

Presentation to the: Virtual School for Computational Science and Engineering

Scaling to Petascale: Concepts & Beyond Scaling to the Present and Future

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Topics

- HPC Applications
- Petaflops Systems
- Enabling Technologies and Trends
- HPC Architectures
- Scaling Factors
- Sources of Performance Degradation
- Parallel Programming Models Condor
- Parallel Programming Models MPI
- Parallel Programming Models OpenMP
- Scaling to a Thousand Petaflops





Aerial & Satellite of Hurricane Katrina







Example of Global Climate Model Simulation Precipitable Water (gray scale) and Precipitation Rate (orange)

October 1 Hour 00

Animation courtesy of NCAR SCD Visualization and Enabling Technologies Section



The U.S. is an official partner in ITER





International Thermonuclear Experimental Reactor

- European Union
- Japan
- United States
- Russia
- Korea
- China
- 500 MW fusion output
- Cost: \$5-10 B
- To begin operation in 2015



Molecular Dynamics





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Road Runner



- First supercomputer to reach sustained 1 PFLOPS performance and current #1 on TOP500
- First hybrid supercomputer (Cell+Opteron)
- System information:
 - 296 racks on 5,200 sq.ft. footprint
 - 18 connected units with 180 nodes each
 - 1.46 PFLOPS peak, 1.1 PFLOPS R_{max}
 - 6,480 AMD Opteron processors
 - 12,960 IBM PowerXCell 8i processors
 - 101 TB memory
 - 216 System x3755 I/O nodes
 - 26 288-port ISR2012 Infiniband 4x DDR switches
 - 2.5 MW power consumption
- Tri-blade compute node:
 - Two QS22 blades (Cell) and one LS21 blade (Opteron)
 - Cell blades host four 3.2 GHz processors with aggregate peak of 435.2 DP GFLOPS
 - Opteron blade contains 2 dual-core 1.8 GHz Opterons 2210 delivering peak of 14.4 GFLOPS
 - Every Opteron core and Cell processor uses 4 GB memory (32 GB per node)















- Second sustained PFLOPS machine (#2 on TOP500)
- System overview
 - Cray XT4 and XT5 nodes over shared network (SION)
 - 284 cabinets in 5,800 sq.ft. floorspace
 - 1.38 PFLOPS peak, 1.06 PFLOPS R_{max} (XT5 only)
 - 26,604 compute nodes with over 181,000 cores
 - 362 TB memory
 - Cray Seastar2+ interconnect configured as 3-D torus
 - 374 TB/s interconnect bandwidth (XT5)
 - 10 PB of RAID6 storage with 240+44 GB/s bandwidth respectively from 214 XT5 and 116 XT4 I/O nodes
 - Power: 6.95 MW, liquid cooling (XT5)
- XT5 node specifications
 - Two quad-core 2356 Barcelona Opterons at 2.3 GHz
 - Peak performance of 73.6 GFLOPS
 - 16GB ECC DDR2-800 SDRAM
 - 6 port Seastar2+ ASIC, 9.6 GB/s per port











FZJ JUGENE (IBM BG/P)



- Most powerful BG/P system (#3 in TOP500)
- System information:
 - 72 racks with 130 m² footprint
 - 73,728 compute nodes with 294,912 processors
 - 1.0 PFLOPS peak, 825.5 TFLOPS R_{max}
 - 144 TB memory
 - Multiple interconnects: 3-D torus, scalable collective network and fast barrier network
 - 600 I/O nodes
 - 1 PB of storage at 16 GB/s
 - Power: 2.5 MW (35 kW per rack)
- Node specification:
 - 4 PowerPC 450 cores at 850 MHz
 - Dual DP FPUs per core
 - 2 GB memory
 - 32-bit mode operation





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Where Does Performance Come From?

