Intro To Parallel Computing

John Urbanic
Pittsburgh Supercomputing Center
Parallel Computing Scientist

Purpose of this talk

- This is the 50,000 ft. view of the parallel computing landscape. We want to orient you a bit before parachuting you down into the trenches to deal with MPI.
- This talk bookends our technical content along with the Outro to Parallel Computing talk. The Intro has a strong emphasis on hardware, as this dictates the reasons that the software has the form and function that is has. Hopefully our programming constraints will seem less arbitrary.
- The Outro talk can discuss alternative software approaches in a meaningful way because you will then have one base of knowledge against which we can compare and contrast.
- The plan is that you walk away with a knowledge of not just MPI, etc. but where it fits into the world of High Performance Computing.

1st Theme

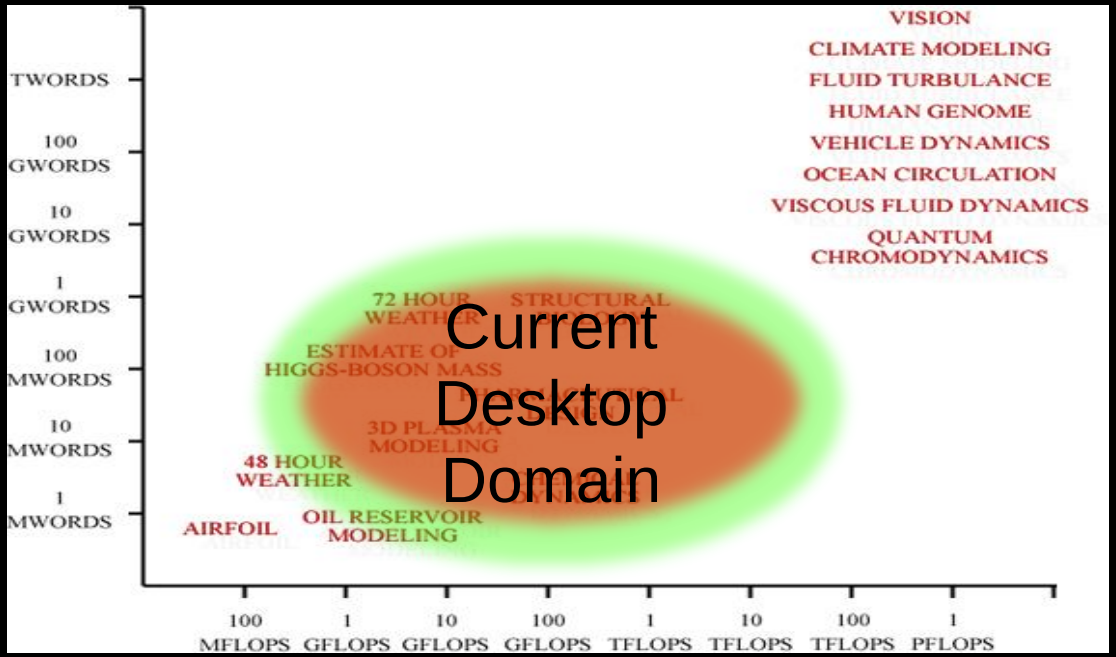
We need Exascale computing

We aren’t getting to Exascale without parallel

What does parallel computing look like

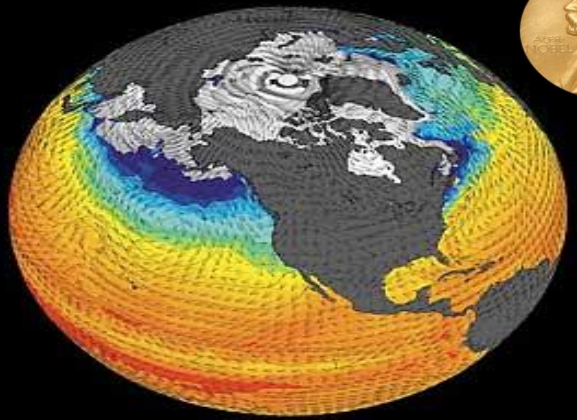
Where is this going

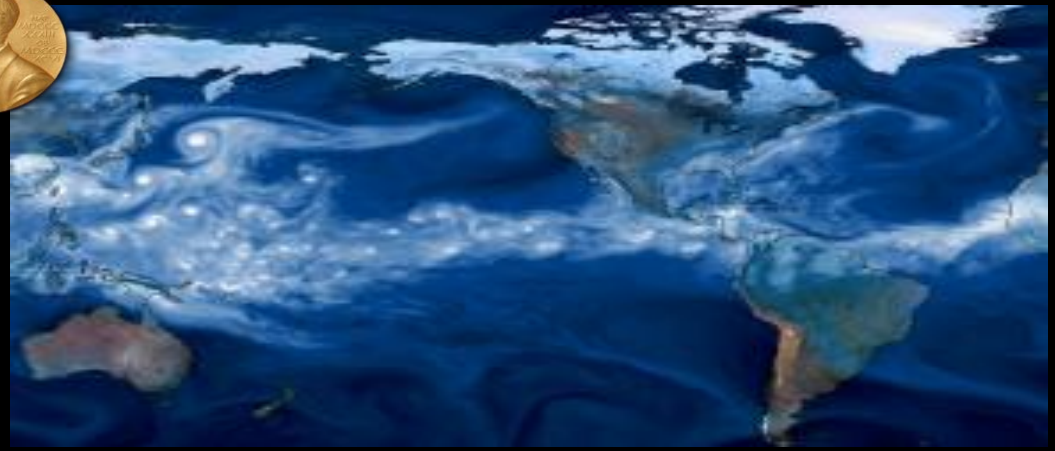
FLOPS we can use now



Which axis is most important?

FLOPS we need: Climate change analysis

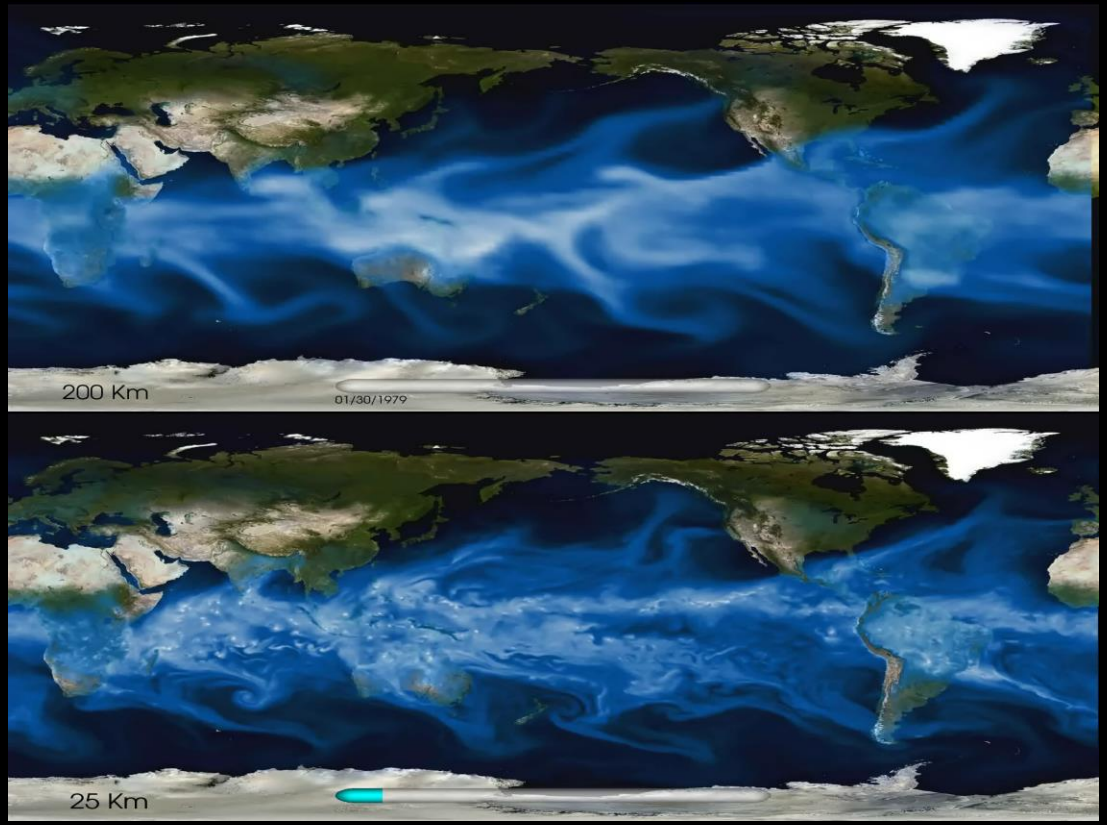




Simulations	Extreme data
• Cloud resolution, quantifying uncertainty, understanding tipping points, etc., will drive climate to exascale platforms • New math, models, and systems support will be needed	• "Reanalysis" projects need 100× more computing to analyze observations • Machine learning and other analytics are needed today for petabyte data sets • Combined simulation/observation will empower policy makers and scientists

Courtesy Horst Simon, LBNL

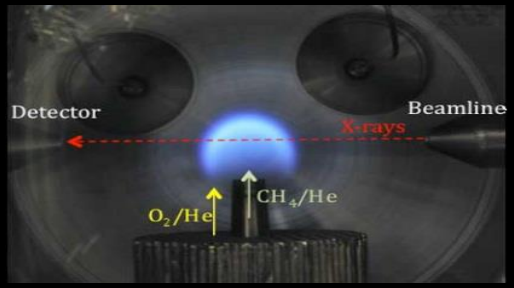
Qualitative Improvement of Simulation with Higher Resolution (2011)

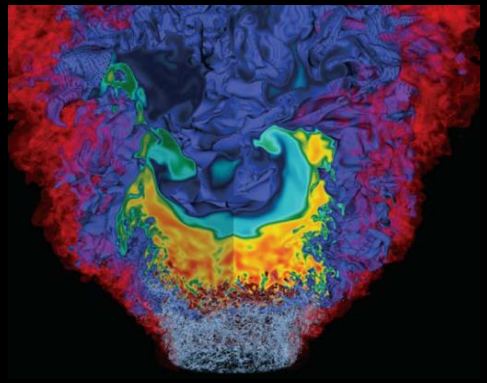


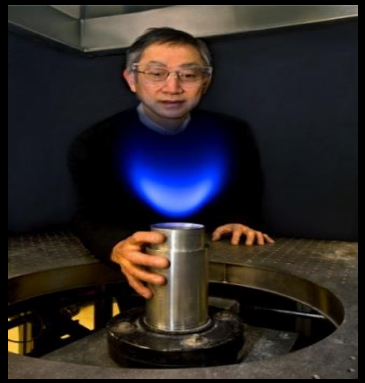
Michael Wehner, Prabhat, Chris Algieri, Fuyu Li, Bill Collins, Lawrence Berkeley National Laboratory; Kevin Reed, University of Michigan; Andrew Gettelman, Julio Bacmeister, Richard Neale, National Center for Atmospheric Research

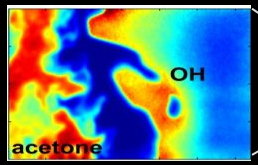
Exascale combustion simulations

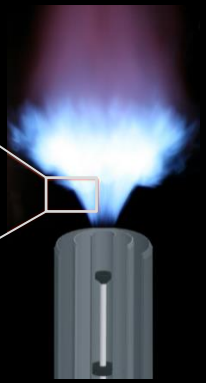
- Goal: 50% improvement in engine efficiency
- Center for Exascale Simulation of Combustion in Turbulence (ExaCT)
  - Combines M&S and experimentation
  - Uses new algorithms, programming models, and computer science

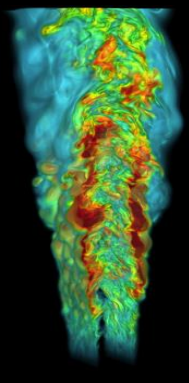










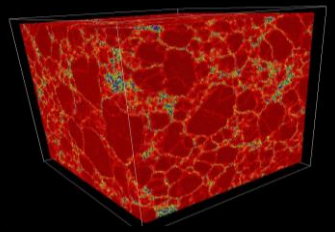


Courtesy Horst Simon, LBNL

Warhead assessment and certification of a smaller nuclear stockpile

Predicting with confidence requires precise understanding of aging and individual life-extended weapons

- **High accuracy in individual weapons calculations:**
  - **Advanced physical models**
  - **3-D to resolve features and phenomena**
  - **Extreme resolution**
- **Uncertainty quantification:**
  - **Massive numbers of high-resolution 3-D simulations to explore impacts of small variations in individual devices**
- **Assessment process: All aspects will require exascale computing to support commitment never to return to underground testing**

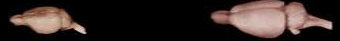


Modeling molten tantalum: 10M atoms required; modeling molten plutonium: 1000× more computing power

Self-steering (a data analysis challenge): Essential to minimize number of simulations

Courtesy Horst Simon, LBNL

Modha Group at IBM Almaden



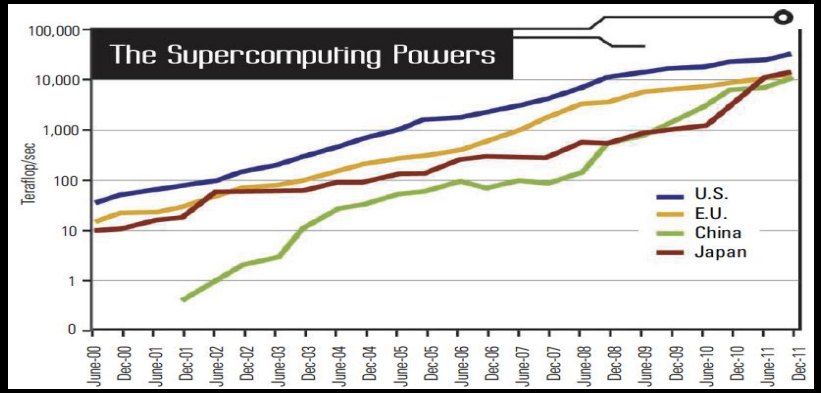
	Mouse	Rat	Cat	Monkey	Human
N:	16×10^6	56×10^6	763×10^6	2×10^9	22×10^9
S:	128×10^9	448×10^9	6.1×10^{12}	20×10^{12}	220×10^{12}

Recent simulations achieve unprecedented scale of $65*10^9$ neurons and $16*10^{12}$ synapses

Almaden	Watson	WatsonShaheen	LLNL Dawn	LLNL Sequoia
BG/L	BG/L	BG/P	BG/P	BG/Q
December, 2006	April, 2007	March, 2009	May, 2009	June, 2012

Courtesy Horst Simon, LBNL

Also important: We aren't going to be left behind.



