First INFN International School on Architectures, tools and methodologies for developing efficient large scale scientific computing applications



1

Ce.U.B. - Bertinoro - Italy, 12 - 17 October 2009

Vincenzo Innocente "Software Architectures For Parallel Programming"

Implemented using

- std::thread
- OpenMP
- MPI

Goal of Today

- Learn a methodology to analyze a computational problem and provide a (optimal) parallel solution
- Review structural building blocks
 - Architectural & Design patterns
 - Algorithmic structures
 - Implementations
- Study few use cases
- Identify pitfalls, use measurement tools, apply optimization strategies

Resources

This lectures is largely based on

the excellent 2009 Par Lab Boot Camp – "Short Course on Parallel Programming"

http://parlab.eecs.berkeley.edu/bootcampagenda

- The OpenLab/Intel courses at CERN
- Examples and exercises use the latest C++0x proposed standard as implemented in gcc 4.4.1
 - Not finalized, implementation incomplete and buggy...
 - Very little doc (best: Anthony Williams <u>ongoing</u> blog)

Top-to-Bottom Parallelism

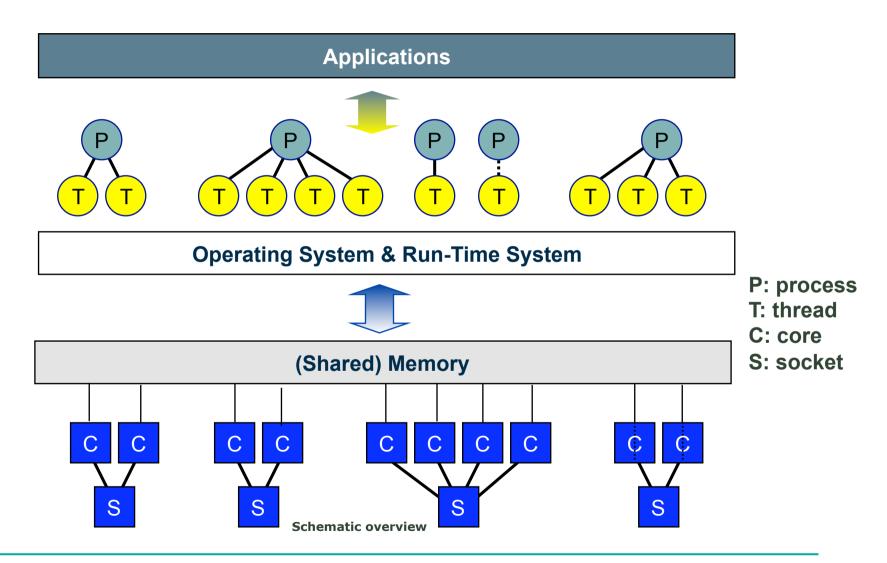
- Cluster/Grid/Cloud
- Multi-socket
- Multi-core
- Hyperthreading
- SIMD/Wide execution
- Pipelining
- Superscalar execution



Our 7 dimensions



Parallel Environments



(Parallel) Software Engineering

Engineering Parallel software follows the "usual" software development process with one difference: Think Parallel!

Analyze, Find & Design

Analyze problem, Finding and designing parallelism

Specify & Implement

How will you express the parallelism (in detail)?

Check correctness

How will you determine if the parallelism is right or wrong?

Check performance

How will you determine if the parallelism improves over sequential performance?

Foster's Design Methodology

Four Steps:

- Partitioning
 - Dividing computation and data
- Communication
 - Sharing data between computations
- Agglomeration
 - Grouping tasks to improve performance
- Mapping
 - Assigning tasks to processors/threads

From "Designing and Building Parallel Programs" by Ian Foster

Designing Threaded Programs

Partition

Divide problem into tasks

Communicate

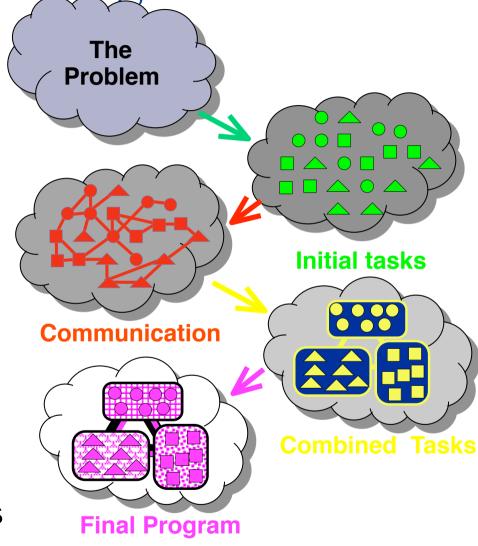
Determine amount and pattern of communication

Agglomerate

Combine tasks

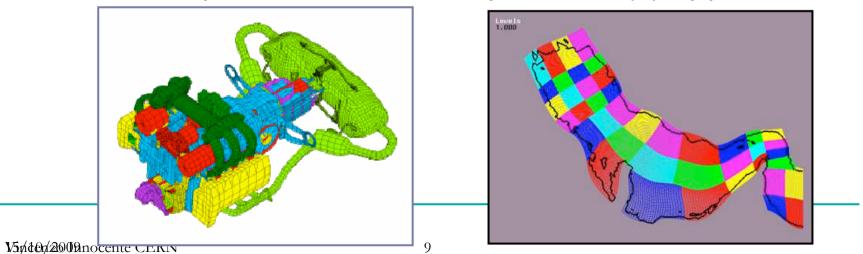
Map

 Assign agglomerated tasks to created threads



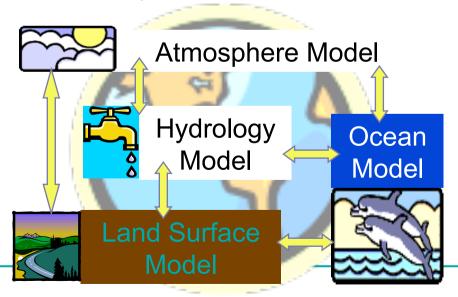
Domain (Data) Decomposition

- Exploit large datasets whose elements can be computed independently
 - Divide data and associated computation amongst threads
 - Focus on largest or most frequently accessed data structures
 - Data parallelism: same operations(s) applied to all