- Device Technology
 - Logic switching speed and device density
 - Memory capacity and access time
 - Communications bandwidth and latency
- Computer Architecture
 - Instruction issue rate
 - Execution pipelining
 - Reservation stations
 - Branch prediction
 - Cache management
 - Parallelism
 - Operations per cycle per processor
 - Instruction level parallelism (ILP)
 - Vector processing
 - Processors per node
 - Number of nodes in a system





Moore's Law









Microprocessor Clock Speed







The SIA ITRS Roadmap





The Memory Wall





THE WALL



Microprocessors no longer realize the full potential of VLSI technology







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The Evolution of HPC







Top 500 List









Top 500: System Architecture



TSUBAME – A Cluster

| Rank | Site | Computer |
|------|---|--|
| 1 | DOE/NNSA/LLNL United States | BlueGene/L - eServer Blue Gene Solution IBM |
| 2 | Forschungszentrum Juelich (FZJ) Germany | JUGENE - Blue Gene/P Solution IBM |
| 3 | SGI/New Mexico Computing Applications Center (NMCAC) United States | SGI Altix ICE 8200, Xeon quad core 3.0 GHz SGI |
| 4 | Computational Research Laboratories, TATA SONS India | EKA - Cluster Platform 3000 BL460c, Xeon 53xx 3GHz, Infiniband Hewlett-Packard |
| 5 | Government Agency Sweden | Cluster Platform 3000 BL460c, Xeon 53xx 2.66GHz, Infiniband Hewlett-Packard |
| 6 | NNSA/Sandia National Laboratories United States | Red Storm - Sandia/ Cray Red Storm, Opteron 2.4 GHz dual core Cray Inc. |
| 7 | Oak Ridge National Laboratory United States | Jaguar - Cray XT4/XT3 Cray Inc. |
| 8 | IBM Thomas J. Watson Research Center United States | BGW - eServer Blue Gene Solution IBM |
| 9 | NERSC/LBNL United States | Franklin - Cray XT4, 2.6 GHz Cray Inc. |
| 10 | Stony Brook/BNL, New York Center for Computational Sciences United States | New York Blue - eServer Blue Gene Solution IBM |





SMP Node Diagram





Comparison of Opteron and Xeon SMP Systems





Source: http://www.devx.com/amd/Article/17437





Multi-Core

- Motivation for Multi-Core
 - Exploits improved feature-size and density
 - Increases functional units per chip (spatial efficiency)
 - Limits energy consumption per operation
 - Constrains growth in processor complexity
- Challenges resulting from multi-core
 - Relies on effective exploitation of multiple-thread parallelism
 - Need for parallel computing model and parallel programming model
 - Aggravates memory wall
 - Memory bandwidth
 - Way to get data out of memory banks
 - Way to get data into multi-core processor array
 - Memory latency
 - Fragments (shared) L3 cache
 - Pins become strangle point
 - Rate of pin growth projected to slow and flatten
 - Rate of bandwidth per pin (pair) projected to grow slowly
 - Requires mechanisms for efficient inter-processor coordination
 - Synchronization
 - Mutual exclusion
 - Context switching









Dual-Core Processor Design



BLC DD 1.0

IRN







Heterogeneous Multicore Architecture

- Combines different types of processors
 - Each optimized for a different operational modality
 - Performance > *N*x better than other *N* processor types
 - Synthesis favors superior performance
 - · For complex computation exhibiting distinct modalities
- Conventional co-processors
 - Graphical processing units (GPU)
 - Network controllers (NIC)
 - Efforts underway to apply existing special purpose components to general applications
- Purpose-designed accelerators
 - Integrated to significantly speedup some critical aspect of one or more important classes of computation
 - IBM Cell architecture
 - ClearSpeed SIMD attached array processor







Data Center Total Concurrency





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Courtesy of Peter Kogge, UND

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Key Terms and Concepts



 <u>Scalable Speedup</u>: Relative reduction of execution time of a fixed size workload through parallel execution

 $Speedup = \frac{execution_time_on_one_processor}{execution_time_on_N_processors}$

<u>Scalable Efficiency</u>: Ratio of the actual performance to the best possible performance.

