Design of Parallel and High-Performance Computing

Fall 2015

Lecture: Introduction

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ETH

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Goals of this lecture

- Motivate you!
- What is parallel computing?
 - And why do we need it?
- What is high-performance computing?
 - What's a Supercomputer and why do we care?
- Basic overview of
 - Programming models
 - Some examples
 - Architectures
 - Some case-studies
- Provide context for coming lectures

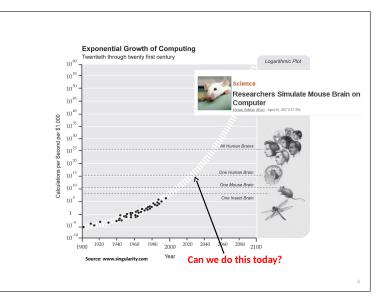
Let us assume ...

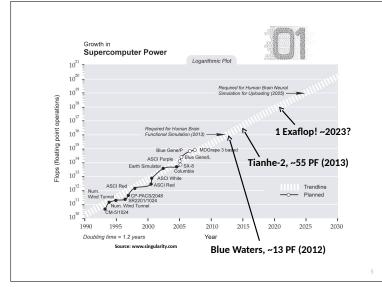
... you were to build a machine like this ...



... we know how each part works

- There are just many of them!
- Question: How many calculations per second are needed to emulate a brain?





Human Brain - No Problem!

... not so fast, we need to understand how to program those machines ...

Human Brain - No Problem!

Simulating 1 second of human brain activity takes 82,944 processors



Scooped!



Forschungszentrum Julich in Germany have managed to simulate a single second of human brain activity in a very, very powerful computer.

Source: extremetech.com

228 Q +1 in Share

Other problem areas: Scientific Computing

biological computing device that ever the fastest supercomputers in the world fail to emulate. Well, that's not

entirely true anymore. Researchers at the Okinawa Institute of Technology

Graduate University in Japan and

- Most natural sciences are simulation driven or are moving towards simulation
 - Theoretical physics (solving the Schrödinger equation, QCD)
 - Biology (Gene sequencing)

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- Chemistry (Material science)
- Astronomy (Colliding black holes)
- Medicine (Protein folding for drug discovery)
- Meteorology (Storm/Tornado prediction)
- Geology (Oil reservoir management, oil exploration)
- and many more ... (even Pringles uses HPC)



Other problem areas: Commercial Computing

- Databases, data mining, search
 - Amazon, Facebook, Google
- Transaction processing
 - Visa, Mastercard
- Decision support
 - Stock markets, Wall Street, Military applications
- Parallelism in high-end systems and back-ends
 - Often throughput-oriented
 - Used equipment varies from COTS (Google) to high-end redundant mainframes (banks)

Other problem areas: Industrial Computing

- Aeronautics (airflow, engine, structural mechanics, electromagnetism)
- Automotive (crash, combustion, airflow)
- Computer-aided design (CAD)
- Pharmaceuticals (molecular modeling, protein folding, drug design)
- Petroleum (Reservoir analysis)
- Visualization (all of the above, movies, 3d)

What can faster computers do for us?

- Solving bigger problems than we could solve before!
 - E.g., Gene sequencing and search, simulation of whole cells, mathematics of the brain, ...
 - The size of the problem grows with the machine power
 Weak Scaling
- Solve today's problems faster!
 - E.g., large (combinatorial) searches, mechanical simulations (aircrafts, cars, weapons, ...)
 - The machine power grows with constant problem size
 Strong Scaling

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High-Performance Computing (HPC)

- a.k.a. "Supercomputing"
- Question: define "Supercomputer"!

