Mitglied der Helmholtz-Gemeinschaft

JÜLICH FORSCHUNGSZENTRUM

Crash Course on High Performance Computing

2012 | Bernd Mohr

Institute for Advanced Simulation (IAS)
Jülich Supercomputing Centre (JSC)

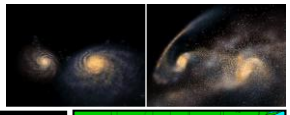
Contents

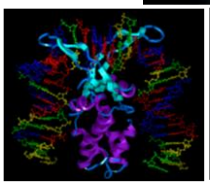
JÜLICH FORSCHUNGSZENTRUM

INTRODUCTION

High-performance computing

- **Computer simulation augments theory and experiments**
  - Needed whenever real experiments would be too large/small, complex, expensive, dangerous, or simply impossible
  - Became third pillar of science
- **Computational science**
  - Multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems
- Challenging applications
  - Protein folding
  - Climate / weather modeling
  - Astrophysics modeling
  - Nano-scale materials
  - . . .





⇨ **Realistic simulations need enormous computer resources (time, memory) !**

Supercomputer

- Supercomputers:
  - Current most powerful and effective computing systems

- Supercomputer (in the 1980's and 1990's)
  - Very expensive, custom-built computer systems

- Supercomputer (since end of 1990's)
  - Large number of "off-the-shelf" components
  - "Parallel Computing"

2012 JSC

Why use Parallel Computers?

- Parallel computers **can** be the only way to achieve specific computational goals at a given time
  - Sequential system is too "slow"
    - ⇨ Calculation takes days, weeks, months, years, …
    - ⇨ **use more than one processor to get calculation faster**
  - Sequential system is too "small"
    - ⇨ Data does not fit into the memory
    - ⇨ **use parallel system to get access to more memory**
- [More and more often] You have a parallel system (⇨ **multicore**) and you want to make use of its special features
- Your advisor / boss tells you to do it ;-)

2012 JSC 6

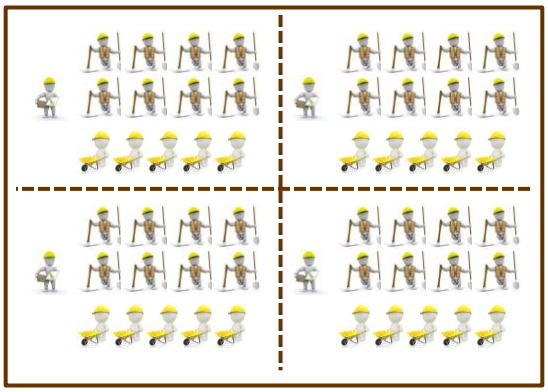
Parallel Computing Thesaurus

- **Parallel Computing**
  - Solving a task by simultaneous use of multiple processors, all components of a unified architecture
- **Distributed Computing (Grid)**
  - Solving a task by simultaneous use of multiple processors of isolated, often heterogeneous computers
- **Embarrassingly Parallel**
  - Solving many similar, but independent, tasks; e.g., parameter sweeps. Also called **farming**
- **Supercomputing**
  - Use of the fastest and biggest machines to solve large problems
- **High Performance Computing (HPC)**
  - Solving a problem via supercomputers + fast networks + large storage + visualization

2012 JSC 7

Programming Parallel Computers

- Application programmer needs to
  - Distribute data to memories
  - Distribute work to processors
  - Organize and synchronize work and dataflow



- Extra constraint
  - Do it with least resources most effective way

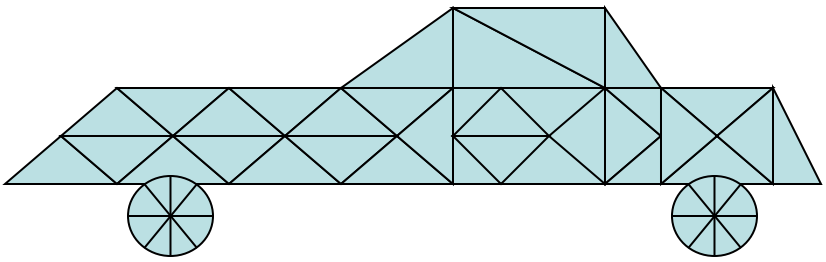
2012 JSC 8

Example: Crash Simulation

- A greatly simplified model based on parallelizing a crash simulation for a car company
- Such simulations save a significant amount of money and time compared to testing real cars
- Example illustrates various phenomena which are common to a great many simulations and other large-scale applications

Finite Element Representation

- Car is modeled by a triangulated surface (the elements)
- The simulation consists of modeling the movement of the elements during each time step, incorporating the forces on them to determine their position
- In each time step, the movement of each element depends on its interaction with the other elements that it is physically adjacent to.



Basic Serial Crash Simulation

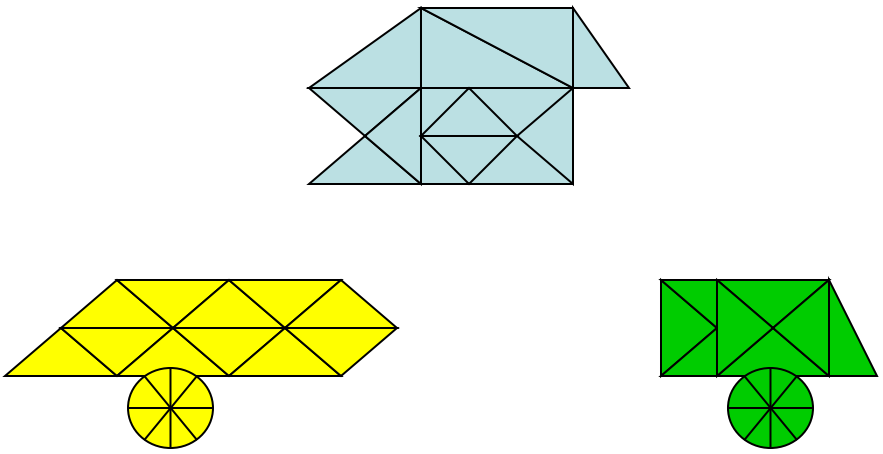
1. For all elements
2. Read State(element), Properties(element), NeighborList(element)

3. For time = 1 to end_of_simulation
4. For element = 1 to num_elements
5. Compute State(element) for next time step based on previous state of element and its neighbors, and on properties of element

Simple Approach to Parallelization

- Parallel computer cluster based on PC-like processors linked with a fast network (⇨ **distributed memory computer**), where processors communicate via messages (⇨ **message passing**)
- Cannot parallelize time, so parallelize space
- Distribute elements to processors (⇨ **data distribution**)
- Each processor updates the positions of the elements stored in its memory (⇨ **owner computes**)
- All machines run the same program (⇨ **SPMD**)

A Distributed Car



Basic Parallel Crash Simulation

- **Concurrently for all processors P**

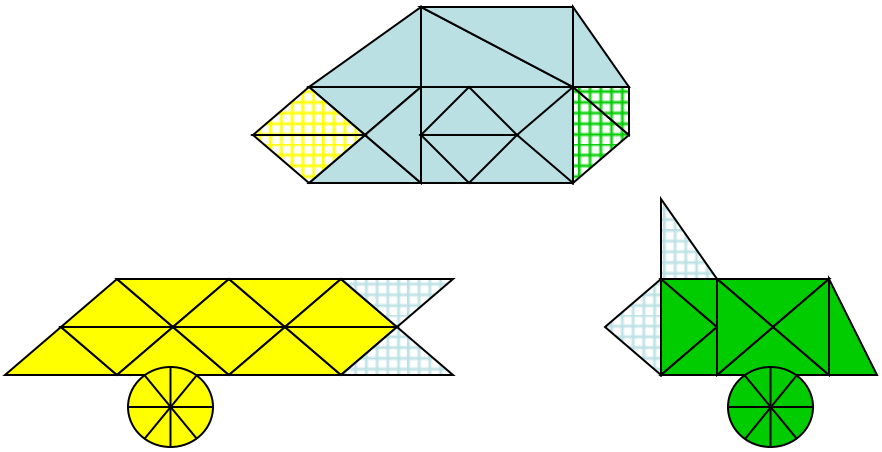
1. For all elements **assigned to P**
2. Read State(element), Properties(element), NeighborList(element)
3. For time = 1 to end_of_simulation
4. For element = 1 to num_elements-**in-P**
5. Compute State(element) for next time step based on previous state of element and its neighbors, and on properties of element
6. **Exchange state information for neighbor elements located in other processors**

Important Issues

- **Allocation**: How are elements assigned to processors?
  - Typically, (initial) element assignment determined by serial preprocessing using domain decomposition approaches
  - Sometimes dynamic re-allocation (⇨ **load-balancing**) necessary
- **Separation**: How does processor keep track of adjacency info for neighbors in other processors?
  - Use **ghost cells** (**halo**) to copy remote neighbors, add transition table to keep track of their location and which local elements are copied elsewhere

2012 JSC 15

Halos



2012 JSC 16

Important Issues II

- **Update**: How does a processor use State(neighbor) when it does not contain the neighbor element?
  - Could request state information from processor containing neighbor. However, more efficient if that processor sends it
- **Coding and Correctness**: How does one manage the software engineering of the parallelization process?
  - Utilize an incremental parallelization approach, building in scaffolding
  - Constantly check test cases to make sure answers correct
- **Efficiency**: How do we evaluate the success of the parallelization?
  - Evaluate via **speedup** or **efficiency** metrics

EVALUATING PROGRAM PERFORMANCE

Evaluating Parallel Programs

- An important component of effective parallel computing is determining whether the program is performing well.
- If it is not running efficiently,
  or cannot be scaled to the targeted number of processors,
  - one needs to determine the causes of the problem
    - ⇨ **performance analysis**
    - ⇨ tool support available
  - and then develop better approaches
    - ⇨ **tuning** or **optimization**
    - ⇨ very little tools support
    - ⇨ difficult as often application and platform specific

Definitions

- For a given problem A, let
  - **SerTime(n)** = Time of the best serial algorithm to solve A for input of size n
  - **ParTime(n,p)** = Time of the parallel algorithm + architecture to solve A for input size n, using p processors
  - Note that SerTime(n) ≤ ParTime(n,1)
- Then
  - **Speedup(p)** = SerTime(n) / ParTime(n,p)
  - **Work(p)** = p • ParTime(n,p)
  - **Efficiency(p)** = SerTime(n) / [p • ParTime(n,p)]

Definitions II

- In general, expect
  - $0 \leq \text{Speedup}(p) \leq p$
  - Serial work $\leq$ Parallel work $< \infty$
  - $0 \leq \text{Efficiency} \leq 1$
- **Linear speedup**: if there is a constant $c > 0$ so that speedup is at least $c \cdot p$. Many use this term to mean $c = 1$.
- **Perfect** or **ideal speedup**: $\text{speedup}(p) = p$
- **Superlinear speedup**: $\text{speedup}(p) > p$ (efficiency > 1)
  - Typical reason: Parallel computer has p times more memory (cache), so higher fraction of program data fits in memory instead of disk (cache instead of memory)
  - Parallel version is solving slightly different, easier problem or provides slightly different answer

Amdahl's Law

- **Amdahl** [1967] noted:
  - Given a program, let f be the fraction of time spent on operations that must be performed serially (not parallelizable work). Then for p processors:

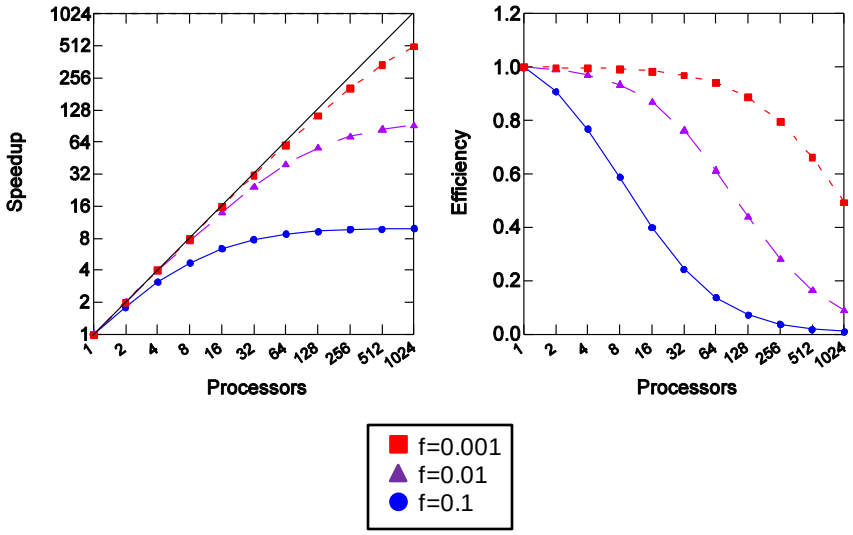
$$\text{Speedup}(p) \leq \frac{1}{f + (1 - f)/p}$$

  - Thus no matter how many processors are used

$$\text{Speedup}(p) \leq 1/f$$

  - Unfortunately, f is typically 5 – 20%

Maximal Possible Speedup / Efficiency

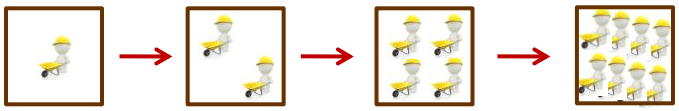


Amdahl's Law II

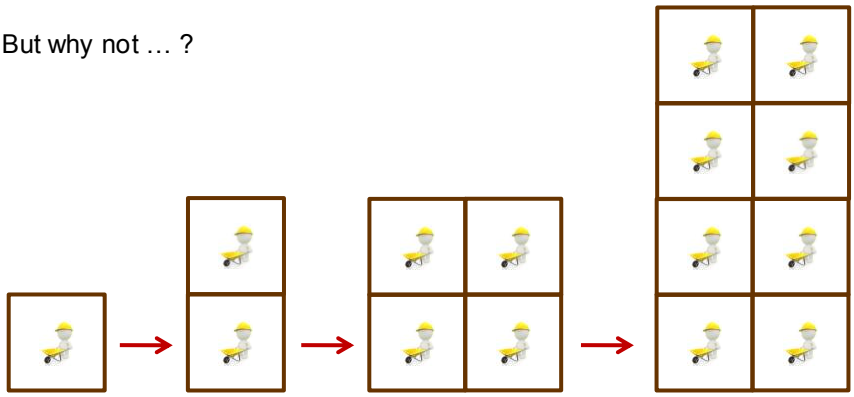
- **Amdahl was an optimist**
  - Parallelization might require extra work, typically
    - Communication
    - Synchronization
    - Load balancing
  - Amdahl convinced many people that general-purpose parallel computing was not viable
- **Amdahl was a pessimist**
  - Fortunately, we can break the law!
  - Find **better (parallel) algorithms** with much smaller values of f
  - **Superlinear speedup** because more data fits cache/memory
  - **Scaling**: exploit large parallel machines by scaling the problem size with the number of processes

Scaling

- Amdahl scaling



- But why not … ?