 $Efficiency = \frac{execution_time_on_one_processor}{(execution_time_on_multiple_processors \times number_of_processors)}$







Strong Scaling, Weak Scaling



- Capability
 - Primary scaling is decrease in response time proportional to increase in resources applied
 - Single job, constant size scaling proportional to machine size
- Cooperative
 - Single job, (different nodes working on different partitions of the same job)
 - Job size scales proportional to machine
 - Granularity per node is fixed
- Capacity
 - Primary scaling is increase in throughput proportional to increase in resources applied
 - Decoupled concurrent tasks, increasing in number of instances scaling proportional to machine.





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- Interlude: the System "hour-glass" Stack
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Sources of Performance Degradation





- <u>Starvation</u>
 - Not enough work to do due to insufficient parallelism or poor load balancing among distributed resources
- <u>Latency</u>
 - Waiting for access to memory or other parts of the system
- <u>Overhead</u>
 - Extra work that has to be done to manage program concurrency and parallel resources the real work you want to perform
- Waiting for Contention
 - Delays due to fighting over what task gets to use a shared resource next. Network bandwidth is a major constraint.





Ideal Speedup Example





Amdahl's Law





Overhead





<u>Assumption</u>: Workload is infinitely divisible

T = v + w





Amdahl's Law with Overhead



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Cache Performance



$$\begin{split} T &= I_{count} \times CPI \times T_{cycle} \\ I_{count} &= I_{ALU} + I_{MEM} \\ CPI &= \left(\frac{I_{ALU}}{I_{count}}\right) \times CPI_{ALU} + \left(\frac{I_{MEM}}{I_{count}}\right) \times CPI_{MEM} \end{split}$$

T = total execution time $T_{\text{cycle}} = \text{time for a single processor cycle}$ $I_{\text{count}} = \text{total number of instructions}$ $I_{\text{ALU}} = \text{number of ALU instructions (e.g. register - register)}$ $I_{\text{MEM}} = \text{number of memory access instructions (e.g. load, store)}$ CPI = average cycles per instructions $CPI_{\text{ALU}} = \text{average cycles per ALU instructions}$

 $\begin{array}{l} \mathsf{CPI}_{\mathsf{MEM}} = \operatorname{average} \ \mathsf{cycles} \ \mathsf{per} \ \mathsf{memory} \ \mathsf{instruction} \\ \mathsf{r}_{\mathsf{miss}} = \mathsf{cache} \ \mathsf{miss} \ \mathsf{rate} \\ \mathsf{r}_{\mathsf{hit}} = \mathsf{cache} \ \mathsf{hit} \ \mathsf{rate} \\ \mathsf{CPI}_{\mathsf{MEM-MISS}} = \mathsf{cycles} \ \mathsf{per} \ \mathsf{cache} \ \mathsf{miss} \\ \mathsf{CPI}_{\mathsf{MEM-HIT}} = \mathsf{cycles} \ \mathsf{per} \ \mathsf{cache} \ \mathsf{hit} \\ \mathsf{M}_{\mathsf{ALU}} = \ \mathsf{instruction} \ \mathsf{mix} \ \mathsf{for} \ \mathsf{ALU} \ \mathsf{instructions} \\ \mathsf{M}_{\mathsf{MEM}} = \ \mathsf{instruction} \ \mathsf{mix} \ \mathsf{for} \ \mathsf{memory} \ \mathsf{access} \ \mathsf{instruction} \end{array}$



Cache Performance



$$\begin{split} CPI_{MEM} &= CPI_{MEM-HIT} + r_{MISS} \times CPI_{MEM-MISS} \\ T &= I_{count} \times \left[\left(M_{ALU} \times CPI_{ALU} \right) + \left(M_{MEM} \times \left(CPI_{MEM-HIT} + r_{MISS} \times CPI_{MEM-MISS} \right) \right) \right] \times T_{cycle} \end{split}$$

T = total execution time $T_{cycle} = \text{time for a single processor cycle}$ $I_{count} = \text{total number of instructions}$ $I_{ALU} = \text{number of ALU instructions (e.g. register - register)}$ $I_{MEM} = \text{number of memory access instructions (e.g. load, store)}$ CPI = average cycles per instructions $CPI_{ALU} = \text{average cycles per ALU instructions}$