High-Performance Computing (HPC)

- a.k.a. "Supercomputing"
- Question: define "Supercomputer"!
 - "A supercomputer is a computer at the frontline of contemporary processing capacity--particularly speed of calculation." (Wikipedia)
 - Usually quite expensive (\$s and kWh) and big (space)
- HPC is a quickly growing niche market
 - Not all "supercomputers", wide base
 - Important enough for vendors to specialize
 - Very important in research settings (up to 40% of university spending)
 - "Goodyear Puts the Rubber to the Road with High Performance Computing"
 "High Performance Computing Helps Create New Treatment For Stroke Victims"
 - "Procter & Gamble: Supercomputers and the Secret Life of Coffee"
 - "Motorola: Driving the Cellular Revolution With the Help of High Performance Computing"
 - "Microsoft: Delivering High Performance Computing to the Masses"

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The Top500 List

- A benchmark, solve Ax=b
 - As fast as possible! _ as big as possible *
 - Reflects **some** applications, not all, not even many
 - Very good historic data!
- Speed comparison for computing centers, states, countries, nations, continents *
 - Politicized (sometimes good, sometimes bad)
 - Yet, fun to watch

RANK	SITE	SYSTEM	CORES	RMAX (TFLOP/S)	RPEAK (TFLOP/S)	POWER (KW)
1	National Super Computer Center in Guangzhou China	Tianhe-2 (MilkyWay-2) - TH-IVB-FEP Cluster, Intel Xeon ES-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
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	27,112.5	8,209
3	DOE/NNSA/LLNL United States	Sequoia - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,660
5	DOE/SC/Argonne National Laboratory United States	Mira - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786,432	8,586.6	10,066.3	3,945
6	Swiss National Supercomputing Centre (CSCS) Switzerland	Piz Daint - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Gray Inc.	115,984	6,271.0	7,788.9	2,325
7	King Abdullah University of Science and Technology Saudi Arabia	Shaheen II - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries interconnect Cray Inc.	196,608	5,537.0	7,235.2	2,834



March 19 2013

Swiss 'GPU Supercomputer' Will Be Fastest in Europe

Tiffany Trader

Page: 1|

The NVIDIA GPU Technology Conference is in full-swing today in San Jose, Calif. The annual event kicked off this morning with a keynote from NVIDIA CEO Jen-Hsun Huang, who revealed that the Swiss National Supercomputing Center (CSCS) is building Europe's fastest GPU-accelerated supercomputer, an extension of a Cray system that was announced last year.

As Cray Vice President, Storage & Data Management Barry Bolding told *HPCwire*, this will be the first Cray supercomputer equipped with Intel Xeon processors and NVIDA GPUs.

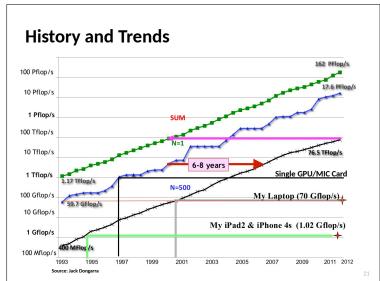


CSCS is part of ETH Zurich, one of the top universities in the world and the alma mater of Albert Einstein. The supercomputing center installed phase one of its shiny new Cray XC30 back in December 2012.



Blue Waters in 2012





High-Performance Computing grows quickly

- Computers are used to automate many tasks
- Still growing exponentially
 - New uses discovered continuously

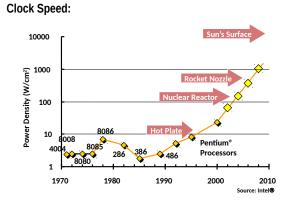
IDC, 2007: "The overall HPC server market grew by 15.5 percent in 2007 to reach \$11.6 billion [...] while the same kinds of boxes that go into HPC machinery but are used for general purpose computing, rose by only 3.6 percent to \$54.4"

IDC, 2009: "expects the HPC technical server market to grow at a healthy 7% to 8% yearly rate to reach revenues of \$13.4 billion by 2015."