Scaling

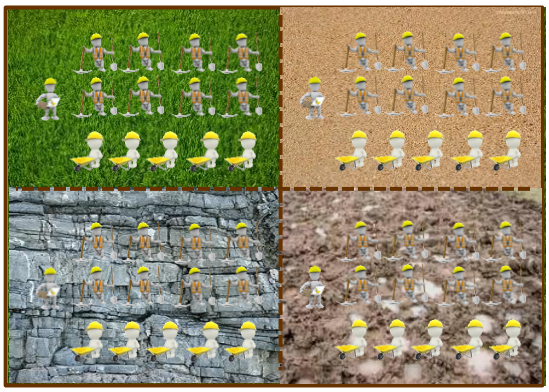
- Sometimes the serial portion
  - is a fixed amount of time independent of problem size
  - grows with problem size but slower than total time
- Thus large parallel machines can often be exploited by scaling the problem size with the number of processes
- Scaling approaches used for speedup reporting/measurements:
  - Fixed problem size (⇨ **strong scaling**)
  - Fixed problem size per processor (⇨ **weak scaling**)
  - Fixed time, find largest solvable problem [Gustafson 1988] Commonly used in evaluating databases (transactions/s)
  - Fixed efficiency: find smallest problem to achieve it (⇨ **isoefficiency analysis**)

Parallelization

- Goal: Divide work and/or communication between processors
- Two approaches:
  - **Domain decomposition**
    - Partition a (perhaps conceptual) space
    - Different processors do similar (same) work on different pieces
    - Examples: harvesting a large farm field with many workers
  - **Functional decomposition**
    - Different processors work on different types of tasks
    - Examples: workers on an assembly line, subcontractors on a project
- Functional decomposition rarely scales to many processors, so most programs are parallelized based on domain decomposition

Parallelization: Load Balancing

- Goal
  - Divide work between processors **equally**
    ⇨ work load on all processors is the same
    ⇨ **load balancing**
- Difficulties
  - Unknown distribution of work
  - Dynamic changes in work load



Load Balancing

- **Ultimate goal**:
  Divide work and/or communication between processors **equally**
  ⇨ work load on all processors is the same
  ⇨ communication load on all processors is the same
  ⇨ **load balancing**

- Many different types of load balancing problems
  - Static (fixed, do it once) or dynamic (changing, adapt to load)
  - Parameterized or data dependent
  - Homogeneous or inhomogeneous
  - Low or high dimensional
  - Graph oriented, geometric, lexicographic, …

- Because of this diversity, many different approaches and tools are needed

Load Balancing: Complicating Factors

- Objects being computed do not have a simple dependency pattern among themselves, so communication load-balancing is difficult to achieve

- Objects do not have uniform computational requirements, and it may not initially be clear which ones need more time

- If objects are repeatedly updated (such as elements in the crash simulation), the computational load of an object may vary over iterations

- Objects may be created dynamically and in an unpredictable manner, complicating both computational and communicational load balance

ARCHITECTURE

Architectural Taxonomies

- The classifications of parallel computers are in terms of hardware; but there are natural software analogues
- These classifications provide ways to think about problems and their solution.
- Note: many real systems blend approaches, and do not exactly correspond to the classifications

Flynn's Instruction/Data Taxonomy

- Flynn 1966: At any point in time can have

$$\left\{ \begin{matrix} S \\ M \end{matrix} \right\} I \left\{ \begin{matrix} S \\ M \end{matrix} \right\} D$$

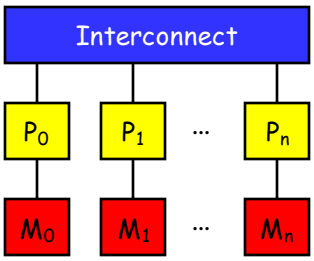
- **SI** **S**ingle **I**nstruction: All processors execute same instruction. Usually involves a central controller
- **MI** **M**ultiple **I**nstruction: Different processors may be executing different instructions
- **SD** **S**ingle **D**ata: All processors are operating on the same data
- **MD** **M**ultiple **D**ata: Different processors may be operating on different data

Flynn's Instruction/Data Taxonomy II

- **SISD** standard serial computer and program
- **MISD** extremely rare; some fault-tolerant schemes, using different computers and programs to operate on same input data
- **MIMD** almost all parallel computers are of this type
- **SIMD** there used to be companies that made such systems (e.g., Thinking Machines' connection machine); only special purpose systems made now

Parallel Architectures: Distributed Memory

- Interconnected nodes (processor + memory)
- All memory is associated with processors
- Advantages
  - Memory is scalable with number of processors
    ⇨ can build very large machines (10000's of nodes)
  - Each processor has rapid access to its own memory without interference or cache coherency problems
  - Cost effective and easier to build: can use commodity parts

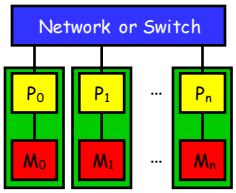


Parallel Architectures: Distributed Memory II

- Disadvantages
  - To retrieve information from another processor's memory a **message** must be sent over the network to the home processor
  - Programmer is responsible for many of the details of the communication; easy to make mistakes
    - **Explicit** data distribution
    - **Explicit** communication via messages
    - **Explicit** synchronization
  - May be difficult to distribute the data structures, often additional data structures needed (ghost cells, location tables, …)
- Programming Models
  - Message passing: **MPI**, PVM, shmem, LAPI, ELAN, …
  - Data parallelism: HPF

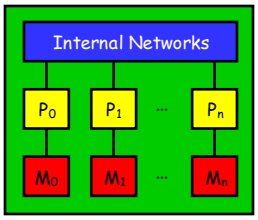
Parallel Architectures: Distributed Memory III

- Further classification based on how memory is accessed
  - NORMA (**NO** **R**emote **M**emory **A**ccess)
    ⇨ Nodes connected via network adaptors to external networks (switches)
    - NOW (**N**etwork **o**f **W**orkstations)
    - COW (**C**luster **o**f **W**orkstations)



Example: PC Cluster

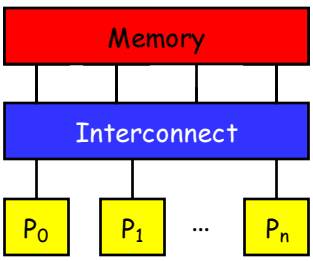
  - RMA (**R**emote **M**emory **A**ccess)
    ⇨ Processors connected via internal special interconnect hardware
    ⇨ Often allows one-sided memory transfers (get, put)
    - MPP (**M**assively **P**arallel **P**rocessing) system



Example: Cray T3E

Parallel Architectures: Shared Memory

- More exact: **shared address space** accessible by all processors
  ⇨ physical memory modules may be distributed



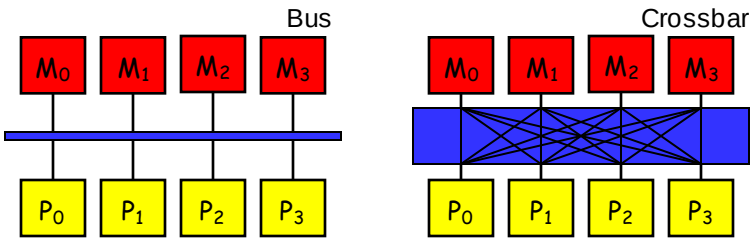
- Processors may have local memory (e.g., caches) to hold copies of some global memory. Consistency of these copies is usually maintained by special hardware
- Programming Models
  - Automatic parallelization via compiler
  - Explicit threading (e.g. POSIX threads)
  - **OpenMP**
  - [MPI]

Parallel Architectures: Shared Memory II

- Advantages
  - Global address space is user-friendly; program may be able to use global data structures efficiently and with little modification
  - Typically easier to program
    - **Implicit** communication via (shared) data
    - **But still explicit synchronization!**
  - Data sharing (communication) between tasks is very fast
- Disadvantages
  - Requires special expensive hardware for efficient (scalable) memory access and cache coherence
  - Therefore not very scalable (10 to 100's of nodes)

Parallel Architectures: Shared Memory III

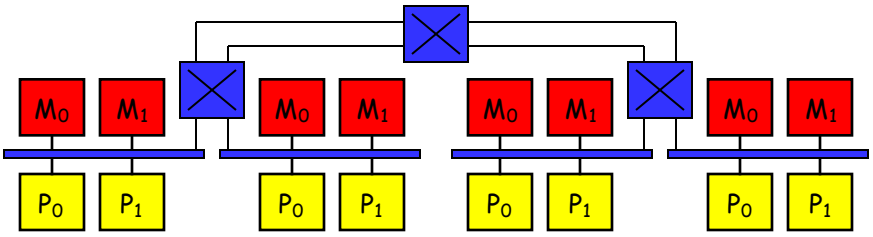
- Further classification based on memory access time:
  - **UMA** (**U**niform **M**emory **A**ccess)
    - Equal access times to memory from each processor
    - Almost always cache-coherent
    - Interconnects:



    - Least scalable architecture
    - Also used: SMP (**S**ymmetrical **M**ulti **P**rocessor)
  - Example: Current Multi-core processors

Parallel Architectures: Shared Memory IV

- Further classification based on memory access time:
  - **NUMA** (**N**on-**U**niform **M**emory **A**ccess)
    - Often made by linking UMA nodes with switching networks
    - One node can directly access memory of another node through special hardware; however this access is typically much slower



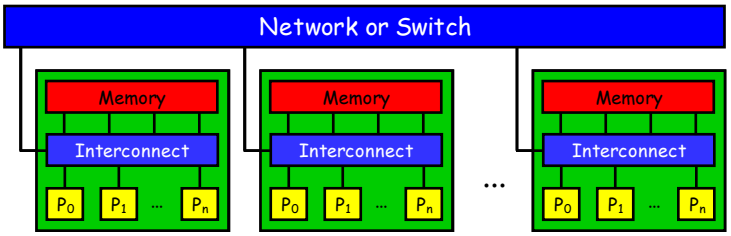
    - cc-NUMA (**c**ache-**c**oherent **NUMA**)
    - Also used: SMP (**S**calable **M**ulti **P**rocessor)
- Examples: SGI Altix

Shared Memory on Distributed Memory

- It is usually easier to parallelize a program on a shared memory system
- However, most systems have distributed memory because of the cost and scalability advantages
- To gain both advantages people investigate using software to emulate shared memory access
  - **Virtual shared memory**: virtualization inside operating system on the memory page level ⇨ **rarely efficient**
  - Special programming languages or libraries providing a **global address space** abstraction
    - Global arrays
    - Unified Parallel C (UPC)
    - Co-Array Fortran (CAF)

Parallel Architectures: Hybrid Systems

- Logical extension of distributed and shared memory architectures



⇨ **Increased complexity in hardware, software, and programming!!!**

- Programming Models
  - Message passing
  - Message passing between nodes + multi-threading within nodes
- Examples: IBM BlueGene/P or Cray XT4

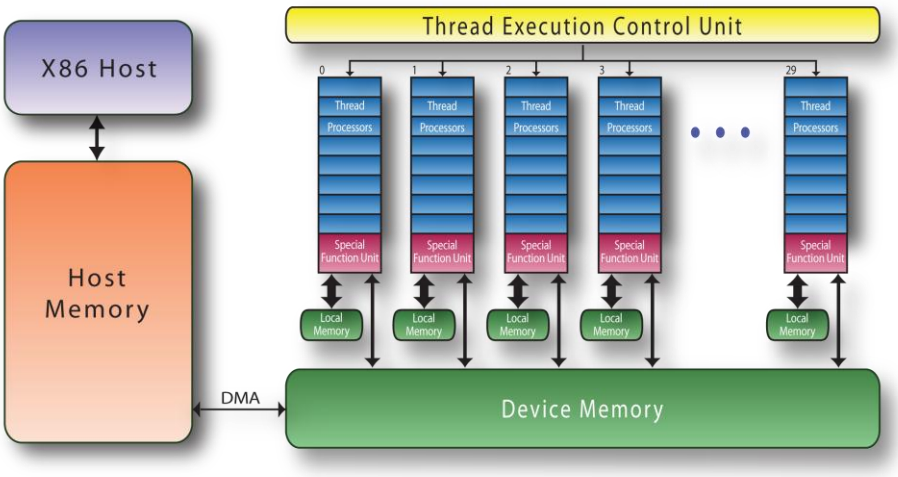
Parallel Architectures: Hybrid Systems II

- Two typical forms:
- **Clusters** of shared memory nodes
  - Number of nodes >> number of processors inside node
  - Often small, cheaper SMP nodes (rack-mounted, blades)
  - Sometimes called **clumps**
  - Often commodity network (e.g., Gigabit Ethernet)
- **Constellation systems**
  - Number of processors inside node > number of nodes
  - Larger, more expensive UMA or cc-NUMA nodes
  - Typically special high performance interconnect networks

Accelerators

- Special hardware for accelerating computations has long tradition in HPC
  - Floating-point units
  - SIMD/vector units
    - MMX, SSE (Intel), 3DNow! (AMD), AltiVec (IBM)
    - BlueGene double hummer, …
  - **FPGA** (**F**ield **P**rogrammable **G**ate **A**rrays)
  - **Cell-Chip**
    - Main PowerPC core + 8 SPE (**S**ynergistic **P**rocessing **E**lements)
    - LLNL RoadRunner (Opteron / Cell heterogeneous system)
- Latest trend in HPC: **GPGPU**
  - **G**eneral **P**urpose computing on **G**raphics **P**rocessing **U**nits

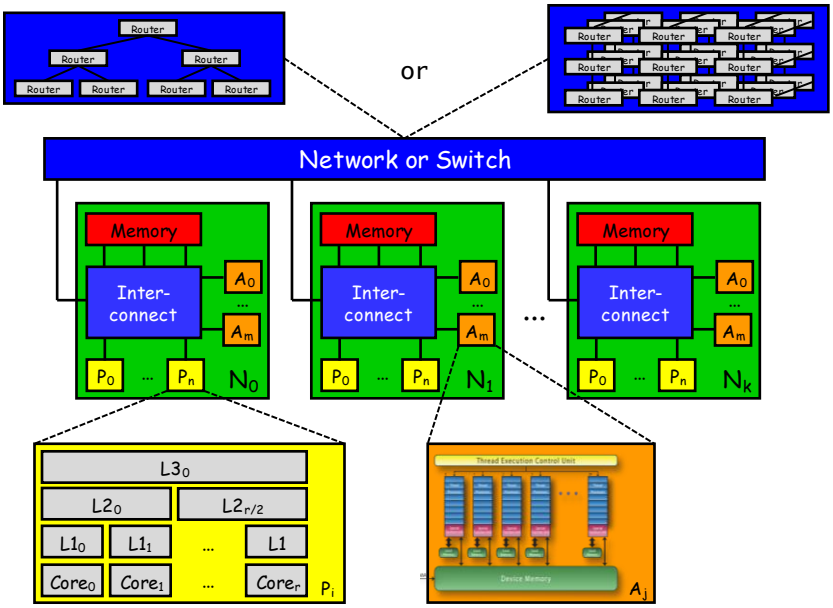
Abstracted x64 + Accelerator Architecture



