I: Performance metrics (cont'd) II: Parallel programming models and mechanics

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Algorithms for 2-D (3-D) Poisson, N=n² (=n³)

Algorithm	Serial	PRAM	Memory	# procs
Dense LU	N ³	Ν	N ²	N ²
Band LU	N ² (N ^{7/3})	Ν	N ^{3/2} (N ^{5/3})	N (N ^{4/3})
Jacobi	N ² (N ^{5/3})	N (N ^{2/3})	Ν	Ν
Explicit inverse	N ²	log N	N ²	N ²
Conj. grad.	N ^{3/2} (N ^{4/3})	N ^{1/2(1/3)} log N	Ν	Ν
RB SOR	N ^{3/2} (N ^{4/3})	N ^{1/2} (N ^{1/3})	Ν	N
Sparse LU	N ^{3/2} (N ²)	N ^{1/2}	N log N (N ^{4/3})	Ν
FFT	N log N	log N	Ν	Ν
Multigrid	Ν	log ² N	Ν	Ν
Lower bound	Ν	log N	Ν	

PRAM = idealized parallel model with zero communication cost. *Source: Demmel (1997)* F

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Sources for today's material

- Mike Heath at UIUC
- CS 267 (Yelick & Demmel, UCB)

Efficiency and scalability metrics (wrap-up)

Example: Summation using a tree algorithm



Efficiency

$$E_p \equiv \frac{C_1}{C_p} \approx \frac{n}{n+p\log p} = \frac{1}{1+\frac{p}{n}\log p}$$

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Basic definitions

M	Memory complexity	Storage for given problem (e.g., words)
W	Computational complexity	Amount of work for given problem (e.g., flops)
V	Processor speed	Ops / time (e.g., flop/s)
T	Execution time	Elapsed wallclock (<i>e.g.</i> , secs)
C	Computational cost	(No. procs) * (exec. time) [e.g., processor-hours]

Parallel scalability

Algorithm is **scalable** if

$$E_p \equiv \frac{C_1}{C_p} = \Theta(1) \text{ as } p \to \infty$$

- Why use more processors?
 - Solve fixed problem in less time
 - Solve larger problem in same time (or any time)
 - Obtain sufficient aggregate memory
 - Tolerate latency and/or use all available bandwidth (Little's Law)

Is this algorithm scalable?

- No, for fixed **problem size**, **exec. time**, and **work / proc.**
- Determine **isoefficiency function** for which efficiency is constant

$$E_p \equiv \frac{C_1}{C_p} \approx \frac{n}{n+p\log p} = \frac{1}{1+\frac{p}{n}\log p} = E \text{ (const.)}$$
$$\implies n(p) = \Theta(p\log p)$$

But then execution time grows with p:

$$T_p = \frac{n}{p} + \log p = \Theta(\log p)$$

A simple model of communication performance



Latency and bandwidth model

Model time to send a message in terms of latency and bandwidth

$$t(n) = \alpha + \frac{n}{\beta}$$

- Usually have cost(flop) << $1/\beta$ << α
 - One long message cheaper than many short ones
 - Can do hundreds or thousands of flops for each message
- Efficiency demands large computation-to-communication ratio

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Empirical latency and (inverse) bandwidth (µsec) on real machines

machine	α	β
T3E/Shm	1.2	0.003
T3E/MPI	6.7	0.003
IBM/LAPI	9.4	0.003
IBM/MPI	7.6	0.004
Quadrics/Get	3.267	0.00498
Quadrics/Shm	1.3	0.005
Quadrics/MPI	7.3	0.005
Myrinet/GM	7.7	0.005
Myrinet/MPI	7.2	0.006
Dolphin/MPI	7.767	0.00529
Giganet/VIPL	3.0	0.010
GigE/VIPL	4.6	0.008
GigE/MPI	5.854	0.00872





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Latency on some current machines (MPI round-trip)





End-to-end latency (1/2 round-trip) over time

Source: Yelick (UCB/LBNL)



Source: Mike Welcome (NERSC)



Parallel programming models

A generic parallel architecture

Physical location of memories, processors? Connectivity?



What is a "parallel programming model?"

- Languages + libraries composing abstract view of machine
- Major constructs
 - **Control**: Create parallelism? Execution model?
 - **Data**: Private vs. shared?
 - **Synchronization**: Coordinating tasks? Atomicity?
- Variations in models
 - Reflect diversity of machine architectures
 - Imply variations in cost

Running example: Summation

Compute the sum,

$$s = \sum_{i=1}^{n} f(a_i)$$

Questions: Where is "A"? Which processors do what? How to combine?



