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T. HOEFLER, M. PUESCHEL

Lecture 1: Introduction

Teaching assistant: Salvatore Di Girolamo

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*
	- **EXARGLE 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?

Source: wikipedia

THE CONTRACTOR

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

By Ryan Whitwam on August 5, 2013 at 1:34 pm | 21 Comments

Share This Article

The brain is a deviously complex biological computing device that even 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

Forschungszentrum Jülich in Germany have managed to simulate a single second of human brain activity in a very, very powerful computer. Source: extremetech.com

Scooped!

Other problem areas: Scientific Computing

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

Quickly emerging areas for HPC/parallel computing technologies

- Big data processing
- **Deep learning**
- HPC was always at the forefront of specialization

Many cloud services require HPC/parallel computing

- Transaction processing/analysis
- Stock markets
- Making movies etc.

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**

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 MW) 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"*

The Top500 List

- **A benchmark, solve Ax=b**
	- As fast as possible! \rightarrow as big as possible \odot
	- 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

The Top500 List (June 2015)

Allen Allen and the

Piz Daint @ CSCS

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spcl.inf.ethz.ch

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More pictures at: http://spcl.inf.ethz.ch/Teaching/2015-dphpc/ 13

spcl.inf.ethz.ch @spcl_eth

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Blue Waters in 2009

Imagine you're designing a \$500 M supercomputer, and all you have is:

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This is why you need to understand performance expectations well!

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MALL

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Albert Williams States

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Blue Waters in 2012

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History and Trends

TANK CONTROL

EMSPEL

Moore's Law – The number of transistors on integrated circuit chips (1971-2016) Our World

in Data Moore's law describes the empirical regularity that the number of transistors on integrated circuits doubles approximately every two years. This advancement is important as other aspects of technological progress – such as processing speed or the price of electronic products – are strongly linked to Moore's law.

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Year of introduction

Source: Wikipedia

Data source: Wikipedia (https://en.wikipedia.org/wiki/Transistor_count) The data visualization is available at OurWorldinData.org. There you find more visualizations and research on this topic.

How to increase the compute power?

Computer Architecture vs. Physics (currently 0:1)

- **Physics (technological constraints)**
	- Cost of data movement
	- Capacity of DRAM cells
	- Clock frequencies (constrained by end of Dennard scaling)
	- Speed of Light
	- Melting point of silicon

- **Computer Architecture (design of the machine)**
	- Power management
	- ISA / Multithreading
	- **SIMD widths**
	- "Computer architecture, like other architecture, is the art of determining the needs of the user of a structure and then designing to meet those needs as effectively as possible within economic and technological constraints." *– Fred Brooks (IBM, 1962)*

Have converted many former "power" problems into "cost" problems

Activity factor (fraction of circuit that switches)

Charles Comments

Voltage

 $P_{dyn} = ACV^2F$

Capacitance (charged/discharged at each clock)

Frequency

Higher voltage is needed to drive higher frequency (due to fixed capacitance). Higher voltage also increases static power dissipation (leakage).

Low-Power Design Principles (2005)

- **Cubic power improvement with lower clock rate due to V²F**
- **Slower clock rates enable use of simpler cores**
- **Simpler cores use less area (lower leakage) and reduce cost**
- **Tailor design to application to REDUCE WASTE**

Low-Power Design Principles (2005)

- **Power5 (server)**
	- 120W@1900MHz
	- Baseline
- **Intel Core2 sc (laptop) :**
	- \blacksquare 15W@1000MHz
	- *4x more FLOPs/watt than baseline*

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- **Intel Atom (handhelds)**
	- 0.625W@800MHz
	- 80x more
- **GPU Core or XTensa/Embedded**
	- 0.09W@600MHz
	- 400x more *(80x-120x sustained)*

Even if each simple core is 1/4th as computationally efficient as complex core, you can fit hundreds of them on a single chip and still be 100x more power efficient.

Heterogeneous computing on the rise!

Big cores (very few) Tiny core

Latency Optimized Core (LOC)

Most energy efficient if you don't have lots of parallelism

Throughput Optimized Core (TOC)

Most energy efficient if you DO have a lot of parallelism!