GPGPU

- **Modern GPUs**
  - Have a parallel many-core architecture
    - Each core capable of running 1000s of threads simultaneously
  - **MIMD blocks with SIMD fine-grain parallelism**
  - Highly parallel structure makes them more effective than general-purpose CPUs for some (vectorizable) algorithms
- Large HPC clusters with GPU acceleration already built (#GPUs):
  - Tianhe-1A (7168), Nebulae (4640), Tokyo Tech (4224), …
- Difficult to use hardware effectively
  - High-level (portable) programming interfaces just evolving
  - Main disadvantage: data must be moved to and from main memory to GPU memory
  - Data locality important, otherwise performance degrades significantly

Parallel Architectures: State of the Art



Example: BSC IBM MareNostrum (2006)

Example: BSC IBM MareNostrum (2006)

- 64-bit IBM PowerPC 970MP 2.3 GHz, 2-way SMP
- 94.21 Teraflop/s peak
  63.83 Teraflop/s Linpack
  Nov06: #5
  Jun12: #465
- 20 TByte memory
- 2,560 JS21 blades
  - 10,240 cores
- Interconnects
  - Myrinet
  - Gigabit Ethernet

Example: LLNL Sequoia computer (2012)

- 64-bit IBM PowerPC A2
  1.6 GHz, 16-way SMP
- 20.13 Petaflop/s peak
  16.32 Petaflop/s Linpack

Jun12: #1

- 1.6 PByte memory
- 96 racks
- 98,304 nodes
- 1,572,864 cores
- 5D interconnect
- Water cooling

2012 JSC 51

Example: RIKEN AICS K computer (2011)

- 64-bit Sparc VIIIfx
  2.0 GHz, 8-way SMP
- 11.28 Petaflop/s peak
  10.51 Petaflop/s Linpack

Nov11: #1
Jun12: #2

- 1.41 PByte memory
- 864 racks
- 88,128 nodes
- 705,024 cores
- 6D interconnect (Tofu)
- Water cooling

2012 JSC 52

Example: RIKEN AICS K computer (2011)

Only supercomputer with its own train station!

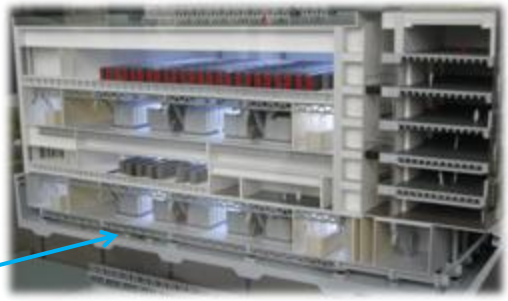
4th floor: K computer

3rd floor: Computer cooling

2nd floor: Disks

1st floor: Disk cooling

Earth quake dampers



Example: RIKEN AICS K computer (2011)

horizontal moves damper

Building
Earth quake
Security

Vertical moves damper

"wiggle" moves damper

flexible pipes

Example: SuperMUC (2012)

JÜLICH FORSCHUNGSZENTRUM

- Fat node
  - 2 x 64-bit Intel Sandy Bridge EP 2.7 GHz, 8-way SMP
- Thin node
  - 4 x Intel Westmere EX 2.4 Ghz, 10-way SMP
- 3.19 Petaflop/s peak
  2.9 Petaflop/s Linpack

TOP500 SUPERCOMPUTER SITES Jun12: #4

- 340 TByte memory
- 9,216 fat / 205 thin nodes
- 155,656 total cores
- Infiniband FDR10 interconnect
- Warm-water cooling (in 30 → out 50)

2012 JSC 55

Example: SuperMUC (2012)

JÜLICH FORSCHUNGSZENTRUM

Water infrastructure

Machine hall raised floor

56

Example: NSCC Tianhe-1A (2010)

- 64-bit Intel Xeon X5670 6C 2.93 GHz, 6-way SMP
- 4.7 Petaflop/s peak
  2.57 Petaflop/s Linpack

  Nov10: #1
  Jun12: #5
- 262 TByte memory

- 112 racks
- 14,336 Xeon
- 86,016 cores
- 7,168 Nvidia Tesla M2050
- 2,048 NUDT FT1000 processors
- Galaxy interconnect (Chinese)

2012 JSC 57

Example: JSC IBM BlueGene/P (2009)

2012 JSC 58

Example: JSC IBM BlueGene/P (2009)

- 32-bit PowerPC 450
  850 MHz, 4-way SMP
- 1,00 Petaflop/s peak
  0,82 Petaflop/s Linpack
  Jun09: #3
  Jun12: #25
- 144 TByte memory
- Numerous hardware
  - 72 racks, 73728 nodes, 294912 cores,
  - 648 power modules, 576 link cards, 144 service cards,
  - 4352 data cables, 288 service cables, … → 4.1 km
- Interconnects
  - 3D-torus, collective (tree), and barrier network
  - 10 GigaBit (I/O), 1 GigaBit (control)

2012 JSC 59

Example: JSC IBM BlueGene/Q (2012)

- 64-bit PowerPC A1
  1.6 GHz, 16-way SMP
  each 4-way SMT
- 1,68 Petaflop/s peak
  1,37 Petaflop/s Linpack
  Jun12: #8
- 131 TByte memory
- 8 racks
- 131072 cores
- 5D-torus interconnect
- 90% water cooled, 10% air

- 6 racks BG/Q more powerful than 72 racks BG/P!

2012 JSC 60

JSC Machine Hall Specifications

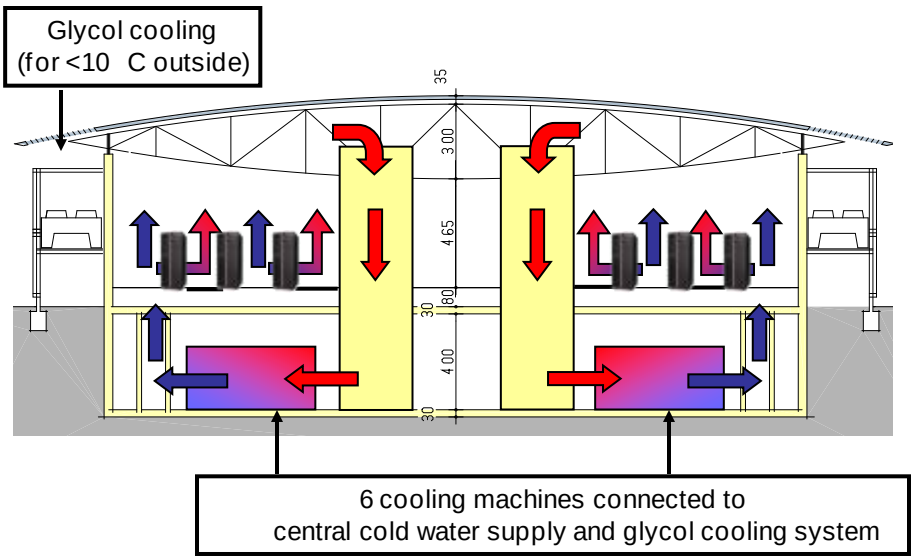
JÜLICH FORSCHUNGSZENTRUM

• Area:	1000 m²
	self supporting roof
• Volume:	6500 m³
• Power supply:	5300 kW
• Floor temperature:	16 C
• Humidity:	40 – 60 %
• Air exchange rate:	38/h
• Air exchange:	250000 m³/h
• UPS:	only for communication and disks

2012 JSC 62

Air Cooling System

JÜLICH FORSCHUNGSZENTRUM



2012 JSC 63

Air + Water Cooling System

JÜLICH FORSCHUNGSZENTRUM

Glycol coolers

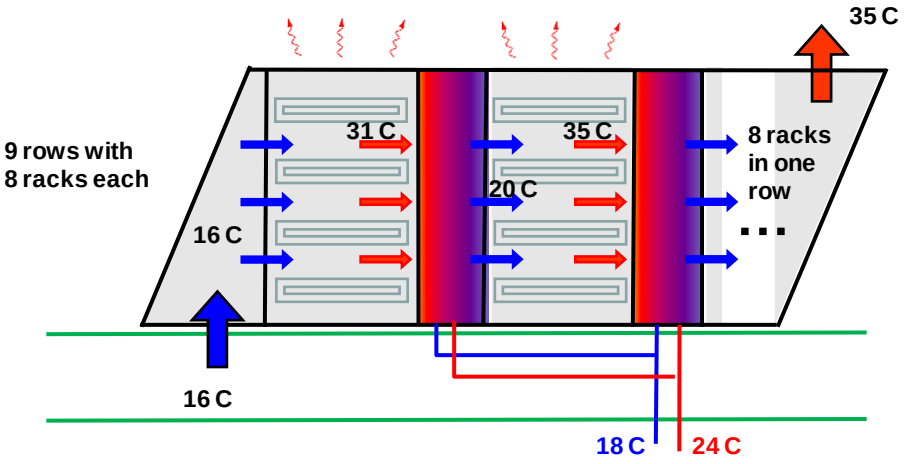
Cooling system

Cold water distribution

Central cold water supply

2012 JSC 64

Water-Cooled Blue Gene/P



JSC: Supply of Cooling Water





Bringing water into basement

Establishing a room with pumps to prepare different inlet temperatures

JSC: Extending the Power Supply

from
1,6 MW

to
5,3 MW

2012 JSC 67

JSC: Power Distribution

30 m power distribution panels

Number of fuses:
- 72x3 125 A
- 220x1 32 A
- 598x1 16 A
- 174x1 32 A
- 12x3 32 A

1244 total

nearly 50 km
length of cables

2012 JSC 68

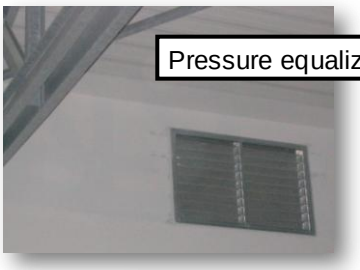
JSC: Supercomputer Networks

Length of the communication cables:

• BG/P:	23 km (copper)
	21 km (fiber)
• JUROPA:	20 km (mixed)
• HPC-FF:	16 km (mixed)
	80 km

2012 JSC 69

JSC: Fire Prevention



2012 JSC 70

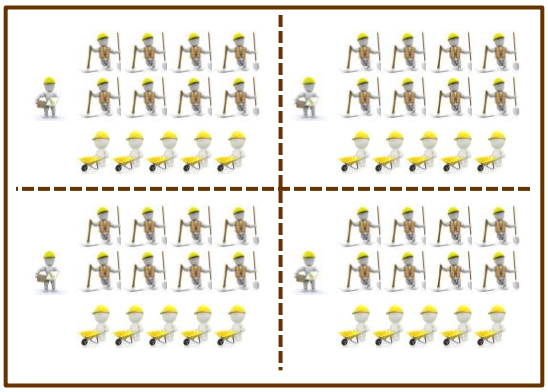
Costs (JSC, 2011)

- **Jugene (IBM BlueGene/P)**
  - 1 Node hour (Quadcore) 0.039 €
  - Typical job (1 day x 2048 nodes) 1916.92 €
  - Maximum (1 day x 73728) 69009.41 €
- **Juropa (Bull/Sun Intel Nehalem/Infiniband cluster)**
  - 1 Node hour (Dual quadcore) 0.39 €
  - Typical job (12h x 128 nodes) 599.04 €
  - Maximum (1 day x 3288) 30775.68 €

PARALLEL PROGRAMMING

RECALL: Programming Parallel Computers

- Application programmer needs to
  - Distribute data to memories
  - Distribute work to processors
  - Organize and synchronize work and dataflow



- Extra constraint
  - Do it with fewest resources in most effective way

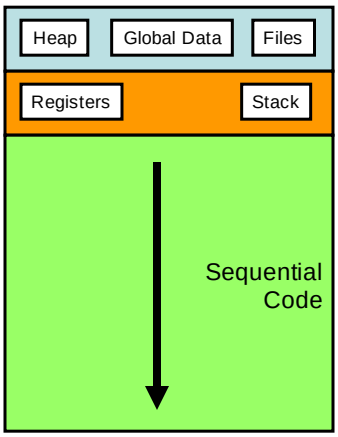
Parallelization Strategies

- Two major computation resources:
  - Processor
  - Memory
- Parallelization means
  - Distributing work among processors
  - Synchronization of the distributed work
- If memory is distributed it also means
  - Distributing data
  - Communicating data between local and remote processors
- Programming models offer combined methods for
  - Distribution of work & data
  - Communication and synchronization

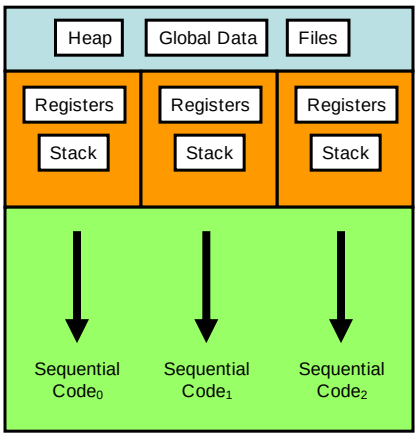
Processes and Threads

- Processes are entities provided by the operating system (OS) to execute programs
- A typical **(sequential) process** consists of a **thread** of execution executing the program starting with main. The thread can access
  - A **stack** for storing local data
  - A **heap** for storing dynamic data (e.g., via allocate/malloc/new)
  - Space for storing **global static data**
- If OS supports **multi-threading**, a process can have multiple **threads**
  - Can be dynamically created and destroyed at run-time
  - Each thread can access the heap and global data
  - Each thread has its own stack!
- Parallel programs
  - Can use multiple processes + mechanism to communicate
  - On shared memory computer, use multi-threading
  - Or combination of both

Single-threaded vs. Multi-threaded



Single-threaded process



Multi-threaded process

Basic Parallel Programming Paradigm: SPMD

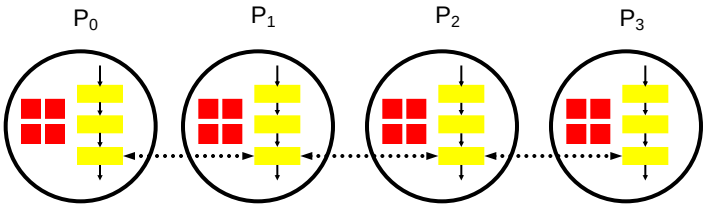
- **SPMD**: **S**ingle **P**rogram **M**ultiple **D**ata
- Basic paradigm for implementing parallel programs

- Programmer writes **one** program
  - Which is executed on **all** processors
  - But written in a way that it works on **different** parts of the data

- Special cases (e.g., different control flow) is handled inside the program

```
if (process_or_thread_id == 42) then
  call do_something()
else
  call do_something_else()
endif
```


