C for Science

Lecture 5 of 5

Sam Bott
http://www2.imperial.ac.uk/~shb104/c
s.bott@imperial.ac.uk

17th April 2013

Imperial College London

Last Week...

- Arrays in C are not limited to two dimensions.
- We can create our own data types using structs.
- Global variables can be accessed anywhere in your program.
- The lifetime of a variable can be extended by making it static.
- A 'Release' build will optimise your program during compile-time.
- Using the bits that make up individual data types can be an efficient alternative the data types themselves.

More Pointers!

- So far, we have seen examples of pointers to:
  - native types (such as `int*`, `float*`, `double*`...)
  - something unknown, which we *can* recast (`void*`)
  - structures (such as `FILE*`)
  - and pointers themselves (such as `int**`, `double**`...)
- There is one more pointer type, a pointer to a *function*.

Why point to functions?

C code is often re-used between projects. Mathematical routines such as ones to find roots of functions, become extremely limited if they are tied down to a specific case.

Declaring a pointer to a function

We do this with a `typedef`:

```
typedef double (* fx)(double x);
```


Function Pointers - An example

```
#include <stdio.h>
typedef double (* fx)(double x);

double newtonSolve(fx func, fx grad, double guess)
{
   unsigned int loop;
   for (loop = 0; loop < 10; loop++) guess -= func(guess)/grad(guess);
   return guess;
}

double sample(double x)
{
   return x*x-2.0;
}

double dsample(double x)
{
   return 2.0*x;
}

int main()
{
   double sol = newtonSolve(sample, dsample, 1.0);
   printf("Solution = %.15lg\n", sol);
   printf("Residue = %lg\n", sample(sol));
   return 0;
}
```

This should get you started with exercise # 5.

Don't Do it All Yourself!

- As you have seen from the exercises, writing functions to solve equations such as cubics can become complicated (especially when rounding error needs to be minimised).
- A lot of people have spent a considerable amount of time attempting to perfect implementations of mathematical functions.
- Routines written by a third party are packaged in *libraries*.
- These are available for you to link your program with.

Using Fortran Code

- In addition to libraries, there is existing source code that can be used...
- Scientific programming has been going on for ≈ 70 years (counting from Colossus) in Britain.
- Unfortunately a lot of this has been carried out in Fortran.

`f2c`

Bell Labs have released a program called `f2c` which converts Fortran source code to C. The output from `f2c` is usually not very human friendly, but it does at least compile.

GNU Scientific Library - GSL

GNU have released their C Scientific Library:

`http://www.gnu.org/software/gsl/`

- It is managed by scientists at Los Alamos, and is very comprehensively documented.
- GSL requires gcc (but "ports" are available - Windows users, see the handouts on my web page)

Licensing

"GSL can be used internally ('in-house') without restriction, but only redistributed in other software that is under the GNU GPL."

GSL Example

```
#include <stdio.h>
#include <gsl/gsl_sf_bessel.h>

int main()
{
   double x = 0.0;

   printf("Enter x \n");
   scanf("%lf", &x);
   printf("J0(%g) = %.18e\n", x, gsl_sf_bessel_J0(x));

   return 0;
}
```

Compile this using the command-line (assuming you have GSL installed):

```
gcc gsl-sample.c -lgsl  -lgslcblas -lm -o gsl-sample
```

NAGLIB

The Numerical Algorithms Group, based in Oxford, maintain a software library called NAGLIB.

- Certain departments in Imperial College have a license for this.
- Check with the Software Shop; you might be covered.

General Numerical Software

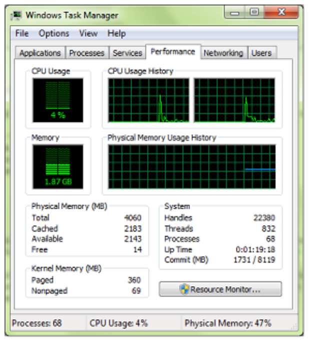
The Netlib Repository contains a lot of very useful numerical code and papers. It is definitely worth having a route through their website:
www.netlib.org

Parallel Computing

What is Parallel Processing?