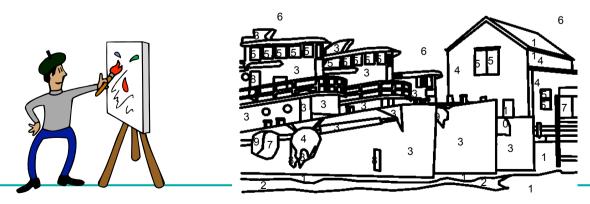
Functional Decomposition

- Divide computation based on a natural set of independent functions
 - Predictable organization and dependencies
 - Assign data for each task as needed
 - Conceptually a single data value or transformation is performed repeatedly



Activity (Task) Decomposition

- Divide computation based on a natural set of independent tasks
 - Non deterministic transformation
 - Assign data for each task as needed
 - Little communication
- Example: Paint-by-numbers
 - Painting a single colour is a single task



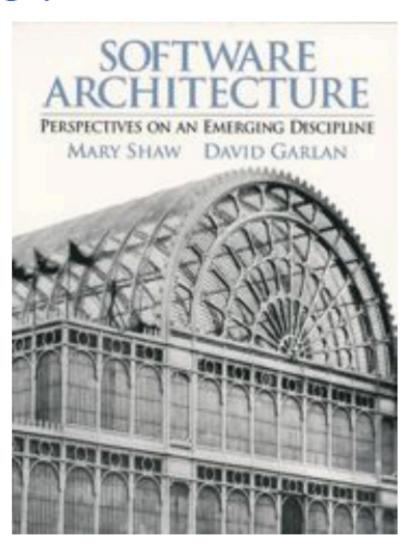
Structural programming patterns



- ■In order to create more complex software it is necessary to compose programming patterns
- ■For this purpose, it has been useful to induct a set of patterns known as "architectural styles"

■Examples:

- pipe and filter
- event based/event driven
- layered
- Agent and repository/ blackboard
- process control
- Model-view-controller

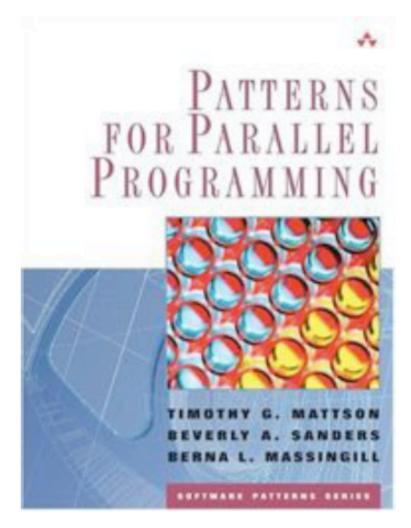




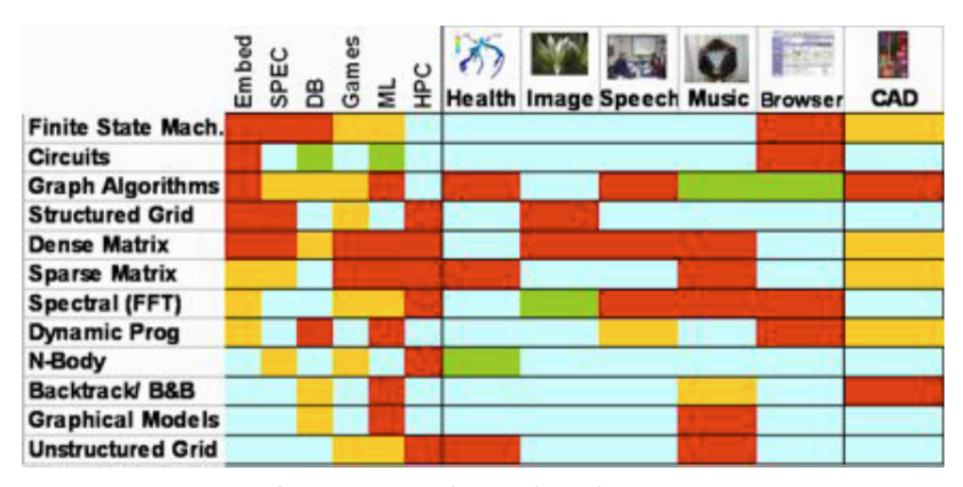
Patterns for Parallel Programming



- PLPP is the first attempt to develop a complete pattern language for parallel software development.
- PLPP is a great model for a pattern language for parallel software
- PLPP mined scientific applications that utilize a monolithic application style
 - PLPP doesn't help us much with horizontal composition
- Much more useful to us than: Design Patterns: Elements of Reusable Object-Oriented Software, Gamma, Helm, Johnson & Vlissides, Addison-Wesley, 1995.



Computational Patters



 Computational patterns describe the key computations but not how they are implemented



Productivity Layer

Our Pattern Language 2.0: Keutzer and Mattson



Applications

Choose your high level structure - what is the structure of my application? Guided expansion

Pipe-and-filter Agent and Repository Process Control Event based, implicit

invocation

Choose you high level architecture? Guided decomposition Task Decomposition ↔ Data Decomposition Group Tasks Order groups data sharing

Model-view controller Iteration Map reduce Layered systems Arbitrary Static Task Graph.

data access

Graph Algorithms Dynamic Programming Dense Linear Algebra Sparse Linear Algebra Unstructured Grids Structured Grids

Identify the key computational patterns - what are my key computations? Guided instantiation

Graphical models Finite state machines Backtrack Branch and Bound N-Body methods Circuits Spectral Methods

