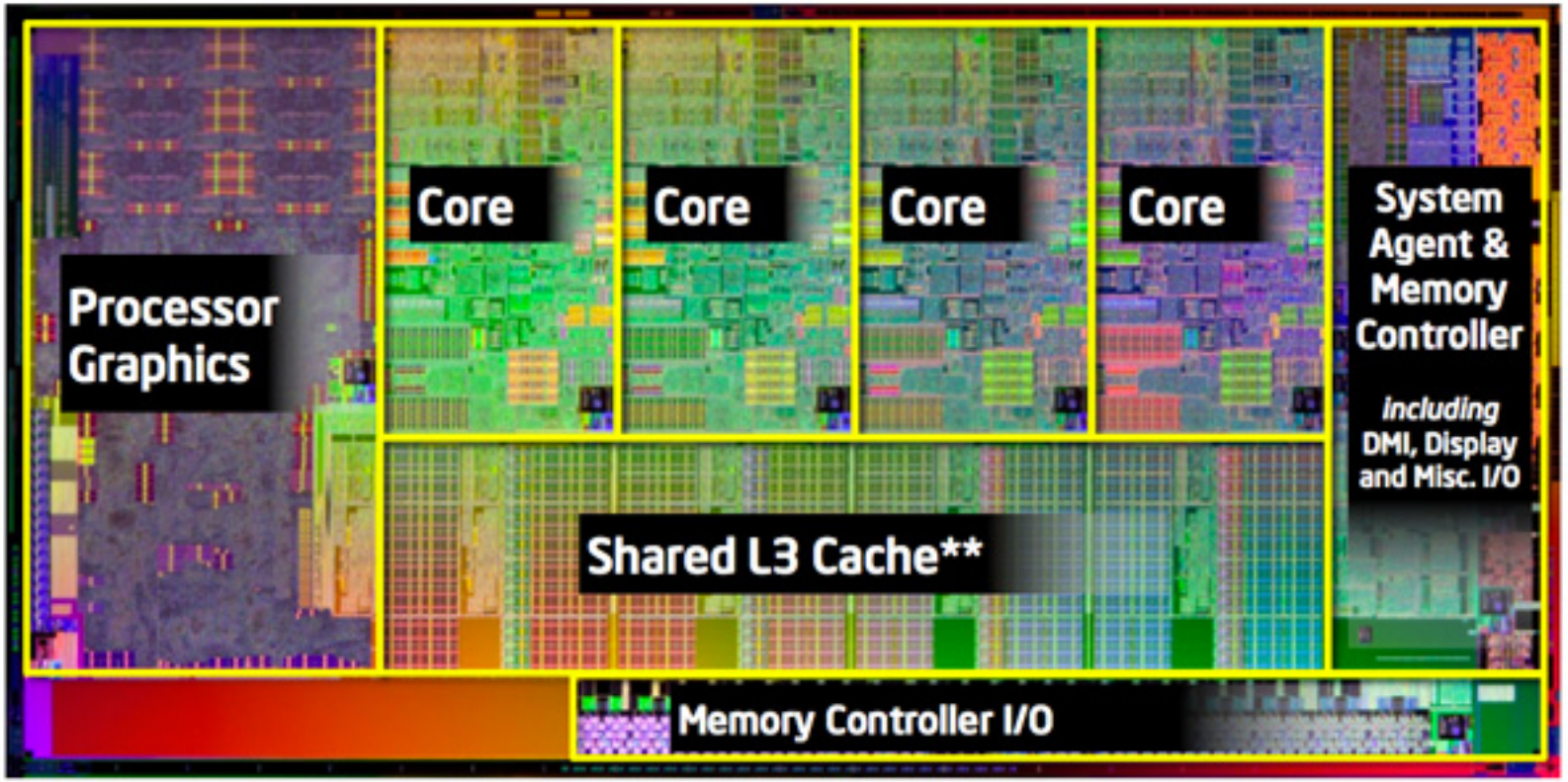
Trends in processor clock speed



Triton's clockspeed is still only 2600 Mhz in 2015!