Courtesy Horst Simon, LBNL

2nd Theme

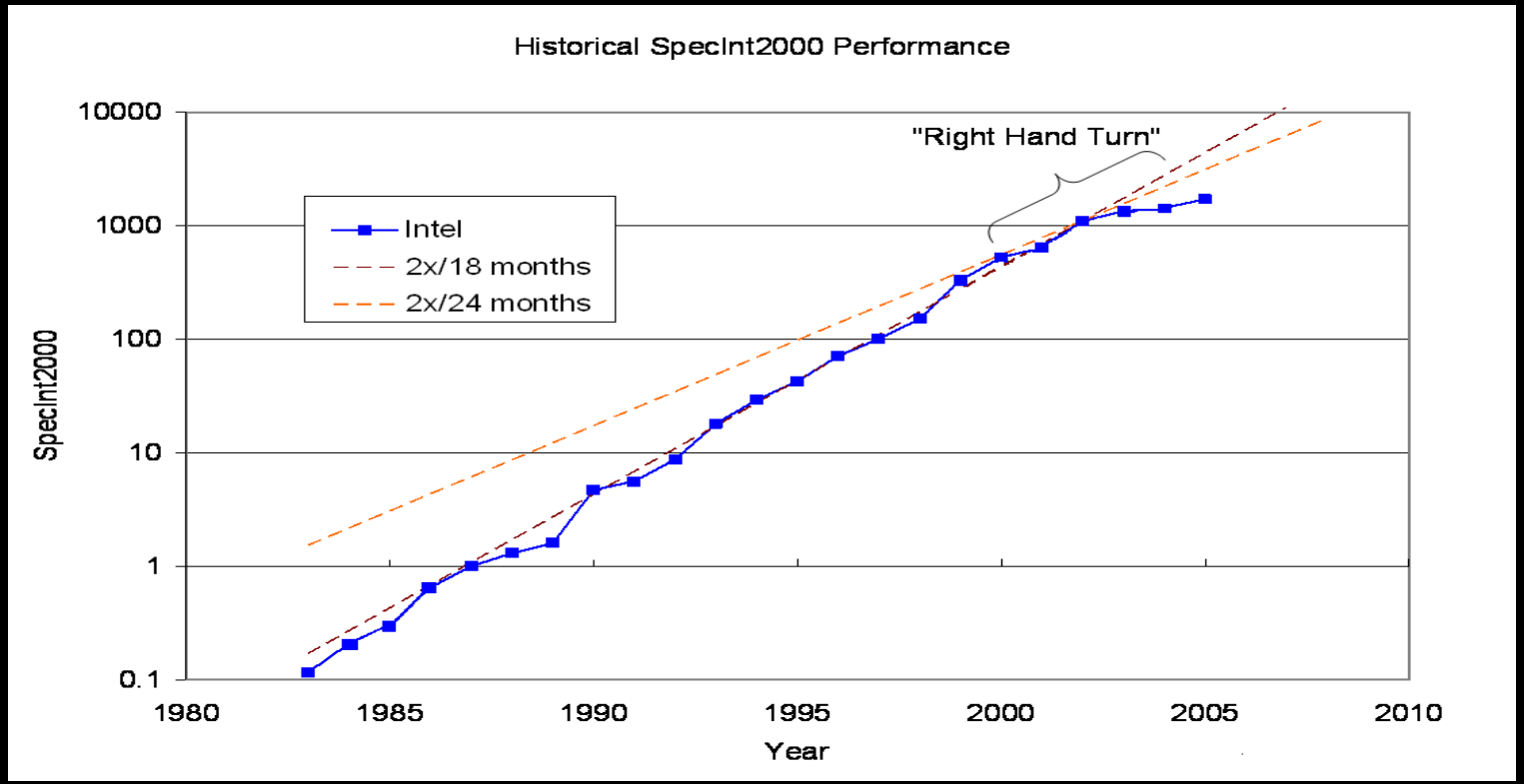
We will have Exascale computing

You aren't getting to Exascale without going very parallel

What does parallel computing look like

Where is this going

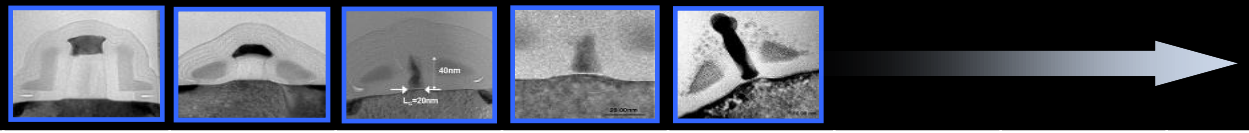
Waiting for Moore's Law to save your serial code start getting bleak in 2004



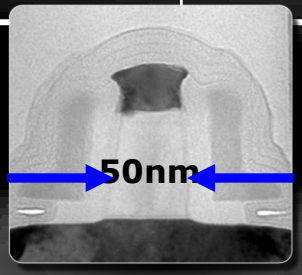
Source: published SPECInt data

Moore's Law is not at all dead…

Intel process technology capabilities

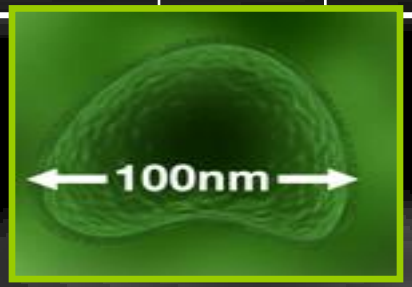


High Volume Manufacturing	2004	2006	2008	2010	2012	2014	2016	2018
Feature Size	90nm	65nm	45nm	32nm	22nm	16nm	11nm	8nm
Integration Capacity (Billions of Transistors)	2	4	8	16	32	64	128	256



Transistor for 90nm Process

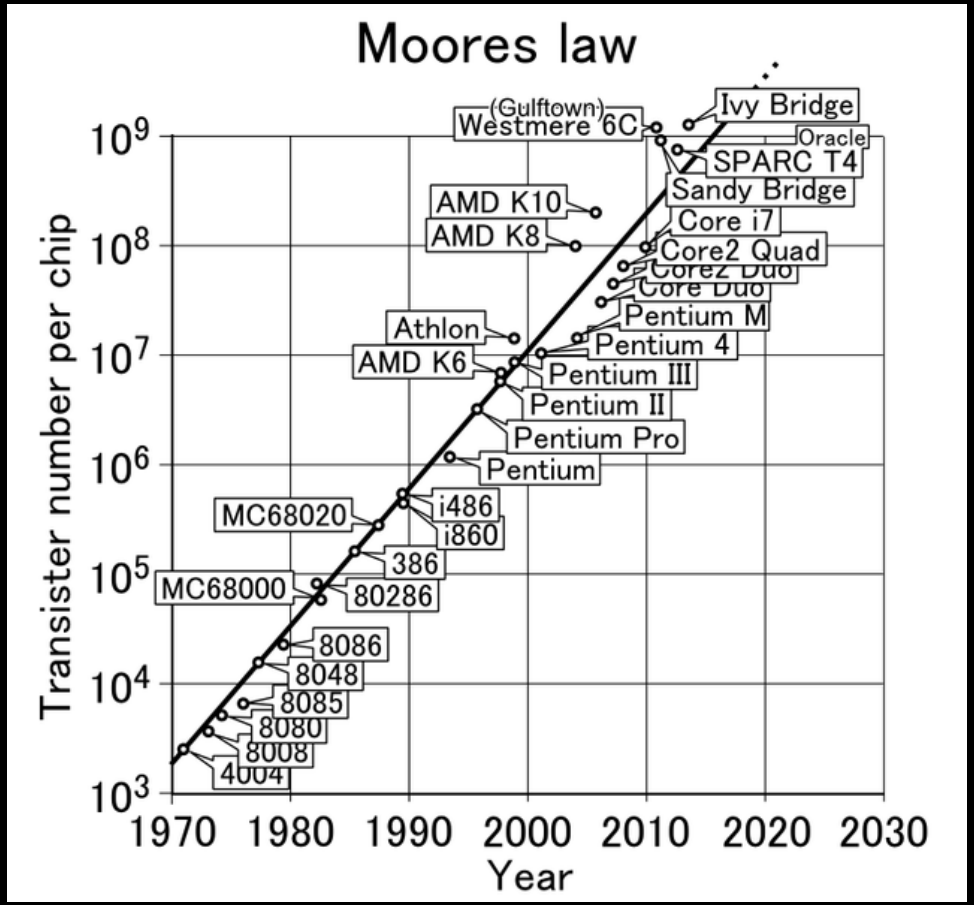
Source: Intel



Influenza Virus

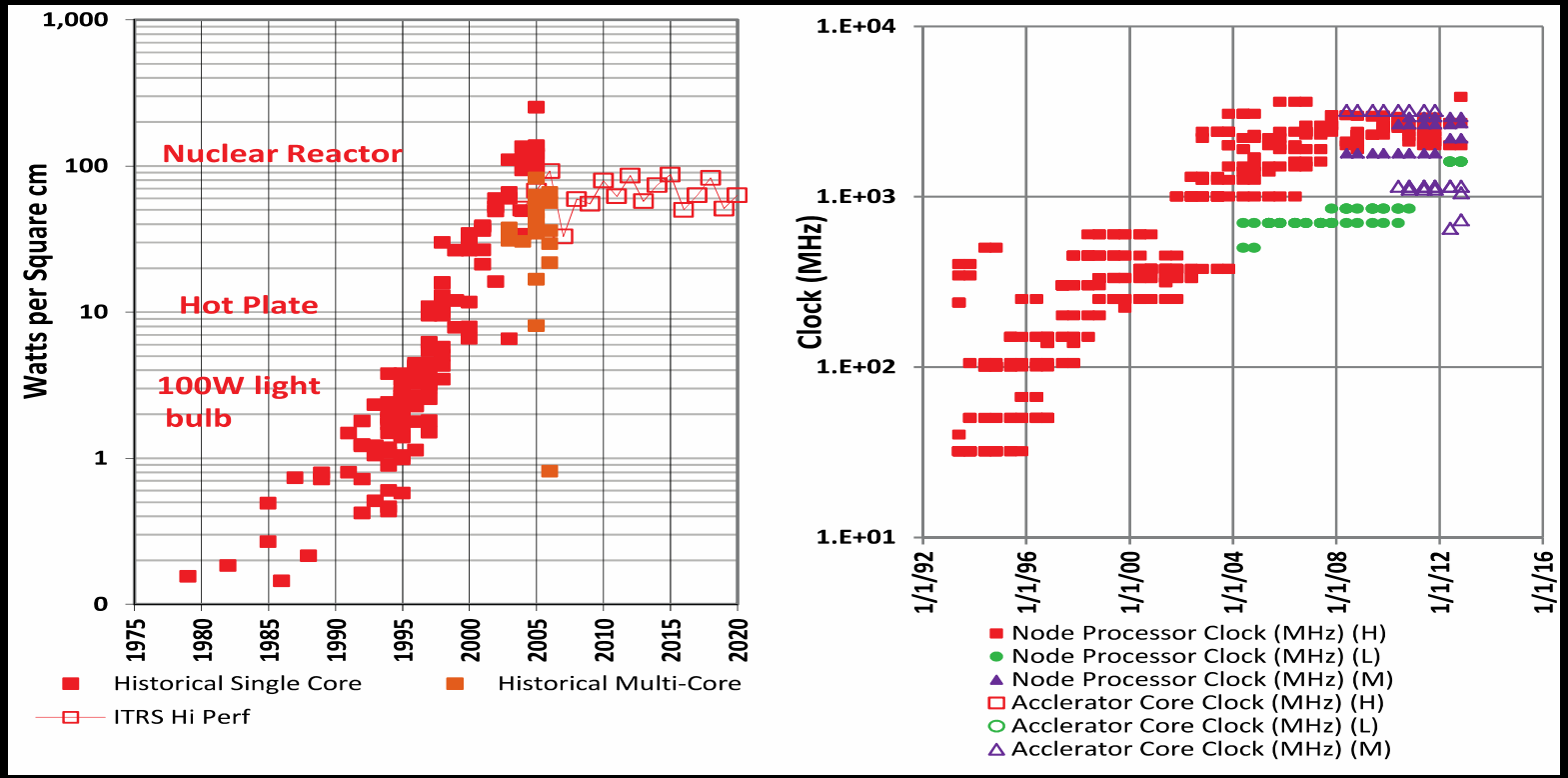
Source: CDC

At end of day, we keep using all those new transistors.



