Parallel Programming Options and Design (Part II)

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### Summary

Topic has been (slightly artificially) split into two Simple solutions are mentioned as they arise

- Reasons for parallelism, and basic design Strengths and weaknesses of each approach Thread pools, client-server, CPU farms etc. Most important models of HPC parallelism
- Available parallel implementations
   OpenMP and other shared-memory models
   PGAS (Fortran coarrays, UPC etc.)
   MPI and other message passing models

### Beyond the Course

Email scientific-computing@ucs for advice

http://www-users.york.ac.uk/~mijp1/teaching/... .../4th\_year\_HPC/notes.shtml

http://www.hector.ac.uk/support/documentation/... .../userguide/hectoruser/hectoruser.html See "References and Further Reading"

http://www.epcc.ed.ac.uk/library/documentation/... .../training/

#### Contents

Some commonly misunderstood terminology

Distributed memory, MPI, etc.

Shared memory, POSIX threads, OpenMP etc.

Fortran coarrays, UPC etc.

Memory models and similar cans of worms

Kernel scheduling issues (for sysadmins only)

### SIMD – The Easy Case

SIMD means Single Instruction, Multiple Data I.e. a serial program runs with parallel data Think of a vector system when you say this This includes indexed and masked arrays

Great advantage: code and debug just like serial Optimisation of it is well–understood and automatic Actually implemented as simplest case of SPMD

It also includes MMX, SSE and Aptivec
But regard them as part of serial optimisation
GPUs will be described later

# MIMD

MIMD means Multiple Instruction, Multiple Data

All modern parallel systems are MIMD And almost all parallel languages and libraries You can run SIMD designs on MIMD systems

• So the term isn't practically useful nowadays Incorrectly used to mean distributed memory

Most MIMD languages are actually SPMD

# **SPMD** (1)

SPMD means Single Program, Multiple Data I.e. exactly the same program runs on all cores But programs are allowed data-dependent logic

So each thread may execute different code Can test the thread identifier or do it explicitly

```
#pragma omp sections
{
    #pragma omp section
    { ... }
    #pragma omp section
    { ... }
}
```

### **SPMD** (2)

The more like SIMD it is, the easier it is At least for coding, debugging and tuning

Minimise thread-specific code as far as possible It isn't a major problem, except for efficiency It makes tuning quite a lot harder

Watch out for locking and communication
 Best to leave all communication to compiler
 Locking indicates SPMD may be wrong model

### Multiple Programs

This is where each process runs independently MPI is a widespread and classic example Term MPMD is almost never used, but could be

• But they usually run a single executable So some people call them SPMD models And, as implied, some people don't ...

 This is not really a meaningful debate
 There is a continuum from SIMD onwards ... to each process running different executables

#### SMP

SMP stands for Shared Memory Processor All threads can access all the memory

• It does NOT guarantee consistency! We will return to this minefield later

It used to mean Symmetric Multi–Processing That use still occasionally crops up

### NUMA

NUMA means Non–Uniform Memory Architecture I.e. not all memory is easily fast to access Usually, some sort of memory/CPU affinity

All large SMP systems are NUMA nowadays Even AMD Opteron ones are

• Caches make even Intel look like it Details are too complicated for this course

### Distributed Memory (1)

This refers to separate CPUs (e.g. clusters) Including separate processes on SMP systems

Each thread is a completely separate process
 No shared memory, real or virtual – see later
 Code and debug each process as if serial

Communication is by message passing
 That is simply a specialist form of I/O
 Usually a library, but may use language syntax

### Distributed Memory (2)

Can trace or time the message passing That is how to do debugging and tuning It is complicated, but no harder than serial

Some parallel debuggers and tuning tools Mostly for MPI – even built–in to libraries

Hardest problem is data distribution
 Each process owns some of the data
 But other processes may need to access it

## Message Passing

Many interfaces used in commerce, Web etc. CORBA, SOAP etc. – let's ignore them

Some languages – Smalltalk, Erlang etc. Few used outside computer science research

MPI (Message Passing Interface) dominates A library callable from Fortran and C/C++ Bindings available for Python, Java etc.