Refine the structure - what concurrent approach do I use? Guided re-organization

Event Based

Data Parallelism

Pipeline

Task Parallelism

Digital Circuits

Divide and Conquer

Geometric Decomposition

Discrete Event

Graph algorithms

Utilize Supporting Structures - how do I implement my concurrency? Guided mapping Master/worker **Efficiency** Layer Fork/Join Distributed Array CSP Shared Data

Shared Queue Shared Hash Table

Loop Parallelism

BSP SPMD

Implementation methods - what are the building blocks of parallel programming? Guided implementation

Thread Creation/destruction Message passing

Speculation

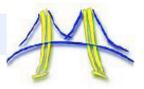
Barriers

Semaphores

Process Creation/destructivollective communication Transactional memory Mutex



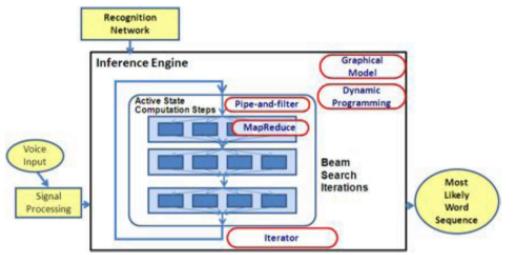
Architecting the Whole Application

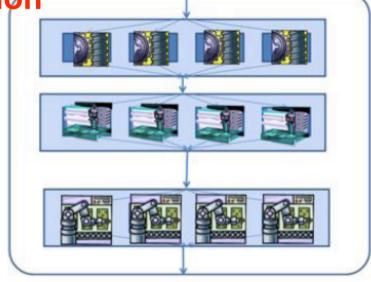


Main Challenge:

Build an architecture that scales

and will survive hardware evolution





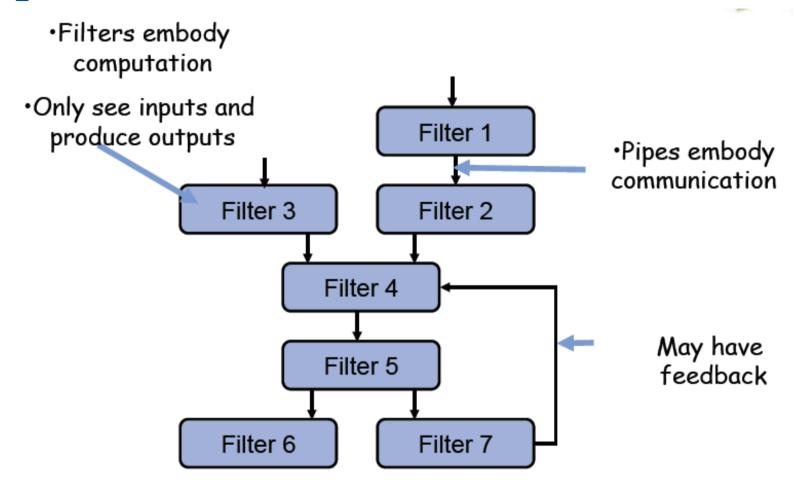
 SW Architecture of Large-Vocabulary Continuous Speech Recognition

Analogous to the design of an entire manufacturing plant

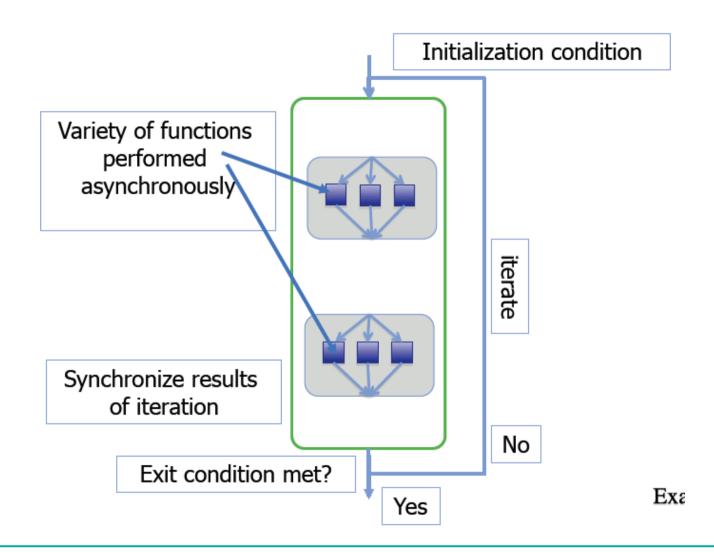
Raises appropriate issues like scheduling, latency, throughput, workflow, resource management, capacity etc.

Think Parallel PATTERNS

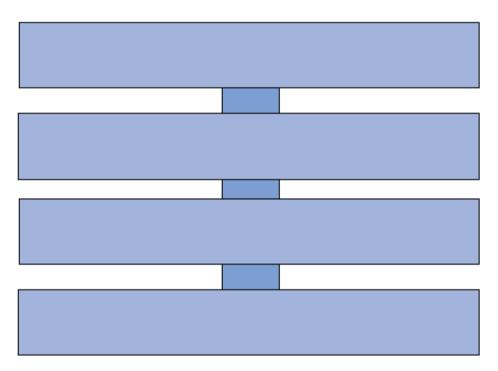
Pipes and Filters



Iteration



Layered Systems



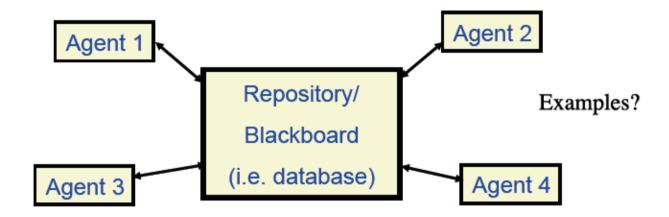
Delegation pattern: Lower layers "work" for the upper ones

- Individual Layers are big
- •Interface between two adjacent layer is narrow
- No communication among not adjacent layers

Challenge:

- •where parallelization shall occur?
- Often lower layers is legacy software

Agents and Repository



Agent and repository: Blackboard structural pattern

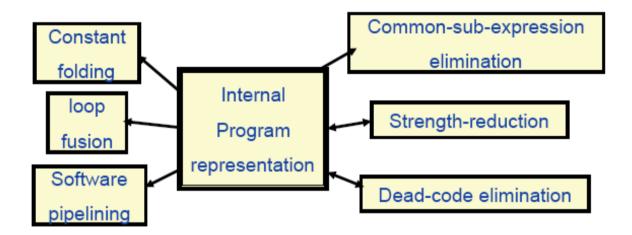
Agents cooperate on a shared medium to produce a result Key elements:

- Blackboard: repository of the resulting creation that is shared by all agents (circuit database)
 - Agents: intelligent agents that will act on blackboard (optimizations)
 - Manager: orchestrates agents access to the blackboard and creation of the aggregate results (scheduler)



Example: Compiler Optimization

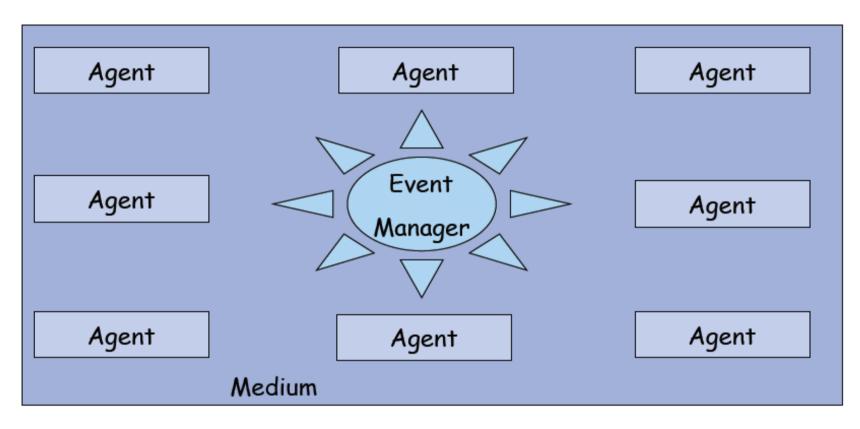




Optimization of a software program

- Intermediate representation of program is stored in the repository
 - Individual agents have heuristics to optimize the program
- Manager orchestrates the access of the optimization agents to the program in the repository
 - Resulting program is left in the repository

Event-Based Systems



Agents interact via events/signals in a medium

Examples?

- Event manager manages events
- Interaction among agents is dynamic no fixed connection

Puppeteer

- Need an efficient way to manage and control the interaction of multiple simulators/computational agents
- Puppeteer Pattern guides the interaction between the simulation codes to guarantee correctness of the overall simulation
- •Difference with agent and repository?
 - No central repository
 - Data transfer between simulators

Simulation 1

Puppeteer

Simulation n

Simulation 2

Examples?

Map/Reduce

Original (google, Hadhoop) Map/Reduce takes a set of input key/value pairs, and produces a set of output key/ value pairs.

- Map (written by the user)
 - takes an input pair and produces a set of intermediate key/value pairs.
- The MapReduce library
 - groups together all intermediate values associated with the same intermediate key I and passes them to the *Reduce function*.
- Reduce, also written by the user,
 - accepts an intermediate key I and a set of values for that key. It merges together these values to form a possibly smaller set of values.

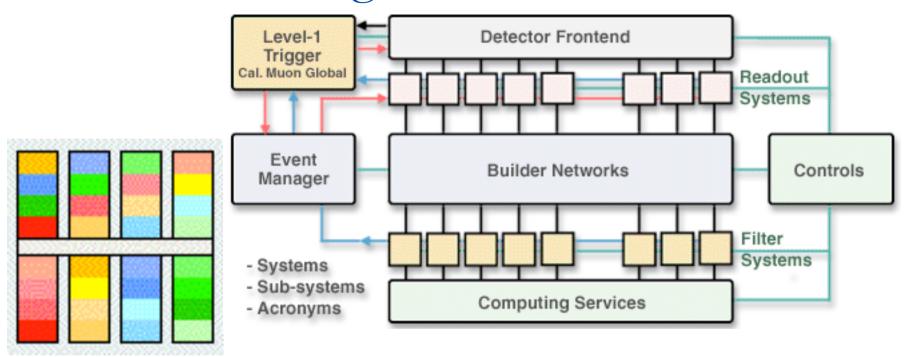
Word count

map(String key, String value):
// key: document name
// value: document contents
for each word w in value:
EmitIntermediate(w, "1");

reduce(String key, Iterator values):
// key: a word
// values: a list of counts
int result = 0;
for each v in values:
result += ParseInt(v);
Emit(AsString(result));

Map Stage Reduce Stage Worker 1 Worker 1 Мар Reduce > Partition Merge Мар Partition Reduce Output Input Split Merge Мар Reduce Partition Мар Partition Reduce Worker M Worker N

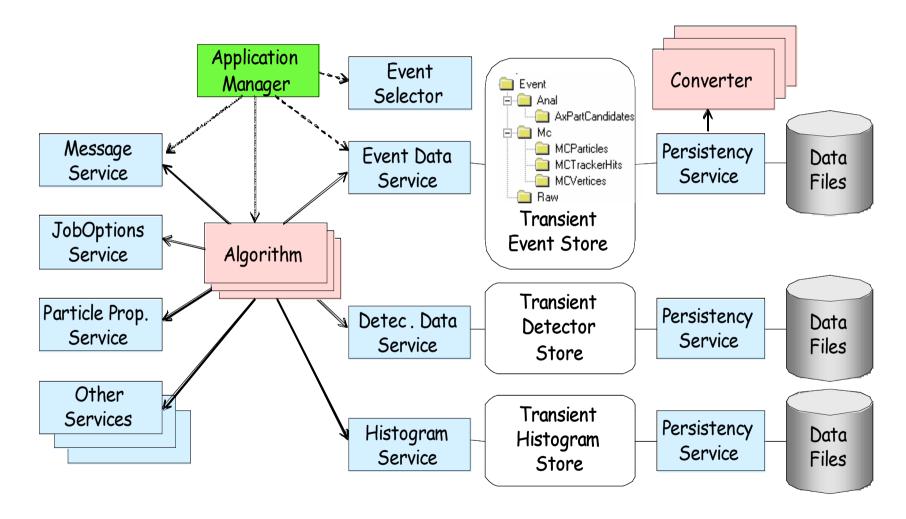
Event Building!