Courtesy Horst Simon, LBNL

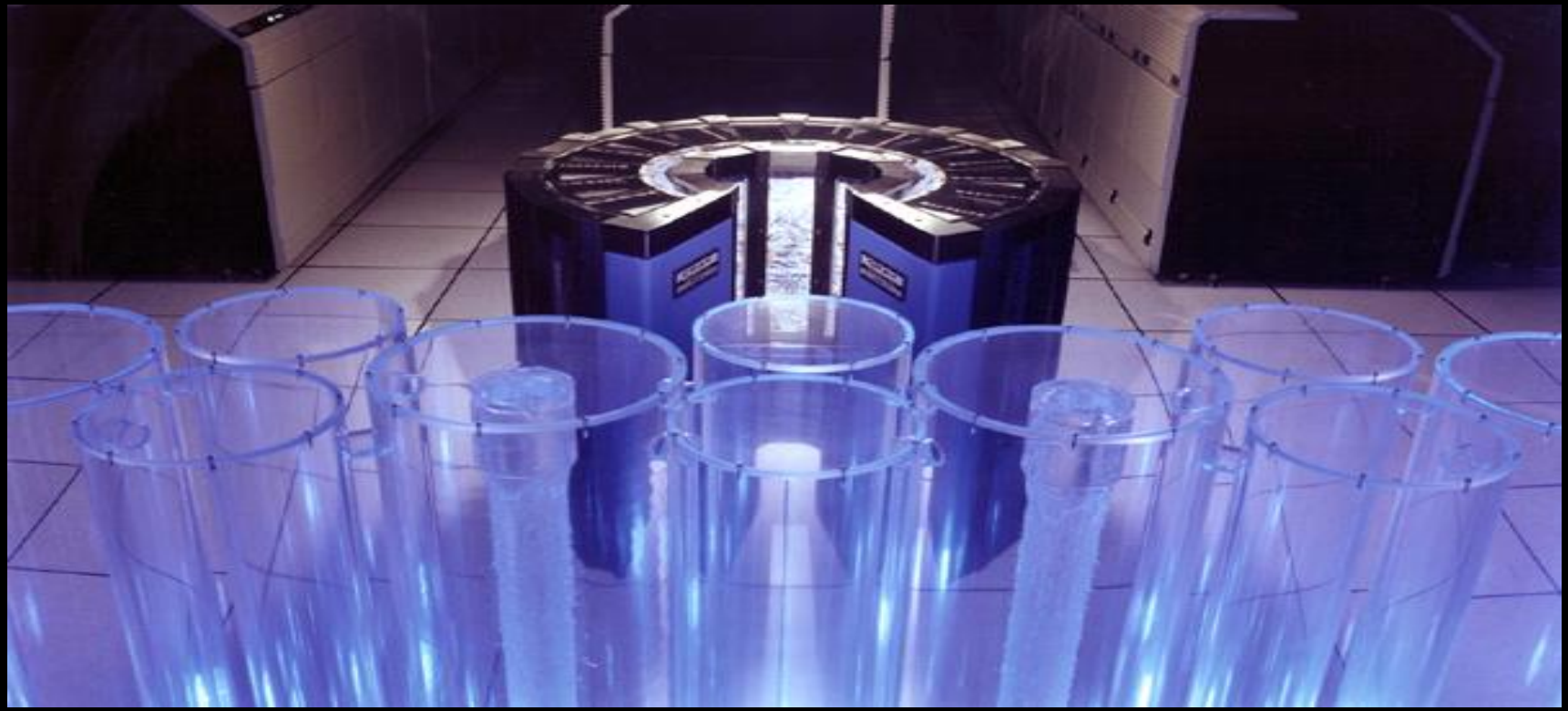
That Power and Clock Inflection Point in 2004… didn't get better.



Fun fact: At 100+ Watts and <1V, currents are beginning to exceed 100A at the point of load!

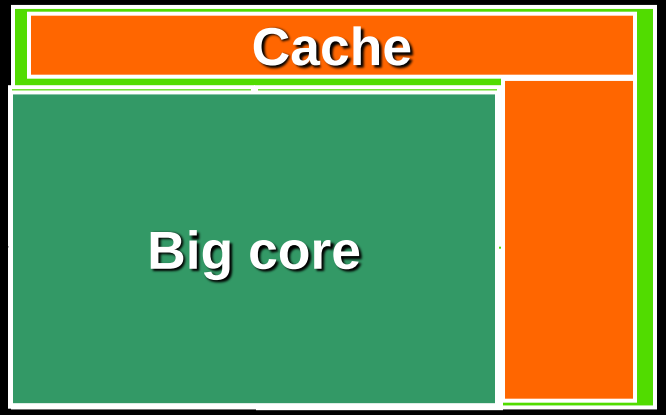
Courtesy Horst Simon, LBNL

Not a new problem, just a new scale…



Cray-2 with cooling tower in foreground, circa 1985

How to get same number of transistors to give us more performance without cranking up power?



Power

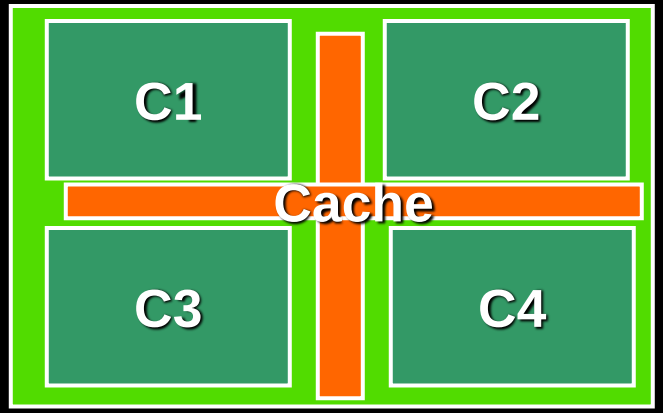
Performance

Key is that

Performance ≈ √ area

Power = ¼

Performance = 1/2



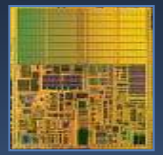
And how to get more performance from more transistors with the same power.

A 15% Reduction In Voltage Yields

RULE OF THUMB

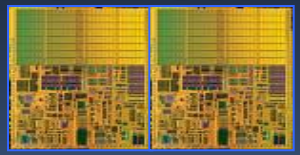
Frequency Reduction	Power Reduction	Performance Reduction
15%	45%	10%

SINGLE CORE



Area = 1
Voltage = 1
Freq = 1
Power = 1
Perf = 1

DUAL CORE



Area = 2
Voltage = 0.85
Freq = 0.85
Power = 1
Perf = ~1.8

3rd Theme

We will have Exascale computing

You will get there by going very parallel

What does parallel computing look like?

Where is this going

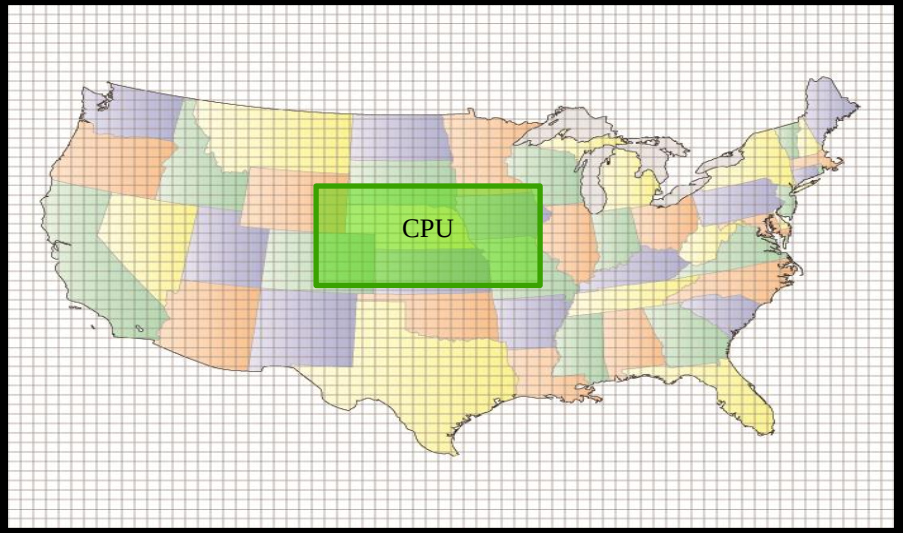
Parallel Computing

One woman can make a baby in 9 months.

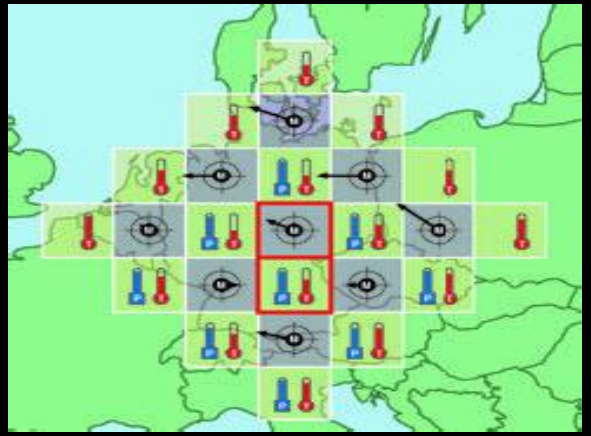
Can 9 woman make a baby in 1 month?

But 9 women can make 9 babies in 9 months.

Prototypical Application: Serial Weather Model

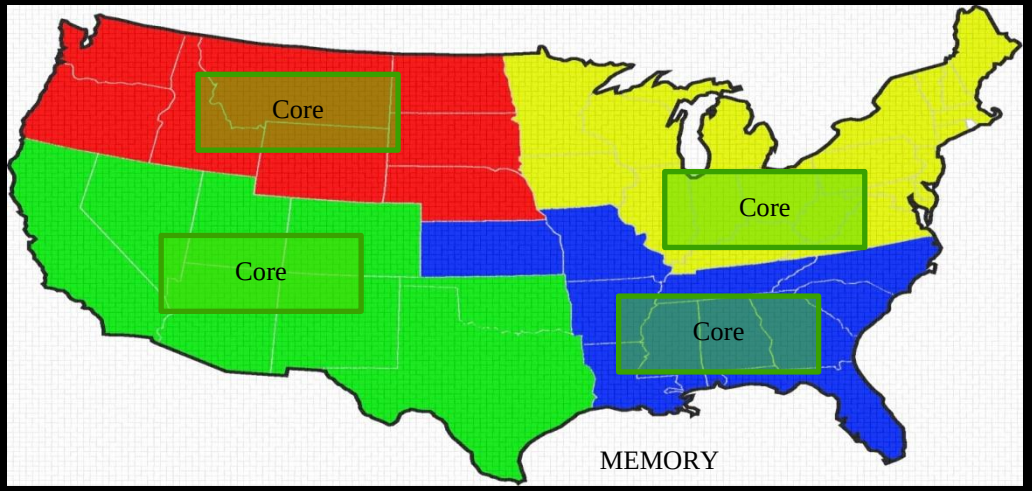


First parallel Weather Modeling algorithm: Richardson in 1917



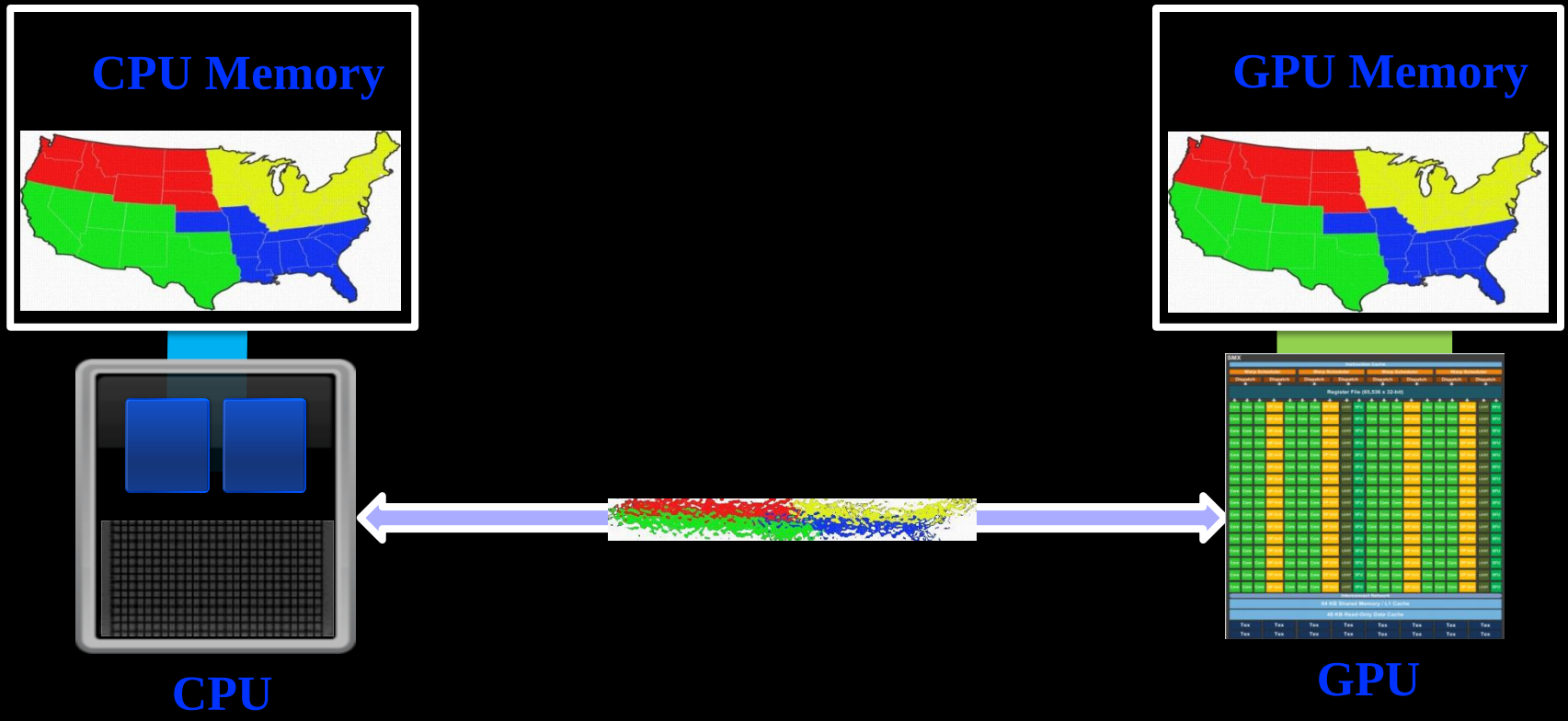
Courtesy John Burkhardt, Virginia Tech

Weather Model: Shared Memory (Today)