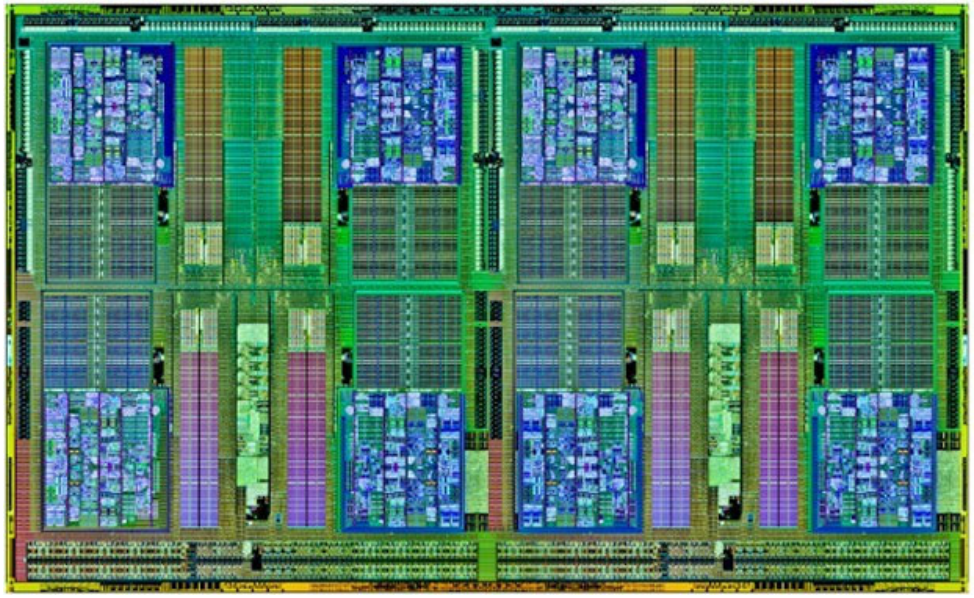
4-core Intel Sandy Bridge

(Triton uses an 8-core version)