Data movement – the wires

- **Energy Efficiency of copper wire:**
	- **Power = Frequency * Length / cross-section-area**

- Wire efficiency *does not improve* as feature size shrinks
- **Energy Efficienc**
	-
	- Capacitance $\sim = A$
	- **Transistor efficiency improves as you shrink it**
	- Power = V^2 * freq the bandwidth-distance limit Photonics could break through

 Net result is that moving data on wires is starting to cost more energy than computing on said data (interest in Silicon Photonics)

Pin Limits

Moore's law doesn't apply to adding pins to package

- 30%+ per year nominal Moore's Law
- Pins grow at $^{\sim}1.5$ -3% per year at best
- **4000 Pins is aggressive pin package**
	- Half of those would need to be for power and ground
	- **•** Of the remaining 2k pins, run as differential pairs
	- Beyond 15Gbps per pin power/complexity costs hurt!
	- \blacksquare 10Gpbs $*$ 1k pins is \sim 1.2TBytes/sec

2.5D Integration gets boost in pin density

- But it's a 1 time boost (how much headroom?)
- 4TB/sec? (maybe 8TB/s with single wire signaling?)

The future?

- **Open-source CPUs?**
	- **RISC-V**
- **Open-source accelerators?**
	- Talk to us if interested!
	- **EX Context of the European Processor Initiative** *Collaboration with L. Benini (ITET)*

Many open research topics

- How to program hardware?
- How to combine IPs into a system
- How to build real high-performance CPUs/systems/accelerators!

A more complete view

The state of the research and

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So how to invest the transistors?

- **Architectural innovations**
	- Branch prediction, out-of-order logic/rename register, speculative execution, ...
	- **Help only so much** \odot
- **What else?**
	- Simplification is beneficial, less transistors per CPU, more CPUs, e.g., Cell B.E., GPUs, MIC, Sunway SW26010
	- We call this "cores" these days
	- Also, more intelligent devices or higher bandwidths (e.g., DMA controller, intelligent NICs)

Source: IBM Source: NVIDIA Source: Intel

Towards the age of massive parallelism

Everything goes parallel

- Desktop computers get more cores
	- *2,4,8, soon dozens, hundreds?*
	- *My watch has four (weak) cores …*
- Supercomputers get more PEs (cores, nodes)
	- *> 10 million today*
	- *> 50 million on the horizon*
	- *1 billion in a couple of years (after 2030?)*
- **Parallel Computing is inevitable!**

Parallel vs. Concurrent computing Concurrent activities *may* be executed in parallel Example: 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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	- **E** Architectures

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Granularity and Resources

Execution Activities

- **Micro-code instruction**
- **Machine-code instruction** (complex or simple)
- Sequence of machine-code instructions:

Blocks

Loops

Loop nests

Functions

Function sequences

Parallel Resource

Report Advisory State

- **Instruction-level parallelism**
	- **Pipelining**
	- **ULIW/EDGE**
	- **Superscalar**
- SIMD operations
	- **Vector operations**
- **Instruction sequences**
	- **Multiprocessors**
	- **Multicores**
	- Multithreading

Programming

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

Historic Architecture Examples

- **Systolic Array**
	- Data-stream driven (data counters)
	- **Multiple streams for parallelism**
	- **Specialized for applications (reconfigurable)**
- **Dataflow Architectures**
	- No program counter, execute instructions when all input arguments are available
	- Fine-grained, high overheads *Example: compute f = (a+b) * (c+d)*
- Both come-back in FPGA computing and EDGE architectures
	- **Interesting research opportunities!** *Talk to us if you're interested (i.e., how to program FPGAs easily and fast)*

Von Neumann Architecture (default today)

Program counter \rightarrow **inherently sequential!**

Retrospectively define parallelism in instructions and data

Parallel Architectures 101 – Multiple Instruction Streams

Today's laptops Today's servers

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… and mixtures of those

Parallel Programming Models 101

- **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)
	- **Nessage 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?*

Answer: P 2 , 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**

UMA

(ETH students): Most of what we covered in Parallel Programming in the 2nd semester! ⁴¹
Shared Memory Machine Programming

- **Threads or processes**
	- **E** 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 (ugs, will see later)**
	- $MPI-3$
	- **DenMP**
	- Others: Java Threads, Qthreads, ...