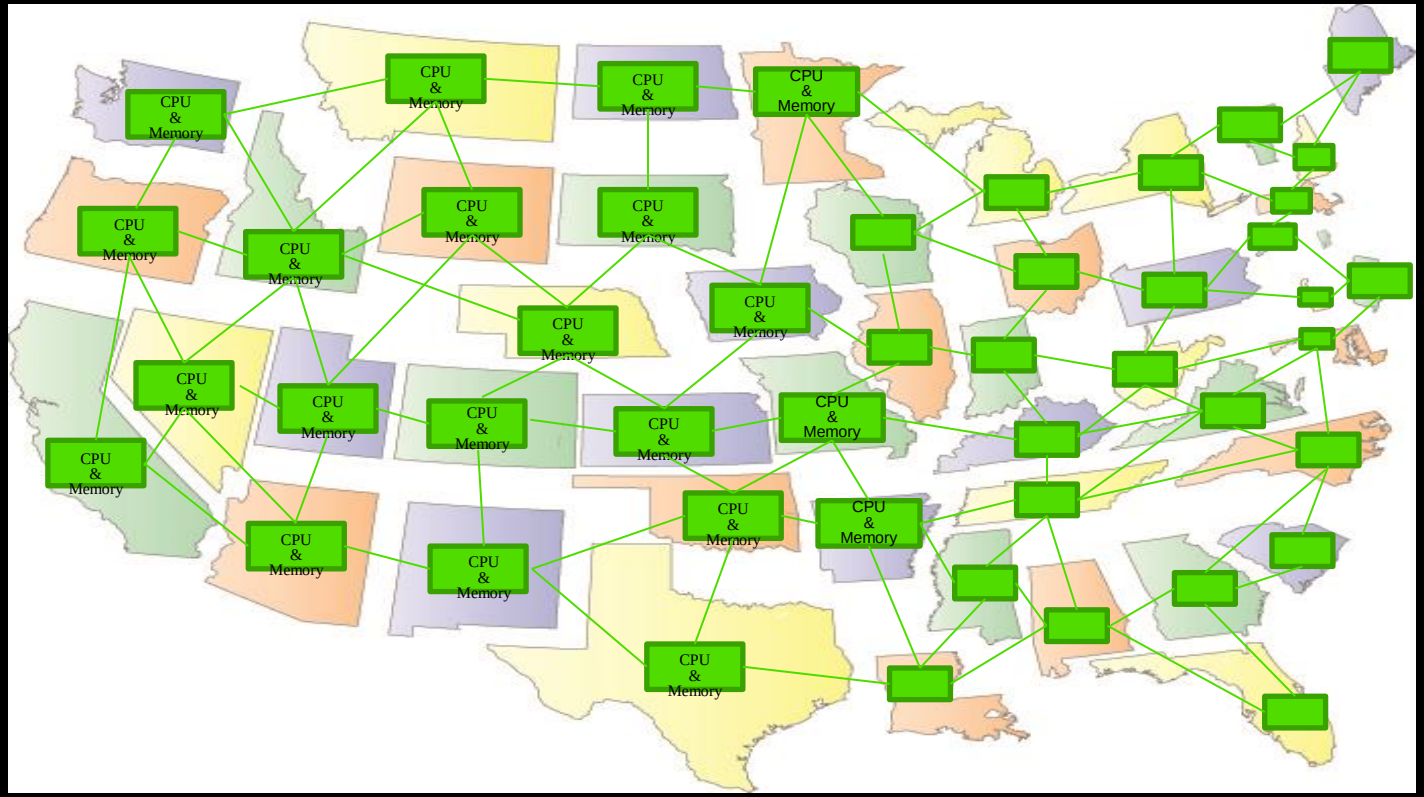
Four guys in the same room sharing the map.

Weather Model: Accelerator (Tomorrow)



1 guy coordinating 1000 using tin cans and a string.

Weather Model: Distributed Memory (Thursday)



50 guys using a telegraph.

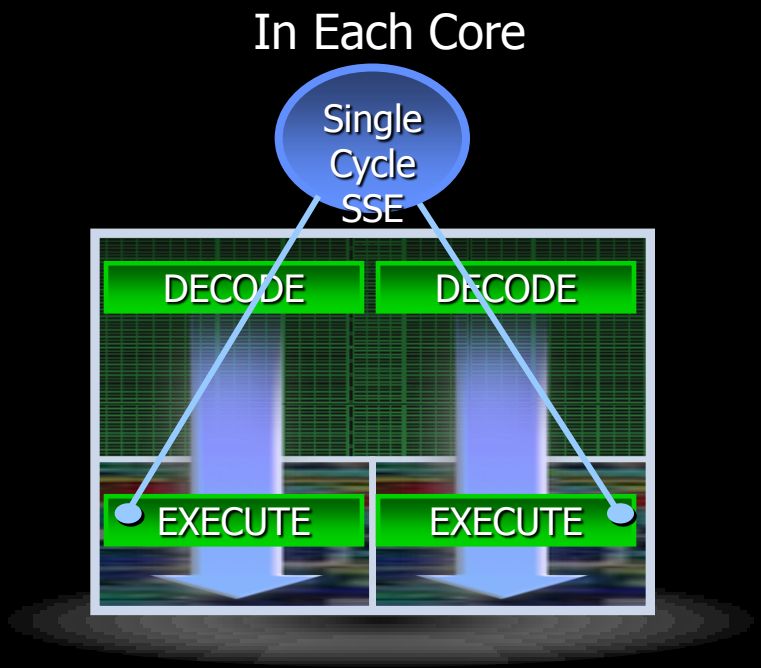
Many levels and types of parallelism:

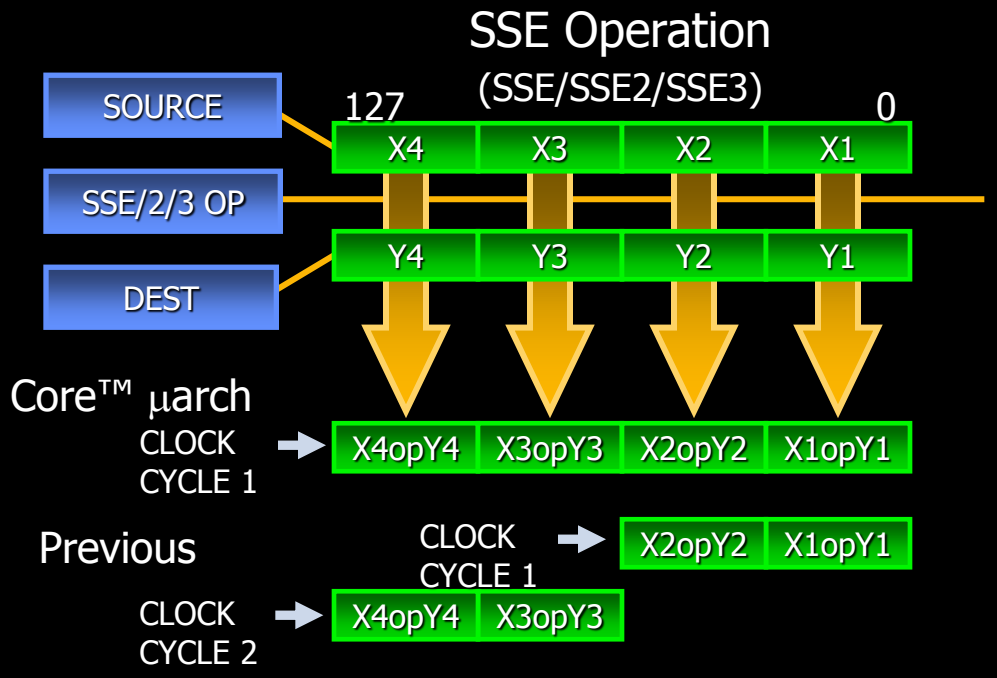
- Instruction
- Multi-Core
- SMP/Multi-socket
- Clusters
- MPPs

- *Accelerators: GPU & MIC, soon APU*

- ASIC/FPGA/DSP
- RAID/IO

Instruction Level: Intel® SSE





Perf ↑

Energy ↓

SIMD instructions compute multiple operations per instruction

*Graphics not representative of actual die photo or relative size

Multi-Core: Just a few of the current offerings

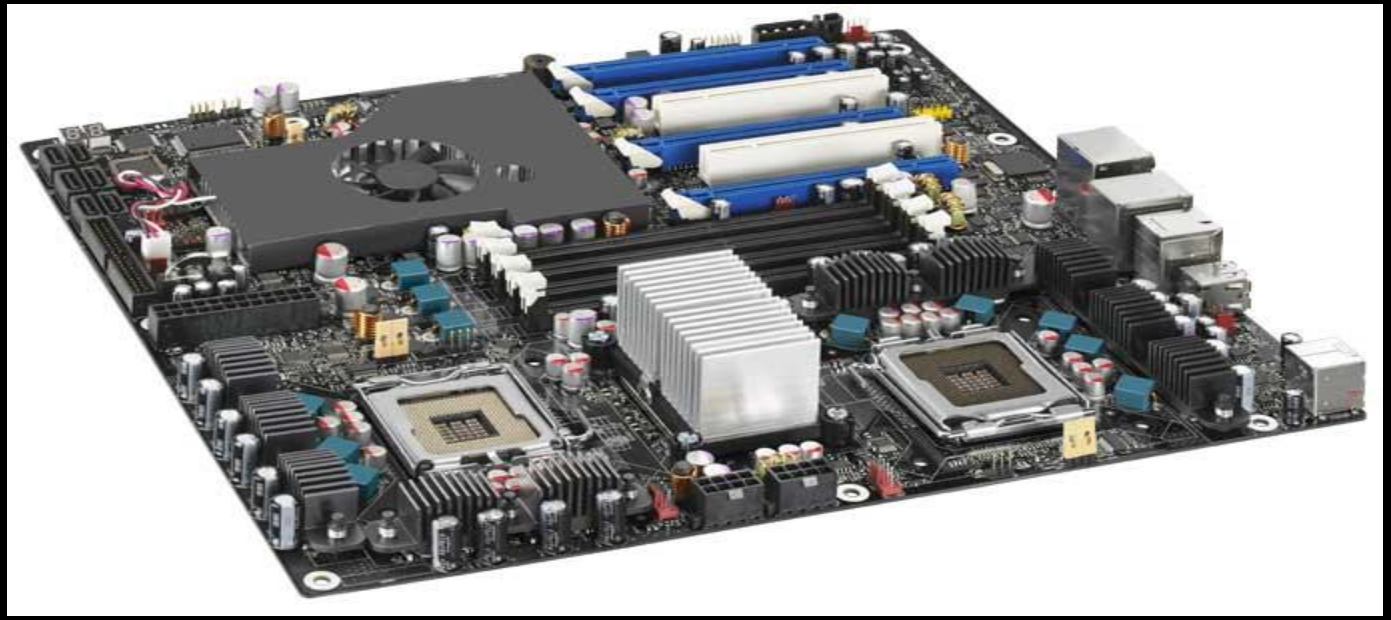
- AMD
  - Opteron (16 core, Bulldozer based Interlagos)
  - Athlon
  - Phenom II
  - Radeon
- ARM
  - MPCore (ARM9 and ARM11)
- Broadcom
  - SiByte
- Cavium Networks
  - Octeon (16 MIPS cores)
- IBM
  - Cell (Sony, and Toshiba)
  - POWER4,5,6,7 (8 core)
- Intel
  - Core i7 (6 core)
  - Xeon (10 core)
  - Itanium 2
  - MIC (60+ core)
- Microsoft
  - Xbox 360 (IBM 3 cores)
- Motorola
  - Freescale dual-core PowerPC
- NetLogic
  - XLP MPIS64 (32 core)
- Picochip
  - DSP devices (300 16-bit processor MIMD cores on one die)
- Stream Processors
  - Storm-1 (2 MIPS CPUs and DSP)
- Sun Microsystems
  - UltraSPARC IV, UltraSPARC IV+,
  - UltraSPARC T1, T2, T3, T5 (16 cores)
- Tilera
  - TILE-Gx (100cores)

Cores, Nodes, Processors, PEs?

- The most unambiguous way to refer to the smallest useful computing device is as a Processing Element, or PE.
- This is usually the same as a single core.
- “Processors” usually have more than one core – as per the previous list.
- “Nodes” is commonly used to refer to an actual physical unit, most commonly a circuit board or blade with a network connection. These often have multiple processors.

I will try to use the term PE consistently here, but I may slip up myself. Get used to it as you will quite often hear all of the above terms used interchangeably where they shouldn’t be.

Multi-socket Motherboards

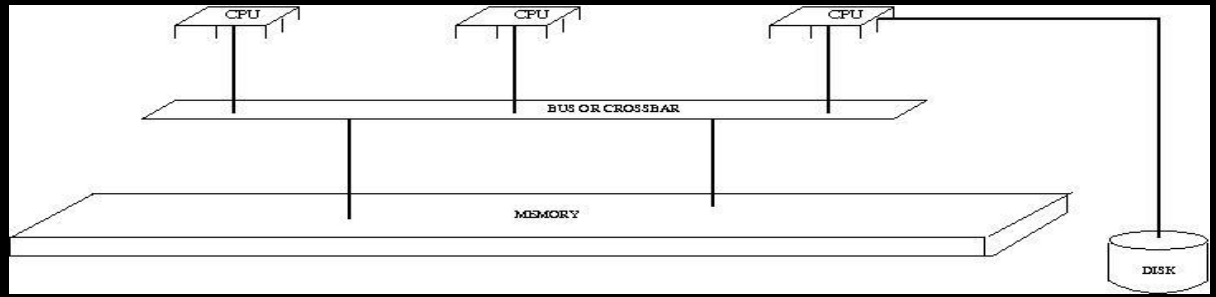


- Dual and Quad socket boards are very common in the enterprise and HPC world.
- Less desirable in consumer world.

Shared-Memory Processing

Each processor can access the entire data space

- Pro's
  - Easier to program
  - Amenable to automatic parallelism
  - Can be used to run large memory serial programs
- Con's
  - Expensive for a lot of cores
  - Difficult to implement on the hardware level
  - Processor count limited by contention/coherency (currently around 512)
  - Watch out for "NU" part of "NUMA"

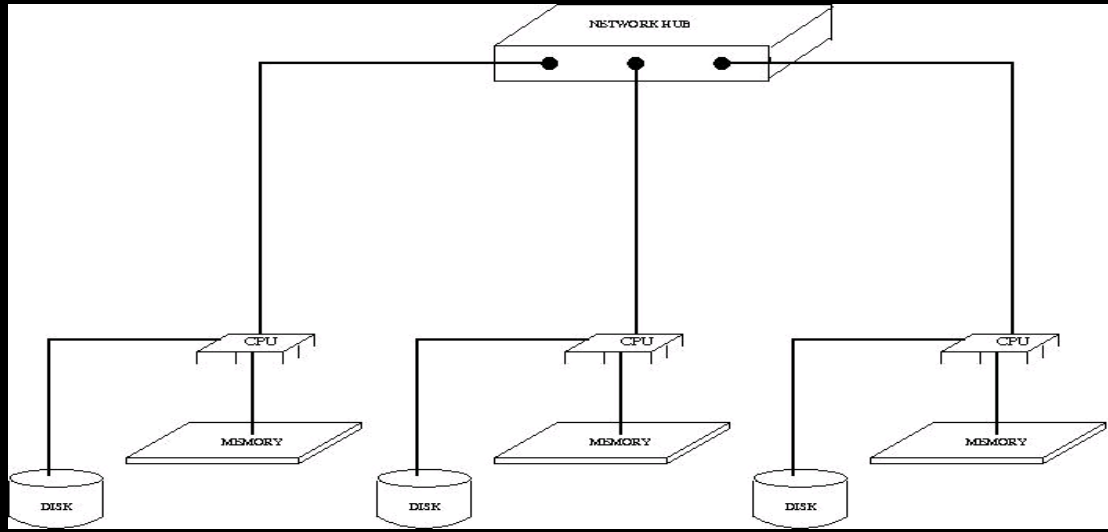


Shared-Memory Processing at Extreme Scale

- Programming
  - OpenMP, Pthreads, Shmem
- Examples
  - All multi-socket motherboards
  - SGI UV (Blacklight!)
    - Intel Xeon 8 dual core processors linked by the UV interconnect
    - 4096 cores sharing 32 TB of memory
    - As big as it gets right now

Distributed – Memory Machines

- Each node in the computer has a locally addressable memory space
- The computers are connected together via some high-speed network
  - Infiniband, Myrinet, Giganet, etc..