Map: Detector frontend assign event-id to each fragment DAQ dispatch all fragment with same id to a given filter node Reduce: filter node assemble the event and process it

PARALLEL ARCHITECTURES FOR HEP EVENT PROCESSING

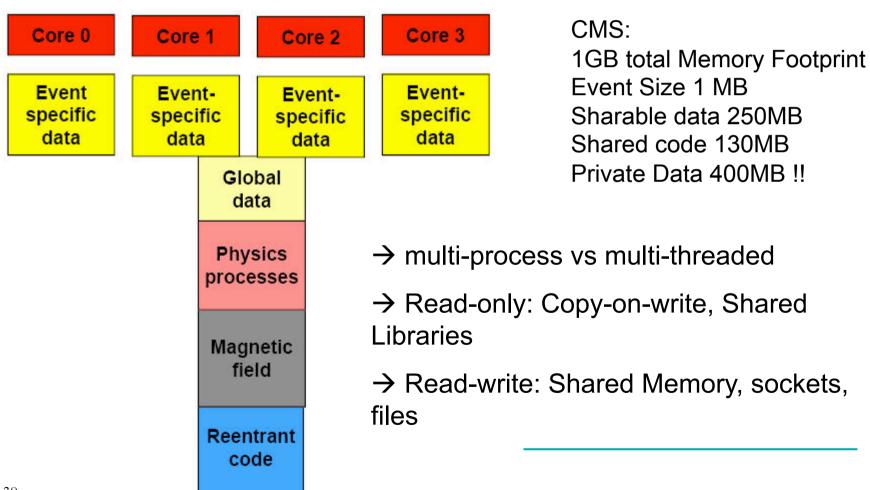
HEP Application



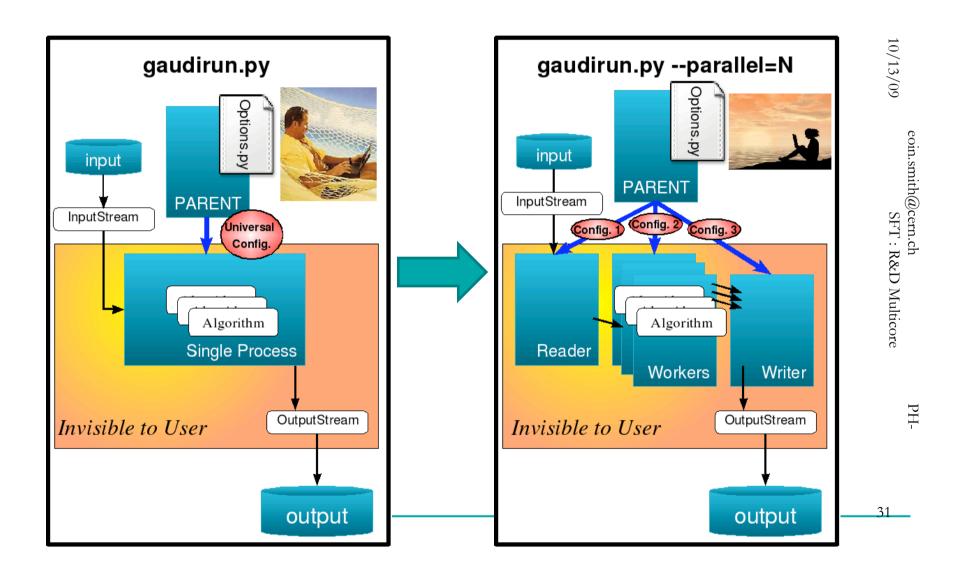
Event parallelism

Opportunity: Reconstruction Memory-Footprint shows large condition data

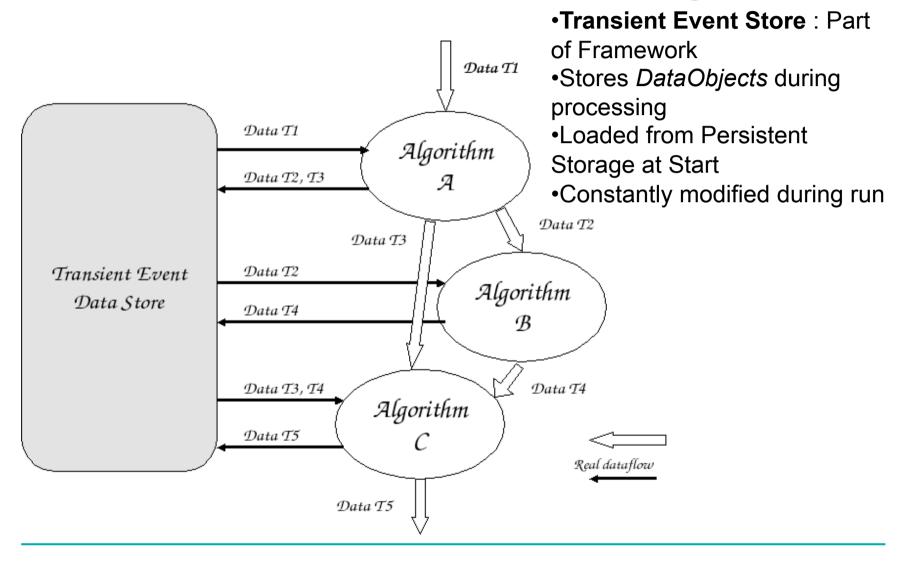
How to share common data between different process?