An SMM Example: Compute Pi

Using Gregory-Leibnitz Series:

In Iterations of sum can be computed in parallel

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Needs to sum all contributions at the end

Pthreads Compute Pi Example

```
int n=10000;
double *resultarr;
pthread t *thread arr;
int nthreads;
void *compute_pi(void *data) {
 int i, j; 
 int myid = (int)(long)data;
 double mypi, h, x, sum; 
 for (j=0; j<n; ++j) { 
   h = 1.0 / (double) n;sum = 0.0;
   for (i = myid + 1; i \leq n; i += nthreads) {
     x = h * ((double)i - 0.5);sum += (4.0 / (1.0 + x*x));} 
   mypi = h * sum;} 
 resultarr[myid] = mypi;}
```

```
int main( int argc, char *argv[] ) 
   // definitions …
   thread_arr = (pthread_t*)malloc(nthreads *sizeof(pthread t));
    resultarr= ( double*)malloc(nthreads * 
                sizeof(double));
   for (i=0; i<nthreads; ++i) {
      int ret = pthread_create( &thread_arr[i], 
                    NULL, compute pi, (void*) i);
    }
   for (i=0; i{th}reads; +i) {
      pthread join( thread arr[i], NULL);
    }
   pi = 0;
   for (i=0; i<nthreads; ++i) pi += resultarr[i];
    printf ("pi is \sim%.16f, Error is %.16f\n",
                  pi, fabs(pi - PI25DT)); 
 }
```
{

TANK COMMENTARY

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)
	- **EXTEND Little tool support (debuggers need some work)**
	- These issues were predominantly discussed in parallel programming in the 2nd semester *We will briefly repeat some but not all!*
- *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)**
	- 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

DM

- 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)**

DMM MPI Compute Pi Example

```
int main( int argc, char *argv[] ) { 
  // definitions
  MPI_Init(&argc,&argv); 
  MPI_Comm_size(MPI_COMM_WORLD, &numprocs); 
  MPI_Comm_rank(MPI_COMM_WORLD, &myid);
```


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```
double t = -MPI Wtime();
for (j=0; j<n; ++j) {
 h = 1.0 / (double) n;sum = 0.0; 
 for (i = myid + 1; i <= n; i += numprocs) { x = h * ((double)i - 0.5); sum += (4.0 / (1.0 + x * x)); }
 mypi = h * sum;
 MPI_Reduce(&mypi, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD); 
} 
t+=MPI_Wtime();
if (!myid) \{printf("pi is approximately %.16f, Error is %.16f\n", pi, fabs(pi - PI25DT)); 
 printf("time: %f\n", t);
}
```

```
MPI Finalize();
```
}

DMM Example: PGAS

- **Partitioned Global Address Space**
	- **Shared memory emulation for DMM** *Usually non-coherent*
	- "Distributed Shared Memory" *Usually coherent*
- **Simplifies shared access to distributed data**
	- Has similar problems as SMM programming
	- Sometimes lacks performance transparency *Local vs. remote accesses*
- **Examples:**
	- UPC, CAF, Titanium, X10, …

- **Interesting research question: how to exploit PGAS/RDMA in practice?**
	- Cf. VLDB'17, Barthels et al.: "Distributed Join Algorithms on Thousands of Cores"

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?, generally MPI+X), ...
- **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)**

Example: Shared Memory Programming with OpenMP

Fork-join model

Example: Shared Memory Programming with OpenMP

Annotate sequential code with pragmas (introduce semantic duplication)

```
#include <omp.h>
main () {
      int var1, var2, var3;
      // Serial code 
      // Beginning of parallel section. Fork a team of threads. Specify variable scoping 
      #pragma omp parallel private(var1, var2) shared(var3)
       {
             // Parallel section executed by all threads 
             // Other OpenMP directives
             // Run-time Library calls
             // All threads join master thread and disband 
       } 
      // Resume serial code 
}
```


Example: Practical PGAS Programming with UPC

PGAS extension to the C99 language

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- **E** Many helper library functions
	- Collective and remote allocation
	- Collective operations
- **E** Complex consistency model

Example: Practical Distributed Memory Programming: MPI-1

TANK CONTROL

Source: Blaise Barney, LLNL

Example: Practical Distributed Memory Programming: MPI-1 – Six Functions!

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```
#include <mpi.h>
int main(int argc, char **argv) {
int myrank, sbuf=23, rbuf=32;
MPI_Init(&argc, &argv);
/* Find out my identity in the default communicator */
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank == 0) {
 MPI_Send(&sbuf, \frac{1}{2} /* message buffer */
      1, /* one data item */
      MPI_INT, / data item is an integer */rank, \frac{1}{2} and \frac{1}{2} are \frac{1}{2} destination process rank \frac{1}{2}99, /* user chosen message tag */
      MPI_COMM_WORLD); /* default communicator */
} else {
 MPI_Recv(&rbuf, MPI_DOUBLE, 0, 99, MPI_COMM_WORLD, &status);
 printf("received: %i\n", rbuf);
 }
```
MPI_Finalize();

}

Example: MPI-2/3 supporting Shared Memory and PGAS-style!

