Lecture 3: Intro to parallel machines and models

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Logistics

Remember:

- Note: the entire class will not be as low-level as lecture 2!
- Crocus cluster setup is in progress.
- If you drop/add, tell me so I can update CMS.
- Lecture slides are posted (in advance) on class web page.

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A little perspective

"We should forget about small efficiencies, say about 97% of the time: premature optimization is the root of all evil."

- C.A.R. Hoare (quoted by Donald Knuth)

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- Best case: good algorithm, efficient design, obvious code
- Speed vs readability, debuggability, maintainability?
- A sense of balance:
 - Only optimize when needed
 - Measure before optimizing
 - Low-hanging fruit: data layouts, libraries, compiler flags
 - Concentrate on the bottleneck
 - Concentrate on inner loops
 - Get correctness (and a test framework) first

Matrix multiply

Consider naive square matrix multiplication:

```
#define A(i,j) AA[j*n+i]
#define B(i,j) BB[j*n+i]
#define C(i,j) CC[j*n+i]
for (i = 0; i < n; ++i) {
  for (j = 0; j < n; ++j) {
    C(i, j) = 0;
    for (k = 0; k < n; ++k)
      C(i,j) += A(i,k) * B(k,j);
  }
```

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How fast can this run?

Two standard matrix layouts:

- Column-major (Fortran): A(i,j) at A+j*n+i
- Row-major (C): A(i,j) at A+i*n+j

I default to column major.

Also note: C doesn't really support matrix storage.

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1000-by-1000 matrix multiply on my laptop

- Theoretical peak: 10 Gflop/s using both cores
- Naive code: 330 MFlops (3.3% peak)
- Vendor library: 7 Gflop/s (70% peak)

Tuned code is $20 \times$ faster than naive!

Can we understand naive performance in terms of membench?

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1000-by-1000 matrix multiply on my laptop

- Matrix sizes: about 8 MB.
- Repeatedly scans B in memory order (column major)
- 2 flops/element read from B
- 3 ns/flop = 6 ns/element read from B
- Check membench gives right order of magnitude!

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Simple model

Consider two types of memory (fast and slow) over which we have complete control.

- m = words read from slow memory
- *t_m* = slow memory op time
- f = number of flops
- t_f = time per flop
- q = f/m = average flops / slow memory access

Time:

$$ft_f + mt_m = ft_f \left(1 + \frac{t_m/t_f}{q}\right)$$

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Larger q means better time.

How big can q be?

- 1. Dot product: *n* data, 2*n* flops
- 2. Matrix-vector multiply: n^2 data, $2n^2$ flops
- 3. Matrix-matrix multiply: $2n^2$ data, $2n^3$ flops

These are examples of level 1, 2, and 3 routines in *Basic Linear Algebra Subroutines* (BLAS). We like building things on level 3 BLAS routines.

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q for naive matrix multiply

 $q \approx$ 2 (on board)

Better locality through blocking

Basic idea: rearrange for smaller working set.

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Q: What do we do with "fringe" blocks?

q for naive matrix multiply

 $q \approx b$ (on board). If M_f words of fast memory, $b \approx \sqrt{M_f/3}$.

Th: (Hong/Kung 1984, Irony/Tishkin/Toledo 2004): Any reorganization of this algorithm that uses only associativity and commutativity of addition is limited to $q = O(\sqrt{M_f})$

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Note: Strassen uses distributivity...

Better locality through blocking



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Truth in advertising



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Coming attractions

HW 1: You will optimize matrix multiply yourself!

Some predictions:

You will make no progress without addressing memory.

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- It will take you longer than you think.
- Your code will be rather complicated.
- Few will get anywhere close to the vendor.
- Some of you will be sold anew on using libraries!

Not all assignments will be this low-level.

Class cluster basics

crocus.csuglab.cornell.edu is a Linux Rocks cluster

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- Six nodes (one head node, five compute nodes)
- Head node is virtual do not overload!
- Compute nodes are dedicated be polite!
- Batch submissions using Sun Grid Engine
- Read docs on assignments page

Class cluster basics

- Compute nodes are dual quad-core Intel Xeon E5504
- Nominal peak per core:
 - 2 SSE instruction/cycle \times
 - 2 flops/instruction \times
 - 2 GHz = 8 GFlop/s per core
- Caches:
 - 1. L1 is 32 KB, 4-way
 - 2. L2 is 256 KB (unshared) per core, 8-way
 - 3. L3 is 4 MB (shared), 16-way associative

L1 is relatively slow, L2 is relatively fast.