- The programs we have been creating compile to machine code which is passed (serially) through a processor.
- Modern desktop computers no longer have just one processor with one processing core within it. They have one or more, multi-cored processors.
- This means there is the ability to run multiple ‘threads’ of a program, each one on its own core, allowing us to take advantage of the full power of the processor.
- There are a few ways to utilise multiple processors, but it can’t be done for all code/algorithms.

How many processors do I have?



In Windows press
`[Ctrl] + [Shift] + [Esc]`
to open Task Manager, then look at the “Performance” tab.

In Linux run:

```
grep -c "^processor" /proc/cpuinfo
```

Ways to utilise Multiple Processors

Wherever our code is running a loop (i.e. doing the same thing across a large data range) we can start to think about parallel execution.
I'm going to mention three of the many ways to take full advantage of your processor:

1. Running multiple instances of the program.
2. Running threads in a shared memory environment.
3. Using MPI in a distributed memory environment.

1. Running Multiple Instances

- Running multiple instances of a serial program is the simplest way to use more than one processor.
- We simply write our code as normal and start n instances of it at the same time, with n being the number of cores to use.
- If your program is running across multiple discrete datasets - for example, processing multiple output files from another program - then running multiple instances, each one targeting separate datasets, might be effective.
- This is only appropriate when no data needs to be shared between processes.

2. Threads in Shared Memory

- Within a program, one can spawn multiple execution threads.
- Threads are all owned by the parent process but are running independently. They can each access their own and shared memory.
- Threads can be spawned arbitrarily, but are particularly useful for splitting up parts of `for` loops between cores and running them in parallel.
- Because running loops in parallel means that they no longer execute sequentially, only algorithms where an iteration does not rely on another can be run in this way.
- Threads in shared memory (not surprisingly) require shared memory. As a "rule of thumb" this is available anywhere where the processors sit in the same physical box.
- We will look at simple use of OpenMP to make our programs run in this way.

3. MPI in Distributed Memory

- Multi-threaded code for shared memory could alternatively be coded for distributed memory.
- A Distributed Memory System is one in which not all processors are addressing the same memory. A common scenario would be using more than one node in a computation cluster.
- Parallel code for distributed memory requires using a Message Passing Interface to send information between the threads/processes.
- This is often more difficult as (unlike with OpenMP) the initial single-threaded code needs to be restructured.
- Programs using MPI can be used on shared and distributed memory systems alike.
- Using MPI is beyond the scope of this course, but you may wish to investigate it for future projects.

OpenMP

OpenMP (Open Multi-Processing) is an API (Application Programming Interface) that can be used to create a multi-threaded program in shared memory with only minor modifications to your initial, single-threaded program.

It is included with the majority of compilers. In `gcc` use the `-fopenmp` switch to enable OpenMP. For Visual Studio or Code::Blocks see the information sheets on my web page.

Multi-threading, and the use of OpenMP, are large topics. We will just cover the use of OpenMP to run `for` loops in parallel; this should be sufficient to create efficient, parallel code for a large number of applicable algorithms.

Writing Multi-Threaded Code

1. Write your algorithm, running on a single thread.
2. Compile, debug and thoroughly test you code.
3. Identify regions that could run in parallel - look for `for`s!
4. Add OpenMP compiler directives.
5. Compile with OpenMP support.

When Can We Multi-Thread?

When one iteration does not depend on another.

Bad Examples

```c
for(i = 1; i <= n; ++i)  //Loop 1
 a[i] = a[i-1] + b[i];
```

```c
for(i = 0; i < n; ++i)   //Loop 2
 x[i] = x[i+1] + b[i];
```

The two above examples could not be run in parallel:

- The first example requires the previous iteration to be finished before it can run the next.
- The second could not be run in parallel as another thread might change the original value of $x[i+1]$ before it has been used to calculate $x[i]$.