 $\begin{aligned} \text{CPI}_{\text{MEM}} &= \text{average cycles per memory instruction} \\ r_{\text{miss}} &= \text{cache miss rate} \\ r_{\text{hit}} &= \text{cache hit rate} \\ \text{CPI}_{\text{MEM-MISS}} &= \text{cycles per cache miss} \\ \text{CPI}_{\text{MEM-HIT}} &= \text{cycles per cache hit} \\ \text{M}_{\text{ALU}} &= \text{instruction mix for ALU instructions} \\ \text{M}_{\text{MEM}} &= \text{instruction mix for memory access instruction} \end{aligned}$



Cache Performance: Example



$$\begin{split} r_{hitA} &= 0.9 & r_{hitB} = 0.5 \\ CPI_{MEM-A} &= CPI_{MEM-HIT} + r_{MISS-A} \times CPI_{MEM-MISS} & CPI_{MEM-B} = CPI_{MEM-HIT} + r_{MISS-B} \times CPI_{MEM-MISS} \\ &= 1 + (1 - 0.9) \times 100 = 11 & = 1 + (1 - 0.5) \times 100 = 51 \\ T_A &= 10^{11} \times ((0.8 \times 1) + (0.2 \times 11)) \times 5 \times 10^{-10} & T_B &= 10^{11} \times ((0.8 \times 1) + (0.2 \times 51)) \times 5 \times 10^{-10} \\ &= 150 \sec & = 550 \sec \end{split}$$





Performance: Locality



- *Temporal Locality* is a property that if a program accesses a memory location, there is a much higher than random probability that the same location would be accessed again.
- Spatial Locality is a property that if a program accesses a memory location, there is a much higher than random probability that the nearby locations would be accessed soon.
- Spatial locality is usually easier to achieve than temporal locality
- A couple of key factors affect the relationship between locality and scheduling :
 - Size of dataset being processed by each processor
 - How much reuse is present in the code processing a chunk of iterations.



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Management Middleware: Condor



Condor MatchMaker

- MatchMaker, a crucial part of the Condor architecture, uses the job description classAd provided by the user and matches the Job to the best resource based on the Machine description classAd
- MatchMaking in Condor is performed in 4 steps :
 - 1. Job Agent (A) and resources (R) advertise themselves.
 - 2. Matchmaker (**M**) processes the known classAds and generates pairs that best match resources and jobs
 - 3. Matchmaker informs each party of the job-resource pair of their prospective match.
 - 4. The Job agent and resource establish connection for further processing. (Matchmaker plays no role in this step, thus ensuring separation between selection of resources and subsequent activities)





Src : Douglas Thain, Todd Tannenbaum, and Miron Livny, "Distributed Computing in Practice: The Condor Experience" *Concurrency and Computation: Practice and Experience*, Vol. 17, No. 2-4, pages 323-356, February-April, 2005. http://www.cs.wisc.edu/condor/doc/condor-practice.pdf



Management Middleware: Condor



Condor Problem Solvers

- **Master-Worker (MW)** is a problem solving system that is useful for solving a coarse grained problem of indeterminate size such as parameter sweep etc.
- The MW Solver in Condor consists of 3 main components : work-list, a tracking module, and a steering module. The work-list keeps track of all pending work that master needs done. The tracking module monitors progress of work currently in progress on the worker nodes. The steering module directs computation based on results gathered and the pending work-list and communicates with the matchmaker to obtain additional worker processes.
- **DAGMan** is used to execute multiple jobs that have dependencies represented as a Directed Acyclic Graph where the nodes correspond to the jobs and edges correspond to the dependencies between the jobs. DAGMan provides various functionalities for job monitori and fault tolerance via creation of rescue DAGs.









condor_status : provides current pool status condor_q : provides current job queue condor_submit : submit a job to condor pool condor_rm : delete a job from job queue



