

Parallel Programming Concepts

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Parallel Background

"Why Bother?"

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- Simultaneous use of multiple 'processors' to solve a single problem
- Use of a group (team) of 'processes' to cooperatively solve a problem
- A demanding challenge that requires programmers to "think in parallel"





Parallel Programming Problems

- Difficult to design, develop, and debug
- Still not entirely portable, but getting better all the time
- Open to more latent bugs based on order of execution and bulk of code
 - "Correct execution of a parallel program once is no guarantee that it will ever execute correctly again." --Jim McGraw, LLNL
- Architectures, and, thus, 'tricks of the trade', are constantly in flux





So Why Do It?

Scientific Demand

- CERN Large Hadron Collider generates 1 Pbyte of raw data per second. It is filtered to 100Mbyte/sec, but, this leaves 1 Pbyte/year to be saved.
- Boeing's idea of a supercomputer is one that will do a complex Airliner flight simulation in 6-7 hours
- ECMWF European Centre for Medium Range Weather
 Forecasting would like a 10km weather forecast, but they will need 50 Tflops sustained to do it.





More Science Demands...

- Estimates for genomics:
 - Biology is big business (\$50 billion/yr)
 - Modeling a prokaryotics cell (no nucleus) requires tracking
 ~30 million structures
 - 40 Tflops sustained to simulate an entire organ
 - Ab initio protein folding requires 1 Pflop/s
 - Director of NCSA estimated biology to be an Exaflop level challenge
- Human brain is a 100 Pflop machine currently are barely past the *mouse brain* level of computing (100 Tflops)





The Demands Quantified

Demand	Result	Computational Increase
Better Remote Sensors	10x Resolution	100 - 1000
Increased resolution for models	10x Resolution	1000 - 10000
Coupled Models	Better Accuracy	2 - 5
Improved Processes	Better Accuracy	2 - 5
Longer Simulations	10-100 times longer	10 - 100
ALL OF THE ABOVE	100x res, 100x longer, more accurate physics	10 ¹⁰





Aside - On Magnitudes

Magnitude	Number of Words
Mega (M)	Small novel
Giga (G)	Pick-up full of paper or 1 DVD
Tera (T)	1 million books (US library of congress in ~10 Tbytes)
Peda (P)	1-2 Pbytes is all academic research libraries combined
Exa (E?)	Probably less than 5 Ebytes of words spoken in human history





Update for 2010

CENTER	SYSTEM	VENDOR	NCPUS	Max TFLOPS
ORNL	Jaguar	Cray XT5	224162	1,759 (1.76 PF)
NSCS	Nebulae	Dawning/GPU	120640	1,271
LANL	Roadrunner	Bladecenter	122400	1,042
NICS	Kraken	Cray XT5	98,928	831.7
ARSC	Pingo	Cray XT5	3456	26.21

Things change quick!

- 11/2008 Pingo debuted at #109
- 06/2009 Pingo was #203
- 06/2010 Pingo is currently #435





Selected Talks At SC10

- Petascale data analytics
- 190 TF Astrophysical N-body Simulation on a cluster of GPUs
- Scalable Earthquake Simulation on Petascale Supercomputers
- Multiscale Simulation of Cardiovascular flows
- Multi-scale Heart Simulation
- Petascale Direct Numerical Simulation of Blood Flow on 200K cores
- Building Exascale GPU-Based Supercomputers
- Exatran: A language for Exascale Computing
- Scaling of a Multimillion-Atom MD Simulation
- Panasas: The Road to Exascale Storage





Update for 2013

CENTER	SYSTEM	VENDOR	NCPUS	Max PFLOPS*
NUDT	Tainhe-2	Xeon CPUs	3.12M	33.86
ORNL	Titan	NVIDIA	261632	17.59
LLNL	Sequoia	IBM	1.57M	17.17
RIKEN	K	SPARC64	705024	10.51
ANL	Mira	IBM	786432	8.59

#1 is Chinese#2, #3, and #5 are DOE machines#4 is Japanese

Note the change to PFLOPS!

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Update for 2015

CENTER	SYSTEM	VENDOR	NCPUS	Max PFLOPS*
NUDT	Tainhe-2	Xeon CPUs	3.12M	33.86
ORNL	Titan	NVIDIA	261632	17.59
LLNL	Sequoia	IBM	1.57M	17.17
RIKEN	K	SPARC64	705024	10.51
ANL	Mira	IBM	786432	8.59

#1 is Chinese#2, #3, and #5 are DOE machines#4 is Japanese

I'm really surprised it is the same as 2013!





Ok - So Why Parallel?

• That's the only way left to go

- Clock speeds are approaching that of light
- Machine level instructions are optimized
- Pipeline technology has limited scope
- Vector processing has scalability limits
- Since they can't build them faster, they're making multi-cpu chips
 - that go into boards,
 - that go into nodes,
 - that go into clusters,
 - » that go into ...





Parallel Architectures

"UMA, NUMA, NORMA?"