Programming Models: Message Passing



- Typically used on distributed memory computer systems
- Local ("distributed") style
  - SPMD-style program runs locally using local data
- **Explicit** data distribution, communication and synchronization

⇨ High programming overhead

⇨ Message passing libraries: **MPI**, PVM, …

Message Passing Performance

- Performance metrics for message passing
  - **Latency**: time to transfer message
  - **Bandwidth**: amount of data which can be transferred in fixed time

  measured for a specific message length

- **Reducing latency** often important for performance. Approaches:
  - Reduce number of messages by mapping communicating entities onto the same processor
  - Combine messages having the same sender and destination
  - If processor P has data needed by processor Q, have P send to Q, rather than Q requesting it. P should send as soon as data ready, Q should read as late as possible to increase probability data has arrived ⇨ **Send early, receive late, don't ask but tell.**
  - Try overlapping communication and calculation (not all systems can do this)

Programming Models: MPI

- MPI: **M**essage **P**assing **I**nterface

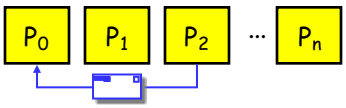
- De-facto **standard** message passing interface
  - MPI 1.0 in 1994
  - MPI 1.2 in 1997
  - MPI 2.0 in 1997
  - MPI 2.1 in 2008
  - MPI 2.2 in 2009

- **Library interface**
- Language bindings for Fortran, C, C++, [Java]
- Typically used in conjunction with SPMD programming style

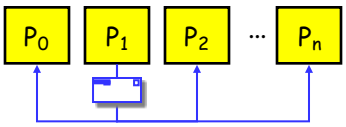
- http://www.mpi-forum.org

MPI Functionality

- **Point-to-point** communication (between 2 processes)



- **Collective** communication (between a group of processes)



- **Barrier** synchronization
- Management of **communicators**, data types, topologies

- **One-sided** communication
- **Parallel I/O**
- F90 and C++ support
- Process creation

} MPI 2.0

MPI Communicators

- **Communicator** consists of a process group and a communication context
- Predefined communicator (representing all processes) is **MPI_COMM_WORLD**

- Each message is sent relative to a communicator
- All processes in the process group of the communicator have to take part in a collective operation

- Operations are provided to:
  - Determine the number of processes in a communicator
  - Determine the **rank** of the executing process relative to a communicator ⇒ **0 to N-1**
  - Build new process groups and communicators

MPI Basic Routines

`MPI_Init()`
- Initialize MPI library
- Needs to be called once, before all other MPI functions

`MPI_Finalize()`
- Wrap-up / terminates MPI usage
- Needs to be called once, after all other MPI functions

`MPI_Comm_size(comm, size)`
- Get total number of processes in communicator `comm`

`MPI_Comm_rank(comm, rank)`
- Get process identification (rank) within `comm`

Example: Hello World (MPI), Fortran

```
program main
include 'mpif.h'
integer :: ierr, myrank, numprocs

call MPI_Init(ierr)
call MPI_Comm_rank(MPI_COMM_WORLD, myrank, ierr)
call MPI_Comm_size(MPI_COMM_WORLD, numprocs, ierr)

write(*,*) "hello from", myrank, "of", numprocs

call MPI_Finalize(ierr)
end program
```

Fortran MPI routines: error code returned in extra parameter!

Example: Hello World (MPI), C I

```
#include <stdio.h>
#include <mpi.h>

int main(int argc, char *argv[])
{
  int ierr, myrank, numprocs;

  ierr = MPI_Init(&argc, &argv);
  ierr = MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
  ierr = MPI_Comm_size(MPI_COMM_WORLD, &numprocs);

  printf("hello from %d of %d\n", myrank, numprocs);

  ierr = MPI_Finalize();
}
```

C MPI_Init: needs access to program parameters

C: error code returned by functions!

Example: Hello World (MPI), C II

```
#include <stdio.h>
#include <mpi.h>

int main(int argc, char *argv[])
{
  int ierr, myrank, numprocs;

  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
  MPI_Comm_size(MPI_COMM_WORLD, &numprocs);

  printf("hello from %d of %d\n", myrank, numprocs);

  MPI_Finalize();
}
```

C MPI_Init: needs access to program parameters

C: error code returned but ignored

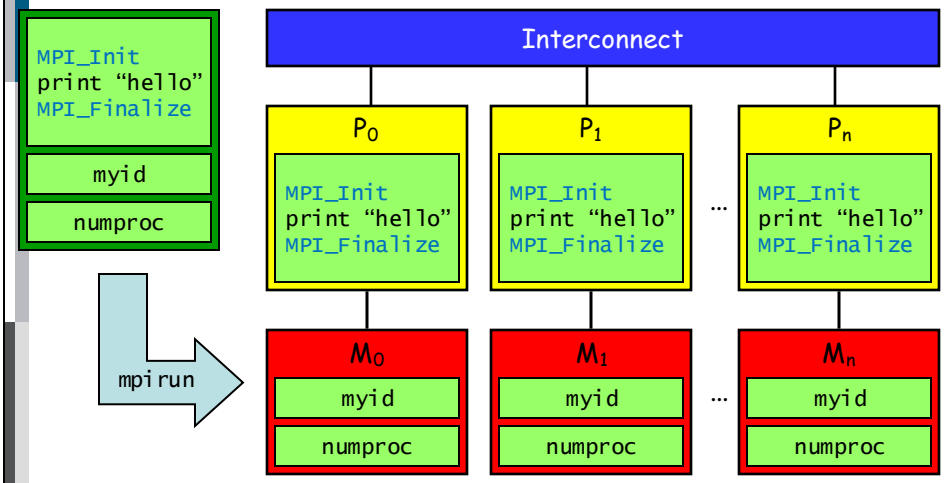
Compiling MPI Programs

- Many implementations provide **special compilation commands** which automatically
  - direct the compilers to the location of MPI header files and modules
  - link in all necessary MPI and network libraries
  - often called:
    - `C:` `mpicc`
    - `C++:` `mpiCC`, `mpicxx`, or `mpic++`
    - `Fortran:` `mpif90`, `mpif77`

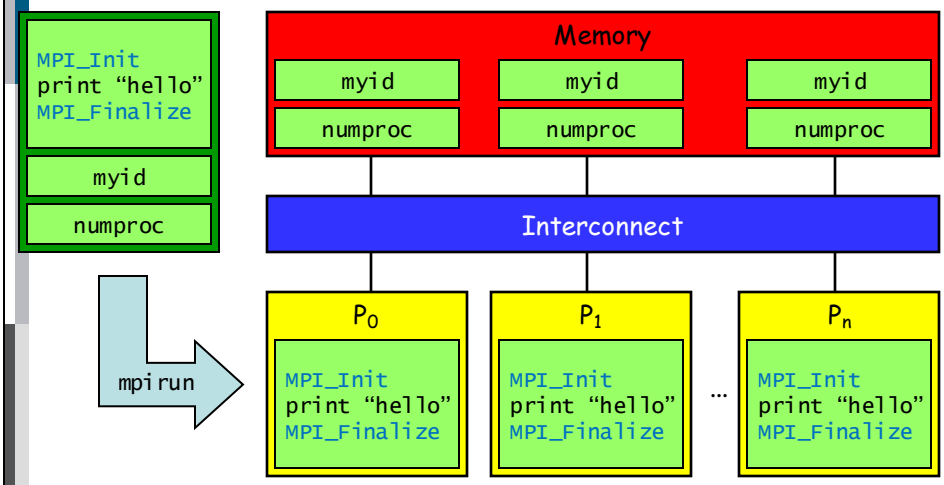
Executing MPI Programs

- Start mechanism is implementation dependent
  - Many implementations:
    - `mpirun -np <numprocs> <executable> [<options>]`
  - MPI-2 standard:
    - `mpiexec -n <numprocs> <executable> [<options>]`
- Possible implementation-dependent differences
  - Options
  - Environment variables
  - Passing runtime parameters, …
- Start mechanism in general different with a batch system like PBS (`qsub` …) or LoadLeveler (`llsubmit` …)

Running MPI on Distributed Memory



Running MPI on Shared Memory



Examples: Executing Hello World (MPI)

- `mpiexec -n 4 helloworld.exe`

```
hello from 0 of 4
hello from 1 of 4
hello from 2 of 4
hello from 3 of 4
```

- `mpiexec -n 4 helloworld.exe`

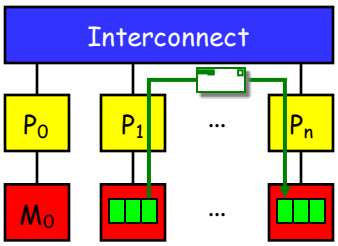
```
hello from 3 of 4
hello from 1 of 4
hello from 0 of 4
hello from 2 of 4
```

- `mpiexec -n 4 helloworld.exe`

```
hehellhelllo from 3
lo from helf 4lo from
1 of 4o fr 2 of 4
om 0 of 4
```

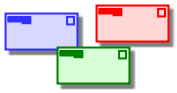

MPI Messages I

- Communication in MPI is done by exchanging **messages**

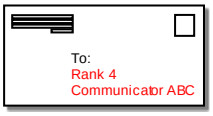


- A message is always described by 3 parameters
  - **buffer**: the address of the object containing the data
  - **num**: number of data elements
  - **datatype**: type of a data element
    - Fortran: `MPI_INTEGER`, `MPI_REAL`, `MPI_DOUBLE_PRECISION`, …
    - C: `MPI_INT`, `MPI_FLOAT`, `MPI_DOUBLE`, …

MPI Messages II



- Point-to-point messages can be **tagged** ("marked") with a user-defined identification number



- Messages are local to communicator
  - ⇨ Source and destination process described by **rank** within **communicator**
    - Special case null process `MPI_PROC_NULL`
      - Message ignored if used as destination or source
      - Useful for non-circular shifts at boundary processes
- Receiving process gets extra information on received message through MPI status object
  - Fortran: `integer :: status(MPI_STATUS_SIZE)`
  - C: `MPI_Status status`

Basic MPI Point-to-Point Routines

`MPI_Send(buffer, num, datatype, dest, tag, comm)`
- Called on sender process
- Pack data inside buffer into a message tagged with `tag` and send it out to rank `dest` within `comm`

`MPI_Recv(buffer, num, datatype, src, tag, comm, status)`
- Called on receiver process
- Receive message tagged with `tag` from rank `src` within `comm` and unpack message into **`data buffer`**

```
MPI_Sendrecv(sendbuf, sendnum, senddtype, dest, sendtag,
             recvbuf, recvnum, recvdtype, src,  recvtag,
             comm, status)
```
- Send a message and receive one at the same time
- Useful for executing shift across a chain of processes

Example: Sending Messages in a Ring, Fortran

```
program shift
include 'mpif.h'
integer :: left, right, ierr, myrank, numprocs
integer :: value=0, tag=42, status(MPI_STATUS_SIZE)

call MPI_Init(ierr)
call MPI_Comm_rank(MPI_COMM_WORLD, myrank, ierr)
call MPI_Comm_size(MPI_COMM_WORLD, numprocs, ierr)

left  = mod(myrank - 1 + numprocs, numprocs)
right = mod(myrank + 1, numprocs)
call MPI_Sendrecv(myrank, 1, MPI_INTEGER, right, tag, &
                  value,  1, MPI_INTEGER, left,  tag, &
                  MPI_COMM_WORLD, status, ierr)
write (*,*) myrank, "received", value

call MPI_Finalize(ierr)
end program
```


Example: Sending Messages in a Ring, C

```
#include <stdio.h>
#include <mpi.h>

int main(int argc, char* argv[]) {
  int left, right, ierr, myrank, numprocs, value=0, tag=42;
  MPI_Status status;

  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
  MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
  left  = (myrank - 1 + numprocs) % numprocs;
  right = (myrank + 1) % numprocs;
  MPI_Sendrecv(&myrank, 1, MPI_INT, right, tag, &value, 1,
               MPI_INT, left, tag, MPI_COMM_WORLD, &status);
  printf("%d received %d\n", myrank, value);
  MPI_Finalize();
  return 0;
}
```

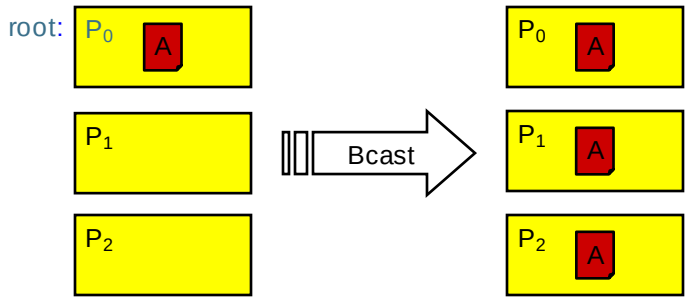
MPI Collective Operations

`MPI_Barrier(comm)`

- Synchronizes all processes in a group

`MPI_Bcast(buffer, num, datatype, root, comm)`

- Distribute same `data` from `root` process to process group



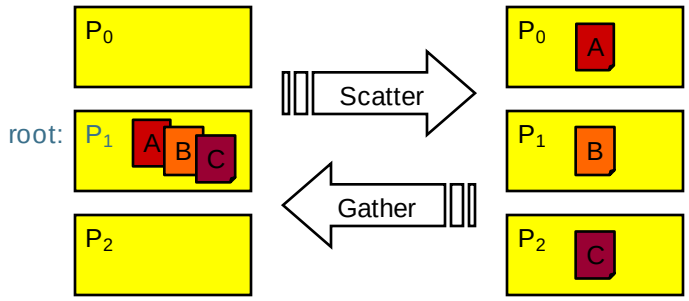
MPI Collective Operations II

`MPI_Scatter(sendbuf, sendnum, senddtype, recvbuf, recvnum, recvdtype, root, comm)`

- Distribute different `data` from `root` to process group

`MPI_Gather(sendbuf, sendnum, senddtype, recvbuf, recvnum, recvdtype, root, comm)`

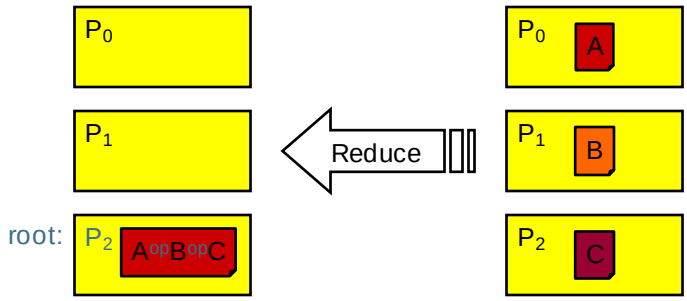
- Collects `data` from process group at `root` process



MPI Collective Operations III

`MPI_Reduce(sendbuf, recvbuf, num, dt, op, root, comm)`

- Collects data from process group at `root` process by reducing it to single value using operation `op` (e.g. sum)



