C for Science

Lecture 1 of 5

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Introduction to the Course

This course has been adapted from its previous incarnation, run by Dr Steve Capper.

Originally, the course was based on the M3SC course run by Dan Moore.

Aims of the Course

- To introduce C programming from scratch.
- To provide insight into scientific computing.
- To write fast, efficient and maybe even multi-threaded code!

- Each afternoon will consist of a ≈ 1 hour lecture
- A \approx 1 hour practical session.



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Five lectures

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Course Content

What we'll cover

- Different number types in C (Integers and Floating Point).
- Operators, operands and their precedence.
- Conversions and casts.
- Mathematical and Logical expressions.
- Statements: if, else, ?, while, do, for, switch. . .
- Functions.
- Pointers, arrays and matrices.
- Characters, strings and interacting with the console.
- Reading and writing files.
- Optimisation and Debugging.
- Scientific C-Libraries and their uses: NAG, GSL, etc.
- An Introduction to Parallel Computing.
- C++ and other languages.



A Rough History of C

Invented ≈ 1970

By Dennis Ritchie working in Bell Labs USA; to facilitate development of a portable UNIX.

C has been standardised

- 1989 ANSI standard ratified ANS X3.159-1989.
- 1990 ISO standard ISO/IEC 9899:1990. Aka C90.
- 2000 ISO standard ISO/IEC 9899:1999. Aka C99.

C++ has evolved from C

Bjarne Stroustrup developed C++ (C with class). Unlike C, C++ is still under very active development (C++11 being the most recent standard at the time of writing).



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Interacting with the Console

Introduction

What is C

What are C and C++?

- C is a cross-platform, compiled, general-purpose language.
- C++ can loosely be thought of as C's object-oriented big brother.

The vast majority of the programs running on your computer (including the operating system kernel), are written in either C or C++. In the case of Windows, another big contender for a lot of the more recent applications is C# (but it isn't appropriate at kernel-level or for fast number-crunching).

Why Use C? (Over Maple, Matlab... Excel(?!)...)

Speed

C programs are compiled to machine code, the resulting routines can run several orders of magnitude quicker than their equivalents in interpreted environments.



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The C language is intrinsically low level, one can manipulate complex data structures with surprisingly little code.



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Flexibility

The C language is intrinsically low level, one can manipulate complex data structures with surprisingly little code.

Portability

A well written C program can target many different environments (Windows PCs, Linux workstations, Apple Macs, DEC Alphas, Embedded devices...).



Getting Started

You will need:

- A C compiler (many different ones to choose from, some are free).
- Some documentation (such as the lecture notes/exercises from this course, a good book, online guides).
- Lots, and lots of time.



Commercial C Compilers

- Intel for Windows or Linux. Compiles highly optimised code for Intel (and AMD) processors. Free for personal use and academic use by students. Full-academic and commercial licenses obtainable from: http://www.polyhedron.com
- Microsoft Visual Studio 2010 Professional -Microsoft's flagship compiler. Ninety day free trial available at: http://www.microsoft.com/visualstudio/en-us/try

Free C Compilers

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Linux

 gcc - The GNU Compiler Collection, C compiler. http://acc.anu.org.

- Visual C++ 2010 Express Microsoft's free compiler,
- Mingw Minimalist GNU for Windows,



Free C Compilers

Getting Started

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- Visual C++ 2010 Express Microsoft's free compiler, http://www.microsoft.com/express/vc/
- Mingw Minimalist GNU for Windows, http://www.mingw.org/.



Integrated Development Environments

Getting Started

gcc (for Linux or MinGW) is a command line driven compiler; an Integrated Development Environment (IDE) is a graphical application that provides tools to assist with editing, compiling and debugging of code. I'd recommend Visual Studio Professional as an IDE, this can be obtained through DreamSpark if you're eligible. For a non-windows or free alternative, I'd recommend:

```
Windows Visual C++ 2010 Express, the free Microsoft IDE.
        http://www.microsoft.com/express/vc/
```

Windows/Linux/Mac Code::Blocks, a cross-platform, open source IDE. http://www.codeblocks.org/



Software

Books for C

Getting Started

Kernighan and Ritchie (K&R2)

The C Programming Language, Second Edition, Prentice Hall. This is a fantastically structured reference book, it is written by the authors of C and is **the** C reference!