- Pros
  - Really large machines
  - Cheaper to build and run
  - Size limited only by gross physical considerations:
    - Room size
    - Cable lengths (10's of meters)
    - Power/cooling capacity
    - Money!
- Cons
  - Harder to program

    Data Locality

Clusters

Thunderbird (Sandia National Labs)

- Dell PowerEdge Series Capacity Cluster
- 4096 dual 3.6 Ghz Intel Xeon processors
- 6 GB DDR-2 RAM per node
- 4x InfiniBand interconnect

System X (Virginia Tech)

- 1100 Dual 2.3 GHz PowerPC 970FX processors
- 4 GB ECC DDR400 (PC3200) RAM
- 80 GB S-ATA hard disk drive
- One Mellanox Cougar InfiniBand 4x HCA*
- Running Mac OS X

MPPs (Massively Parallel Processors)

Distributed memory at largest scale. Often shared memory at lower level.

- **Sequoia (LLNL)**
  - **16.32475 petaflops Rmax and 20.13266 petaflops Rpeak**
  - **IBM Blue Gene/Q**
  - **98,304 compute nodes**
  - **1.6 million processor cores**
  - **1.6 PB of memory**

- **Titan (ORNL)**
  - **AMD Opteron 6274 processors (Interlagos)**
  - **560,640 cores**
  - **Gemini interconnect** (3-D Torus)
  - **Accelerated node design using NVIDIA multi-core accelerators**
  - **20+ PFlops peak system performance**

Compute Nodes	18,688
Login & I/O Nodes	512
Memory per node	32 GB + 6 GB
# of Fermi chips (2012)	960
# of NVIDIA “Kepler” (2013)	14,592
Total System Memory	688 TB
Total System Peak Performance	20+ Petaflops
Liquid cooling at the cabinet level	Cray EcoPHLex

Networks

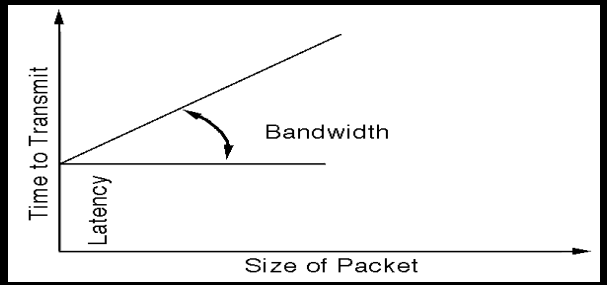
3 characteristics sum up the network:

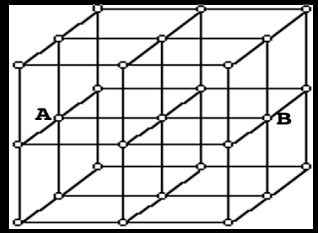
- **Latency**

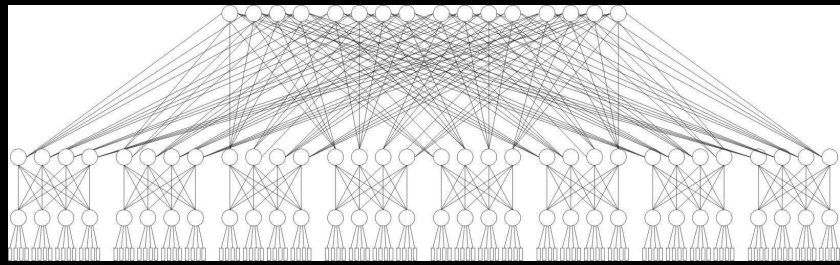
  The time to send a 0 byte packet of data on the network

- **Bandwidth**

  The rate at which a very large packet of information can be sent



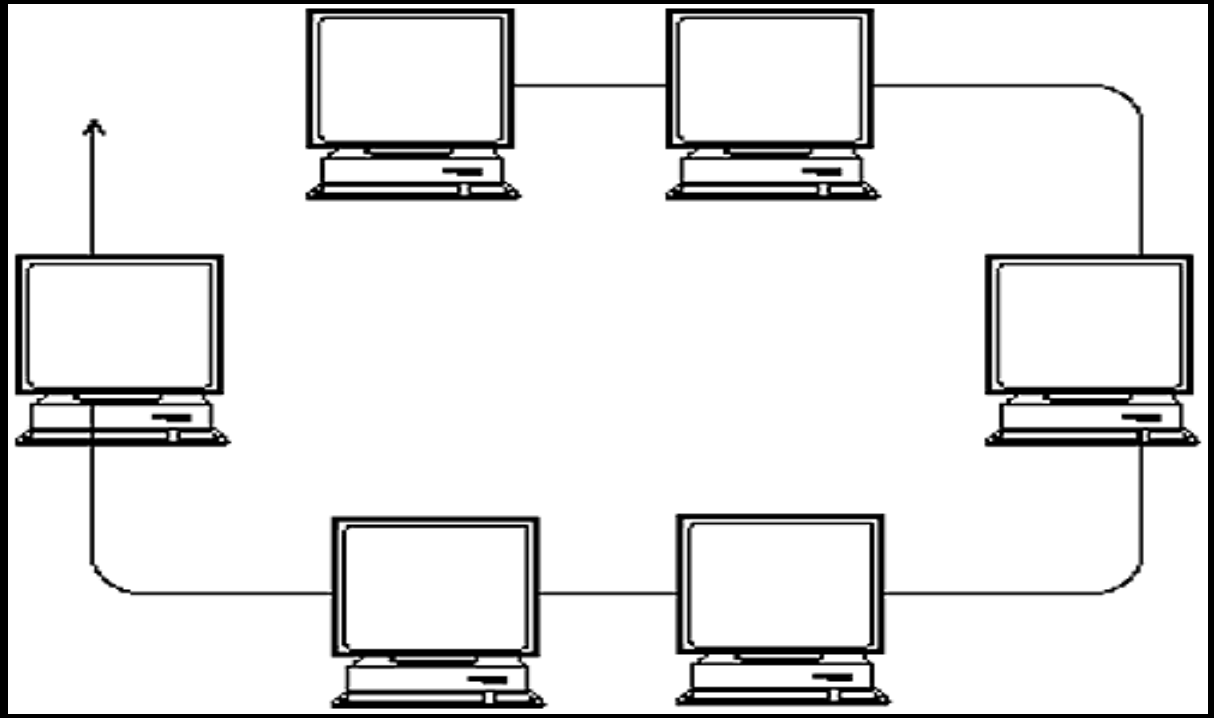




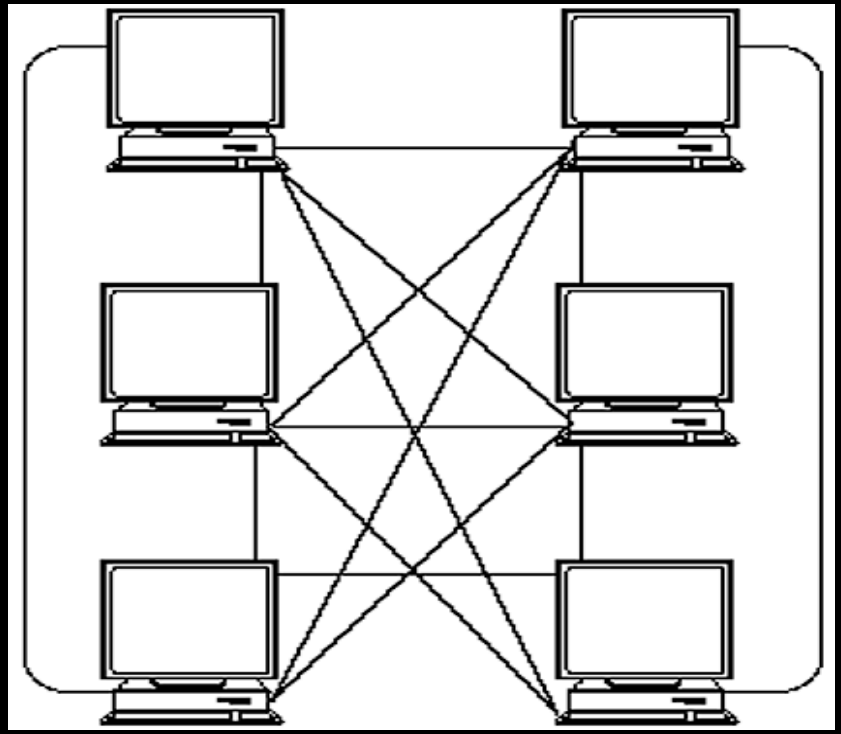
- **Topology**

  The configuration of the network that determines how processing units are directly connected.