`MPI_Allreduce(sendbuf, recvbuf, num, dt, op, comm)`

- Variant of `MPI_Reduce` where all processes receive the result

Example: Max value of Polynomial (serial)

```
program poly_max_serial
integer           :: i,nsteps
double precision  :: x,y,ymax,step,coeff(4),xmin,xmax

open(1, file="poly.dat")
read(1,*) coeff, xmin, xmax, nsteps

ymax = -huge(x)
   x = xmin
step = (xmax - xmin) / (nsteps - 1)
do i = 1, nsteps
   y = coeff(4)*x**3 + coeff(3)*x**2 + coeff(2)*x + coeff(1)
   ymax = max(ymax, y)
   x = x + step
end do

write(*,*) "Maximum is ", ymax
end program
```

MPI Work Distribution

JÜLICH FORSCHUNGSZENTRUM

Sequential 0

```
do i = 1, N
   call work(i)
end do
```

Cyclic 0 1 2 3 4 5 6 7 8 9

```
do i = rank+1, N, numprocs
   call work(i)
end do
```

Block 0 1 2 3 4 5 6 7 8 9

```
c    = N / numprocs
low  = rank*c + 1
high = low + c - 1
if (rank==numprocs-1) &
  high = N

do i = low, high
   call work(i)
end do
```

Block balanced 0 1 2 3 4 5 6 7 8 9

```
c    = N / numprocs
r    = mod(N,numprocs)
low = rank*c + min(rank,r) + 1
if (rank<r) c = c + 1
high = low + c - 1

do i = low, high
   call work(i)
end do
```


Work Distribution of Polynomial Example

JÜLICH FORSCHUNGSZENTRUM

```
   x = xmin
step = (xmax - xmin) / (nsteps - 1)
do i = 1, nsteps
   y = coeff(4)*x**3 + coeff(3)*x**2 + coeff(2)*x + coeff(1)
   ymax = max(ymax, y)
   x = x + step
end do
```

```
step = (xmax - xmin) / (nsteps - 1)
do i = myrank+1, nsteps, numprocs
   x = xmin + (i-1) * step
   y = coeff(4)*x**3 + coeff(3)*x**2 + coeff(2)*x + coeff(1)
   lmax = max(lmax, y)
end do
```

Example: Max value of Polynomial (MPI) I

```
program poly_max_mpi
include 'mpif.h'
integer          :: i,ierr,myrank,numprocs
double precision :: x,y,ymax,lmax,step,coeff(4),domain(3)

call MPI_Init(ierr)
call MPI_Comm_rank(MPI_COMM_WORLD, myrank, ierr)
call MPI_Comm_size(MPI_COMM_WORLD, numprocs, ierr)

if ( myrank == 0 ) then
  open(1, file="poly.dat")
  read(1,*) coeff, domain
endif

call MPI_Bcast(coeff, 4, MPI_DOUBLE_PRECISION, 0, &
               MPI_COMM_WORLD, ierr)
call MPI_Bcast(domain, 3, MPI_DOUBLE_PRECISION, 0, &
               MPI_COMM_WORLD, ierr)
```


Example: Max value of Polynomial (MPI) II

```
lmax = -huge(x)
step = (domain(2) - domain(1)) /  (domain(3) - 1)
do i = myrank+1, domain(3), numprocs
   x = domain(1) + (i-1) * step
   y = coeff(4)*x**3 + coeff(3)*x**2 + coeff(2)*x + coeff(1)
   lmax = max(lmax, y)
end do

call MPI_Reduce(lmax, ymax, 1, MPI_DOUBLE_PRECISION, &
                MPI_MAX, 0, MPI_COMM_WORLD, ierr)

if ( myrank == 0 ) then
  write(*,*) "Maximum is ", ymax
endif

call MPI_Finalize(ierr)
end program
```

Example: PI Calculation (serial)

```
program pi_serial                    ! Approximate π with
integer          :: i,n              ! n-point rectangle
double precision :: x,sum,pi,h       ! quadrature rule

open(1, file="pi.dat")
read(1,*) n                          ! Number of rectangles

h = 1.0d0 / n
sum = 0.0d0
do i = 1, n
   x = (i - 0.5d0)*h
   sum = sum + (4.d0/(1.d0 + x*x))
end do
pi = h * sum

write(*, fmt="(A, F16.12)") "Value of pi is ", pi
end program
```


Example: PI Calculation (MPI) I

```
program pi_mpi
include 'mpif.h'
integer          :: i,n,ierr,myrank,numprocs
double precision :: x,sum,pi,h,mypi

call MPI_Init(ierr)
call MPI_Comm_rank(MPI_COMM_WORLD, myrank, ierr)
call MPI_Comm_size(MPI_COMM_WORLD, numprocs, ierr)

if ( myrank == 0 ) then
   open(1, file="pi.dat")
   read(1,*) n
end if

call MPI_Bcast(n, 1, MPI_INTEGER, 0, MPI_COMM_WORLD, ierr)

...
```

Example: PI Calculation (MPI) II

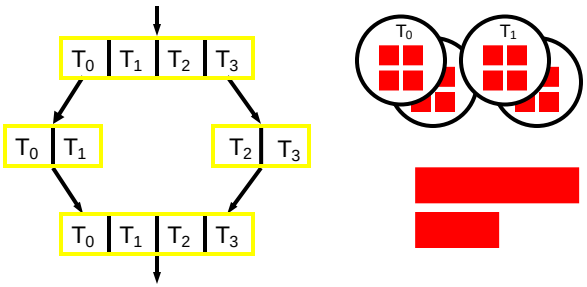
```
...
h = 1.0d0 / n
sum = 0.0d0
do i = myrank+1, n, numprocs
   x = (i - 0.5d0)*h
   sum = sum + (4.d0/(1.d0 + x*x))
end do
mypi = h * sum

call MPI_Reduce(mypi, pi, 1, MPI_DOUBLE_PRECISION, &
                MPI_SUM, 0, MPI_COMM_WORLD, ierr)

if ( myrank == 0 ) then
  write(*, fmt="(A, F16.12)") "Value of pi is ", pi
endif

call MPI_Finalize(ierr)
end program
```


MPI Evaluation

- **Advantages**
  - Supplies communication, synchronization, and I/O variations and optimized functions for a wide range of needs
  - Supported by all major parallel computer vendors; optimized for the vendor's hardware
  - Free open-source versions available (MPICH, OpenMPI,…)
  - About 130 functions (MPI 1), now 320 functions (MPI 2)
  - But basic programs can be implemented with 10 to 20 functions ⇨ gentle learning curve
- **Disadvantages**
  - High programming overhead
    - explicit data distribution, communication, and synchronization
  - Separate sequential and parallel version of program necessary

⇨ **MPI codes help preserve your investment as systems change!**

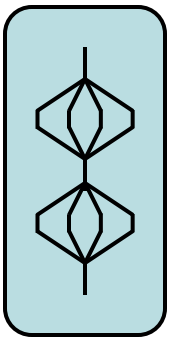
Programming Models: Shared Memory



- Global ("sequential") style
- Work distribution onto **threads** for global operations
- Domain decomposition determines work distribution
- All processors can access all memory: however **shared + private data**
- Directive-based programming with **OpenMP** or explicit threading (e.g. POSIX threads)

OpenMP Overview

- OpenMP: **Open** specification for **M**ulti **P**rocessing
- De-facto **standard** programming interface for portable **shared memory** programming
  - ⇨ **Does NOT work on distributed memory systems!**
- Based on **Directives** for Fortran 77/90 and **pragmas** for C/C++, library routines and environment variables
- Explicit (not automatic) programming model
  - ⇨ **Does NOT check correctness of directives!**
- **Fork-join model** resulting in a global program
- http://www.openmp.org
- http://www.compunity.org



History

- Proprietary designs by some vendors (SGI, CRAY, SUN, IBM, …) end of the 1980's
- Different unsuccessful attempts to standardize API
  - PCF
  - ANSI X3H5
- OpenMP-Forum founded to define portable API
  - 1997 first API for Fortran (V1.0)
  - 1998 first API for C/C++ (V1.0)
  - 2000 Fortran V2.0
  - 2002 C/C++ V2.0
  - 2005 combined C/C++/Fortran specification V2.5
  - 2008 V3.0
  - 2011 V3.1

OpenMP Functionality

- Directives/pragmas
  - **Parallel regions** (execute the same code in parallel)
  - **Parallel loops** (execute loop iterations in parallel)
  - **Parallel sections** (execute different sections in parallel)
  - **Tasks** (dynamically create and execute tasks in parallel, since V3.0)
  - Execution by exactly one single or master thread
  - Shared and private data
  - Reductions
  - Synchronization primitives (Barrier, Critical region, Atomic)
- Run-time library functions
  - omp_get_num_threads(), omp_get_thread_num()
  - omp_set_lock(), omp_unset_lock(), …
- Environment variables
  - OMP_NUM_THREADS, …

OpenMP Execution Model

JÜLICH FORSCHUNGSZENTRUM

Program:

```
a = 1

a = 2

do i = 1,9
   call work(i)
enddo

a = 3
```

(Sequential) Execution:

Thread$_0$

```
a = 1

a = 2

i=1..9:
  work(i)
enddo

a = 3
```


OpenMP Execution Model

JÜLICH FORSCHUNGSZENTRUM

Program:

```
a = 1
!$omp parallel
a = 2

do i = 1,9
   call work(i)
enddo
!$omp end parallel
a = 3
```

(Parallel) Execution:

Thread$_0$ Thread$_1$ Thread$_2$

```
a = 1
```

parallel region

```
a = 2        a = 2        a = 2

i=1..9:      i=1..9:      i=1..9:
  work(i)      work(i)      work(i)
enddo        enddo        enddo
```

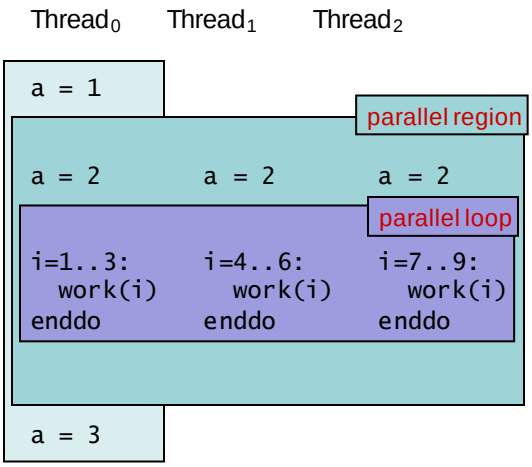
```
a = 3
```

OpenMP Execution Model

Program:

```
a = 1
!$omp parallel
a = 2
!$omp do
do i = 1,9
   call work(i)
enddo
!$omp end parallel
a = 3
```

(Parallel) Execution:



Example: Hello World (OpenMP), Fortran

```
program main
integer :: myid, nthreads
integer :: OMP_Get_num_threads, OMP_Get_thread_num

!$omp parallel private(myid, nthreads)
myid = OMP_Get_thread_num()
nthreads = OMP_Get_num_threads()

write(*,*) "hello from", myid, "of", nthreads
!$omp end parallel

end program
```

Example: Hello World (OpenMP), C

```
#include <stdio.h>
#include <omp.h>

int main() {
  int myid, nthreads;

  #pragma omp parallel private(myid, nthreads)
  {
    myid = omp_get_thread_num();
    nthreads = omp_get_num_threads();

    printf("hello from %d of %d\n", myid, nthreads);
  }
}
```


OpenMP 3.0 – Introducing Tasks

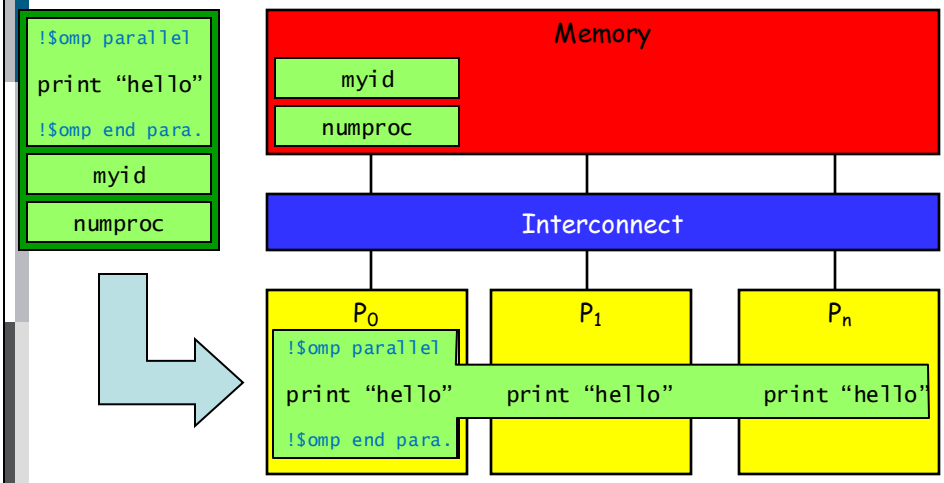
- Tasks describe independent chunks of work
- Useful for:
  - Tree traversals
  - Linked lists
  - Recursive algorithms
- Basic usage (C):

```
void process_leaf(int nodeID)
{
...
  #pragma omp task
  {
    process_leaf( left_childID[ nodeID ] );
  }
...
}
```

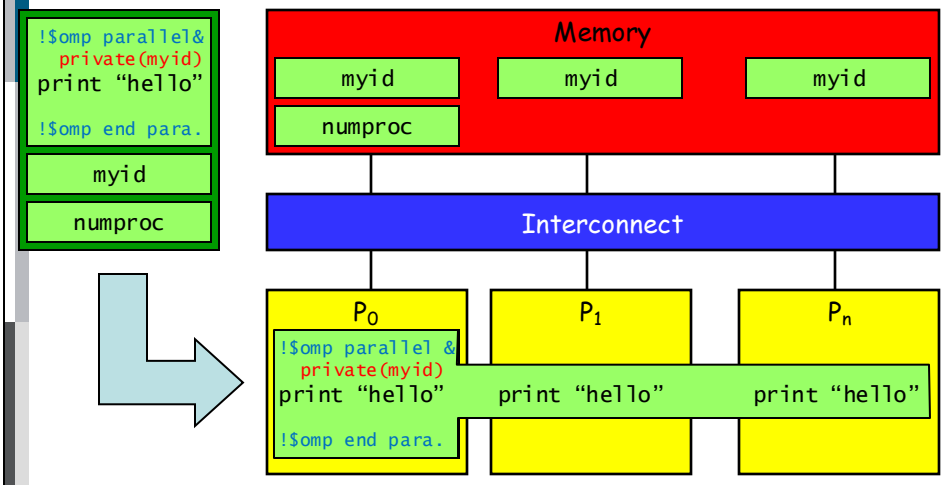
Compiling and Executing OpenMP Programs

- OpenMP compilation triggered by **compiler options**
  - otherwise OpenMP directives/pragmas get ignored
  - option is compiler-specific:
    - GNU: `-fopenmp`
    - Intel: `-openmp`
    - IBM XL: `-qsmp=omp`
    - PGI: `-mp`
    - Oracle: `-xopenmp`
    - NEC: `-Popenmp`
- OpenMP programs are executed **like sequential programs**
  - Parallelism specified by environment variable `OMP_NUM_THREADS`
  - Batch jobs: allocate extra cores for additional threads