Parallelization of Gaudi Framework



Gaudi: HEP Event Processing



HEP data processing

- No need of a coherent event state:
 - Algorithms
 - read specific event-fragments, store new fragments: never modify existing ones
 - Storage:
 - Fragments map root branches: independent of each other
- Conditions shared among events and (some) algorithms
 - Event parallelism will profit of coherent shared conditions
 - Algorithm parallelism can make them private to each of them

Act Parallel ALGORITHMIC STRUCTURE

Hello Word!

```
void hello() {
    std::thread t1(hi);
    std::thread t2(hi);
    hi();
    t1.join();
    t2.join();
}

Create (Fork) new Threads
    where hi will run

Run hi in the "main" thread

wait for Threads to
    terminate
```

OO Hello Word!

```
void hello() {
                                                                             Thread
class Hi {
                                                      std::thread t1(hi);
public:
                                                      std::thread t2(Hi(3));
 Hi(): j(0) \{\}
                                                      hi();
 explicit Hi(int i) : j(i){}
 void operator()() {
                                                      Hi oneHi;
  ++j;
                                                      std::thread t3(std::ref(oneHi));
  std::cout << "Hello World from "
                                                      std::thread t4(std::ref(oneHi));
               << std::this_thread::get_id()
                                                      oneHi();
        << " where j is " << j << std::endla
                                                      1.join();
                                                                             Create local Hi object
 int j;
                                                      t2.join();
                                                                             Pass it by reference
                                                     t3.join();
                                                                             to Threads
Create (Fork) new Threads
                                                      t4.join();
where Hi::operator() will
                                                      std::cout << "j is " << oneHi.j <
run
                                                    std::endl;
wait for Threads to
terminate
```

Create local Hi object

Pass it by copy to

What Happens?

Hello World from Hello World from 140186020210544

Hello World from 1090701632 where j is 4 start is 0

[pcphsft60] ~/public/Bertinoro \$./a.out

1113024832

start is 3 Hello World Hello Hello World from from World from \ 1090701632 where j is 11130248321401860202105442 \ where j is where j is 11 start is start is start is 00 start is 0 i is 2 [pcphsft60] ~/public/Bertinoro \$./a.out Hello World from 1091725632Hello World from Hello World from 1102555456 where j is 4 start is 0 139953850718064 start is 2 Hello World from Hello 139953850718064Hello where j is \ World 1 start is World 0from start is 0 from 1102555456 where j is 2 start is 0 1091725632 where j is 3 start is 0 i is 3

```
[pcphsft60] ~/public/Bertinoro $ ./a.out
Hello World from Hello 139882834876272World from
1108351296 where i is 4 start is 0
Hello World from 1084438848
start is 2
Hello World Hello Hello World from from 1398828348762721108351296
where j is where j is 1 start is 0World
from start is 0
3 start is 0
1084438848 where j is 2 start is 0
i is 3
[pcphsft60] ~/public/Bertinoro $ ./a.out
Hello World from Hello 140206101608304World from 1093429568 where j
4 start is Hello World from 0
1085036864
start is 2
Hello Hello World World from World from 140206101608304 where j
is from 110934295681085036864 where j is start is where j is 0
start is 0
1 start is 0
2 start is 0
i is 2
```

Synchronization

- Critical sections
 - A critical section is a portion of code that shall be executed by only one thread at a time.
 - Used to protect access to shared resources (memory)
 - In C++0x, a critical section can be protected by a "guard" that takes care to lock and then release a "Mutual exclusion object (mutex)"

```
typedef std::mutex Mutex;
typedef std::unique_lock<std::mutex> Guard;
Mutex lock;
{
    Guard guard(lock);
    std::cout....
}
Constructor locks the mutex
Destructor unlocks it
```

Optimize Critical Sessions (and avoid pitfalls)

- Critical sections may introduce a significant fraction of sequential (non parallel) operations
 - Granularity shall be chosen properly
 - Make critical sections small
 - Use different mutex to guard independent sections
 - Major Pitfall: DeadLock
 - Are sections really independent?



Basic Types of Synchronization: Barrier



Barrier -- global synchronization

- Especially common when running multiple copies of the same function in parallel
 - » SPMD "Single Program Multiple Data"
- simple use of barriers -- all threads hit the same one

```
work_on_my_subgrid();
barrier;
read_neighboring_values();
barrier;
```

- more complicated -- barriers on branches (or loops)

```
if (tid % 2 == 0) {
  work1();
  barrier
} else { barrier }
```

- barriers are not provided in all thread libraries

No "barrier in C++0x: use modified boost::barrier

Explicit Synchronization

C++0x provides a simple explicit synchronization mechanism based on "condition variable"s

```
typedef std::mutex Mutex;
typedef std::unique_lock<std::mutex> Guard;
typedef std::condition_variable Condition;

Mutex goLock;
Condition go;
```

```
Guard guard(goLock);
go.wait(guard);
// do something
}
```

```
{
    Guard guard(goLock);
    // prepare data
    go.notify_all();
}
```

release mutex, put thread in wait When notified re-acquire mutex

Barrier implementation

```
#include <thread>
#include <exception>
class barrier {
 public:
  typedef std::mutex Mutex;
  typedef std::unique_lock<std::mutex> Guard;
  typedef std::condition_variable Condition;
     barrier(unsigned int count)
            : m_threshold(count),
m_count(count), m_generation(0) {
   if (count == 0)
           throw std::invalid_argument("count
cannot be zero.");
```

```
bool wait() {
   Guard guard(m_mutex);
   unsigned int gen = m_generation;
   if (--m_count == 0) {
           m_generation++;
           m_count = m_threshold;
           m_cond.notify_all();
           return true:
   while (gen == m_generation)
          m_cond.wait(guard);
   return false:
 private:
  Mutex m_mutex; Condition m_cond;
  unsigned int m threshold, m count;
  unsigned int m_generation;
 };
```