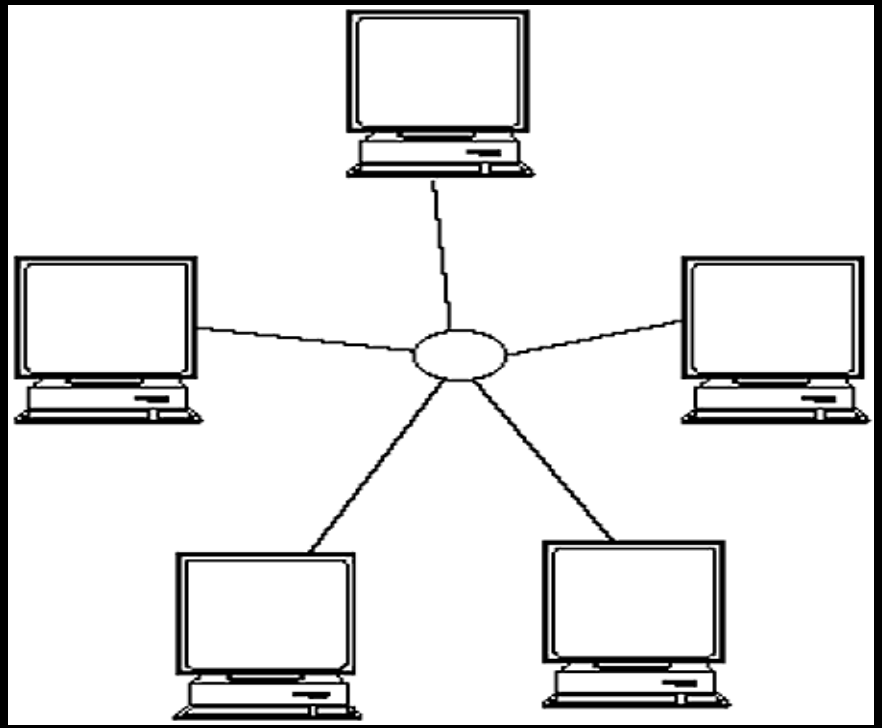
Ethernet with Workstations



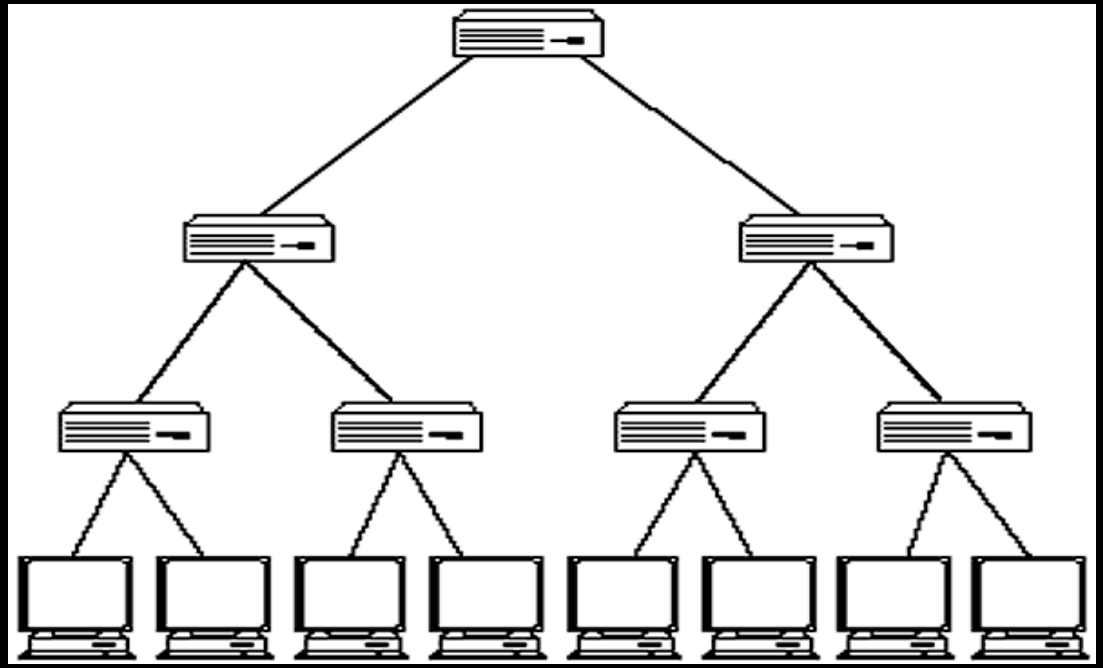
Complete Connectivity



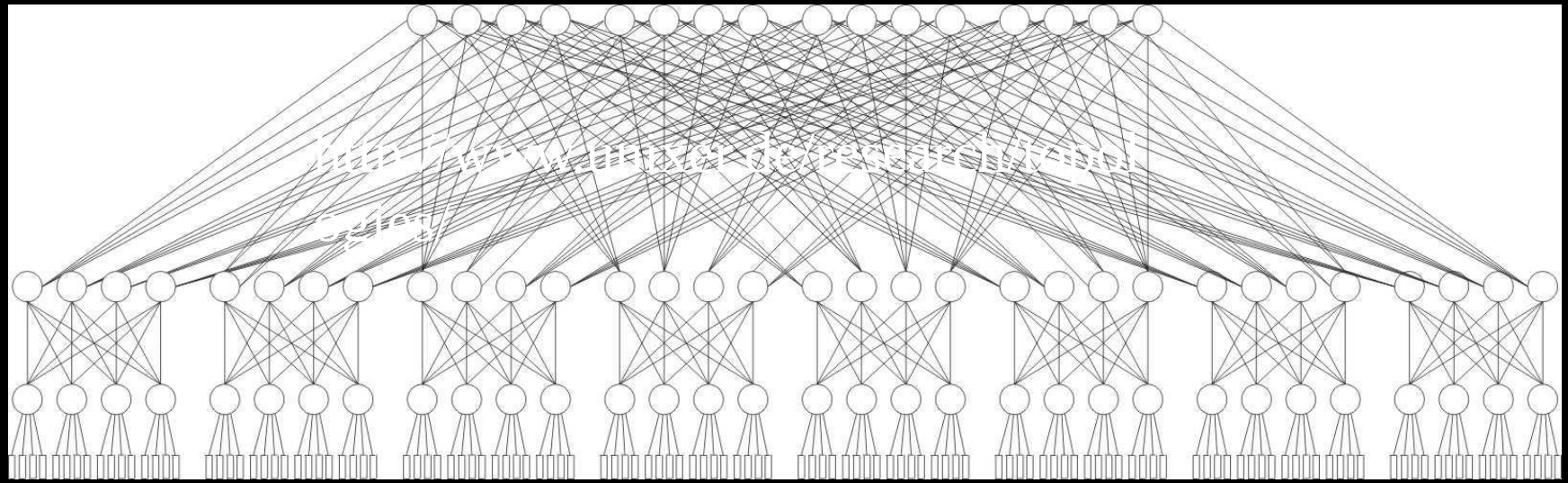
Crossbar



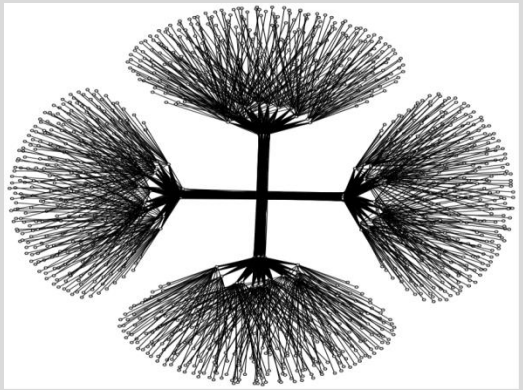
Binary Tree



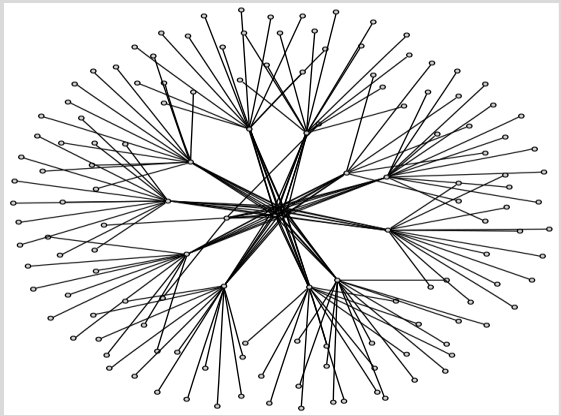
Fat Tree



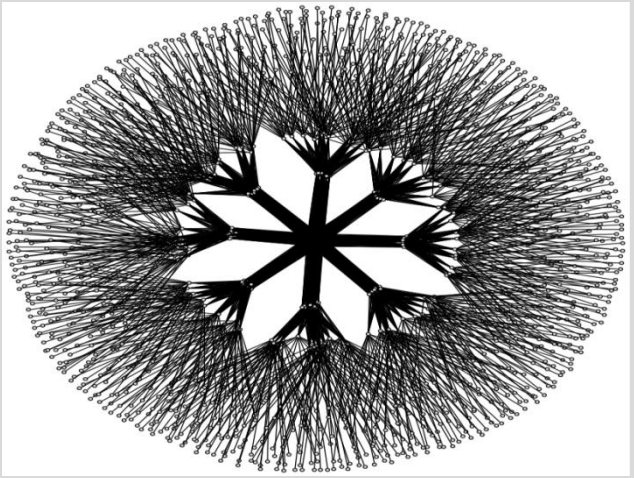
Other Fat Trees



Big Red @ IU

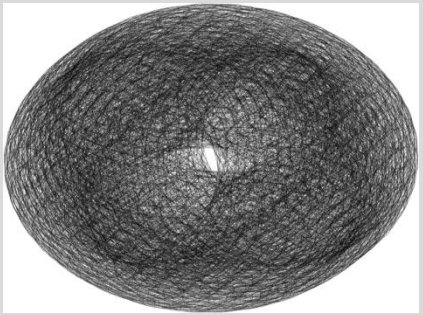


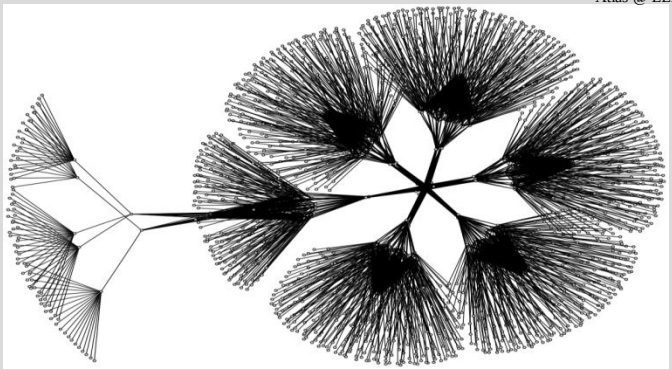
Odin @ IU



Atlas @ LLNL

Jaguar @ ORNL

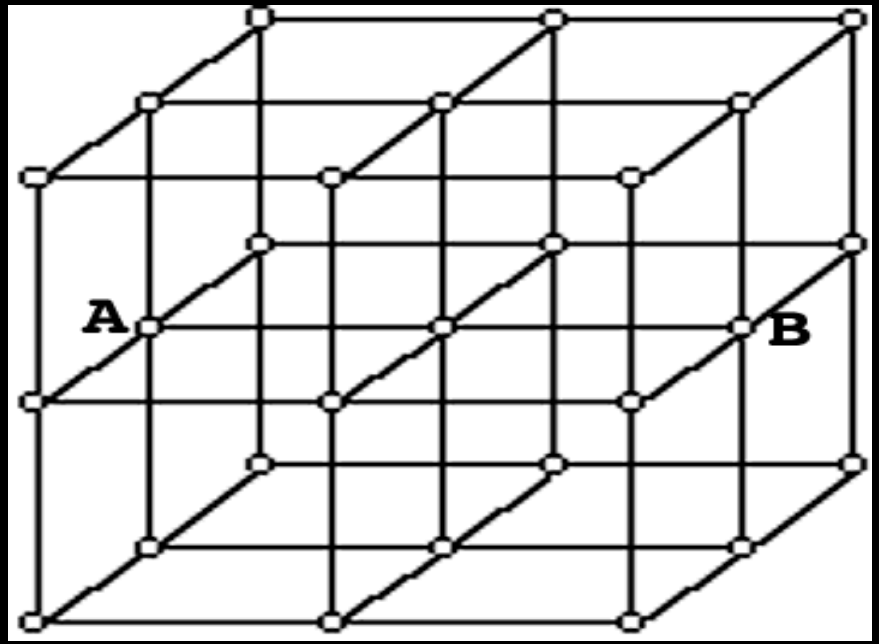




Tsubame @ Tokyo Inst. of Tech

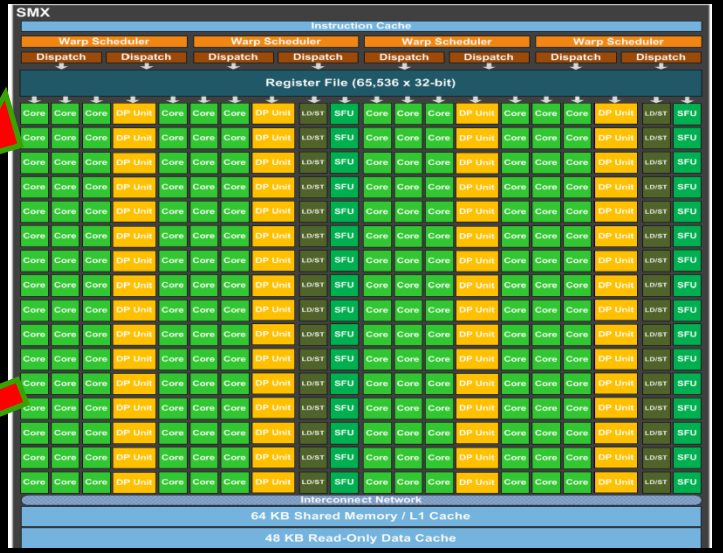
From Torsten Hoefler's Network Topology Repository at
http://www.unixer.de/research/topologies/

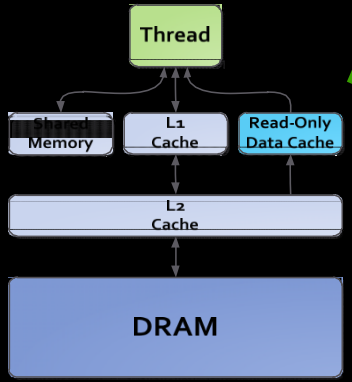
3-D Torus (T3D – XT7…)



- XT3 has Global Addressing hardware, and this helps to simulate shared memory.
- Torus means that “ends” are connected. This means A is really connected to B and the cube has no real boundary.

GPU Architecture - GK110 Kepler





From a document you should read if you are interested in this:

http://www.nvidia.com/content/PDF/kepler/NVIDIA-Kepler-GK110-Architecture-Whitepaper.pdf

Intel’s MIC Approach

Since the days of RISC vs. CISC, Intel has mastered the art of figuring out what is important about a new processing technology, and saying “why can’t we do this in x86?”

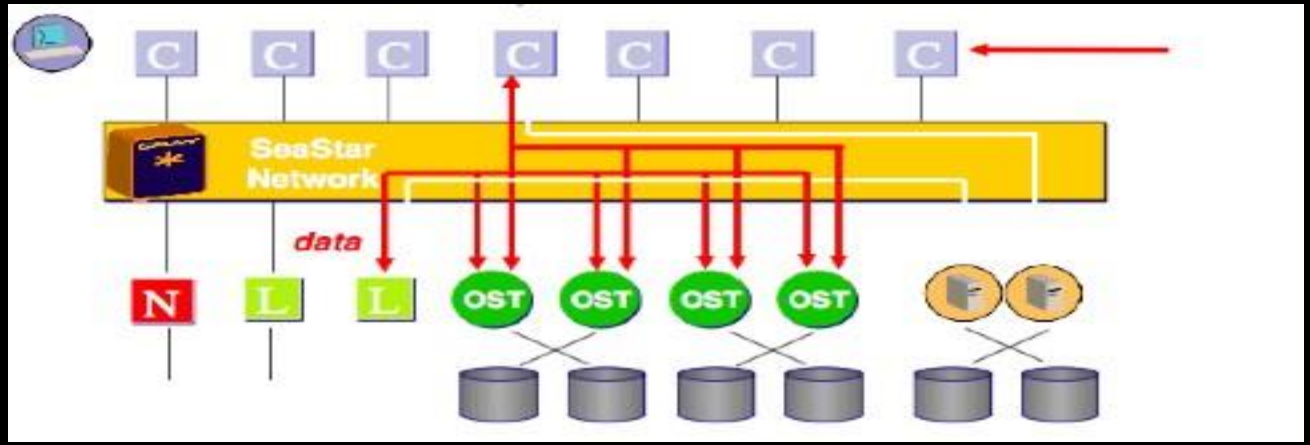
The Intel Many Integrated Core (MIC) architecture is about large die, simpler circuit, much more parallelism, in the x86 line.

Top 10 Systems as of November 2015

#	Site	Manufacturer	Computer	CPU Interconnect [Accelerator]	Cores	Rmax (Tflops)	Rpeak (Tflops)	Power (MW)
1	National Super Computer Center in Guangzhou **China**	NUDT	Tianhe-2 (MilkyWay)	Intel Xeon E5-2692 2.2 GHz TH Express-2 Intel Xeon Phi 31S1P	**3,120,000**	**33,862**	**54,902**	**17.8**
2	DOE/SC/Oak Ridge National Laboratory **United States**	Cray	Titan Cray XK7	Opteron 6274 2.2 GHz Gemini NVIDIA K20x	**560,640**	**17,590**	**27,112**	**8.2**
3	DOE/NNSA/LLNL **United States**	IBM	Sequoia BlueGene/Q	Power BQC 1.6 GHz Custom	**1,572,864**	**17,173**	**20,132**	**7.8**
4	RIKEN Advanced Institute for Computational Science (AICS) **Japan**	Fujitsu	K Computer	SPARC64 VIIIfx 2.0 GHz Tofu	**705,024**	**10,510**	**11,280**	**12.6**
5	DOE/SC/Argonne National Laboratory **United States**	IBM	Mira BlueGene/Q	Power BQC 1.6 GHz Custom	**786,432**	**8,586**	**10,066**	**3.9**
6	DOE/NNSA/LANL/SNL **United States**	Cray	Trinity Cray XC40	Xeon E5-2698v3 2.3 GHz Aries	**301,056**	**8,100**	**11,078**	
7	Swiss National Supercomputing Centre (CSCS) **Switzerland**	Cray	Piz Daint Cray XC30	Xeon E5-2670 2.6 GHz Aries NVIDIA K20x	**115,984**	**6,271**	**7,788**	**2.3**
8	HLRS **Germany**	Cray	Hazel Hen Cray XC40	Xeon E5-2680 2.5 GHz Aries	**185,088**	**5,640**	**7,403**	
9	King Abdullah University of Science and Technology **Saudi Arabia**	Cray	Shaheen II Cray XC40	Xeon E5-2698v3 2.3 GHz Aries	**196,608**	**5,537**	**7,235**	**2.8**
10	Texas Advanced Computing Center/Univ. of Texas	Dell	Stampede PowerEdge C8220	Xeon E5-2680 2.7 GHz Infiniband FDR	**462,462**	**5,168**	**8,520**	**4.5**

Parallel IO (RAID…)

- There are increasing numbers of applications for which many PB of Data need to be written.
- Checkpointing is also becoming very important due to MTBF issues (a whole ‘nother talk).
- Build a large, fast, reliable filesystem from a collection of smaller drives.
- Supposed to be transparent to the programmer.
- Increasingly mixing in SSD.