Running OpenMP I



Running OpenMP II



Example: Max value of Polynomial (OpenMP)

```
program poly_max_omp
integer           :: i,nsteps
double precision  :: x,y,ymax,step,coeff(4),xmin,xmax

open(1, file="poly.dat")
read(1,*) coeff, xmin, xmax, nsteps

ymax = -huge(x)
step = (xmax - xmin) / (nsteps - 1)
!$omp parallel do private(x,y) reduction(max:ymax)
do i = 1, nsteps
   x = xmin + (i-1) * step
   y = coeff(4)*x**3 + coeff(3)*x**2 + coeff(2)*x + coeff(1)
   ymax = max(ymax, y)
end do

write(*,*) "Maximum is ", ymax
end program
```

Example: PI Calculation (OpenMP)

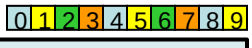
```
program pi_omp
integer          :: i,n
double precision :: x,sum,pi,h

open(1, file="pi.dat")
read(1,*) n

h = 1.0d0 / n
sum = 0.0d0
!$omp parallel do private(x) reduction(+:sum)
do i = 1, n
   x = (i - 0.5d0)*h
   sum = sum + (4.d0/(1.d0 + x*x))
end do
pi = h * sum

write(*, fmt="(A, F16.12)") "Value of pi is ", pi
end program
```


OpenMP Work Distribution

Sequential

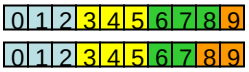

```
do i = 1, N
   call work(i)
end do
```

Cyclic




```
!$omp do schedule(static,1)
do i = 1, N
   call work(i)
end do
```

Block




```
!$omp do schedule(static)
do i = 1, N
   call work(i)
end do
```

- OpenMP also provides:
  - `schedule(dynamic [, chunk])`
  - `schedule(guided [, chunk])`

OpenMP Evaluation

JÜLICH FORSCHUNGSZENTRUM

- **Advantages**
  - Stable standard
  - Supported by all major parallel computer + compiler vendors; optimized for the vendor's hardware
  - Lean: simple and limited set of compiler directives
  - Ease of use
    - supports incremental parallelization
    - Sequential version = parallel version
- **Disadvantages**
  - Only works on shared memory machines
  - Requires special compiler
    - ⇨ GNU OpenMP since V4.2
  - Danger of missing or incorrect synchronization
  - Getting efficient parallel implementation often hard

2012 JSC 125

Low-Level GPGPU Programming

JÜLICH FORSCHUNGSZENTRUM

- Proprietary programming languages or extensions
  - NVIDIA: **CUDA** (C/C++ based)
  - AMD: StreamSDK or **Brooks+** (C/C++ based)
- **OpenCL** (Open Computing Language)
  - Open standard for portable, parallel programming of heterogeneous parallel computing
  - CPUs, GPUs, and other processors
- **Major rewriting of the code required, not portable**

⇨ Best performance, usually only needed for
  - Important kernels
  - Libraries

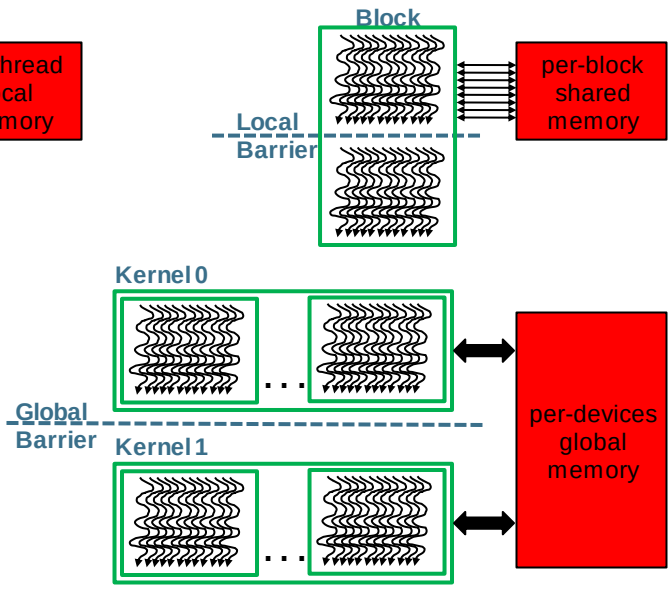
2012 JSC 126

High-Level GPGPU Programming

- Compilation systems with (OpenMP-like) **directives for GPU programming**
  - User tells compiler which part of code to accelerate
  - Portland Group Fortran and C compilers
    - http://www.pgroup.com/resources/accel.htm
  - CAPS HMPP (Fortran, C)
    - http://www.caps-enterprise.com/hmpp.html
  - **OpenACC** joint-venture by:
    - NVIDIA
    - Portland Group
    - CRAY
    - CAPS
    - http://www.openacc-standard.org

OpenACC DIRECTIVES FOR ACCELERATORS

CUDA Hierarchical Programming Model



- **Threads** are grouped into **blocks**
- **Blocks** are grouped into a **grid**
- A **kernel** is executed as a **grid** of **blocks** of **threads**

EXAMPLE: CUDA saxpy Code

```
/* -- Sequential Version ------------------------------- */
void saxpy_s(int n, float a, float x[], float y[])
{
   for (int i=0; i<n; ++i)
      y[i] = a * x[i] + y[i];
}
saxpy_s(n, 2.0, x, y);

/* -- CUDA Parallel Version ----------------------------- */
__global__ void saxpy_p(int n, float a, float x[], float y[])
{
   int i = blockIdx.x * blockDim.x + threadIdx.x;
   if (i < n) y[i] = a * x[i] + y[i];
}
/* -- Invoke kernel with 256 threads/block
int nblocks = (n + 255) / 256;
saxpy_p<<<nblocks, 256>>>(n, 2.0, x, y);
```


EXAMPLE: Jacobi Relaxation

The Portland Group

```
change = tolerance + 1.0
do while(change > tolerance)
  change = 0
  do i = 2, m-1
    do j = 2, n-1
      newa(i,j) = w0*a(i,j) + &
          w1 * (a(i-1,j) + a(i,j-1) + &
                a(i+1,j) + a(i,j+1)) + &
          w2 * (a(i-1,j-1) + a(i-1,j+1) + &
                a(i+1,j-1) + a(i+1,j+1))
      change = max(change,abs(newa(i,j)-a(i,j)))
    enddo
  enddo
  a(2:m-1,2:n-1) = newa(2:m-1,2:n-1)
enddo
```

EXAMPLE: Device-side CUDA C Kernel Ia

The Portland Group

```
extern "C" __global__ void
jacobikernel( float* a, float* anew, float* lchange, int n, int m )
{
  int ti = threadIdx.x, tj = threadIdx.y; /* local indices */
  int i = blockIdx.x*16+ti;               /* global indices */
  int j = blockIdx.y*16+tj;
  __shared__ float mychange[16*16], b[18][18];

  b[tj][ti] = a[(j-1)*m+i-1];
  if(i<2) b[tj][ti+16] = a[(j-1)*m+i+15];
  if(j<2) b[tj+16][ti] = a[(j+15)*m+i-1];
  if(i<2&&j<2) b[tj+16][ti+16] = a[(j+15)*m+i+15];
  __syncthreads();

  mya = w0 * b[tj+1][ti+1]  +
        w1 * (b[tj+1][ti]   + b[tj][ti+1]    +
              b[tj+1][ti+2] + b[tj+2][ti+1]) +
        w2 * (b[tj][ti]     + b[tj+2][ti]    +
              b[tj][ti+2]   + b[tj+2][ti+2]);
  newa[j][i] = mya;
```


EXAMPLE: Device-side CUDA C Kernel Ib

The Portland Group

```
/* this thread's "change" */
  mychange[ti+16*tj] = fabs(mya,b[tj+1][ti+2]);
  __syncthreads();

  /* reduce all "change" values for this thread block
   * to a single value */
  n = 256;
  while( n <<= 1 ){
    if( tx+ty*16 < n )
    mychange[ti+tj*16] = fmaxf( mychange[ti+tj*16],
                                mychange[ti+tj*16+n]);
    __syncthreads();
  }
  /* store this thread block's "change" */
  if(tx==0&&ty==0)
    lchange[blockIdx.x+blockDim.x*blockIdx.y]
                                      = mychange[0];
}
```

EXAMPLE: Device-side CUDA C Kernel II

The Portland Group

```
/*reduce all thread block's "change" values*/
extern “C” __global__ void
reduction( float* lchange, int n )
{
  __shared__ float mychange[256];
  float mych = lchange[i];
  int i = threadIdx.x, m = n;
  while( m <= n ){
    mych = fmaxf(mych,lchange[m]);
    m += n;
  }
  mychange[i] = mych;
  __syncthreads();
  n = 256;
  while( n <<= 1 ){
    if(i<n) mychange[i] = fmaxf(mychange[i],mychange[i+n]);
    __syncthreads();
  }
  if(i==0) change = mychange[0];
}
```


EXAMPLE: Device-side CUDA C Kernel III

The Portland Group

```
/* Update 'a' from 'newa */
extern "C" __global__ void
updatekernel( float* a, float* anew, int n, int m )
{
  int i = blockIdx.x*16 + threadIdx.x;
  int j = blockIdx.y*16 + threadIdx.y;
  a[j*m+i] = newa[j*m+i];
}
```

EXAMPLE: Host-side CUDA C GPU Control Code

The Portland Group

```
__device__ float dchange;  float change;

memsize = sizeof(float)*n*m

cudaMalloc( &da, memsize );  cudaMalloc( &dnewa, memsize );
cudaMalloc( &lchange, (n/16)*(m/16) );
cudaMemcpy( da, a, memsize, cudaMemcpyHostToDevice );

do{
  dim3 threads( 16, 16 );  dim3 blocks( n/16, m/16 );
  jacobikernel<<<blocks,threads>>>( da, dnewa, lchange, n, m );
  reduction<<<1,256>>>( lchange, (n/16)*(m/16) );
  updatekernel<<<blocks,threads>>>( da, dnewa, n, m );
  cudaMemcpy( &change, &dchange, sizeof(float),
        cudaMemcpyDevicetoHost );
}while( change > tolerance );

cudaMemcpy( a, dnewa, memsize, cudaMemcpyDeviceToHost );
cudaFree( da ); cudaFree( dnewa ); cudaFree( lchange );
```


OpenACC

OpenACC DIRECTIVES FOR ACCELERATORS

- High-level programming model, similar to OpenMP
- Joint-venture to develop an open, portable standard
- All members are part of the OpenMP language committee
- Compilers have preliminary support, full support announced for Q4/2012

- Tuning is done by specifying data regions for which data:
  - Can reside on the GPU over several iterations
  - Can be shared between different loop regions
  - Is only needed locally on the GPU
- Compiler developers focus on implementing good optimization schemes themselves

CAPS CRAY THE SUPERCOMPUTER COMPANY NVIDIA The Portland Group

OpenACC – Basic Usage

OpenACC DIRECTIVES FOR ACCELERATORS

JÜLICH FORSCHUNGSZENTRUM

- Manage **execution** on device:

```
#pragma acc parallel [clauses]
#pragma acc kernels [clauses]
#pragma acc loop [clauses]
```

Combined directives:

```
#pragma acc parallel loop [clauses]
#pragma acc kernels loop [clauses]
```

- Implicit **data movement** with „hints“ from the programmer:

```
#pragma acc data [clauses]
```

- Internal Control Variables (ICVs)
  - Set via environment variables
  - Query and set via runtime functions

EXAMPLE: OpenACC Version

JÜLICH FORSCHUNGSZENTRUM

```
!$acc data copy(a) create(newa)
  do while(change > tolerance)
    !$acc kernels
    change = 0
    !$acc loop collapse(2) reduction(max:change)
    do i = 2, m-1
      do j = 2, n-1
        newa(i,j) = w0*a(i,j) + &
            w1 * (a(i-1,j) + a(i,j-1) + &
                  a(i+1,j) + a(i,j+1)) + &
            w2 * (a(i-1,j-1) + a(i-1,j+1) + &
                  a(i+1,j-1) + a(i+1,j+1))
        change = max(change,abs(newa(i,j)-a(i,j)))
      enddo
    enddo
    a(2:m-1,2:n-1) = newa(2:m-1,2:n-1)
    !$acc end kernels
  enddo
!$acc end data
```

CAPS HMPP Directives

- **Codelet** is a pure function that can be remotely executed on a GPU

```
#pragma hmpp myfunc codelet, target=GPU, …
void saxpy(int n, float alpha, float x[n], float y[n]){
  #pragma hmppcg parallel
  for(int i = 0; i<n; ++i)
    y[i] = alpha*x[i] + y[i];
}
```

- **Regions** are a short cut for writing codelets
- **Target clause** specifies what GPU code to generate
  - *GPU* can be CUDA or OpenCL
  - The runtime selects out of the available hardware and code

```
#pragma hmpp myreg region, …
{
  for(int i = 0; i<n; ++i)
    y[i] = alpha*x[i] + y[i];
}
```

- Parallel loops are the code constructs converted in GPU threads
  - **Directive hmppcg parallel** forces parallelization
  - Two levels of parallelism can be used to generate the threads

CAPS HMPP: Tuning

- Tuning hybrid CPU/GPU code consists of
  - Reducing penalty when allocating and releasing GPUs
  - Reducing data transfer time
    - Reduce data transfer occurrences
    - Share data on the GPU between codelets
    - Map codelet arguments to the same GPU space
    - Perform partial data transfers
  - Optimizing performance of the GPU kernels
    - Loop tiling, splitting, …
    - Reductions
    - Select right level of GPU memory (global, local, …)
  - Using CPU cores in parallel with the GPU
- **HMPP provides a set of directives to address these optimizations**

Advantages of Pragma/directives-based GPU Programming

- "Only" need to add pragmas/directives
  - Single Code for "normal" and accelerated version
  - Incremental program migration
  - Minimal code changes
- Auto-generated
  - Data allocation and transfers
  - Reductions
  - (Partially) Heuristics for thread block size and shape
- "Standard" tool chain
- Potential for future portability

Dual Level Parallelism

- Often: Applications have two natural levels of parallelism.
  - If possible, take advantage of it and exploit by using OpenMP within an SMP node and by using MPI between nodes
- Why ?
  - MPI performance degrades when
    - Domains become too small
    - Message latency dominates computation
    - Parallelism is exhausted
  - OpenMP
    - Typically has lower latency
    - Can maintain speedup at finer granularity
- **Drawback:**
  - Programmer must know MPI and OpenMP
  - Code might be harder to debug, analyze and maintain