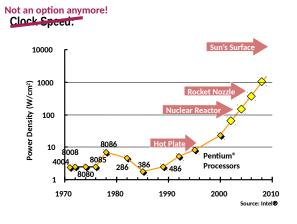
"The non-HPC portion of the server market was actually down 20.5 per cent, to \$34.6bn"

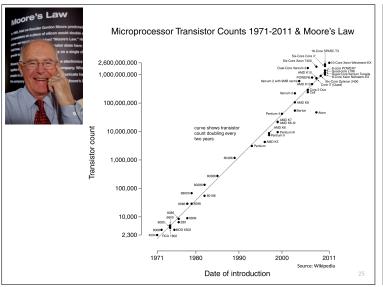


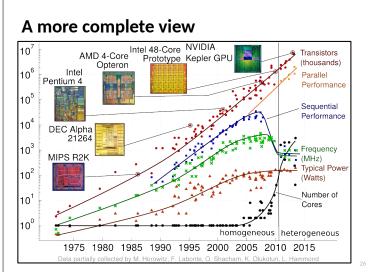
How to increase the compute power?



How to increase the compute power?







So how to invest the transistors?

- **Architectural innovations**
 - Branch prediction, Tomasulo logic/rename register, speculative execution,
 - Help only so much →
- What else?
 - Simplification is beneficial, less transistors per CPU, more CPUs, e.g., Cell B.E., GPUs, MIC
 - We call this "cores" these days
 - Also, more intelligent devices or higher bandwidths (e.g., DMA controller, intelligent NICs)







Towards the age of massive parallelism

- **Everything goes parallel**
 - Desktop computers get more cores 2,4,8, soon dozens, hundreds?
 - Supercomputers get more PEs (cores, nodes)
 - > 3 million today
 - > 50 million on the horizon
 - ▶1 billion in a couple of years (after 2020)
- Parallel Computing is inevitable!

Parallel vs. Concurrent computing Concurrent activities may be executed in parallel

A1 starts at T1, ends at T2: A2 starts at T3, ends at T4 Intervals (T1,T2) and (T3,T4) may overlap!

Parallel activities:

A1 is executed while A2 is running

Usually requires separate resources!

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 - Architectures

Some case-studies

Provide context for coming lectures

Granularity and Resources

Activities

- Micro-code instruction
- Machine-code instruction (complex or simple)
- instructions:

Blocks

Loops

Loop nests

Functions

Function sequences

Parallel Resource

- Instruction-level parallelism
- Pipelining
- VLIW
- Superscalar SIMD operations
- Vector operations
- Instruction sequences
 - Multiprocessors Multicores

Multithreading

Resources and Programming

Parallel Resource

- Instruction-level parallelism
 - Pipelining
 - VIIW
- Superscalar
- SIMD operations
- Vector operations
- Instruction sequences
 - Multiprocessors
 - Multicores
 - Multithreading

Programming

- - (inline assembly)
 - Hardware scheduling
- Compiler (inline assembly)
- Libraries
- Compilers (very limited)
- **Expert programmers**
 - Parallel languages
 - Parallel libraries

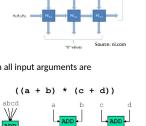
 - Hints

Historic Architecture Examples

- Systolic Array
 - Data-stream driven (data counters)
 - Multiple streams for parallelism
 - Specialized for applications (reconfigurable)



- No program counter, execute instructions when all input arguments are available
- Fine-grained, high overheads Example: compute f = (a+b) * (c+d)

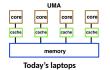


Von Neumann Architecture

Program counter H Inherently serial! Retrospectively define parallelism in instructions and data



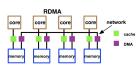
Parallel Architectures 101





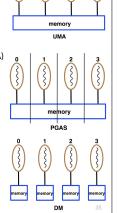
... and mixtures of those





Programming Models

- Shared Memory Programming (SM/UMA)
 - Shared address space
 - Implicit communication
 - Hardware for cache-coherent remote memory access
 - Cache-coherent Non Uniform Memory Access (cc NUMA)
- (Partitioned) Global Address Space (PGAS)
 - Remote Memory Access
 - Remote vs. local memory (cf. ncc-NUMA)
- Distributed Memory Programming (DM)
 - Explicit communication (typically messages)
 - Message Passing



Shared Memory Machines

Two historical architectures:

■ "Mainframe" – all-to-all connection between memory, I/O and PEs Often used if PE is the most expensive part Bandwidth scales with P

PE Cost scales with P, Question: what about network cost?