Programming model 1: Shared memory

- Program = collection of threads of control
- Each thread has **private** variables
- May access **shared** variables, for communicating implicitly and synchronizing



Need to avoid race conditions: Use locks

Race condition (data race): Two threads access a variable, with at least one writing and concurrent accesses

shared int s = 0;



Thread 2 for i = n/2, n-1 s = s + f(A[i])

Need to avoid race conditions: Use locks

Explicitly lock to guarantee atomic operations



Machine model 1a: Symmetric multiprocessors (SMPs)

All processors connect to large shared memory

Challenging to scale both hardware & software > 32 procs





Source: Pat Worley (ORNL)

Machine model 1b: Simultaneous multithreaded processor (SMT)

Multiple thread contexts share memory and functional units

Switch among threads during long-latency memory ops





Source: John Feo (Cray)

Machine model 1c: Distributed shared memory

Memory logically shared, but physically distributed

Challenge to scale **cache coherency protocols** > 512 procs



Cache lines (pages) must be large to amortize overhead → locality is critical to performance

Programming model 2: Message passing

- Program = named processes
- **No shared** address space
- Processes communicate via **explicit send/receive** operations



Example: Computing A[1]+A[2]

```
Processor 1:

x = A[1]

SEND x \rightarrow Proc. 2

RECEIVE y \leftarrow Proc. 2

s = x + y
```

```
Processor 2:

x = A[2]

SEND x \rightarrow Proc. 1

RECEIVE y \leftarrow Proc. 1

s = x + y
```

- What could go wrong in the following code?
 - Scenario A: Send/receive is like the **telephone** system
 - Scenario B: Send/receive is like the **post office**

Machine model 2a: Distributed memory

- **Separate** processing nodes, memory
- Communicate through **network interface** over interconnect



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Programming model 2b: Global address space (GAS)

- Program = **named** threads
- Shared data, but **partitioned** over local processes
- Implied cost model: **remote accesses cost more**



Machine model 2b: Global address space

- Same as distributed, but NI can access memory w/o interrupting CPU
- **One-sided** communication; remote direct memory access (RDMA)



Programming model 3: Data parallel

- Program = **single thread** performing **parallel operations** on data
- **Implicit** communication and coordination; easy to understand
- Drawback: Not always applicable
- Examples: HPF, MATLAB/StarP



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Machine model 3a: Single instruction, multiple data (SIMD)

- Control processor issues instruction, (usually) simpler processors execute
- May "turn off" some processors
- Examples: CM2, Maspar



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Machine model 3b: Vector processors

- Single processor with multiple functional units
 - Perform same operation
 - Instruction specifies large amount of parallelism, hardware executes on a subset
- **Rely on compiler** to find parallelism
- Resurgent interest
 - Large scale: Earth Simulator, Cray X1
 - Small scale: SIMD units (e.g., SSE, Altivec, VIS)

Vector hardware

Operations on vector registers, O(10-100) elements / register



Actual hardware has 2-4 vector **pipes** or **lanes**

Programming model 4: Hybrid

- May mix any combination of preceeding models
 - MPI + threads
 - DARPA HPCS languages mix threads and data parallel in global address space

Machine model 4: Clusters of SMPs (CLUMPs)

- Use SMPs as building block nodes
- Many clusters (*e.g.*, GT "warp" cluster)
- Best programming model?
 - Flat" MPI
 - Shared mem in SMP, MPI between nodes

Administrivia

Administrative stuff

- No office hours today (maybe "virtual" only—AIM: **VuducOfficeHours**)
- **Accounts**: Apparently, you already have them or will soon (!)
 - Try logging into 'warp1' with your UNIX account password
 - If it doesn't work, go see TSO Help Desk (and **good luck!**)
 - CCB 148 / M-F 7a-5p / 404.894.7065 / AIM:tsohlpdsk
 - IHPCL mailing list:
 - https://mailman.cc.gatech.edu/mailman/listinfo/ihpc-lab

Shared memory programming: POSIX Threads and OpenMP

Programming model 1: Shared memory

- Program = collection of threads of control
- Each thread has **private** variables
- May access **shared** variables, for communicating implicitly and synchronizing



Shared memory programming

- Libraries for existing languages
 - POSIX Threads (PThreads), Solaris Threads: Portable, Iow-level library
 - OpenMP: Pragma-based, targets scientific computing apps
 - Intel Thread Building Blocks (TBB): pThreads + OpenMP
- Language extensions

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Common notions of thread creation

cobegin

task1 (a1);
task2 (a2);
coend

id = fork (task1, a1); task2 (a2); join (id);

POSIX Threads (PThreads)

- Portable system call interface for creating and synchronizing threads
- Threads share all global variables
- Fork/join style

```
errcode = pthread_create (&thread_id,
&thread_attribute,
&thread_fun,
&fun_arg)
```

errcode = pthread_join (thread_id, NULL);

Reference: <u>https://computing.llnl.gov/tutorials/pthreads/</u>

Loop-level parallelism

May fork threads at any time, *e.g.*, within a loop

```
... A[n];
for (i = 0; i < n; ++i)
    pthread_create (..., &task, &i);
...</pre>
```