Numerical Recipes in C

By Press, Teukolsky, Vetterling & Flannery, Second Edition, CUP. Full of high quality example scientific C code. A free online edition can be found at:

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• To *build* an executable from source, we carry out the following three steps:

Edit Source

Use a text editor to create a . c file.

Compile

With a C compiler, this creates *object file(s)*.

Link

Combine the object files together into an executable.

 These steps are can be automated by Integrated Development Environments (IDEs).



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Building a C Program

 To build an executable from source, we carry out the following three steps:

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Building a C Program

 To build an executable from source, we carry out the following three steps:

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Use a text editor to create a . c file.

Compile

With a C compiler, this creates *object file(s)*.

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Combine the object files together into an executable.

 These steps are can be automated by Integrated Development Environments (IDEs).



```
1 #include <stdio.h>
2
3 int main(void)
4 {
5    printf("Hello World!\n");
6    return 0;
7 }
```

The "Hello World" Program

A traditional first program started by Ritchie. This is one of the smallest possible C programs that demonstrates some functionality (printing to screen).

```
#include <stdio.h>
  int main(void)
5
     printf("Hello World!\n");
6
     return 0;
```

Line 1

A pre-processor directive (it begins with a #) advertising extra routines to the compiler.

```
1 #include <stdio.h>
2
3 int main(void)
4 {
5    printf("Hello World!\n");
6    return 0;
7 }
```

Line 2

An empty line, or equivalently, a line consisting solely of *whitespace*. This is ignored by the compiler but makes the source code more readable.

```
1 #include <stdio.h>
2
3 int main(void)
4 {
5    printf("Hello World!\n");
6    return 0;
7 }
```

Line 3

A function declaration, defining our main function. The main function is where our program starts and is known as an *entry point*. Our main function takes *no parameters* (void) and *returns* an integer (int).

```
#include <stdio.h>
  int main(void)
5
     printf("Hello World!\n");
6
     return 0;
```

Line 4

Opening brace, all statements enclosed between the braces {, } belong to the main function.

```
#include <stdio.h>
  int main(void)
5
     printf("Hello World!\n");
6
     return 0;
```

Line 5

A statement; the printf (print formatted) function is called with the argument "Hello World!\n". This prints:

```
Hello World!
```

to standard output (usually a text console).



```
#include <stdio.h>
  int main(void)
5
     printf("Hello World!\n");
6
     return 0;
```

Line 6

A return statement, we exit main with a return code of 0. The system interprets 0 as "success".

```
#include <stdio.h>
  int main(void)
5
     printf("Hello World!\n");
6
     return 0;
```

Line 7

A *closing brace*, everything after this line does not belong to main.

```
#include <stdio.h>
   int main(void)
 5
       int low=-40, high=140, step=5, f, c;
 6
       c = low;
       while (c <= high)
 8
          f = 32 + 9 * c/5;
          printf("%6d \t %6d\n", c, f);
11
          c = c + step;
12
13
       return 0;
14 }
```

```
#include <stdio.h>
int main(void)
   int low=-40, high=140, step=5, f, c;
   c = low;
```

Lines 1, 2, 3 & 4

Identical meaning as in the previous program.

```
#include <stdio.h>
  int main(void)
5
     int low=-40, high=140, step=5, f, c;
     c = low:
```

Line 5

Local variable declarations; the integers low, high, step, f and c are declared. These are local to main. The variables low, high and step are initialised with the values; whilst f and c are undefined.

```
#include <stdio.h>
  int main(void)
5
     int low=-40, high=140, step=5, f, c;
6
     c = low;
```