Future

C++0x provides a data exchange mechanism among threads based on *promise-future* pattern Able to transfer exceptions too!

```
std::promise<T> promise;
```

```
try {
    // prepare data
    promise.set_value(result);
    }catch (...){
    m_promise.set_exception(std::current_exception());
    }

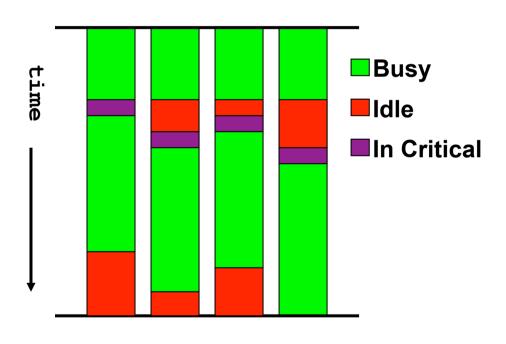
    // continue processing

try {
    unique_future<T> input = promise.get_future();
    // now I need the result of the other thread
    try {
        T data = input.get();
        // continue processing
    }
} catch (...) {
    //*handle error*/}

Wait till other thread does not set value
    (or exception) in promise
```

Synchronization

Lost time waiting for locks



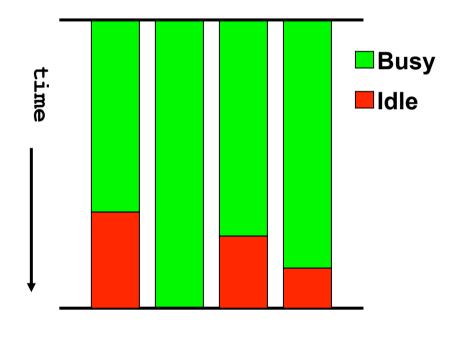
Load Imbalance

 Unequal work loads lead to idle threads and wasted time

```
#pragma omp parallel
{

#pragma omp for
  for(;;){

  }
}
```



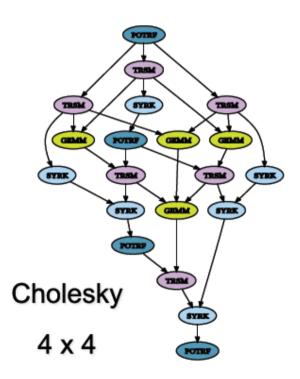


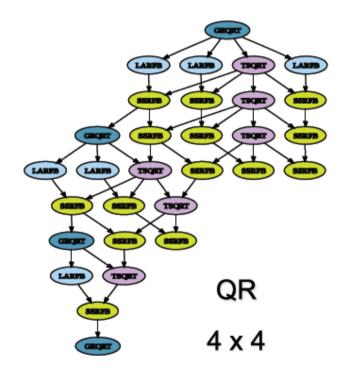
Performance Pitfall: too many Barriers



Computations as DAGs

View parallel executions as the directed acyclic graph of the computation





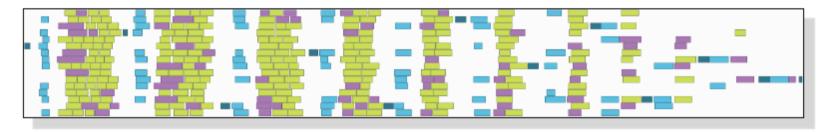
Slide source: Jack Dongarra



Illustration from PLASMA Project



Nested fork-join parallelism (e.g., Cilk, TBB)



Arbitrary DAG scheduling (e.g., PLASMA,



SuperMatrix)

Performance Calculations

 T_{s}

Best serial code timing (single thread/core)

 $T_p(n)$

Parallel code timing using n threads/cores (p fraction parallel, $p \in [0,1]$)

 $T_p(1)$

Parallel code timing using 1 thread/core

 $\frac{T_p(1)}{T_s}$

Indication of parallel overhead

$$S_p(n) = \frac{T_s}{T_p(n)}$$

Actual Speedup over single thread using *n* threads/cores (*p* fraction parallel)

$$E_p(n) = \frac{S_p(n)}{n}$$

Efficiency using *n* threads/cores (*p* fraction parallel)

$$S_p^{\max}(n) = \frac{1}{1 - p + \frac{p}{n}}$$

Max. Speedup over single thread using n threads/cores (p fraction parallel)

Speedup

Maximum speedup defined by Amdahl's law:



$$S_p^{\max}(n) = \frac{1}{1 - p + \frac{p}{n}}$$

n=#threads, p=parallel fraction

- Which just state the obvious:
 - A bare 10% non-parallel fraction limits the speedup to a factor 10!

Classical parallel Algorithms

- Single Program Multiple Data (SPMD)
- Loop parallelism

Wait for OpenMP/MPI presentation!

Divide&Conquer by Fork&Join

```
/* re-entrant function Mattson el al. 5.29 page 170 */
template<typename Iter, typename Compare>
void parallel_sort(Iter b, Iter e, Compare c) {
 size_t n = std::distance(b,e);
 // final exit
 if (n < SORT_THRESHOLD) return std::sort(b,e,c);
// Divide
 Iter pivot = b + n/2;
 // Conquer
 // fork first half
 Thread forked(parallel_sort<lter,Compare>,b,pivot,c);
// process locally second half
 parallel_sort(pivot,e,c);
// wait for the other half
 forked.join();
 // merge...
 std::inplace_merge(b,pivot,e);
```

Exercise: rewrite Map-Reduce-Like Eventually using OpenMP

What about returning data, error management, exceptions?
Wait for future!

Master/Worker

Workers

Workers

Master/ Orchestrator

Workers ers

- Master distribute tasks to workers
 - No communication among workers
 - Many possible data access patterns
- Scheduling and queue theory applies!
 - Single queue multiple workers
 - Multiple queues
 - Dedicated queues/workers
 - Roundrobin, priorities,...