Using OpenMP

To make a `for` loop run on multiple cores, use the `parallel for` OpenMP compiler directive on the line above:

```c
#pragma omp parallel for
for (i = 0; i < max_i; i++)
 {
     a[i] = b[i] + c[i+1];
 }
```

This will automatically split up the `for` loop, and run it on all available cores.

Private and Shared Variables

By default all variables are shared, this means any thread has access to them. There are three exceptions:

- The loop index.
- Variables that are declared within the for loop.
- Variables explicitly listed as private or a reduction.

No other thread can read or write to another thread's private variables. This is important for loop indexes as each thread needs to keep track of its own position in the loop. It is also useful for intermediate values in a calculation

To explicitly list a variable such as `sqrt_q` as private we modify our compiler directive:

```
#pragma omp parallel for private(sqrt_q)
```


Reductions

Two threads modifying the same variable at the same time can cause problems. To overcome this potential problem we can use a "reduction". A reduction makes a variable private in each thread and then uses a rule operator (`+, -, *, |, &, ^, &&`) to reduce all the private values back to the original variable after the for loop.

An Example

```
int i = 1, factorial;
#pragma omp parallel for reduction(*: factorial)
for (i = 1; i <= x; i++)
{
    factorial *= i;
}
```


Bringing it all together: An Example

Single-Threaded Loop

```
int **Matrix, i, col, sum;
for (i=0; i<rows; i++)
{
     col = WhichColumn(i);
     sum += Matrix[i][col];
}
```

Multi-Threaded Loop

```
int **Matrix, i, row, sum;
#pragma omp parallel for private(col) reduction(+: sum)
for (i=0; i<rows; i++)
{
     col = WhichColumn(i);
     sum += Matrix[i][col];
}
```


High Performance Computing

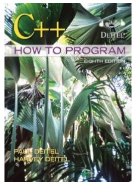
- Once you have made a good multi-threaded program, if it is still taking a long time to compute and you need results faster, you may wish to run it on an HPC.
- An HPC is a large computing cluster containing many, many, fast processors across multiple nodes (physical computers).
- Threading in shared memory can utilise all the processors in one node, code using MPI can be run across multiple processors and multiple nodes.
- Imperial College has a very large HPC and CPU time can be rented from them, for information see: http://www3.imperial.ac.uk/ict/services/hpc

Moving on to C++

What is it?

- C++ can be thought of very loosely as an object oriented extension to C.
- The C++ standard is over twice as big as the C standard.
- C++ is still actively developed and maintained.

References



- One good book that has been brought to my attention is “C++ How to Program, 8th Edition” by Harvey and Paul Deitel published in 2011.
- Before buying any C++ book, make sure that it is recent, and that you like the writing style.

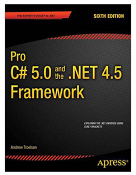
Moving on to C#

C# belongs to a different class of language.

- C# targets the .NET framework. This can be thought of as an **extensive** library of well-maintained and (mostly) stable general-purpose functions.
- .NET runs in software, rather than directly on hardware. This results in slower code, but a consistent and safe execution environment.
- C# is *my* language of choice. The language, together with .NET, favours fast and intuitive development of powerful programs.
- Pointers are hidden from the user in C#. Most memory allocation and de-allocation is done automatically, via *garbage collection*.
- To combine the execution speed of C and the development power of C# I have previously written fast algorithms into C libraries and written a program around it in C#.
- C# is less portable than C; C# can only be run on .NET for windows, or Mono for Linux, Mac, Android and iOS.

C# References

Book



- “Pro C# and the .NET 4.5 Framework, 6th Edition” by Andrew Troelsen, appears to be up-to-date and comprehensive.

MSDN

The definitive (and free) source of information for Microsoft Platforms is the MSDN, the C# documentation is browsable at:
http://msdn.microsoft.com/en-gb/library/kx37x362.aspx

Summary

- We can create pointers to functions. This enables us to pass functions to another function.
- There exist function libraries that you can use rather than write your own versions of established algorithms.
- By running multiple instances of your program, or writing a multi-threaded program, you can use the full processing power of your computer.
- An HPC is a very powerful computer-processing cluster and can be hired to run CPU intensive code.