Essentially all HPC work on clusters uses MPI

#### Take a Breather

That has covered most of the terminology

Will mention a few high–level design guidelines About how to structure your application

Then will cover what MPI can do

Then move onto the shared memory morass Sorry, but that is very complicated

# Designing for Distribution (1)

A good rule of thumb is the following:

- Design for **SIMD** if it makes sense
- Design for lock-free SPMD if possible
- Design as independent processes otherwise

For correctness – order of increasing difficulty Not about performance – that is different Not about shared versus distributed memory

• Performance may be the converse There Ain't No Such Thing As A Free Lunch

# Designing for Distribution (2)

Next stage is to design the data distribution
 SIMD is usually easy – just chop into sections

Then work out need for communication
 Which threads need which data and when
 Do a back of the envelope efficiency estimate

• If too slow, need to redesign distribution Often the stage where SIMD models rejected

# Designing for Distribution (3)

• Don't skimp on this design process Data distribution is the key to success

• You may need to use new data structures And, of course, different algorithms

• Above all, KISS – Keep It Simple and Stupid Not doing that is the main failure of ScaLAPACK Most people find it very hard to use and debug

### MPI

This was a genuinely open specification process Mainly during the second half of the 1990s

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

MPI-1 is basic facilities – all most people use Most people use only a small fraction of it!

MPI-2 is extensions (other facilities) Also includes the MPI 1.2 update

MPI-3 is currently being worked on Non-blocking collectives and Fortran 90 support

# MPI-1 (1)

- Bindings for Fortran and C
   Trivial to use for arrays of basic types
   Tricky for Fortran 90 and C++ derived types
- Point-to-point and collective transfers
   Latter are where all processes interoperate
   Can define process subsets for communication
- Blocking and non-blocking transfers
   Not always clear which are more efficient
   Issues are beyond scope of this course

# MPI-1 (2)

Two open source versions – MPICH and OpenMPI Most vendors have own, inc. Intel and Microsoft

Wide range of tuning and debugging tools Mostly commercial, but not all Or can use built-in profiling interface Easy to use and can help with debugging

• Not ideal, but consensus is pretty good Some higher-level interfaces built on top of it

# I/O in MPI

Applies to all distributed memory interfaces

No problem with separate files for each process Or if they all read the same file at once

• Provided that the file server is adequate!

Problems occur with stdin, stdout and stderr Immense variation in ways that is implemented

Best to do their I/O only from primary process
 Use MPI calls to transfer data to and from that

### Some Sordid Details

There may be a separate thread for I/O Or the master thread may handle stdout Or each thread may write directly, and lock

All can cause severe scheduling problems

stdin may be copied or shared stdout and stderr may interleave badly

Causes programs to fail when changing systems

# MPI-2 (1)

- Not all implementations support all of this Use only the extensions you actually need
- Miscellaneous extensions (gaps in MPI-1) Some of these are useful, but rarely essential

One-sided communications
 Some people find these much easier, but I don't
 Explaining the issues is beyond this course

• C++ bindings – now being deprecated But using the C bindings in C++ works, too

### MPI-2 (2)

These extensions are less likely to be available

• Dynamic process handling – to supersede PVM Few, if any, people use this, and I don't advise it

• Parallel I/O – direct and sequential Few people here do I/O intensive HPC

#### PVM – Parallel Virtual Machine

This was a predecessor of MPI Based around a cycle stealing design But with inter-processor communication, too CPUs could leave and join the processor pool

It's effectively dead – thank heavens!
 A pain to use, with unrealistic assumptions
 A positive nightmare to administer and debug

MPI-2 includes all of PVM's facilities

### Shared-Memory Terminology

Atomic means an action happens or doesn't It will never overlap with another atomic action

Locked means software makes it look atomic Usually a lot less efficient, and can deadlock

A data race is when two non-atomic actions overlap The effect is completely undefined – often chaos

Synchronisation is coding to prevent data races

### Shared Memory (1)

All threads have access to all memory
Unfortunately, that isn't exactly right ...
There are three general classes of shared memory

• Fully shared within single process As in POSIX threads and OpenMP

• Shared memory segments, POSIX mmap etc. Shared between processes on same system

• Virtual shared memory (rarely called that) Cray SHMEM, PGAS, even BSP etc. – see later

Shared Memory (2)

Shared memory has memory model problems Will return to that in more detail later

If two threads/processes access same location:

- Either all accesses must be reads
- Or both threads must be synchronised
- Or all accesses must be atomic or locked

Details depend on the interface you are using

• Critical to read specification carefully

### Shared Memory (3)

Updates may not transfer until you synchronise But they may, which is deceptive

Memory will synchronise itself automatically

• Now, later, sometime, mañana, faoi dheireadh

So incorrect programs often work – usually But may fail, occasionally and unpredictably

Makes it utterly evil investigating data races

Any diagnostics will often cause them to vanish

### **Fully Shared Memory**

POSIX/Microsoft threads, Java and OpenMP No other interface is used much at present

Plus some computer science research, of course There are also a few specialist ones

Most SMP libraries implemented using OpenMP See later about the consequences of this

OpenMP is implemented using POSIX threads And Microsoft threads when relevant, I assume

#### Shared Memory I/O

POSIX is seriously self-inconsistent
 I/O is thread-safe (2.9.1) but not atomic (2.9.7)
 Can you guess what that means? I can't

Don't even think of relying on **SIGPIPE** 

Most other interfaces are built on POSIX Some interfaces may implement I/O like MPI Warnings on that may apply here, too

Do all your I/O from the initial thread

# OpenMP (1)

A language extension, not just a library Designed by a closed commercial consortium "Open" just means no fee to use specification Dating from about 1997, still active

http://www.openmp.org

Specifications for Fortran, C and C++ Most compilers have some OpenMP support

• This is the default to use for SMP HPC Unfortunately the specification is ghastly

## OpenMP (2)

- The compiler handles the synchronisation
   Covers up problems in underlying implementation
   E.g. ambiguities in the threading memory model
- Mainly directives in the form of comments
   They indicate what can be run in parallel, and how
   Also a library of utility functions

OpenMP permits (not requires) autoparallelisation I.e. when the compiler inserts the directives Available in many Fortran compilers, rarely in C

# OpenMP (3)

- Easiest way of parallelising a serial program Can just modify the areas that take the most time
- Can usually mix SMP libraries and OpenMP Start with calls to parallel library functions And set compiler options for autoparallelisation
- Then use SIMD or SPMD directives Finally, worry about more advanced parallelism

Too good to be true? I am afraid so

# OpenMP (4)

- Inserting directives trickier than it seems Make even a minor mistake, and chaos ensues
- That is why I advise 'pure' SPMD mode No synchronization, locking or atomic Will get the best diagnostics and other help
- Debugging and tuning can be nightmares It is MUCH easier to avoid them in design

Too complicated to go into details here
OpenMP Debugging (1)

- Aliasing is when two variables overlap
   And the compiler hasn't been told that
   Bugs often show up only when run in parallel
- Must declare variables as shared or not And obviously must declare that correctly!
   Note that shared objects need synchronisation
- Failure is often unpredictably incorrect behaviour
- Serial debuggers will usually get confused

## OpenMP Debugging (2)

 Variables can change value 'for no reason' Failures are critically time-dependent

• Many parallel debuggers get confused Especially if you have an aliasing bug

• A debugger changes a program's behaviour Same applies to diagnostic code or output Problems can change, disappear and appear

Try to avoid ever needing a debugger

## OpenMP Tuning (1)

• Unbelievably, tuning is much worse

Most compilers will help with parallel efficiency
 I.e. proportion of time in parallel (Amdahl's Law)
 Most users know that from their initial design!

- Below that, hardware performance counters Not easy to use and not available under Linux
- The debugging remarks also apply to profiling

## OpenMP Tuning (2)

- Can also lose a factor of 2+ in overheads Manually analyse the assembler for efficiency
- Worst problems are scheduling glitches
   You have NO tools for those!

Most people who try tuning OpenMP retire hurt [I have succeeded, but not often]

 Same applies to POSIX threads, incidentally and Microsoft and Java ones ...

## C++ Threads (1)

- Forthcoming C++ standard will define threading The design is good, but compilers don't support it yet
- Ordinary memory accesses must not conflict Roughly, you must write-once or read many

Atomic memory accesses impose synchronisation
 Default is sequentially consistent – so not scalable
 Beyond that is definitely for experts only

Standard Template Library (STL) is still serial It currently has only low-level facilities

#### C++ Threads (2)

Inherited C facilities are full of gotchas

Often not behave as you expect or simply not work
 Includes all I/O – so use from only one thread

Some bad ideas – e.g. cross-thread exceptions Issues too complicated for this course

Using it will be no easier than using OpenMP

The C standard is copying it – if anyone cares!