4th Theme

We will have Exascale computing

You will get there by going very parallel

What does parallel computing look like?

Where is this going?

Today

- Pflops computing fully established with more than 50 machines
- The field is thriving
- Interest in supercomputing is now worldwide, and growing in many new markets
- Exascale projects in many countries and regions

Exascale?

exa = 10^{18} = 1,000,000,000,000,000,000 = quintillion

23,800 X

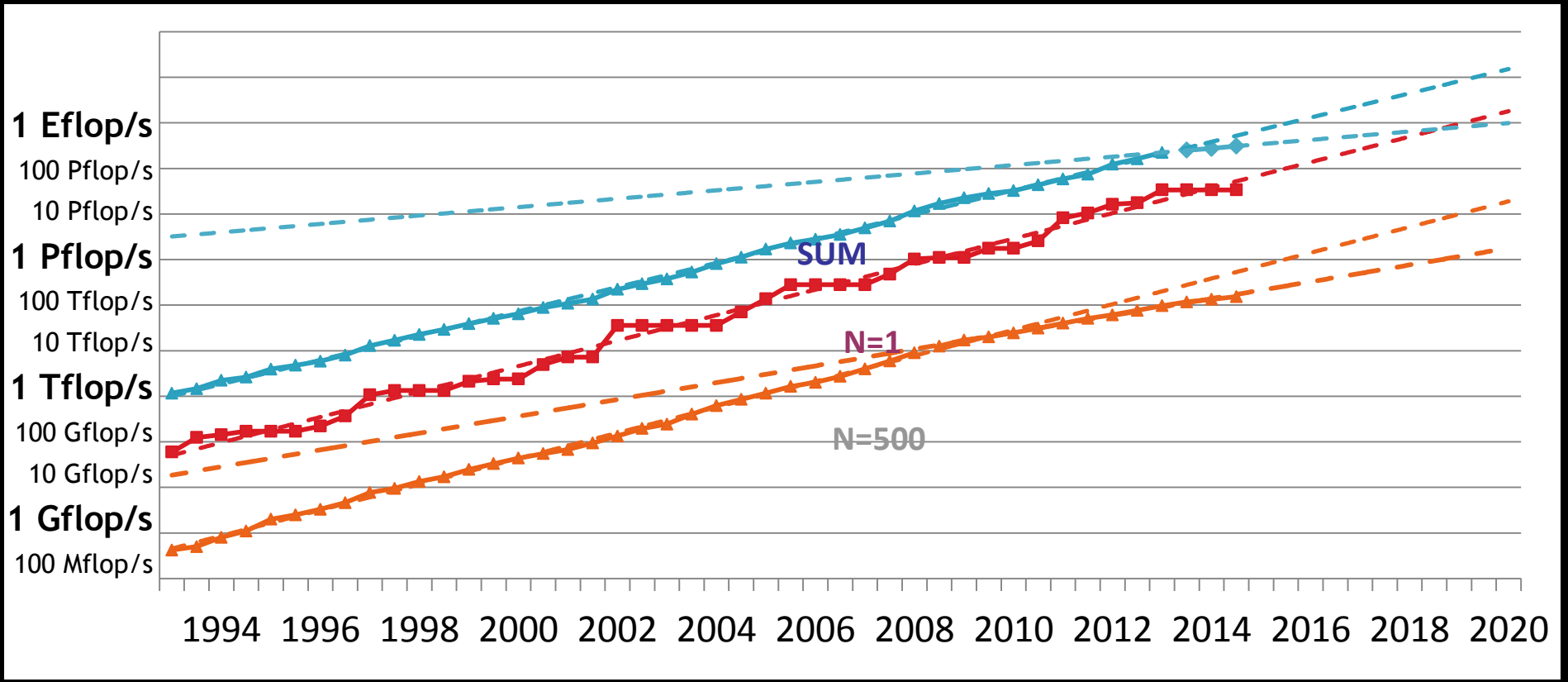
Cray Red Storm
2004
42 Tflops

or

833,000 X

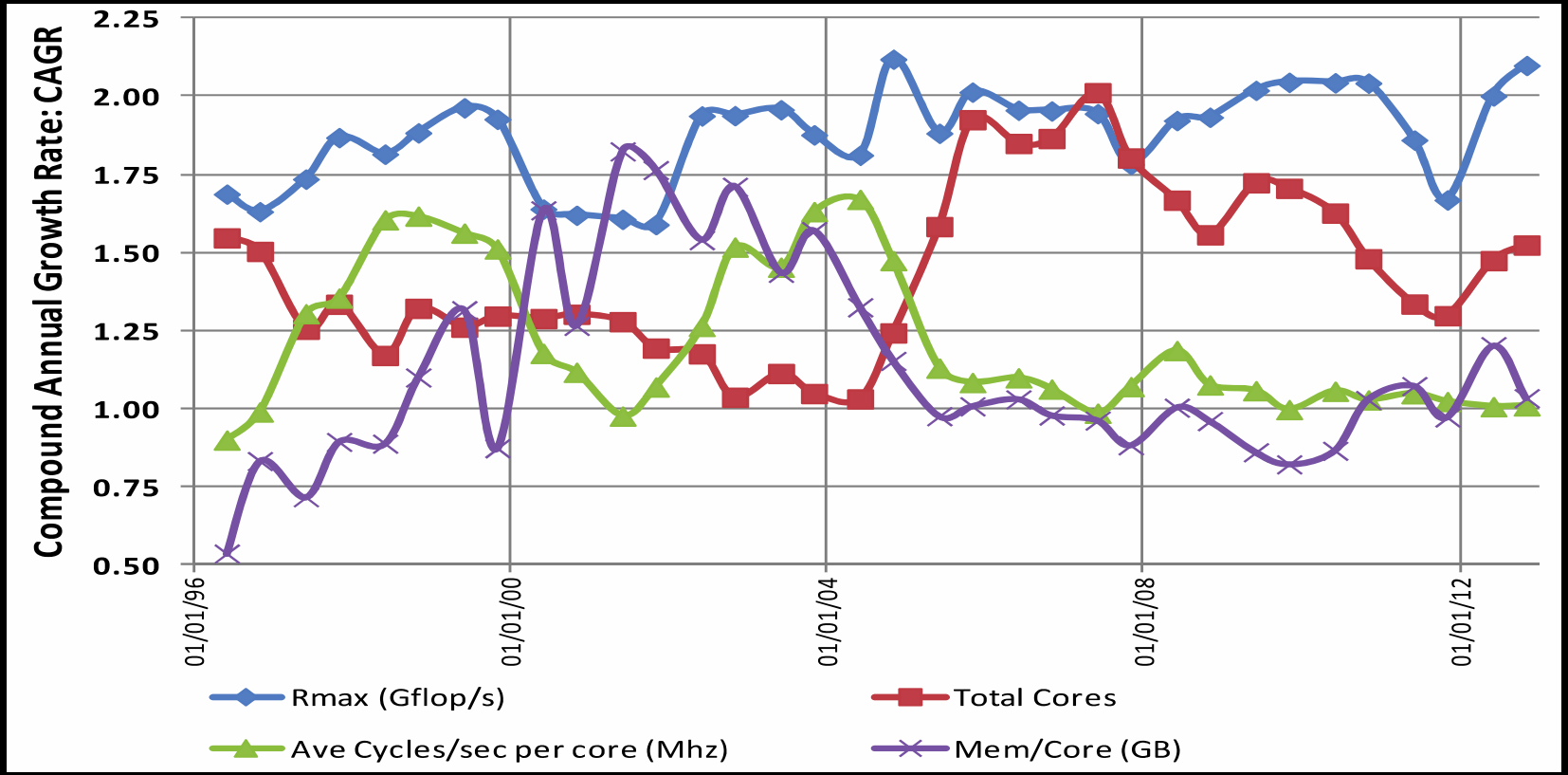
NVIDIA K40
1.2 Tflops

Projected Performance Development



TOP500

Trends with ends.



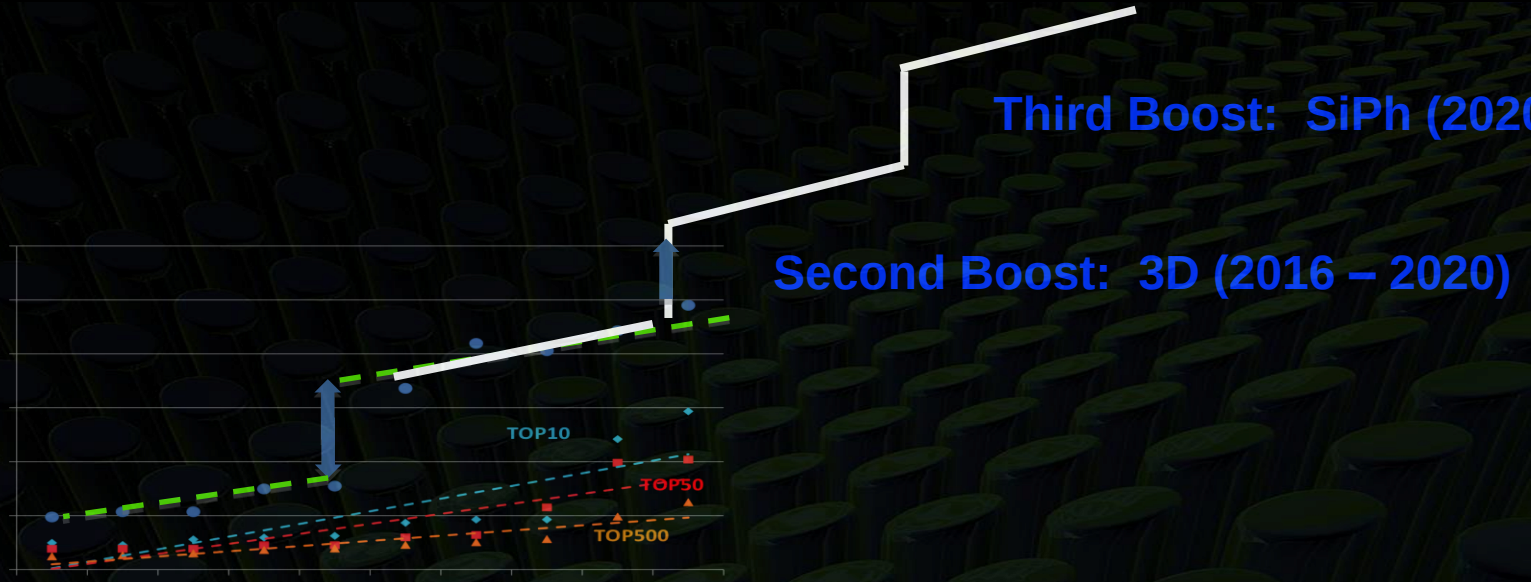
Courtesy Horst Simon, LBNL

Obstacles?

One of the many groups established to enable this outcome (the Advanced Scientific Computing Advisory Committee) puts forward this list of 10 technical challenges.

- Energy efficient circuit, power and cooling technologies.
- High performance interconnect technologies.
- Advanced memory technologies to dramatically improve capacity and bandwidth.
- Scalable system software that is power and resilience aware.
- Data management software that can handle the volume, velocity and diversity of data-storage
- Programming environments to express massive parallelism, data locality, and resilience.
- Reformulating science problems and refactoring solution algorithms for exascale.
- Ensuring correctness in the face of faults, reproducibility, and algorithm verification.
- Mathematical optimization and uncertainty quantification for discovery, design, and decision.
- Software engineering and supporting structures to enable scientific productivity.

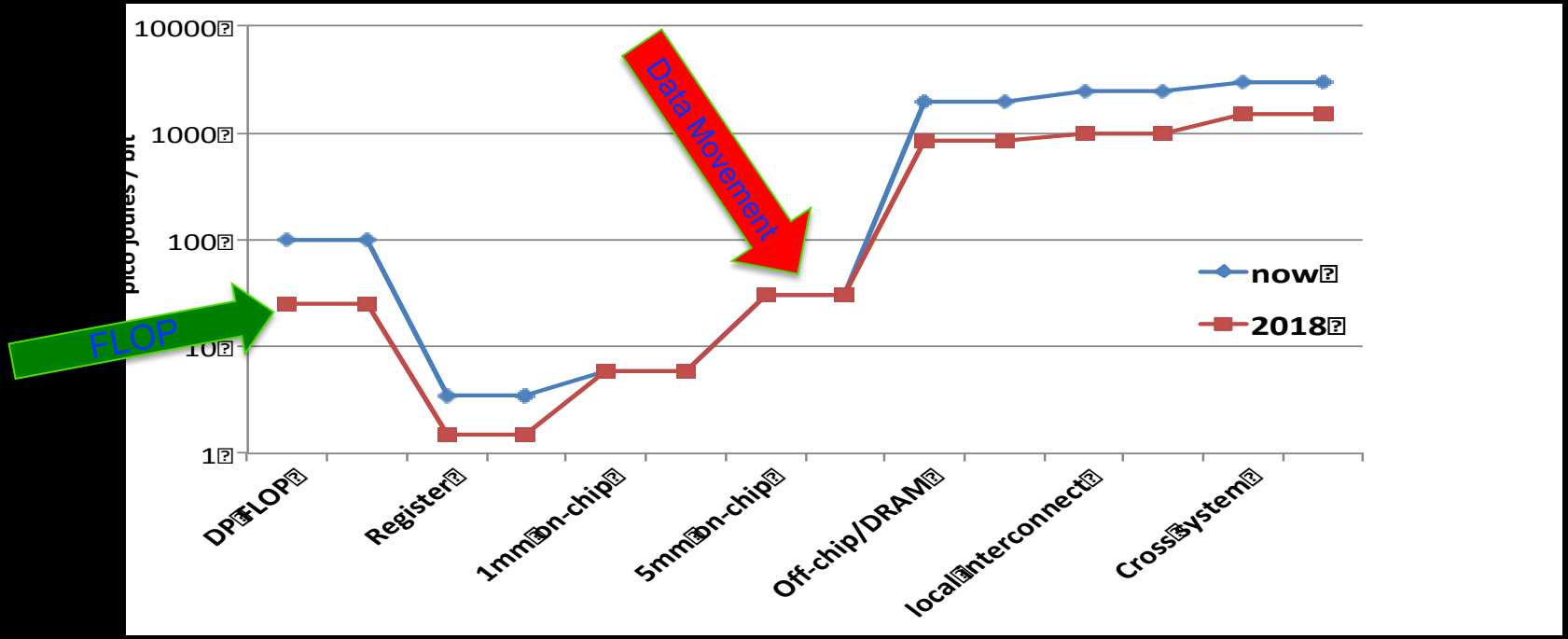
Two Additional Boosts to Improve Flops/Watt and Reach Exascale Target



Courtesy Horst Simon, LBNL

Power Issues by 2018

FLOPs will cost less than on-chip data movement!