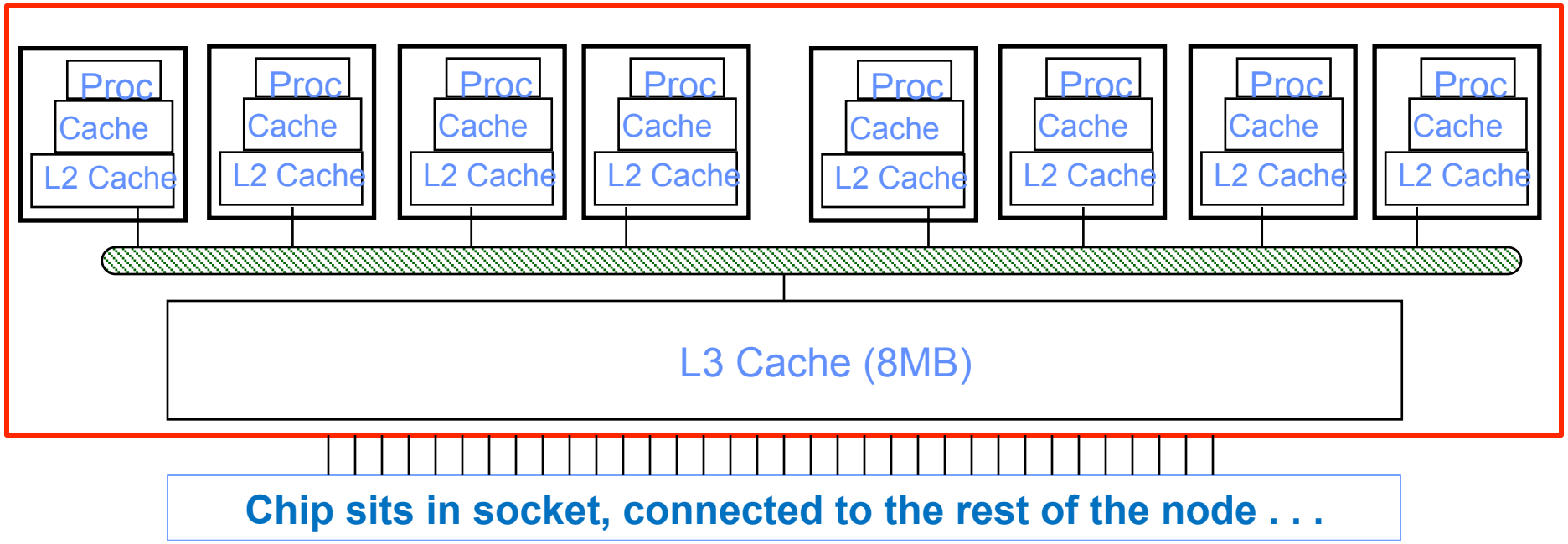


2600 Mhz clock speed

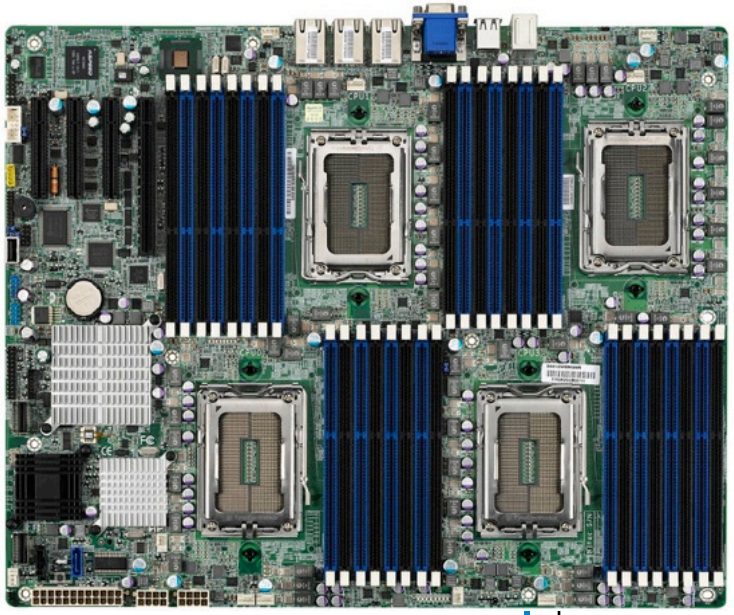
Triton memory hierarchy: I (Chip level)