Shared Memory Machines

Two historical architectures:

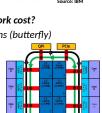
 "Mainframe" – all-to-all connection between memory, I/O and PEs

Often used if PE is the most expensive part Bandwidth scales with P

PE Cost scales with P, Question: what about network cost?

Answer: Cost can be cut with multistage connections (butterfly)

"Minicomputer" – bus-based connection
 All traditional SMP systems
 High latency, low bandwidth (cache is important)
 Tricky to achieve highest performance (contention)
 Low cost, extensible

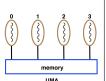


Shared Memory Machine Abstractions

- Any PE can access all memory
 - Any I/O can access all memory (maybe limited)
- OS (resource management) can run on any PE
 - Can run multiple threads in shared memory
 - Used since 40+ years

Communication through shared memory

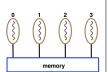
- Load/store commands to memory controller
- Communication is implicit
- Requires coordination
- Coordination through shared memory
 - Complex topic
 - Memory models



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Shared Memory Machine Programming

- Threads or processes
 - Communication through memory
- Synchronization through memory or OS objects
 - Lock/mutex (protect critical region)
 - Semaphore (generalization of mutex (binary sem.))
 - Barrier (synchronize a group of activities)
 - Atomic Operations (CAS, Fetch-and-add)
 - Transactional Memory (execute regions atomically)
- Practical Models:
 - Posix threads
 - MPI-3
 - OpenMP
 - Others: Java Threads, Qthreads, ...

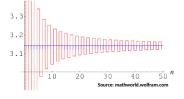


An SMM Example: Compute Pi

Using Gregory-Leibnitz Series:

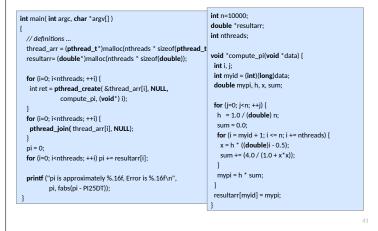
$$4\sum_{k=0}^{\infty} \frac{(-1)^k}{2k+1}$$

- Iterations of sum can be computed in parallel
- Needs to sum all contributions at the end



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Pthreads Compute Pi Example

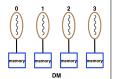


Additional comments on SMM

- OpenMP would allow to implement this example much simpler (but has other issues)
- Transparent shared memory has some issues in practice:
 - False sharing (e.g., resultarr[])
 - Race conditions (complex mutual exclusion protocols)
 - Little tool support (debuggers need some work)
- Achieving performance is harder than it seems!

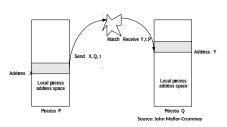
Distributed Memory Machine Programming

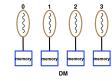
- Explicit communication between PEs
 - Message passing or channels
- Only local memory access, no direct access to remote memory
 - No shared resources (well, the network)



- Programming model: Message Passing (MPI, PVM)
 - Communication through messages or group operations (broadcast, reduce, etc.)
 - Synchronization through messages (sometimes unwanted side effect) or group operations (barrier)
 - Typically supports message matching and communication contexts

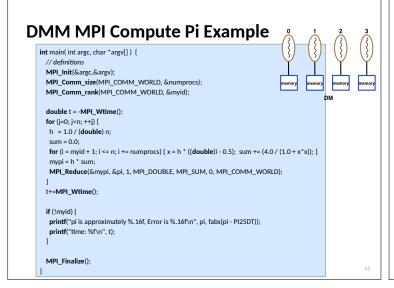
DMM Example: Message Passing





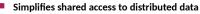
- Send specifies buffer to be transmitted
- Recv specifies buffer to receive into
- Implies copy operation between named PEs
- Optional tag matching
- Pair-wise synchronization (cf. happens before)