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RSC RSC Parallel Architecture Models

Shared Memory Multiprocessor

- N processors share a common memory
- Ideal is UMA (Uniform Memory Access)
- Reality is NUMA (Non-Uniform Memory Access)
- To program this machine, use OpenMP
- Distributed Memory Multicomputer
 - N computers interconnected by a network
 - NORMA (NO-Remote Memory Access)
 - To program this machine, use MPI
- Distributed Shared Memory
 - To program , use OpenMP and/or MPI





Acronyms

• UMA - Uniform Memory Access

physical memory equidistant from all PEs

NUMA - Non-Uniform Memory Access

physical memory is distributed to processors, thus access time varies with the location of the word

NORMA - No-Remote-Memory-Access

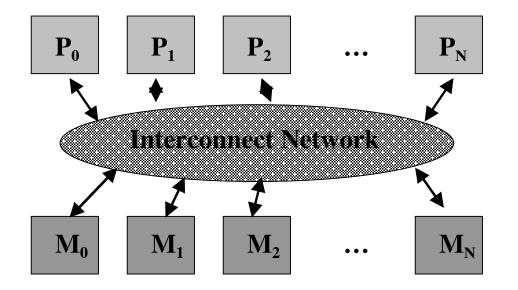
physical memory is distributed to processors





Shared Memory

- Large globally shared memory space
- These are single nodes in modern systems
- Examples include SGI O2000, CRAY SV1, IBM Regatta, Cray/NEC SX-6, IBM P690+

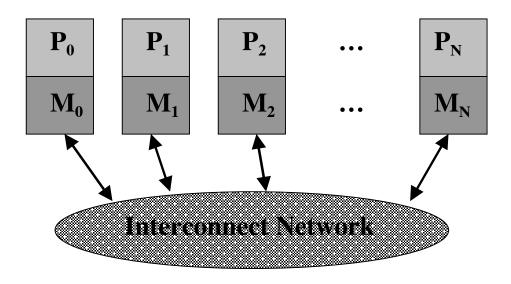






Distributed Memory

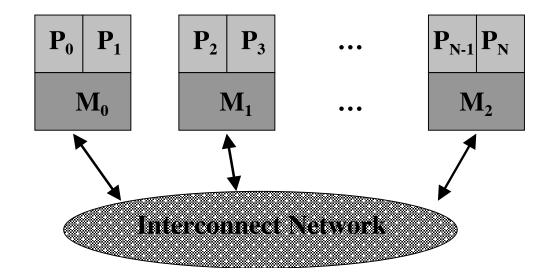
- Each node contains one processor with its own memory.
- Nodes are interconnected by message passing network (switches or routers)
- Examples include typical linux clusters







- Modest number of processors share memory within a single node
- Distributed memory among nodes
- Example is IBM Winterhawk, p655, p690







Architecture Comparison

Memory Latency

- Time to access a memory location
- Local memory access is low latency (SM, DSM)
- Remote memory access is high latency and may be possible only through message passing (DM, DSM)





Architecture Comparison

Memory Contention

- Occurs when multiple processors attempt to access a single memory location particularly for update
- No memory contention for distributed memory - only a single processor can access local memory
- Potential for a high level of memory contention for shared memory systems





- Sharing/False Sharing 2 (or more) PEs updating variable(s) on the same cache line
 - PE 1 wants to write to cache line X, but PE 2 owns it
 - request PE 2 to flush cache line X to main memory
 - invalidate all other PEs cache line X
 - read cache line X from main memory
 - update local cache line with value
 - PE 2 wants to write to cache line X, but PE 1 owns it
 - Request ...
 - PE 3 wants to write to ...
 - And so on, and so on, ...





Parallel Algorithms

"Thinking In Parallel"

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Algorithm Requirements

- Concurrency ability to work on a problem with separate simultaneous tasks
- Scalability ability to produce increased speed up as the number of processors is increased
- Locality ability to minimize remote memory access by accessing local data as frequently as possible





Parallel Programming Models

Shared Memory

- Communication via memory constructs
- SPMD (single program multiple data) is the most common form
- For our purposes, the majority of shared memory programming will be splitting main loops into the available PEs

(sounds simple enough, right?)



ARSC Parallel Programming Models

Distributed Mem/Message Passing

- Communication is explicit using messages
- SPMD is most common form of code for a homogeneous environment
- Adapts well to MPMD (multiple program multiple data) codes in heterogeneous computing systems





Example - Global Reduction

Global Reduction - parallel operation on an array

- commutative binary operations only
 - OK: SUM, PRODUCT(?), MIN, MAX, AVE
 - NOT OK: division, subtraction
- usually defined in standard parallel programming libraries



ARSC Global Sum - Shared Memory

Shared Memory

\$OMP private(my_sum)
Do j=my_start,my_stop
 my_sum = my_sum+data[j]
End do
\$OMP critical
 sum = sum + my_sum
\$OMP end critical

Notes

- Must declare variable scope
- Calculate global indices (usually automatically done)
- Global memory must be protected in order to avoid race conditions, i.e. EXPLICIT SYNCHRONIZATION is required.
- Each synchronization construct slows code and has potential to reduce performance to serial (or worse)





Global Sum - Message Passing

Message Passing

Do j=start,stop

my_sum = *my_sum* + *data[j] End do*

```
If (my_pe==0) then
```

```
sum = my_sum
```

do j=1,NUM_PE-1

Recv(j,remote_sum)

sum = sum + remote_sum

end do

Else

```
Send(0,my_sum)
End if
```

• Notes

- Local memory access only
- Message passing can be orders of magnitude slower than memory access
- Synchronization is implicit
- Boss/Worker paradigm leads to load imbalance and, once again, has the potential to reduce performance to serial (or worse)
- How could this be done better?