Hybrid Programming

- Many of today's most powerful computers employ both shared memory and distributed memory architectures
  ⇨ **hybrid systems**
- The corresponding hybrid programming model is a combination of shared and distributed memory programming
  - MPI and OpenMP
  - MPI and POSIX threads
  - MPI and multi-threaded libraries
- **Can** give better scalability than pure MPI or OpenMP
- Upcoming systems with accelerators complicate the situation:
  - Hybrid programming will become the norm:
    - Multi-threaded + accelerators
    - MPI + multi-threaded + accelerators

DEBUGGING AND PERFORMANCE ANALYSIS

Performance Properties of Parallel Programs

- Factors which influence performance of parallel programs
  - "Sequential" factors
    - Computation
    - ⇨ **Choose right algorithm, use optimizing compiler**
    - Cache and memory
    - ⇨ **Tough! Not many tools yet, hope compiler gets it right**
    - Input / output
    - ⇨ **Not given enough attention**
  - "Parallel" factors
    - Communication (Message passing)
    - Threading
    - Synchronization
    - ⇨ **More or less understood, tool support**
    - Accelerators
    - ⇨ **Tough! Very little, simple tools for now**

Metrics of Performance

- What can be measured?
  - A **count** of how many times an event occurs
  - The **duration** of some time interval
  - The **size** of some parameter
- Derived metrics (e.g., rates) needed for normalization
- Typical metrics
  - **Execution** time
  - **MIPS**
    - Millions of instructions executed per second
  - **MFLOPS/GFLOPS**
    - Millions/billions of floating-point operations per second
  - Cache or TLB misses
  - …

"math" Operations?
HW Operations?
HW Instructions?
32-/64-bit? …

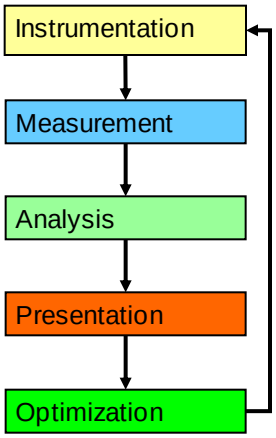
Example: Time Measurement (MPI)

```
program main
include 'mpif.h'
integer :: ierr, myrank, numprocs
double precision :: starttime, endtime  !double in C/C++

call MPI_Init(ierr)
call MPI_Comm_rank(MPI_COMM_WORLD, myrank, ierr)
call MPI_Comm_size(MPI_COMM_WORLD, numprocs, ierr)

starttime = MPI_Wtime()
write(*,*) "hello from", myrank, "of", numprocs
endtime = MPI_Wtime()
write(*,*) myrank, "used", endtime-starttime, "seconds"

call MPI_Finalize(ierr)
end program
```


Example: Time Measurement (OpenMP)

```
program main
integer :: myid, nthreads
integer :: OMP_Get_num_threads, OMP_Get_thread_num
double precision :: OMP_Get_wtime, starttime, endtime

starttime = OMP_Get_wtime()
!$omp parallel private(myid)
myid = OMP_Get_thread_num()
nthreads = OMP_Get_num_threads()

write(*,*) "hello from", myid, "of", nthreads
!$omp end parallel
endtime = OMP_Get_wtime()
write(*,*)"used", endtime-starttime, "seconds"

end program
```

Performance Measurement Cycle



- Insertion of extra code (probes, hooks) into application
- Collection of data relevant to performance analysis
- Calculation of metrics, identification of performance problems
- Transformation of the results into a representation that can be easily understood by a human user
- Elimination of performance problems

Performance Measurement

- Two dimensions
  - **When** performance measurement is triggered
    - **Externally** (asynchronous) ⇨ indirect measurement
      - Sampling
        - » Timer interrupt
        - » Hardware counters overflow
    - **Internally** (synchronous) ⇨ direct measurement
      - Code instrumentation
        - » Automatic or manual instrumentation
  - **How** performance data is recorded
    - **Profile** ::= Summation of events over time
      - run time summarization (functions, call sites, loops, …)
    - **Trace file** ::= Sequence of events over time

Measurement Methods: Profiling I

- Recording of **aggregated information**
  - Time
  - Counts
    - Calls
    - Hardware counters
- **about program and system entities**
  - Functions, call sites, loops, basic blocks, …
  - Processes, threads
- Statistical information: min, max, mean and total number of values

- Methods to create a profile
  - PC sampling (statistical approach)
  - Interval timer / direct measurement (deterministic approach)

Profiling II

- **Sampling**
  - General **statistical** measurement technique based on the assumption that a subset of a population being examined is representative for the whole population
  - Running program is interrupted periodically
    - Operating system signal or Hardware counter overflow
    - Interrupt service routine examines return-address stack to find address of instruction being executed when interrupt occurred
      - Using symbol-table information this address is mapped onto specific subroutine
  - Requires long-running programs
- **Interval timing**
  - Time measurement at the beginning and at the end of a code region
  - Requires instrumentation + high-resolution / low-overhead clock

Profiling Tools

- **gprof**
  - Available on many systems
- **mpiP** (LLNL et al)
  - http://mpip.sourceforge.net
  - MPI profiler
  - single output file: data for all ranks
- **FPMPI-2** (ANL)
  - http://www.mcs.anl.gov/fpmpi/
  - MPI profiler
  - **special**: Optionally **identifies synchronization time**
  - single output file: count, sum, avg, min, max over ranks

Profiling Tools II

- **ompP** (UC Berkeley)
  - http://www.ompp-tool.com
  - OpenMP profiler
- **HPCToolkit** (Rice University)
  - http://www.hpctoolkit.org
  - Multi-platform sampling-based callpath profiler
  - Works on un-modified, optimized executables
- **Open|SpeedShop** (Krell Institute with support of LANL, SNL, LLNL)
  - http://www.openspeedshop.org
  - Comprehensive performance analysis environment

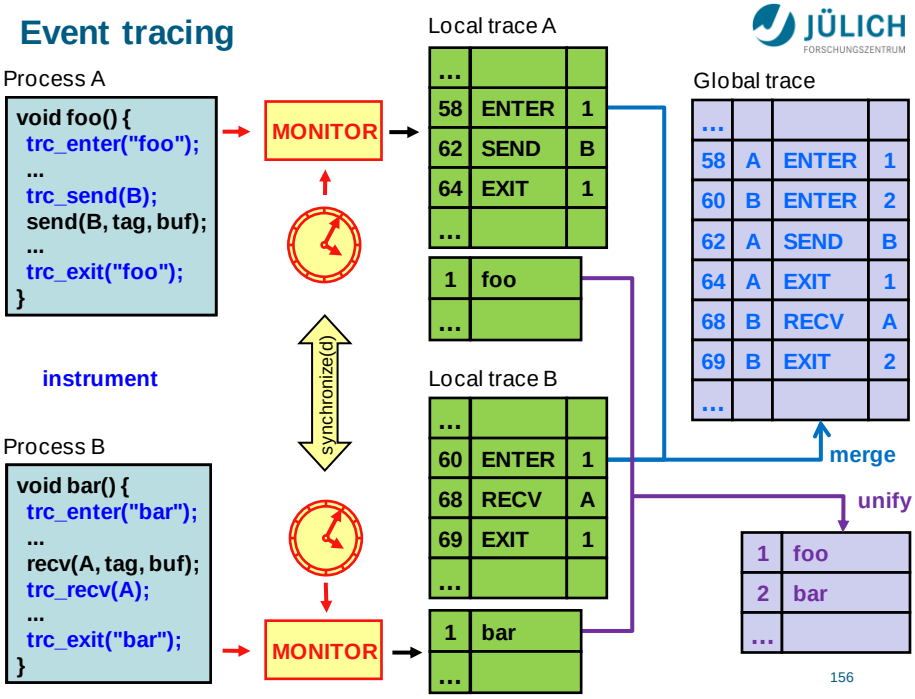
Measurement Methods: Tracing

- Recording **information about** significant points (**events**) during execution of the program
  - Enter/leave a code region (function, loop, …)
  - Send/receive a message …
- Save information in **event record**
  - Timestamp, location ID, event type
  - plus event specific information
- **Event trace** := stream of event records sorted by time

- Can be used to reconstruct the **dynamic behavior**
  ⇨ Abstract execution model on level of defined events

2012 JSC 155

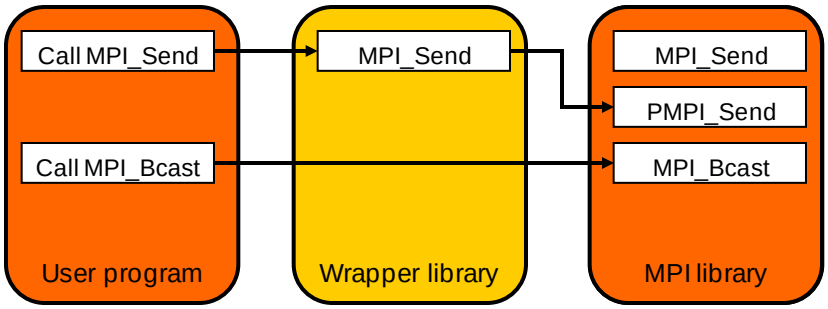
Event tracing



156

PMPI: The MPI Profiling Interface

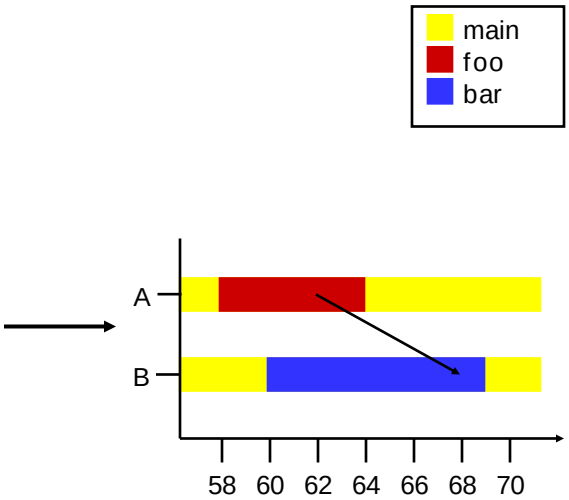
- PMPI allows selective replacement of MPI routines at link time
  ⇒ no re-compilation necessary
- Uses technique of **"wrapper"** function libraries
- Used by most MPI performance tools



Event Tracing: "Timeline" Visualization

1	foo
2	bar
3	...

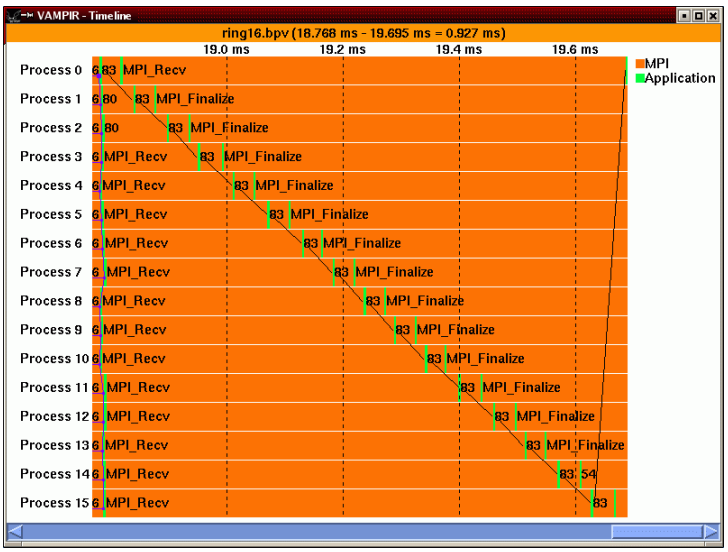
...			
58	A	ENTER	1
60	B	ENTER	2
62	A	SEND	B
64	A	EXIT	1
68	B	RECV	A
69	B	EXIT	2
...			



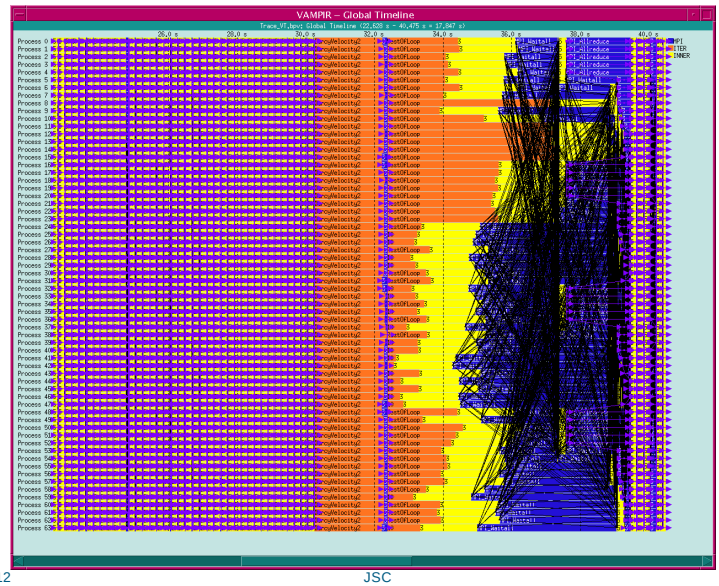
Tracing Tools

- **MPE / Jumpshot** (ANL)
  - Part of MPICH2
  - Only supports MPI P2P and collectives; SLOG2 trace format
- **VampirTrace / Vampir** (TU Dresden, ZIH)
  - http://www.tu-dresden.de/zih/vampirtrace/
  - http://www.vampir.eu
  - Open-source measurement system (VampirTrace) + commercial trace visualizer (Vampir); OTF trace format
- **Extrae / Paraver** (BSC/UPC)
  - http://www.bsc.es/paraver
  - Measurement system (Extrae) and visualizer (Paraver)
  - Powerful filter and summarization features
  - Very configurable visualization