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DMM Example: PGAS

- Partitioned Global Address Space
 - Shared memory emulation for DMM Usually non-coherent
 - "Distributed Shared Memory"
 Usually coherent



- Has similar problems as SMM programming
- Sometimes lacks performance transparency
 Local vs. remote accesses
- Examples:
 - UPC, CAF, Titanium, X10, ...

0 1 2 3

How to Tame the Beast?

- How to program large machines?
- No single approach, PMs are not converging yet
 - MPI, PGAS, OpenMP, Hybrid (MPI+OpenMP, MPI+MPI, MPI+PGAS?), ...
- Architectures converge
 - General purpose nodes connected by general purpose or specialized networks
 - Small scale often uses commodity networks
 - Specialized networks become necessary at scale
- Even worse: accelerators (not covered in this class, yet)

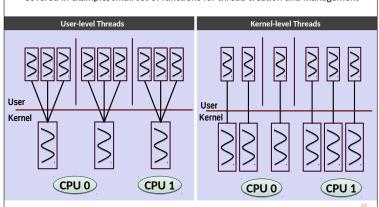


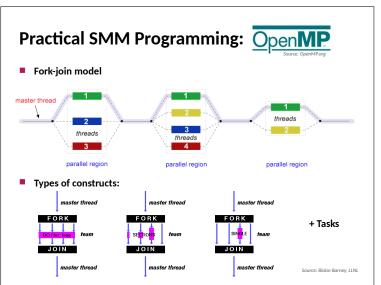


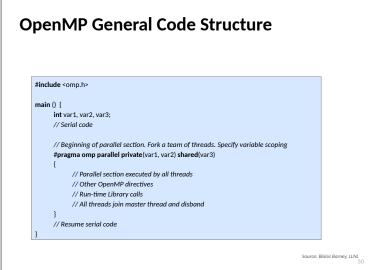


Practical SMM Programming: Pthreads

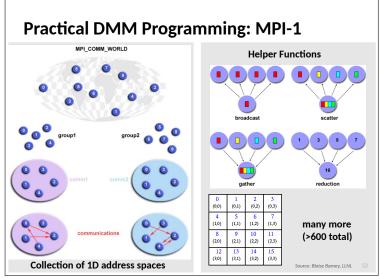
Covered in example, small set of functions for thread creation and management

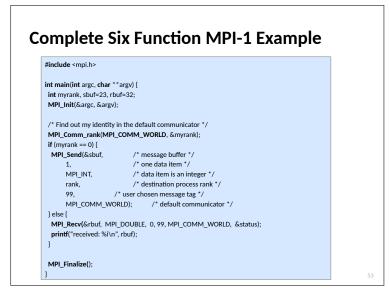


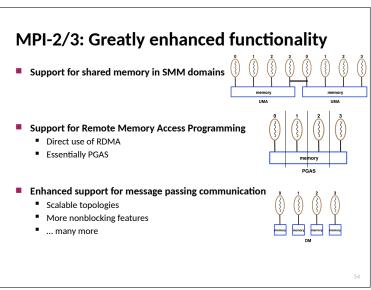




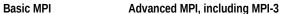
Practical PGAS Programming: UPC PGAS extension to the C99 language Thread 0 Thread 1 Thread 2 Thread 3 Shared c[0], c[4],... a c[1], c[5],... a c[2], c[6],... a c[3], c[7],... a c[3], c[7],.