Parallel Performance Issues

(Yep, they' ve got issues)

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Speedup

Definition

speedup = unimproved run-time / improved run-time
(Also called application speedup)

• Example

- Program ported to X1 runs in 20 hours
- Core loop is modified to vectorize, bringing run-time down to 5 hours
- Therefore, speedup = 20 / 5 = 4





What's the Big Deal?

- If we have a program that takes time T_1 to run on one processor, why don't we just use p processors to run it in time T_1/p ?
 - 1. To use more than one processor requires coordination and communication between them, and
 - 2. Almost all "real" programs contain portions that cannot utilize multiple processors.





Speed Up Goal

- Goal: Get N speed up for N processors
- Nearly always, Speed Up < N
- Fixed problem size has a fixed speed up

$$S_N = T_1 / T_N \qquad S_N$$





Speedup Revisited

- If we can see a speedup of p for p processors, we call that a *linear* speedup
 - In general, that is the best we can hope for
 - However, there are pathological cases of superlinear speedup
- Often though, speedup tails off so that adding more processors could even cause a slowdown





Amdahl's Law

- Speedup is limited by the fraction of the code that does not benefit
- E.g., suppose we have a parallel machine. Let
 - $-F_s$ = fraction of code that is inherently serial
 - $-F_p$ = fraction of code that is parallelizable

$$- So F_{s} + F_{p} = 1$$

 $-T_1 = time to run on 1 processor$

• Therefore

speedup = $T_1 / (F_s T_1 + (F_p T_1 / N) = 1 / (F_s + ((1-F_s) / N))$





Amdahl's Law (cont.)

• Implication of Amdahl's Law

speedup = 1 / (Fs + (Fp / N))

- Suppose a program runs in 10 hours on one processor and 80% of the code can be executed in parallel on 1000 processors. Then
 - Tp = 0.2(10) + (0.8(10) / 1000) = 2.0 + 0.008 = 2.008 and
 - speedup = 1 / (0.2 + 0.8 / 1000) = 1 / 0.2008 = 4.98

• What if

- Fp drops to 50% ?
- N goes to infinity?

Fs	20%	10%	5%	1%
4	2.5	3.1	3.5	3.9
16	4.0	6.4	9.1	13.9
64	4.7	8.8	15.4	39.3
256	4.9	9.7	18.6	72.1
8	5.0	10.0	20.0	100.0





Efficiency

- Ratio of actual speed up to perfect speed up
- Measure of a parallel program's ability to use multiple processors
- Goal is to achieve 100% efficiency
- Reality is that Efficiency < 1
- Remember Amdahl's Law? Here's the impact on efficiency:

	<i>f</i> = 0.2	<i>f</i> = 0.1	<i>f</i> = 0.05	<i>f</i> = 0.01
N = 4	63%	78%	88%	98%
N = 16	25%	40%	57%	87%
N = 64	7%	14%	24%	61%
N = 256	2%	4%	7%	28%





Data Access Issues

• Data Scoping: Private vs. Shared

- Refers to the accessibility of data to processes
- Private data is accessible only to owning process
- Shared data is accessible to all processes in group
 - ☺allows work-sharing by multiple processes☺allows memory contention and data races
- DM architectures are all private memory
- DSM & SM architectures allow both private & shared





Data Access Issues

- Atomic operation: an operation that can be performed in a single step
- Few operations are truly atomic Example: j = j + 1
 - Step 1: Load contents of memory location j into register
 - **Step 2: Increment the contents of the register**
 - Step 3: Store contents of register to memory location j

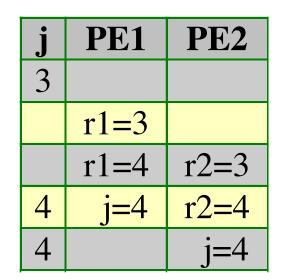




Data Access Issues

 Data races occur when multiple PEs attempt simultaneous modification of a shared variable using a non-atomic operation

Time	PE1	PE2
0		
1	Load r1, j	
2	Incr r1	Load r2, j
3	Store j,r1	Incr r2
4		Store j,r2







- *Granularity* measure of the amount of computation involved in a software process. e.g. # of instructions, usually
 - fine (instruction level),
 - medium (loop level), or
 - coarse (subroutine/program level)
- Load Balancing assignment of tasks to equalize the work load across multiple processors