Must have sufficient granularity to mask thread-creation overhead

Low-level policy control

- Detached state: Avoid pthread_join calls
- Scheduling parameters: priority, policy (FIFO vs. round-robin)
- Contention scope: With what thread does this thread compete for CPU

Barriers for global synchronization (Optional extension)

Usage outline

```
pthread_barrier_t b;
pthread_barrier_init (&b, NULL, 3); // 3 threads
...
pthread_barrier_wait (&b); // All threads wait
...
```

pthread_barrier_destroy (&b);

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Mutual exclusion locks (mutexes)

Basic usage

```
pthread_mutex_t lock = PTHREAD_MUTEX_INITIALIZER;
pthread_mutex_init (&lock, NULL);
...
pthread_mutex_lock (&lock);
    // ... do critical work ...
pthread_mutex_unlock (&lock);
```

Beware of **deadlock**

Thread 1	Thread 2
lock (a);	lock (b);
lock (b);	lock (a);

OpenMP: An API for multithreaded shared-memory programming

Programmer identifies **serial** and **parallel regions**, not threads



- Library + directives (requires compiler support)
- Official website: <u>http://www.openmp.org</u>
 - Also: <u>https://computing.llnl.gov/tutorials/openMP/</u>

Simple example

int main() {

}

printf ("hello, world!\n"); // Execute in parallel
return 0;

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Simple example

```
int main()
{
    omp_set_num_threads (16);
    #pragma omp parallel
    {
        printf ("hello, world!\n"); // Execute in parallel
        } // Implicit barrier/join
        return 0;
}
```

Concurrent loops

May parallelize a loop, but **you must check dependencies**

#pragma omp parallel for \
 shared (s)
for (i = 0; i < n; ++i)
 #pragma omp critical
 s += x[i];</pre>

#pragma omp parallel for \
 reduction(+: s)
for (i = 0; i < n; ++i)
 s += x[i];</pre>

Loop scheduling

- Use "schedule" clause to partition loop iterations
- Static: k iterations per thread, assigned statically
 #pragma omp parallel for schedule static(k) ...
- **Dynamic**: *k* iterations per thread, using logical work queue

#pragma omp parallel for schedule dynamic(k) ...

- Guided: k iterations per thread initially, reduced with each allocation #pragma omp parallel for schedule guided(k) ...
- **Run-time**: Use value of environment variable, **OMP_SCHEDULE**

Synchronization primitives

Critical sections	No explicit locks	<pre>#pragma omp critical { }</pre>
Barriers		#pragma omp barrier
Explicit locks	May require flushing	<pre>omp_set_lock (1); omp_unset_lock (1);</pre>
Single-thread regions	Inside parallel regions	<pre>#pragma omp single { /* executed once */ }</pre>



"In conclusion..."



Backup slides

Network topology

- Of great interest historically, particularly in mapping algorithms to networks
 - Key metric: Minimize hops
 - Modern networks hide hop cost, so topology less important
- Large gap in hardware/software latency: On IBM SP, *cf*. 1.5 usec to 36 usec
- Topology affects bisection bandwidth, so still relevant

Bisection bandwidth

- Bandwidth across smallest cut that divides network in two equal halves
- Important for all-to-all communication patterns



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Linear and ring networks

Linear Diameter ~ n/3 Bisection = 1

Ring/Torus Diameter ~ n/4 Bisection = 2



Multidimensional meshes and tori

2-D mesh Diameter ~ 2*sqrt(*n*) Bisection = sqrt(*n*)



2-D torus

Diameter ~ sqrt(n)Bisection = $2^sqrt(n)$



Hypercubes

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- No. of nodes = 2^d for dimension d
 - Diameter = d

Bisection = n/2



Trees

- Diameter = $\log n$
- Bisection bandwidth = 1
- **Fat trees**: Avoid bisection problem using fatter links at top



Butterfly networks

- Diameter = $\log n$
- Bisection = n
- Cost: Wiring



Topologies in real machines

	Machine	Network
1	Cray XT3, XT4	3D torus
	BG/L	3D torus
	SGI Altix	Fat tree
Nowor	Cray X1	4D hypercube*
newer	Millennium (UCB, Myricom)	Arbitrary*
Older	HP Alphaserver (Quadrics)	Fat tree
	IBM SP	~ Fat tree
	SGI Origin	Hypercube
	Intel Paragon	2D mesh
\downarrow	BBN Butterfly	Butterfly

Evolution of distributed memory machine networks

- Message queues replaced by direct memory access (DMA)
- **Wormhole** routing: Processor packs/copies, initiates transfer, then goes on
- Message passing libraries provide store-and-forward abstraction
 - May send/receive between any pair of nodes
 - Time proportional to distance since each processor along path participates