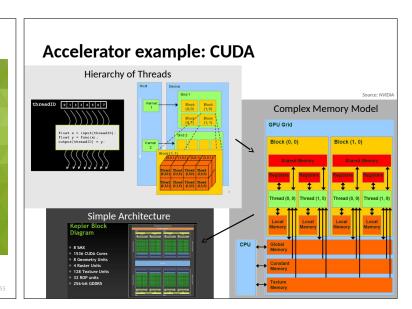


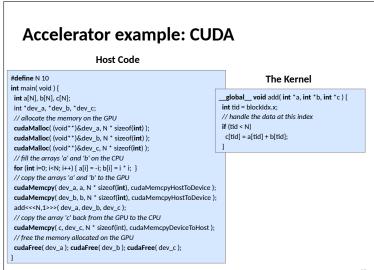


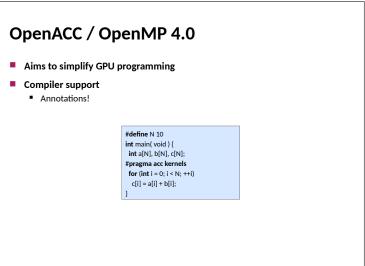












More programming models/frameworks

- Not covered:
 - SMM: Intel Cilk / Cilk Plus, Intel TBB, ...
 - Directives: OpenHMPP, PVM, ...
 - PGAS: Coarray Fortran (Fortran 2008), ...
 - HPCS: IBM X10, Fortress, Chapel, ...
 - Accelerator: OpenCL, C++AMP, ...
- This class will not describe any model in more detail!
 - There are too many and they will change quickly (only MPI made it >15 yrs)
- No consensus, but fundamental questions remain:
 - Data movement
 - Synchronization
 - Memory Models
 - Algorithmics
 - Foundations

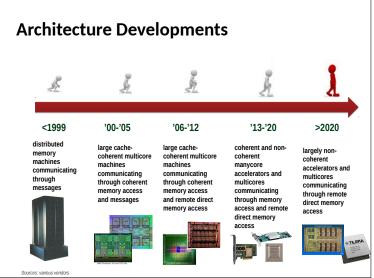
Goals of this lecture

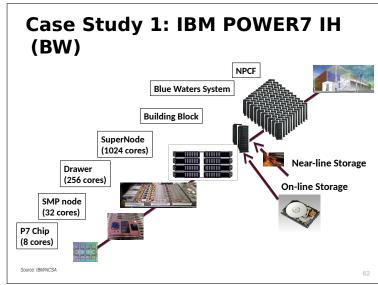
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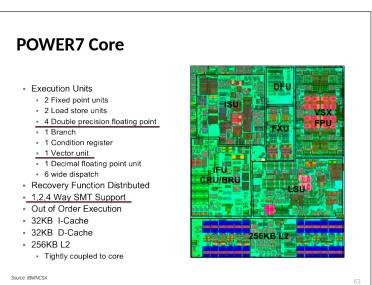
Some case-studies

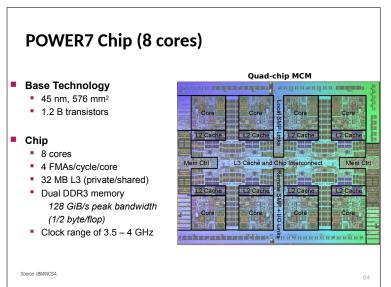
Provide context for coming lectures

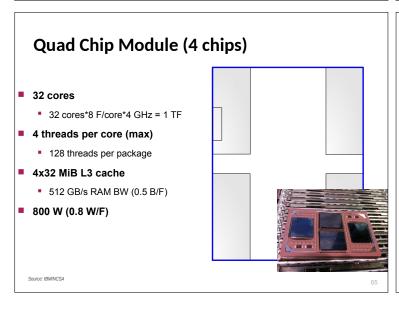
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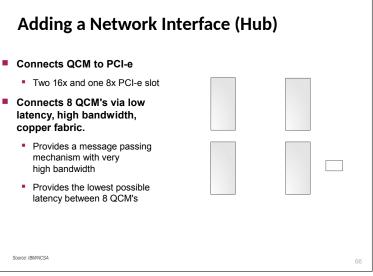