• I don't really recommend it for most people

#### POSIX/Microsoft/Java Threads

Using threads like processes usually works
 I.e. minimal, explicit thread communication
 Precisely how most threaded applications work

 Beyond that, is task for real experts only Morass of conflicting, misleading specifications
 With more gotchas than you believe possible

Mention some of the issues, usually in passing Details are too complicated for this course

Please ask for help if you need it here

#### Java Threads

The first version was a failure, and was redesigned Reports of the merits of the second one are mixed

http://java.sun.com/docs/books/tutorial/... .../essential/concurrency

Essential to read sections Thread Interference and Memory Consistency Errors

Also applies to **POSIX** and **Microsoft**, of course

Users of those should read those sections, too

#### **POSIX** Threads

C90 and C99 are entirely serial languages Legal C optimisations break POSIX threads

Neither C nor POSIX defines a memory model Reasons why one is essential are covered later

No way of synchronising non-memory effects Not just I/O, but signals, process state etc. Even simple ones like clock() values and locales

http://www.opengroup.org/onlinepubs/... .../009695399/toc.htm

#### **Microsoft Threads**

I failed to find a suitable Web reference Finding the API was easy enough

But I failed to find a proper specification Or even a decent tutorial, like Java's

Searching threads "memory model" From \*.microsoft.com had 167 hits, but ...

I have reason to think it is currently in flux Yes, I do mean that it is about to change

## Others

If you are really interested, try: http://en.wikipedia.org/wiki/Concurrent\_computing

The following look potentially useful for scientists: Both have been used for production code

Cilk – possibly useful for irregular problems Based on C, and needs disciplined coding Extended language now supported by Intel compilers

GNU Ada – a largely checked language Reported to be safest open source compiler

## **GPUs**

Extending GPUs to use for HPC Will describe current leader (NVIDIA Tesla)

Hundreds of cores, usable in SPMD fashion Cores are grouped into SIMD sections Can be expensive to synchronise and share data

Can be 50–100 times as fast as CPUs

Only for some applications, after tuning

And that is only for single precision code NVIDIA Fermi should be better in this respect

# NVIDIA GPU Design



### CUDA and OpenCL

Based on extended C99/C++ languages Some Fortran prototypes are available

Programming is reported to be fairly easy Rules for sharing memory are trickiest part

Tuning is where the problems arise
 Can be anywhere from easy and fiendish
 Critically dependent on details of application

■ Don't forget CPU⇔GPU transfer time

### **Precision Issues**

Graphics is numerically very undemanding Double precision is very much slower

• But most scientific codes critically need it!

#### Watch out!

There are some techniques to help with this

Dating from the 1950s to 1970s

Look for books on numerical programming of that date Or ask one of the people who was active in that area

## Shared Memory Segments (1)

A way of sharing memory between processes Almost always on a single SMP system

POSIX mmap, 'SysV shmem' (POSIX shmat) etc. Surprising, NOT most variants of Cray SHMEM

Best regarded as communication mechanisms
 Several are actually memory-mapped I/O

## Shared Memory Segments (2)

Synchronisation may need to be in both processes Or just in sender or just in receiver POSIX §4.10 is seriously ambiguous – do both

Once transferred, can use just as ordinary memory
Don't update if in use by another process
It is your responsibility to obey constraints

Often used to implement other interfaces Including message-passing ones, like MPI!

#### Virtual Shared Memory

This is SPMD with separate processes Possibly even running on different systems

You program it a bit like true shared memory
But synchronisation is mandatory
Getting that wrong causes almost all bugs

But some systems may transfer automatically
You can't rely on transfers being queued
Except, with the right options, for BSP

## **Cray SHMEM and Variants**

This is actually one-sided communication
 I.e. one process calls put or get
 All threads must call barrier to synchronise

May assume same local and remote addresses
 Or may need to call a mapping function

Use them much like shared memory segments
Be sure to check correct documentation
A zillion variants, even just on Cray systems

## **BSP** (1)

Stands for Bulk Synchronous Parallel http://www.bsp-worldwide.org/

• Similar, but much simpler and cleaner Designed by Hoare's group at Oxford

Series of computation steps and barriers
 All communication is done at the barriers
 All threads are involved (i.e. no subsets)

Failures like deadlock cannot occur
 Considerably simplifies debugging and tuning

## **BSP** (2)

It is used much like Cray SHMEM I.e. it uses put, get, map\_address calls The data are queued for transfer

• Advantages derive from its restrictions Flexibility has its cost (TANSTAAFL)

Only a few people have used it at Cambridge I haven't, but it is so simple I know I could!