- Inter-node communication is switched gigabit Ethernet
- 16 GB memory per node

Consider:

- Each core has vector parallelism
- Each chip has four cores, shares memory with others
- Each box has two chips, shares memory
- Cluster has five compute nodes, communicate via Ethernet

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How did we get here? Why this type of structure? And how does the programming model match the hardware?

Parallel computer hardware

Physical machine has processors, memory, interconnect.

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- Where is memory physically?
- Is it attached to processors?
- What is the network connectivity?

Parallel programming model

Programming model through languages, libraries.

- Control
 - How is parallelism created?
 - What ordering is there between operations?
- Data
 - What data is private or shared?
 - How is data logically shared or communicated?

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- Synchronization
 - What operations are used to coordinate?
 - What operations are atomic?
- Cost: how do we reason about each of above?

Consider dot product of x and y.

Where do arrays x and y live? One CPU? Partitioned?

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- Who does what work?
- How do we combine to get a single final result?

Shared memory programming model

Program consists of *threads* of control.

- Can be created dynamically
- Each has private variables (e.g. local)
- Each has shared variables (e.g. heap)
- Communication through shared variables
- Coordinate by synchronizing on variables

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Examples: OpenMP, pthreads

Shared memory dot product

Dot product of two *n* vectors on $p \ll n$ processors:

1. Each CPU evaluates partial sum (n/p elements, local)

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2. Everyone tallies partial sums

Can we go home now?

A race condition:

► Two threads access same variable, at least one write.

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- Access are concurrent no ordering guarantees
 - Could happen simultaneously!

Need synchronization via lock or barrier.

Race to the dot

Consider S += partial_sum on 2 CPU:

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- P1: Load S
- P1: Add partial_sum
- P2: Load S
- P1: Store new S
- P2: Add partial_sum
- P2: Store new S

Shared memory dot with locks

Solution: consider S += partial_sum a critical section

- Only one CPU at a time allowed in critical section
- Can violate invariants locally
- Enforce via a lock or mutex (mutual exclusion variable)

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Dot product with mutex:

- 1. Create global mutex 1
- 2. Compute partial_sum
- 3. Lock 1
- 4. S += partial_sum
- 5. Unlock 1

Shared memory with barriers

- Lots of scientific codes have distinct phases (e.g. time steps)
- Communication only needed at end of phases
- Idea: synchronize on end of phase with barrier
 - More restrictive (less efficient?) than small locks
 - But much easier to think through! (e.g. less chance of deadlocks)

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Sometimes called bulk synchronous programming

Shared memory machine model

- Processors and memories talk through a bus
- Symmetric Multiprocessor (SMP)
- Hard to scale to lots of processors (think \leq 32)

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- Bus becomes bottleneck
- Cache coherence is a pain
- Example: Quad-core chips on cluster

Multithreaded processor machine

 May have more threads than processors! Switch threads on long latency ops.

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- Called hyperthreading by Intel
- Cray MTA was one example

Distributed shared memory

- Non-Uniform Memory Access (NUMA)
- Can logically share memory while physically distributing
- Any processor can access any address
- Cache coherence is still a pain
- Example: SGI Origin (or multiprocessor nodes on cluster)

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Message-passing programming model

- Collection of named processes
- Data is partitioned
- Communication by send/receive of explicit message

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Lingua franca: MPI (Message Passing Interface)

Message passing dot product: v1

Processor 1:

- 1. Partial sum s1
- 2. Send s1 to P2
- 3. Receive s2 from P2

4. s = s1 + s2

Processor 2:

- 1. Partial sum s2
- 2. Send s2 to P1
- 3. Receive s1 from P1

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4. s = s1 + s2

What could go wrong? Think of phones vs letters...

Message passing dot product: v1

Processor 1:

- 1. Partial sum s1
- 2. Send s1 to P2
- 3. Receive s2 from P2

4. s = s1 + s2

Processor 2:

- 1. Partial sum s2
- 2. Receive s1 from P1

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3. Send s2 to P1

4. s = s1 + s2

Better, but what if more than two processors?

MPI: the de facto standard

- Pro: Portability
- Con: least-common-denominator for mid 80s

The "assembly language" (or C?) of parallelism... but, alas, assembly language can be high performance.

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Distributed memory machines

- Each node has local memory
 - ... and no direct access to memory on other nodes

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- Nodes communicate via network interface
- Example: our cluster!
- Other examples: IBM SP, Cray T3E

Why clusters?

Clusters of SMPs are everywhere

 Commodity hardware – economics! Even supercomputers now use commodity CPUs (though specialized interconnects).

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- Relatively simple to set up and administer (?)
- But still costs room, power, ...
- Will grid/cloud computing take over next?