Line 6

The local variable c is assigned the value of low.

```
while (c <= high)
          f = 32 + 9 * c/5;
          printf("%6d \t %6d\n", c, f);
11
          c = c + step;
12
13
       return 0;
14
```

Lines 7, 8 & 12

A *while* loop is defined. For as long as the variable c is less than or equal to high, the code between the braces on lines 8 and 12 is executed.

```
while (c <= high)
          f = 32 + 9 * c/5;
10
          printf("%6d \t %6d\n", c, f);
11
          c = c + step;
12
13
       return 0;
14 }
```

Line 9

The local variable f is assigned a value from the integer arithmetic expression involving c.

Another C Program - What does this do?

```
while (c <= high)
          f = 32 + 9 * c/5;
10
          printf("%6d \t %6d\n", c, f);
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12
13
       return 0;
14 }
```

Line 10

The variables c and f are printed to standard out, each six characters wide, separated by a tab and two spaces.

Another C Program - What does this do?

```
while (c <= high)
8
          f = 32 + 9 * c/5;
10
          printf("%6d \t %6d\n", c, f);
11
          c = c + step;
12
13
       return 0;
14 }
```

Line 11

The local variable c is incremented by step.

Another C Program - What does this do?

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11
          c = c + step;
12
13
       return 0;
14 }
```

Lines 13 & 14

Have an identical meaning as in the last program.

Commenting C Programs

Getting Started

A comment is text in the source file that gets ignored by the compiler. This is useful for providing human-readable notes about what the code is doing, or removing lines of code temporarily. There are two ways of commenting files in C:

Traditional Way

```
Anything between /* and */ is a comment, i.e. /* This function is used to compute the roots of a quadratic equation */
```

C++ Style