Shared Queue

Full chapter in Mattson el al.

```
bool pop(T & t) {
  Guard g(m_lock);
  while (empty()) {
    if (m_drain) return false;
    m_empty.wait(g);
  t = m_q.front();
  m_q.pop();
  if ( !full() ) m_full.notify_all(); // (or
notify_one?)
  return true;
```

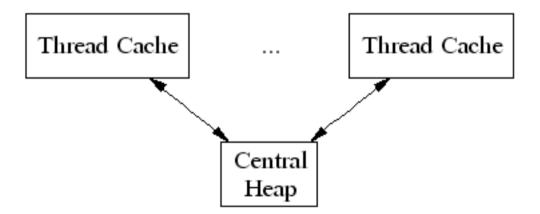
```
void push(T const & t) {
  Guard g(m_lock);
  if (full()) m_full.wait(g);
  m_q.push(t);
  m_empty.notify_all(); // (or notify_one?)
         std::queue (?)
```

(managing) shared data

- Single Lock:
 - Last resort (in case of legacy data-structures)
- Distributed Locks
 - Optimize granularity
 - Heuristic: #locks = #threads
- Distributed data
 - Map-Reduce:
 - overhead of reduce vs overhead of locks
- Transactional memory access
 - Atomic operations
 - No lock, unroll if fails
 - Promising technology...

TCMalloc (Google Malloc)

- TCMalloc assigns each thread a thread-local cache.
 - Small allocations are satisfied from the thread-local cache.
 - Objects are moved from central data structures into a thread-local cache as needed,
 - Periodic garbage collections are used to migrate memory back from a thread-local cache into the central data structures.



Not the end of the story...

Read Phenix Rebirth about porting on a 256-thread UltraSPARC T2+ system.

http://csl.stanford.edu/~christos/publications/2009.scalable_phoenix.iiswc.pdf

Atomic operation

- Modern architectures provide atomic operations
 - Guaranteed to be fully completed by just one thread
- gcc intrinsics on x86_64

http://gcc.gnu.org/onlinedocs/gcc-4.4.1/gcc/Atomic-Builtins.html

- CAS
 - __sync_bool_compare_and_swap(addr,expected,new)
 - sync_val_compare_and_swap(addr,expected,new)
- Op and fetch (also fetch and op)
 - sync_add_and_fetch(addr,n)
- Swap
 - sync_lock_test_and_set(addr,n)

Atomic operation

C++0x std::atomic<type>

```
#include <cstdatomic> std::atomic<int> x;
```

- CAS
 - x.compare_exchange_strong(expected,new)
- Fetch and op ; Op and fetch
 - x.fetch add(n); x++; x+=n; etc
- Swap
 - x.exchange(n); x=n;

Atomics in use

Barrier with spinlock

```
struct barrier {
  void wait() {
    __sync_add_and_fetch(m_n,-1);
    while(m_n) {/* std::this_thread::yield(); */}
  }
  volatile long m_n;
};
```

Shared linked list

```
pointer insert(pointer p, value_type const & value) {
  Node * me = new Node; me->value=value;
  if (p==0) p=&head;
  while (true) {
    me->next = p->next; // next sequential code p->next=me;
    if (__sync_bool_compare_and_swap(&(p->next),me->next,me)) break;
  }
```

next

Non Blocking Shared Queue

// circular buffer T container[last+1];

```
bool pop(T&t) {
    while (true) {
        if(waitEmpty()) return false; //
    include a signal to drain and terminate
        volatile size_t cur=tail;
        if (cur==head) continue;
        t = container[cur];
        if
        (__sync_bool_compare_and_swap(&tail,cur,cur==0 ?last : cur-1)) break;
     }
    return true;
}
```

```
// single producer only
void push(T const & t) {
  while (true) {
   waitFull(); // head always empty...
   volatile size_t cur=head;
   container[cur] = t; // shall be done first to
avoid popping wrong value
   _sync_bool_compare_and_swap(&head,c
ur,cur==0 ? last : cur-1 )) {
           // container[cur] = t; // too late
pop already occured!
           break;
```

Lock Free Hash Table

(Cliff Click at Google Camp 2007)

- Insert: CAS as before
- Delete: just mark
- The difficult part is to implement lock free resizing
 - Do not block operation from other threads
 - Allow other threads to collaborate in resizing
- Memory management is the other big issue
- Read slides and papers: very instructive

Singleton, Services

- Very unclear, static seems to introduce a full memory barrier in any case
- Will not be covered
- Slide will be deleted

(Sorting)
Word count
Histograming
Clustering
N-body dynamics

USE CASES

Histograming

Produce amplitude histogram (0-255) for each 10MPixel image

- Throughput: process images in parallel
 - Embarrassingly parallel
- Latency: process each image in parallel!
- Input: vector<uchar> image(10000000);
- Output: vector<int> histogram(256);
- Function: ++histogram[image[i]];

Word count

Count the number of occurrences of each word in a text

- Input: Sequence<char> text(N); N large
- Output: AssociativeContainer<string,int> words;
- Function: WordIterator word(text); ++words[*(++word)];

Clusterize

Clusterize points in 3D using Kmeans

- Input vector<Points3D> points
- Output vector<Cluster> clusters

Algorithm

- Start with a set of seeds
- Associate points to closest seed: (clusters)
- Compute mean (cluster position, new seed)
- iterate

Bibliography

- Google, wikipedia
- Architecture:
 - http://www.cs.berkeley.edu/~volkov/cs267.sp09/
 - http://parlab.eecs.berkeley.edu/wiki/patterns/pattern1 0
 - http://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.55.3594
 - http://www.sigsoft.org/phdDissertations/theses/JorgeOrtega.pdf
- Computational Patterns
 - http://www.eecs.berkeley.edu/Pubs/TechRpts/2006/EECS-2006-183.pdf
- Map-Reduce
 - http://hadoop.apache.org/ (distributed: cluster, grid, cloud)
 - Phoenix http://mapreduce.stanford.edu/ (multicore)
- C++0X
 - http://www.justsoftwaresolutions.co.uk/threading/multithreading-in-c++0xpart-1-starting-threads.html
 - http://www.stdthread.co.uk/doc/