• Consider using its design, at least Please tell me of any experiences with it

## **PGAS** (1)

May stand for Partitioned Global Address Space Or Parallel Global Array Storage, or ... [ Don't confuse with Parallel Genetic Algorithms ]

• Shared arrays are spread across threads Each block is owned by exactly one thread Typically, scalars are owned by thread zero

• All threads can access all memory The compiler handles the data transfer All accesses must be synchronised

## **PGAS (2)**

• Usually provided using language extensions Claimed by believers to be much easier to use

Very trendy at present – the current bandwagon Mostly used to publish research papers on it

 Little used outside ASCI ASCI = Accelerated SuperComputer Initiative USA government's 'Son of Star Wars' project

Some people in Cambridge share codes with ASCI

## HPF

HPF stands for High Performance Fortran First attempt at a standard for parallel Fortran http://hpff.rice.edu/

Originated about 1992, never really took off Superseded by OpenMP by about 2000

- You may still some across code written in it
- Some compilers still have HPF options Of course, they don't always actually work ...
- It's dead, a zombie, a late parrot don't use it

## Fortran Coarrays (1)

Being driven by Cray/ASCI/DoD Some of it available on Cray systems since 1998

• In forthcoming Fortran 2008 standard I am not a great fan of it, but was closely involved

ftp://ftp.nag.co.uk/sc22wg5/... .../N1801-N1850/N1824.pdf http://www.co-array.org/

Starting to appear in compilers

#### Fortran Coarrays (2)

Cray and Intel have released, IBM will soon Most other compilers will follow in due course

g95 supports some of the proposal Only an intermittently active project, though

The Rice U. open-source project is a bit dubious http://www.hipersoft.rice.edu/caf/

gfortran is currently adding syntax checking Starting to work on a simple MPI implementation

#### Fortran Coarrays (3)

Threads are called images Code looks like the following:

> real, dimension(1000)[\*] :: x,y x(:) = y(:)[q]

The square brackets index the thread Indicate you are copying across threads On the owning image, you can omit them:

x(:) = y[9](:)+y(:)

## UPC (1)

Unified Parallel C – a C99 extension A lot of activity, mainly in USA CS depts Started in 1999 – open–source compiler since 2003

Lots of predictions of future successes Little evidence of actual use, even in ASCI

Specification even more ambiguous than C99 However, it does define its memory model

http://upc.gwu.edu/ and http://upc.lbl.gov/

## UPC (2)

Lots of scope for making obscure errors The very thought of debugging it makes me blench

Syntax is just like C99 arrays – e.g. a[n][k] Semantics and constraints are not like arrays

The '[n]' indexes the thread for shared objects Uses of a[n][k] undefined if not on thread 'n' Must call library functions to copy between threads

• However, I do NOT recommend using it Often recommended on basis of no experience

## Language Support

Fortran does very well, for a serial language Why OpenMP Fortran is the leader in this area

C was mentioned earlier, under POSIX

C++ is currently defining its memory model

Java was described earlier

C# is probably following Java

## Memory Models (1)

Shared memory seems simple, but isn't 'Obvious orderings' often fail to hold Parallel time is very like relativistic time

Too complicated (and evil) to cover in this course Suitable key phrases to look up include:

Data Races / Race Conditions Sequential Consistency Strong and Weak Memory Models Dekker's Algorithm

## Main Consistency Problem



Now did A get set first or did B? 0 – i.e. A did 0 – i.e. B did

Intel x86 allows that – yes, really So do Sparc and POWER

## Another Consistency Problem



Thread 3 X = AY = Bprint X, Y

Now, did A get set first or did B? Thread 4 Y = B X = Aprint X, Y

#### 1 0 - i.e. Adid

0 1 – i.e. **B** did

## How That Happens



## Memory Models (2)

 Easiest to use language that prevents problems No current one does that automatically and safely Some can help, if you code in a disciplined way Reasons for OpenMP+Fortran and SIMD design