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Basic MPI Calls



- In review, the 6 main MPI calls:
 - MPI_Init
 - MPI_Finalize
 - MPI_Comm_size
 - MPI_Comm_rank
 - MPI_Send
 - MPI_Recv
- Include MPI Header file
 - #include "mpi.h"
- Basic MPI Datatypes
 - MPI_INT, MPI_FLOAT,





Example : communicators







Example : Communicator & Rank

• Compiling :

mpicc -o hello2 hello2.c

• Result :

| Hello, | World! | from | 4 | of | 8 |
|--------|--------|------|---|----|---|
| Hello, | World! | from | 3 | of | 8 |
| Hello, | World! | from | 1 | of | 8 |
| Hello, | World! | from | 0 | of | 8 |
| Hello, | World! | from | 5 | of | 8 |
| Hello, | World! | from | 6 | of | 8 |
| Hello, | World! | from | 7 | of | 8 |
| | | - | | _ | |



MPI : Point to Point Communication primitives



- The basic communication mechanism of MPI between a pair of processes in which one process is sending data and the other process receiving the data, is called "*point to point communication*"
- Message passing in MPI program is carried out by 2 main MPI functions
 - MPI_Send sends message to a designated process
 - MPI_Recv receives a message from a process
- Each of the send and recv calls is appended with information to the data that needs to be exchanged between application programs
- The message envelope consists of the following information
 - The rank of the receiver
 - The rank of the sender
 - A tag
 - A communicator
- The source argument is used to distinguish messages received from different processes
- Tag is user-specified *int* that can be used to distinguish messages from a single process



Collective Calls



- A communication pattern that encompasses all processes within a communicator is known as collective communication
- MPI has several collective communication calls, the most frequently used are:
 - Synchronization
 - Barrier
 - Communication
 - Broadcast
 - Gather & Scatter
 - All Gather
 - Reduction
 - Reduce
 - AllReduce



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OpenMP: Basic Constructs



OpenMP Execution Model (FORK/JOIN): Sequential Part (master thread)

Parallel Region (FORK : group of threads)

Sequential Part (JOIN: master thread)

Parallel Region (FORK: group of threads)

Sequential Part (JOIN : master thread)

To invoke library routines in C/C++ add #include <omp.h>

near the top of your code





C / C++ :

#pragma omp parallel {
 parallel block
} /* omp end parallel */



OpenMP for directive

- *for* directive helps share iterations of a loop between a group of threads
- If *nowait* is specified then the threads do not wait for synchronization at the end of a parallel loop
- The *schedule* clause describes how iterations of a loop are divided among the threads in the team (discussed in detail in the next few slides)







OpenMP sections directive

- *sections* directive is a non iterative work sharing construct.
- Independent section of code are nested within a sections directive
- It specifies enclosed *section* of codes between different threads
- Code enclosed within a *section* directive is executed by a thread within the pool of threads

```
#pragma omp parallel private(p)
{
#pragma omp sections
{{ a=...;
    b=...;}
#pragma omp section
{ p=...;
    q=...;}
#pragma omp section
{ x=...;
    y=...;}
} /* omp end sections */
} /* omp end parallel */
```





OpenMP *critical* directive: Explicit Synchronization



- Race conditions can be avoided by controlling access to shared variables by allowing threads to have exclusive access to the variables
- Exclusive access to shared variables allows the thread to *atomically* perform read, modify and update operations on the variable.
- Mutual exclusion synchronization is provided by the critical directive of OpenMP
- Code block within the *critical region* defined by critical /end critical directives can be executed only by one thread at a time.
- Other threads in the group must wait until the current thread exits the critical region. Thus only one thread can manipulate values in the critical region.