Flops are free?

At exascale, >99% of power is consumed by moving operands across machine.

Does it make sense to focus on flops, or should we optimize around data movement?

To those that say the future will simply be Big Data:

“All science is either physics or stamp collecting.”

- Ernest Rutherford

It is not just “exaflops” – we are changing the whole computational model

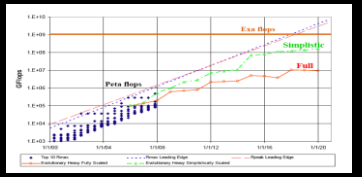
Current programming systems have WRONG optimization targets

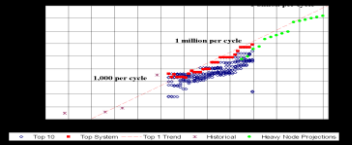
Old Constraints

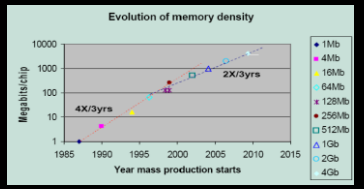
- **Peak clock frequency** ***as primary limiter for performance improvement***
- **Cost:** ***FLOPs*** **are biggest cost for system:** ***optimize for compute***
- **Concurrency: Modest growth of parallelism by adding nodes**
- **Memory scaling*: maintain byte per flop capacity and bandwidth***
- **Locality*: MPI+X model (uniform costs within node & between nodes)***
- **Uniformity:** ***Assume uniform system performance***
- **Reliability*: It’s the hardware’s problem***

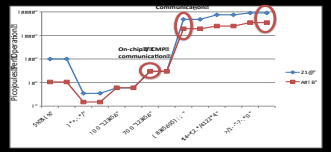
New Constraints

- **Power** *is primary design constraint for future HPC system design*
- **Cost:** *Data movement dominates: optimize to minimize data movement*
- **Concurrency:** *Exponential growth of parallelism within chips*
- **Memory Scaling:** *Compute growing 2x faster than capacity or bandwidth*
- **Locality***: must reason about data locality and possibly topology*
- **Heterogeneity**: *Architectural and performance non-uniformity increase*
- **Reliability**: *Cannot count on hardware protection alone*







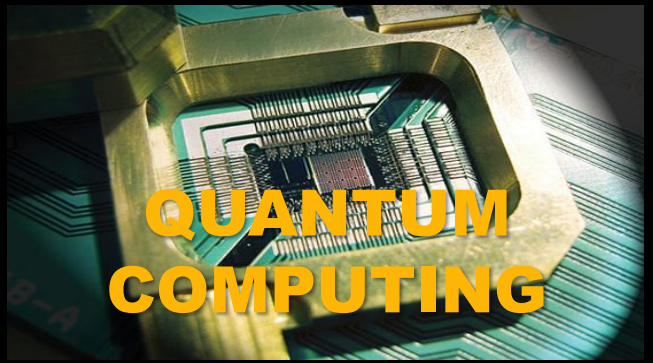


Fundamentally breaks our current programming paradigm and computing ecosystem

Adapted from John Shalf

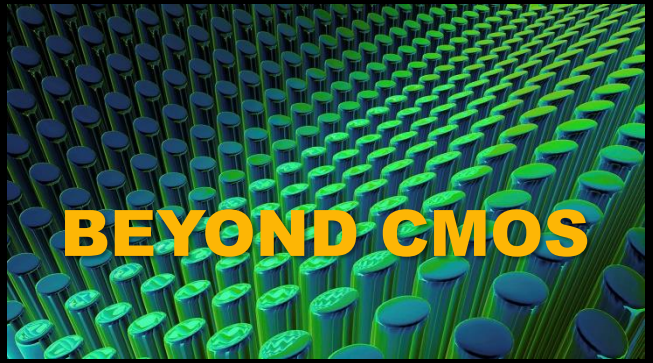
End of Moore's Law Will Lead to New Architectures

Non-von Neumann



ARCHITECTURE

von Neumann

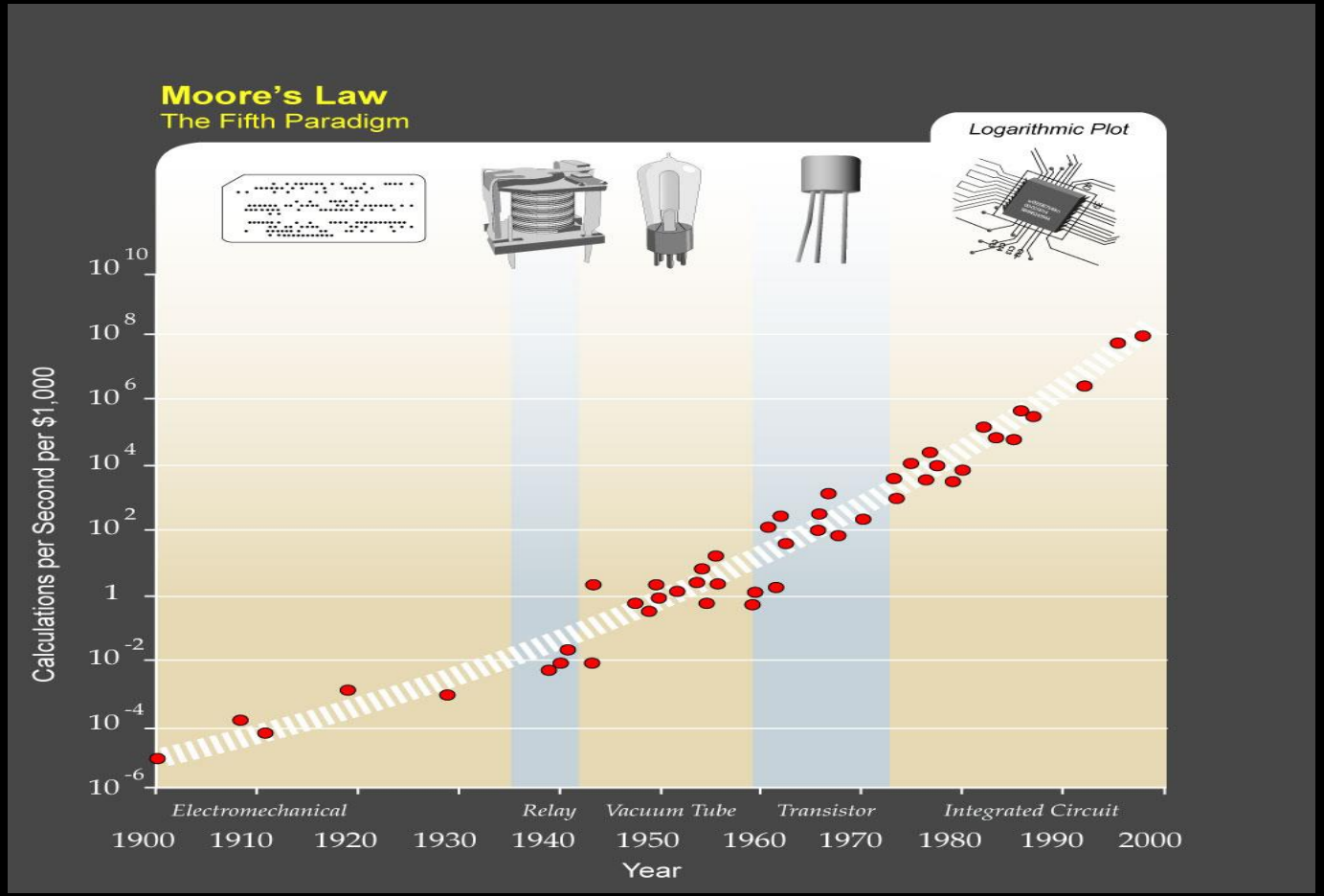


CMOS

Beyond CMOS

TECHNOLOGY

It would only be the 6th paradigm.



As a last resort, we ~~could~~ will learn to program again.

It has become a mantra of contemporary programming philosophy that developer hours are so much more valuable than hardware, that the best design compromise is to throw more hardware at slower code.

This might well be valid for some Java dashboard app used twice week by the CEO. But this has spread and results in…

The common observation that a modern PC (or phone) seems to be more laggy than one from a few generations ago that had literally 1 thousandth the processing power.

Moore's Law has been the biggest enabler (or more accurately rationalization) for this trend. If Moore's Law does indeed end, then progress will require good programming.

No more garbage collecting, script languages. I am looking at you, Java, Python, Matlab,

We can do better. We have a role model.

- Straight forward extrapolation results in a real time human brain scale simulation at about 1 - 10 Exaflop/s with 4 PB of memory
- Current predictions envision Exascale computers in 2022+ with a power consumption of at best 20 - 30 MW
- The human brain takes 20W
- Even under best assumptions in 2020 our brain will still be a million times more power efficient

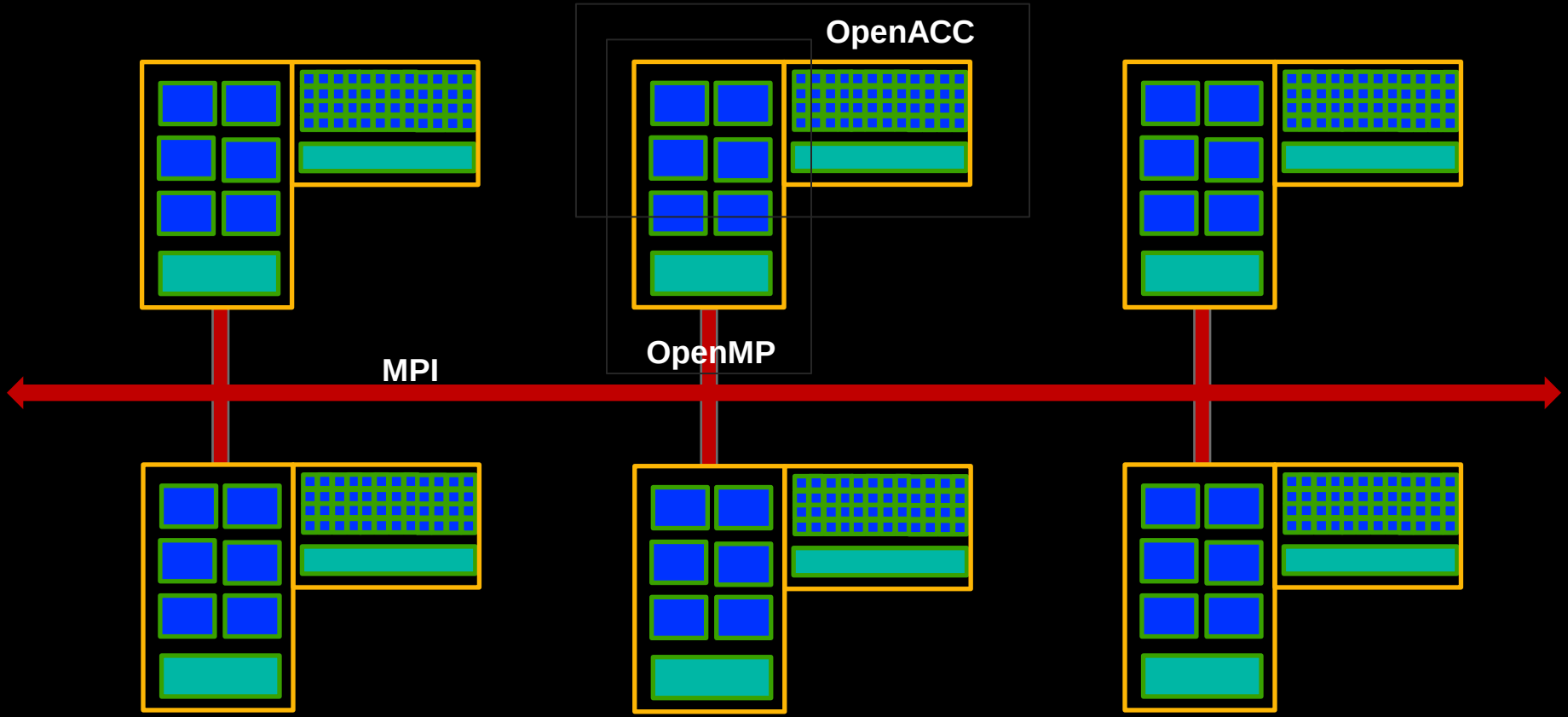
Courtesy Horst Simon, LBNL

Why you should be (extra) motivated.

- This parallel computing thing is no fad.
- The laws of physics are drawing this roadmap.
- If you get on board (the right bus), you can ride this trend for a long, exciting trip.

Let’s learn how to use these things!

In Conclusion…



Credits

- Horst Simon of LBNL
  - His many beautiful graphics are a result of his insightful perspectives
  - He puts his money where his mouth is: $2000 bet in 2012 that Exascale machine would not exist by end of decade
- Intel
  - Many datapoints flirting with NDA territory
- Top500.org
  - Data and tools
- Supporting cast:

Erich Strohmaier (LBNL)
Jack Dongarra (UTK)
Rob Leland (Sandia)
John Shalf (LBNL)
Scott Aronson (MIT)
Bob Lucas (USC-ISI)
John Kubiatowicz (UC Berkeley)
Dharmendra Modha and team(IBM)
Karlheinz Meier (Univ. Heidelberg)