Next easiest solution is explicit synchronisation
 Don't assume data transfer is automatic
 This is model used by Cray SHMEM and BSP

 Beyond that, KISS – Keep It Simple and Stupid Check you don't assume more than is specified Even Hoare regards this as tricky and deceptive

## For Masochists Only

http://www.cl.cam.ac.uk/~pes20/... .../weakmemory/index.html

Intel(R) 64 and IA-32 Architectures Software Developer's Manual, Volume 3A: System Programming Guide, Part 1, 8.2 Memory Ordering

http://developer.intel.com/products/... .../processor/manuals/index.htm

Follow the guidelines here, and can ignore them

Start to be clever and you had better study them
#### Valid Memory Accesses

• Virtual shared memory is the easy one All you need to do is to synchronise correctly Trivial in theory, not so easy in practice

• True shared and segments are tricky You don't always need to synchronise But when do you and when don't you?

In theory, can synchronise like virtual

That is how I recommend most people to do it
 OpenMP without locks does it automatically

### Atomicity (1)

Thread 1: <type> A; A = <value1>; A = <value2>; Thread 2: <type> B; B = A;

Will B get either <value1> or<value2>?

Don't bet on it – it's not that simple

Probably OK, IF <type> is scalar and aligned But depends on compiler and hardware Structures (e.g. complex) are not scalar

Best to use explicitly atomic operations
 These are language and compiler dependent

## Atomicity (2)

Killer is heterogeneous accesses of any form

- Don't mix explicitly atomic and any other
- Don't mix RDMA transfers and CPU access
- Don't even mix scalar and vector accesses
   SSE probably works, now, but might not
- Don't trust atomic to synchronise

#### Cache Line Sharing

int A[N];
Thread i: A[i] = <value\_i>;

• That can be **Bad News** in critical code Leads to cache thrashing and dire performance

Each thread's data should be well separated Cache lines are 32–256 bytes long

• Don't bother for occasional accesses The code works – it just runs very slowly

### Kernel Scheduling

Following slides are rather esoteric Why low-level parallel tuning is not easy

They cover points that are normally ignored But are a common cause of inefficiency

• Try to avoid them, not to solve them Some hints given of how to do that

#### Kernel Scheduler Problems

• In both shared memory and message passing Both on SMP systems and separate CPUs

Investigation can be simple to impossible MPI on separate CPUs can be simple Shared memory and SMP systems are nasty Often need kernel tools (e.g. Solaris dtrace)

Very often tricky for programmer to fix

May need to tweak system configuration

## Gang Scheduling (1)

Almost all HPC models assume gang scheduling Details are system-dependent and complicated

• Principles are generic and very important

Ideal is that each thread 'owns' a core
 I.e. that the core is always available, immediately
 Even a slight delay can have major knock-on effects

Most system tuning is ensuring threads  $\leq$  cores

Don't make that impossible when programming

## Gang Scheduling (2)

- Avoid running other daemons or interaction Effect can be to reduce effective number of CPUs
- Remember there may be extra controlling thread Describing details is way beyond this course
- Don't want threads to wander between cores
   Their active data has to be copied between caches
   Can be caused by too few CPUs for threads

### Optimal all-to-all



#### Near-optimal all-to-all



Only 17% slower + 1 thread swap / core

# Near-pessimal all-to-all



This is 100% slower (a factor of two)

#### Near-pessimal all-to-all



This has 5 thread swaps / core

Scheduler Glitches (1)

Threads being delayed can be far worse It may drop the library into 'slow' mode This uses sleeping rather than spinning

Most kernel schedulers have a 10 mS cycle Will often change thread state once per cycle This can degrade to a cycle of scheduler delays

• Ask for help if you have trouble here Solution is to avoid starting the cycle

## Scheduler Glitches (2)



#### Scheduler Glitches (3)

- Most I/O calls trigger long sleeps And quite a few other 'waiting' system calls
- Don't include them in performance-critical code
   One thread/process can hold up others

Other solutions involve system configuration
 Search terms include spin loops, nanosleep
 Too complicated for course – ask offline