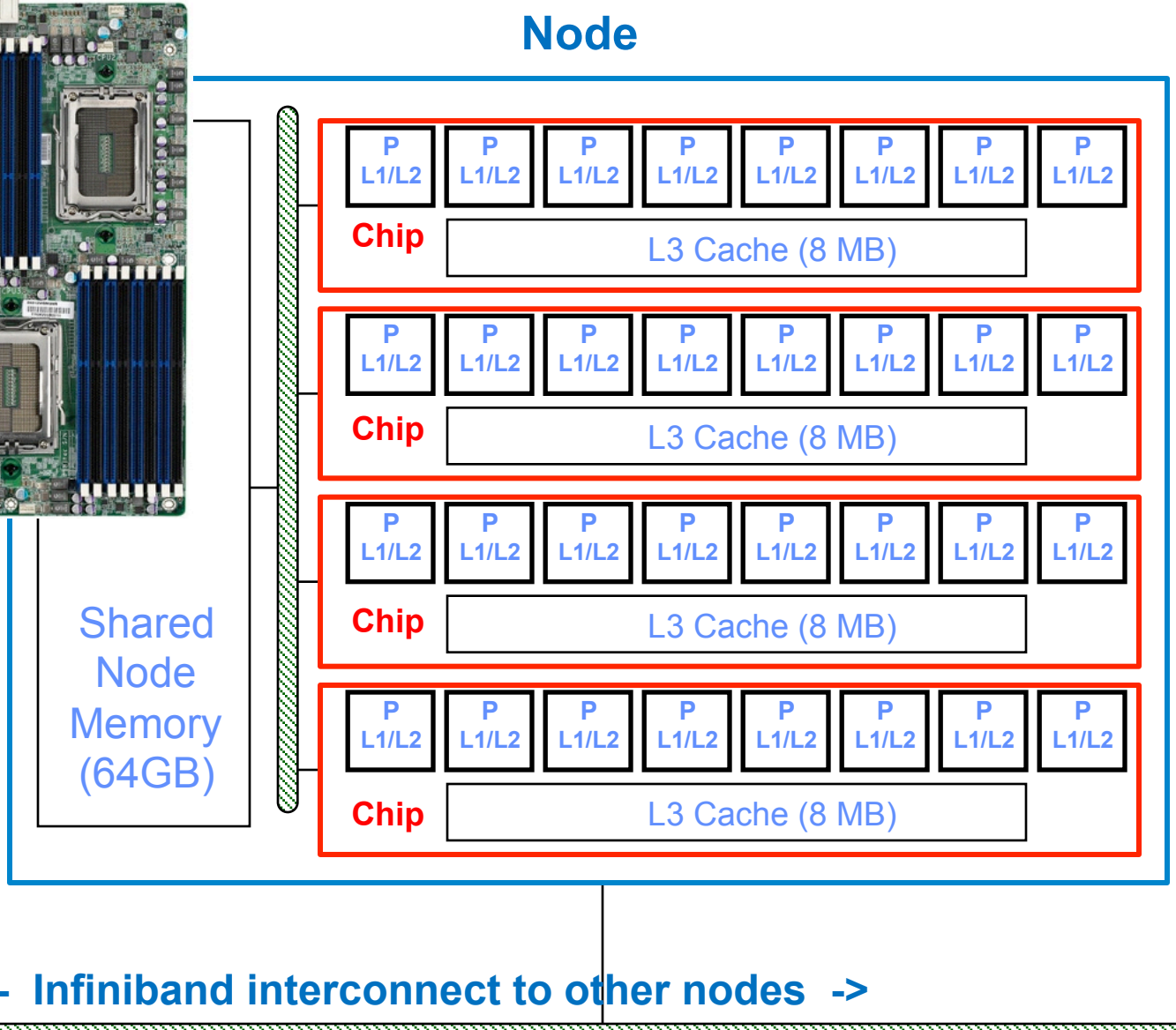


(AMD Opteron 8-core Magny-Cours, similar to Tritons' Intel Sandy Bridge)

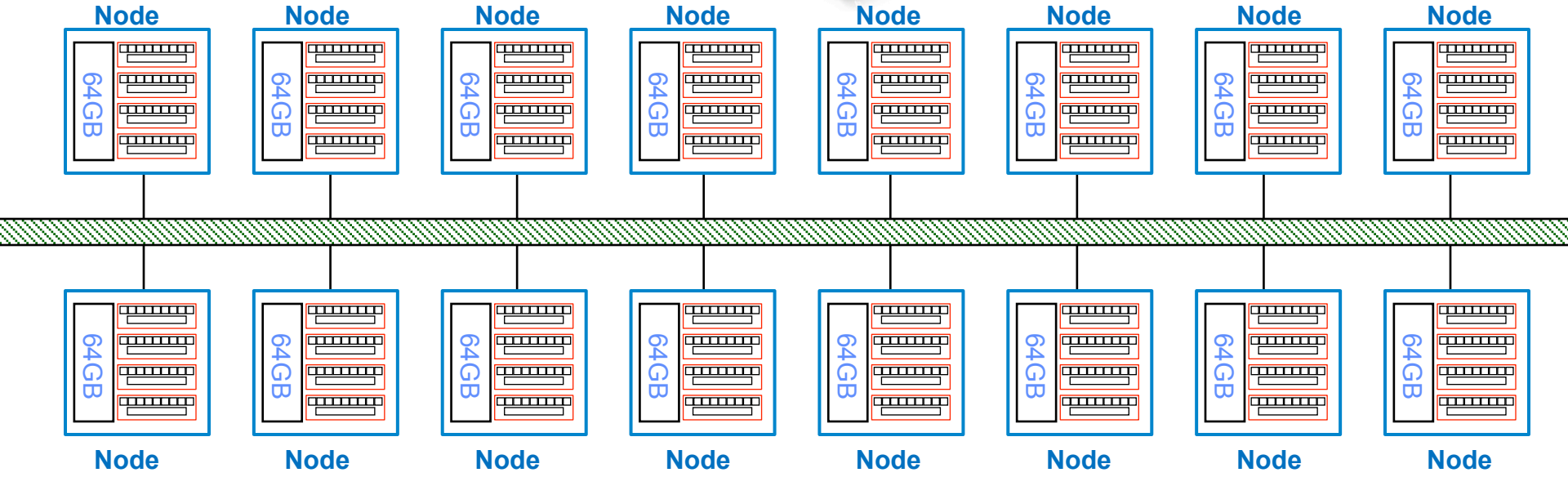


Triton memory hierarchy II (Node level)





Triton memory hierarchy III (System level)



324 nodes, message-passing communication, no shared memory