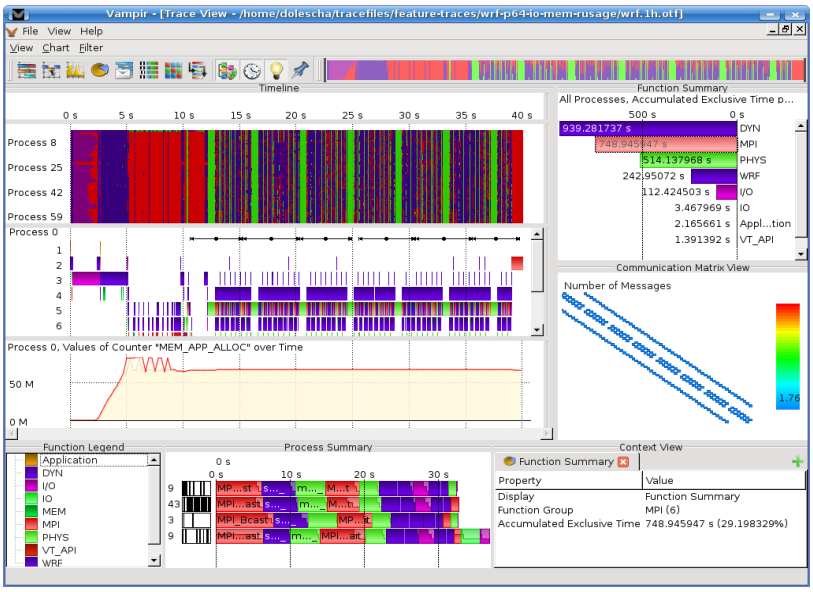
Example: Timeline of MPI Ring Program



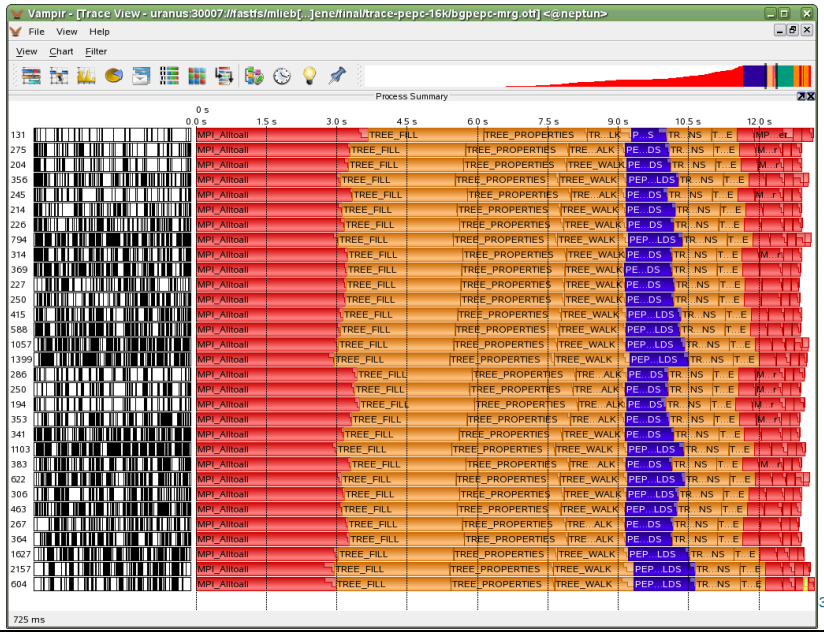
“Real World” Example



Vampir Event-Trace Displays



VampirServer: PEPC, 16384 PEs, Cluster Analysis

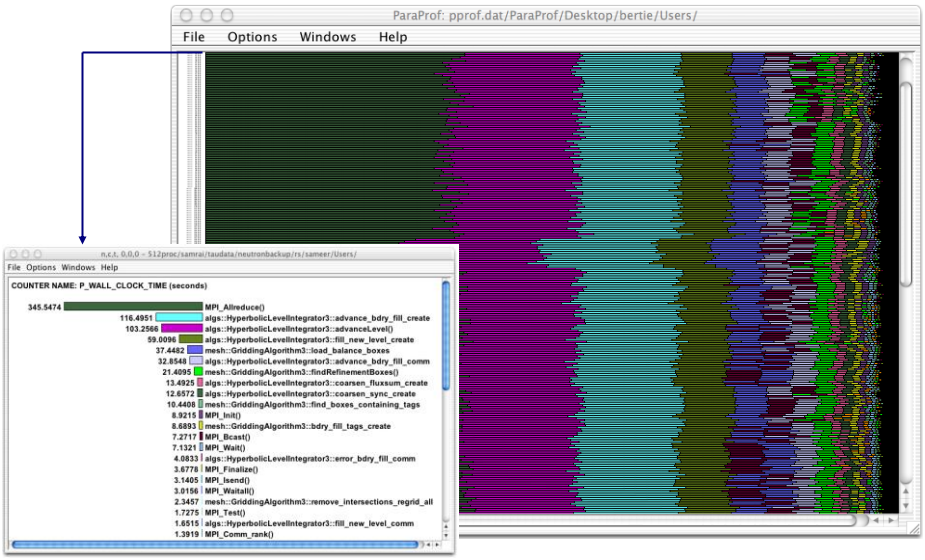


3

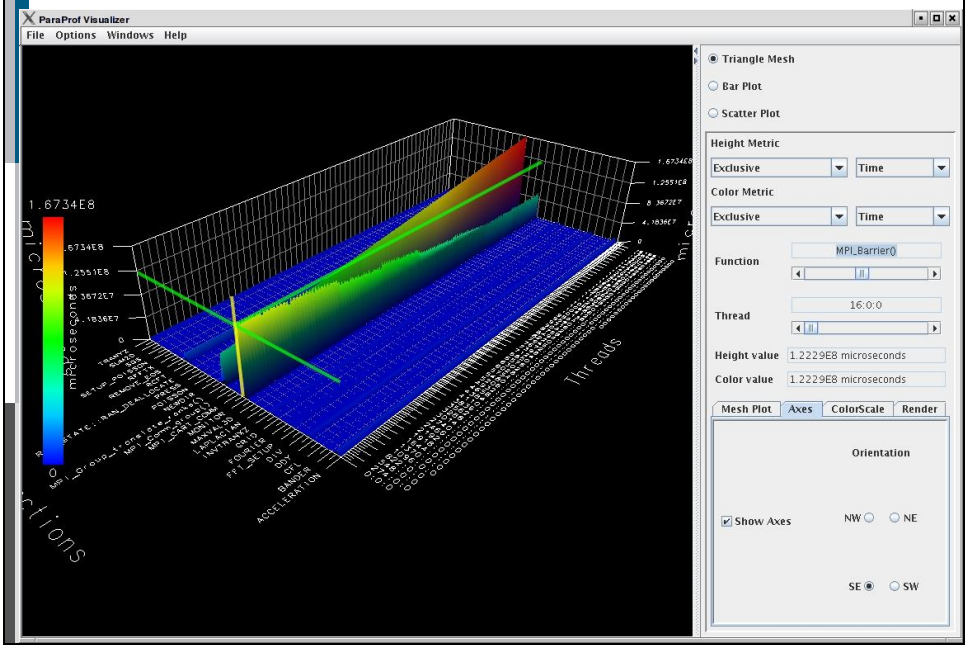
Profiling + Tracing Toolsets

- **TAU** (University of Oregon)
  - http://tau.uoregon.edu
  - Very versatile performance analysis toolset for profiling and tracing
  - Supports many platforms, programming paradigms, and languages
- **Scalasca** (JSC)
  - http://www.scalasca.org
  - Highly scalable call-path profiling
  - Automatic trace-based performance analysis
    - Detection, classification and ranking of common parallel programming bottlenecks
  - Supports many platforms, programming paradigms, and languages

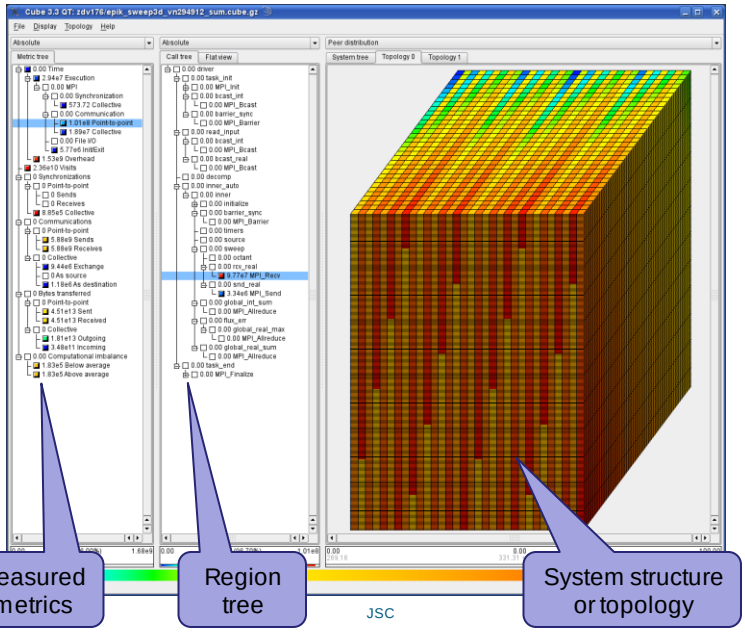
TAU Profiling, Large System



TAU ParaProf: 3D Profile, Miranda, 16K PEs



Scalasca Analysis sweep3D(294,912 Cores)



UNITE

- **UN**ified **I**ntegrated **T**ool **E**nvironment
- **http://apps.fz-juelich.de/unite/**
- Lower bar for inexperienced users and admins
  - Common usage and installation documentation
  - Download, build and install all the following tools from one package:
    - UNITE package installer and module package
    - Cube-3.4.2
    - Extrae-2.2.1
    - Marmot-2.4.0
    - OTF-1.10.2
    - Paraver-4.3.2
    - Pdtoolkit-3.17
    - Scalasca-1.4.2
    - TAU-2.21.2
    - UniMCI-1.0.1
    - Vampirtrace-5.12.2
    - Vampir-5.x or 7.x
    - VampirServer-1.x or 7.x

Debugging of Parallel Programs

- **… is much more difficult than sequential debugging!**
- Reasons
  - Multiplication of sequential bugs on multiple processes
  - Amount of resources to control and data to handle
  - Additional kind of bugs in parallel programs, e.g., **deadlocks**
  - **Non-deterministic behavior** ⇨ non reproducible behavior
    - **Race conditions**
    - **Heisenbugs**: bugs appear/disappear under debugging
- Commercial parallel debuggers (supporting MPI, threads, CUDA, …)
  - **DDT** (Allinea, UK)
    - http://www.allinea.com
  - **Totalview** (TotalView Technologies, Rogue Wave, USA)
    - http://totalviewtech.com

FUTURE ISSUES FOR HPC

Increasing Importance of Scaling

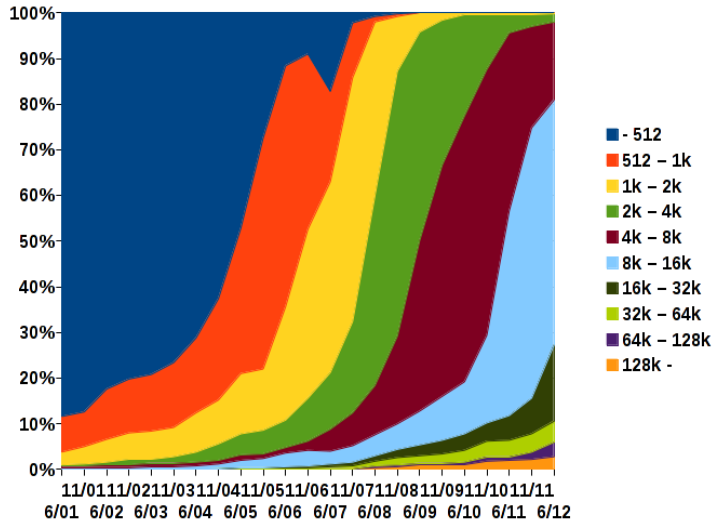
- Number of Cores share for TOP 500 Nov 2012

NCore	Count	Share	∑Rmax	Share	∑NCore
1025-2048	1	0.2%	122 TF	0.1%	1,280
2049-4096	9	1.8%	623 TF	0.5%	30,520
4097-8192	85	17.0%	7,500 TF	6.1%	581,728
8193-16384	268	53.6%	24,852 TF	20.1%	3,319,798
> 16384	137	27.4%	90,376 TF	73.2%	9,519,131
Total	500	100%	123,473 TF	100%	13,452,457

- **Average** system size: **26,904 cores**
- **Median** system size: **13,104 cores**

Increasing Importance of Scaling II

- Number of Cores share for TOP 500 Jun 2001 – Jun 2012



Observations

SOFTWARE DEVELOPMENT TOOLS FOR PETASCALE COMPUTING WORKSHOP
WASHINGTON, DC

From workshop report
SDTPC Aug 2007
http://www.csm.ornl.gov/workshops/Petascale07/

- **Petascale is not terascale scaled up!**
  - More than linear increase of scale
  - Multi-core processors
    - ⇨ Multi-mode parallelism
    - ⇨ Reduced memory per core
  - Heterogeneity via HW acceleration (Cell, FPGA, GPU, …)
    - ⇨ New programming models (needed)
    - ⇨ Higher system diversity
- More emphasis on
  - **Fault-tolerance** and **performability**
  - **Automated diagnosis and remediation**

2012 JSC 173

Projection for a Exascale System*

JÜLICH FORSCHUNGSZENTRUM

System attributes	2010	"2015"		"2018"		Difference 2010 & 2018
System peak	2 Pflop/s	200 Pflop/s		1 Eflop/sec		O(1000)
Power	6 MW	15 MW		~20 MW		
System memory	0.3 PB	5 PB		32-64 PB		O(100)
Node performance	125 GF	0.5 TF	7 TF	1 TF	10 TF	O(10) – O(100)
Node memory BW	25 GB/s	0.1 TB/sec	1 TB/sec	0.4 TB/sec	4 TB/sec	O(100)
Node concurrency	12	O(100)	O(1,000)	O(1,000)	O(10,000)	O(100) – O(1000)
Total Concurrency	225,000	$O(10^8)$		$O(10^9)$		O(10,000)
Total Node Interconnect BW	1.5 GB/s	20 GB/sec		200 GB/sec		O(100)
MTTI	days	O(1day)		O(1 day)		- O(10)

2012 * From http://www.exascale.org 174

IESP

- **International Exascale Software Project**
- International collaboration
  - Started Apr 2009
- http://www.exascale.org/

- Objectives
  - Develop international exascale (system) software roadmap
  - Investigate opportunities for international collaborations and funding
  - Explore governance structure and models for IESP

Roadmap Components

4.1 Systems Software
- 4.1.1 Operating systems
- 4.1.2 Runtime Systems
- 4.1.3 I/O systems
- 4.1.4 Systems Management
- 4.1.5 External Environments

4.2 Development Environments
- 4.2.1 Programming Models
- 4.2.2 Frameworks
- 4.2.3 Compilers
- 4.2.4 Numerical Libraries
- 4.2.5 Debugging Tools

4.3 Applications
- 4.3.1 Application Element: Algorithms
- 4.3.2 Application Support: Data Analysis and Visualization
- 4.3.3 Application Support: Scientific Data Management

4.4 Crosscutting Dimensions
- 4.4.1 Resilience
- 4.4.2 Power Management
- 4.4.3 Performance Optimization
- 4.4.4 Programmability

see IJHPCA, Feb 2011, http://hpc.sagepub.com/content/25/1/3

EESI

- **European Exascale Software Initiative**
- EU FP7
  - Funded Jun 2010 to Nov 2011
- http://www.eesi-project.eu/
- Objectives
  - Develop European exascale system and application software vision and roadmap
  - Investigate Europe's strengths and weaknesses
  - Identify sources of competitiveness for Europe
  - Investigate and propose programs in education and training for the next generation of computational scientists
- EESI2 will start September 2012

2012 JSC 177

Conclusion

- We **can** do performance analysis on the tera- and petascale, however…
  - Parallel Computing (PC?) might have reached the masses …

  - but remember, we do **High** Performance Computing (HPC!)

⇨ We need integrated teams / simulation labs / end stations / ..
⇨ To get integrated, customized tool support
⇨ Tool community needs to build up interoperable, reusable tool components implementing the various basic technologies

2012 JSC 178