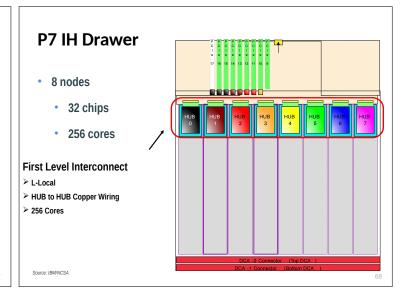


1.1 TB/s POWER7 IH HUB

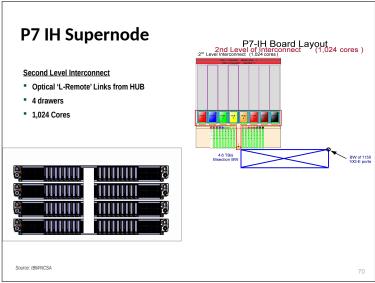
- 192 GB/s Host Connection
- 336 GB/s to 7 other local nodes
- 240 GB/s to local-remote nodes
- 320 GB/s to remote nodes
- 40 GB/s to general purpose I/O
- cf. "The PERCS interconnect" @Hotl'10

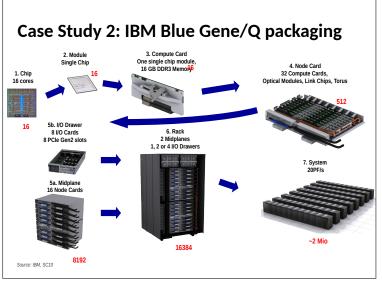


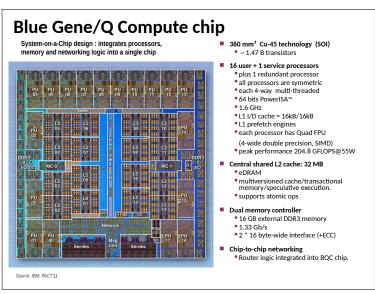
Source: IBM/NCSA 67









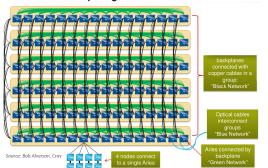


Blue Gene/Q Network

- On-chip external network
 - Message UnitTorus Switch
- Torus Switch
 Serdes
 Everything!
 Only 55-60 W per node
 Top of Green500 and GreenGraph500

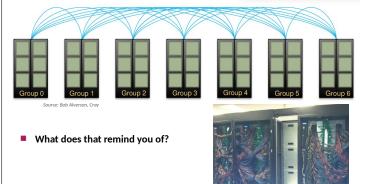
Case Study 3: Cray Cascade (XC30)

- Biggest current installation at CSCS!
 - >2k nodes
- Standard Intel x86 Sandy Bridge Server-class CPUs



Cray Cascade Network Topology

All-to-all connection among groups ("blue network")



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- What is parallel computing?
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- What is high-performance computing?

Provide context for coming lectures

- What's a Supercomputer and why do we care?
- Basic overview of
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DPHPC Lecture

- You will most likely not have access to the largest machines
 - But our desktop/laptop will be a "large machine" soon
 - HPC is often seen as "Formula 1" of computing (architecture experiments)
- DPHPC will teach you concepts!
 - Enable to understand and use all parallel architectures
 - From a quad-core mobile phone to the largest machine on the planet! MCAPI vs. MPI - same concepts, different syntax
 - No particular language (but you should pick/learn one for your project!) Parallelism is the future:



Related classes in the SE focus

263-2910-00L Program Analysis

http://www.srl.inf.ethz.ch/pa.php

Spring 2016

Lecturer: Prof. M. Vechev

263-2300-00L How to Write Fast Numerical Code

www.inf.ethz.ch/personal/markusp/teaching/263-2300-ETH-spring16 /course.html

Spring 2016

Lecturer: Prof. M. Pueschel

This list is not exhaustive!