Support for shared memory in SMM domains

- **Support for Remote Memory Access Programming**
	- **Direct use of RDMA**
	- **Essentially PGAS**
- **Enhanced support for message passing communication**
	- **Scalable topologies**
	- **Nore nonblocking features**
	- ... many more

MPI: de-facto large-scale prog. standard

Note that the Sea

SCIENTIFIC

Basic MPI Advanced MPI, including MPI-3

Example: Accelerator programming with CUDA

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Example: Accelerator programming with CUDA

Host Code

The Kernel

```
\Boxglobal\Box void add( int *a, int *b, int *c) {
int tid = blockIdx.x;
// handle the data at this index
if (tid < N)
 c[tid] = a[tid] + b[tid];}
```


Example: OpenACC / OpenMP 4.0

- **Aims to simplify GPU programming**
- **E** Compiler support
	- Annotations! More pragmas and semantic duplication

Many many 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 (I/O complexity)
	- Synchronization (avoiding races, deadlock etc.)
	- Memory Models (read/write ordering)
	- Algorithmics (parallel design/thinking)
	- Foundations (conflict minimization, models, static vs. dynamic scheduling etc.)

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	- **EXP** Architectures

Some case-studies

Provide context for coming lectures

Architecture Developments

memory machines communicating through messages

large cachecoherent multicore machines communicating through coherent memory access and messages

machines communicating through coherent memory access and remote direct memory access

coherent and noncoherent manycore accelerators and multicores communicating through memory access and remote direct memory access

largely noncoherent

accelerators and multicores communicating through remote direct memory access

Sources: various vendors

Case Study 1: Cray Cascade (XC30) – Piz Daint!

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

Contract of Contract Only 1975

Case Study 1: Cray Cascade Network Topology

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

Source: Bob Alverson, Cray

- **Interesting research opportunities!**
- **Topology design?**
	- E.g., Besta, TH: Slim Fly: A Cost Effective Low-Diameter Network Topology
- **Interference analysis (can we provide isolation)?**
- **How to route low-diameter topologies?**

Case Study 2: IBM POWER7 IH (BW)

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POWER7 Core

- **Execution Units**
	- 2 Fixed point units
	- 2 Load store units
	- 4 Double precision floating point
	- 1 Branch
	- 1 Condition register
	- 1 Vector unit
	- 1 Decimal floating point unit
	- 6 wide dispatch
- Recovery Function Distributed
- 1,2,4 Way SMT Support
- Out of Order Execution
- 32KB I-Cache
- 32KB D-Cache
- $-256KBL2$
	- Tightly coupled to core

POWER7 Chip (8 cores)

Base Technology

- \blacksquare 45 nm, 576 mm²
- 1.2 B transistors

Chip

- 8 cores
- 4 FMAs/cycle/core
- 32 MB L3 (private/shared)
- Dual DDR3 memory *128 GiB/s peak bandwidth (1/2 byte/flop)*
- Clock range of $3.5 4$ GHz

Quad-chip MCM

Quad Chip Module (4 chips)

- **32 cores**
	- $\overline{}$ 32 cores*8 F/core*4 GHz = 1 TF
- **4 threads per core (max)**
	- 128 threads per package
- **4x32 MiB L3 cache**
	- 512 GB/s RAM BW (0.5 B/F)
- **800 W (0.8 W/F)**

PARTIES

Adding a Network Interface (Hub)

- - Two 16x and one 8x PCI-e slot
- Connects 8 QCM's via low latency, high bandwidth, copper fabric.
	- **Provides a message passing** mechanism with very high bandwidth
	- **Provides the lowest possible** latency between 8 QCM's

1.1 TB/s POWER7 IH HUB

P7 IH Drawer

- 8 nodes
	- 32 chips
	- 256 cores

First Level Interconnect

L-Local

≻HUB to HUB Copper Wiring

256 Cores

POWER7 IH Drawer @ SC09

aller alle cheese to use

CONTRACTOR

P7 IH Supernode

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Some case-studies

Provide context for coming lectures

DPHPC Lecture

- **You will likely not have access to the largest machines (unless you specialize to HPC)**
	- 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 2017 Lecturer: Prof. M. Vechev**
- **263-2300-00L How to Write Fast Numerical Code <http://www.inf.ethz.ch/personal/markusp/teaching/263-2300-ETH-spring16/course.html> Spring 2017 Lecturer: Prof. M. Pueschel**
- **This list is not exhaustive!**

DPHPC Overview

SEATER CONTINUES OF