OpenMP: Reduction



- performs reduction on *shared variables* in list based on the operator provided.
- for C/C++ operator can be any one of :
 - +, *, -, ^, |, ||, & or &&
 - At the end of a reduction, the shared variable contains the result obtained upon combination of the list of variables processed using the operator specified.

```
sum = 0.0
#pragma omp parallel for
reduction(+:sum)
for (i=0; i < 20; i++)
sum = sum + (a[i] * b[i]);</pre>
```





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In Review



- 3 classes of parallel/distributed computing
 - Capacity
 - Capability
 - Cooperative
- 3 classes of parallel architectures (respectively)
 - Loosely coupled clusters and workstation farms
 - Tightly coupled vector, SIMD, SMP
 - Distributed memory MPPs (and some clusters)
- 3 classes of parallel execution models (respectively)
 - Workflow, throughput, SPMD
 - Multithreaded with shared memory semantics
 - Communicating Sequential Processes
- 3 classes of programming models
 - Condor
 - MPI
 - OpenMP









| Cabinet | | | | |
|-------------------------------|---|--|--|--|
| Organization | 4x 8U compute cages | | | |
| | 1x 1U optical switch | | | |
| | 3x 4U secondary storage array | | | |
| Peak performance | 1.18 PFLOPS | | | |
| Memory | 192 TB | | | |
| Secondary storage (effective) | 2.25 PB | | | |
| Compute Cage | | | | |
| Blades per cage | 14 | | | |
| Blade housing width | 30 mm | | | |
| Blade type | 12x system nodes | | | |
| | 1x spare system node or conventional node | | | |
| | 1x cage-level optical switch | | | |
| Storage Array | | | | |
| Raw capacity | 960 TB | | | |
| Effective capacity | 768 TB | | | |
| Number of disks | 80 | | | |
| Disk type | 3.5", 12 TB, 7200 RPM | | | |
| Redundancy | RAID 6, 8+2 parity | | | |







| System Node | | |
|--------------------------------------|-------------|--|
| Processor nodes | 16 | |
| Peak performance | 24.5 TFLOPS | |
| Memory | 4 TB | |
| Board dimensions | 450x330 mm | |
| Fraction of board area for processor | 75% | |
| nodes with local interconnect | | |

| Processor Node | | | | |
|---------------------------------|--------------|--|--|--|
| Processor modules | 8 | | | |
| Peak performance | 1536 GFLOPS | | | |
| Total memory | 256 GB | | | |
| Aggregate streaming performance | 128 GFLOPS | | | |
| Carrier dimensions | 58.4x86.2 mm | | | |











Speedup with Memory Accelerators







| Processor Module | | | | |
|---|--|--|--|--|
| Organization | 1 TSV stack (low power density) | | | |
| | 1 standalone chip (high power density), side by side | | | |
| Aggregate performance | 192 GFLOPS | | | |
| Aggregate EMP performance | 64 GFLOPS | | | |
| Aggregate streaming performance | 128 GFLOPS | | | |
| Number of EMPs | 128 | | | |
| Number of streaming processors | 8 | | | |
| Memory capacity | 32 GB | | | |
| TSV stack footprint | 150 mm ² | | | |
| Standalone chip footprint | 150 mm ² | | | |
| Combined silicon outline | 14.6x20.6 mm | | | |
| Silicon outline to package outline area | 90% | | | |
| ratio | | | | |
| Package dimensions | 15.3x21.7 mm | | | |
| EMP | | | | |
| Clock frequency | 512 MHz | | | |
| Floating-point op. issue per cycle | 1 | | | |
| Silicon area | 0.5 mm ² | | | |
| Streaming Processor | | | | |
| Clock frequency 2 GHz | | | | |
| Peak floating-point ops per cycle | 8 | | | |





Active Global Address Space (AGAS)

- Distributed
- Assumes no coherence between localities
- User variables
- Synchronization variables and objects
- Threads as first-class objects
- Moves virtual named elements in physical space
- Parcel sets (but not parcels!)
- Process
 - First class object
 - Specifies a broad task
 - Defines a distributed environment
 - Spans multiple localities
 - Need not be contiguous





Parcels may utilize underlying communication protocol fields to minimize the message footprint (e.g. destination address, checksum)



Latency Hiding with Parcels Idle Time with respect to Degree of Parallelism



Idle Time/Node (number of nodes in black)