```
These are single line only, anything after // is a comment, i.e. int c = 3; // set c to 3
```

Technically, C++ style comments aren't in the C standard. (But they are ubiquitous to C code anyway).

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Variable Names

From K&R

"... Is a sequence of letters and digits. The first character must be a letter; the underscore _ counts as a letter. Upper and lower case letters are different"

- Punctuation or any other symbols are not allowed in variable
- The modern C standard discourages the use of an underscore



Variable Names

From K&R

"... Is a sequence of letters and digits. The first character must be a letter; the underscore _ counts as a letter. Upper and lower case letters are different."

What to Avoid...

- Punctuation or any other symbols are not allowed in variable names.
- The modern C standard discourages the use of an underscore as the first character of a variable name.



One example is:

#include <stdio.h>

Which tells the compiler to search <stdio.h> for functions.

• Another example is:

#define MAXSIZE 1024

This replaces all occurrences of MAXSIZE with 1024

- Define statements can be named in a similar way to variables, but
- It is convention to use upper case for #define statements.
- Or even simpler:

#define NDEBU

Meaning NDEBUG is defined. This will be expanded later on



Preprocessor Directives

One example is:

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Numbers in C

There are two types of number in C:

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Integers

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Floating Point Numbers

Floating point numbers are more flexible and provide an approximation to real numbers. They store a representation of a number in a form with a similar concept to scientific notation.



Integers

Integer types in C can be thought of as rings of different sizes (i.e. hours on a clock face). They hold one of the range of integers in the ring and once the highest value in the ring is reached the next incremental value will be the lowest value in that ring.

- As integers lose all fractional data, multiplication is not always the inverse of division.
- Products higher than the size of the ring will wrap to the smallest value in the ring; division is not necessarily the inverse of multiplication.

Integer Types

short, unsigned short, int, unsigned int, long, unsigned long, long long, unsigned long long



Integer Types - For a 32 bit program

Туре	Min	Max
short	-32768	32767
unsigned short	0	65535
int	-2147483648	2147483647
unsigned int	0	4294967295
long	-2147483648	2147483647
unsigned long	0	4294967295
long long	-9223372036854775808	9223372036854775807
unsigned long long	0	18446744073709551615

For example, here are two bit patterns for short:



(for more information see imits.h>)



Integers

- Two main subtypes signed and unsigned. Signed types use a sign bit.
- For signed types we, usually, have:
 - minimum value: -2^{size-1}
 - maximum value: 2^{size-1} 1
- For unsigned types we have:
 - minimum value: 0
 - maximum value: 2^{size} 1
- short is often used to conserve memory.
- int represents the native CPU integer type so is used for speed. (If in doubt use int).
- long and long long are used to maintain accuracy.



Integer Arithmetic

Base Operators

The four usual operators are defined +, -, \star and /.

Ring arithmetic

Division is not always the reverse of multiplication:

$$1/2=0$$
, $0 \star 2=0$.

Also, any result of a computation must lie within the ring, any number outside the range of the current data type will "wrap" around. (i.e. 11am + 3 hours gives 2pm).

Modulo Operator

The remainder operator % is unique to integer types, it acts as expected: 7 % 2 = 1.



Floats

These are much more flexible numbers, but still *NOT* the same as \mathbb{R} .

- Because of the way the number is stored, even fairly simple-looking base-10 numbers (0.1, 0.2, 0.3...) are only stored as an approximation.
- Because numbers are kept as approximations: associativity and commutativity don't always apply and multiplicative inverses don't always exist.
- The way in which the numbers are stored can result in a loss of the least significant parts of numbers. This causes problems when adding/subtracting big and small numbers together.
- Programming floats well for numerical problems, especially with large/small numbers, is an art form!

Float Types

float, double, long double



Getting Started

Floating Point Numbers (IEEE 754 Standard)

On my machine, a float (single precision) looks like:

It consists of three parts, the sign bit(b), the biased exponent(e) and the fraction(f). We break down a number x:

$$x^{\text{float}} = (-1)^b \times 2^{e-127} \times (1 + f \times 2^{-23}), \quad 0 < e < 255, \\ 0 \le f \le 2^{23} - 1,$$

We have four special numbers, $-Inf(-\infty)$, $Inf(\infty)$, NaN (Not a Number) and zero.

For double (double precision) we have:

$$x^{\text{double}} = (-1)^b \times 2^{e-1023} \times (1 + f \times 2^{-52}), \quad 0 < e < 2047 \\ 0 \le f \le 2^{52} - 1.$$



Floating Point

Base Operators

As with integers, we have +, -, * and /.

Floating point code

- It looks like integer code but with a decimal point suffix.
- Scientific notation is achieved with e: double speedofLight = 2.997e8; (2.997×10^8)

Float Arithmetic

- Division is not always the reverse of multiplication.
- Operators may not be commutative!

$$A + B + C \neq A + C + B$$
 (sometimes)



Getting Started

More Mathematical Functions in <math.h>

 Maths functions come with the ANSI Standard C Library, which contains many maths functions. To use them we need a:

```
#include <math.h>
```

Here some example functions:

```
\sin(x) asin(x) \sinh(x) exp(x)

\cos(x) acos(x) \cosh(x) log(x)

\tan(x) atan(x) \tanh(x) log10(x)

\operatorname{sqrt}(x) atan2(x,y) \operatorname{pow}(x,y) fabs(x)
```

(all the trigonometric functions use radians!)

The pow(x, y) function (declared in <math.h>)

Exponentiation

Getting Started

There is no exponentiation operator (e.g. \wedge , $\star\star$) in C. Instead we have the following:

$$x^{y} = pow(x, y)$$

This assumes x and y are of type double.

Beware

The pow function is often implemented as:

$$exp(y*ln(x))$$

For whole integer powers (i.e. x^2), one should perform the multiplication explicitly (x * x).



Simple Logical Expressions

```
7 while (c <= high)
```

- Are used to carry out branches (if statement) and loops (such as for, and while).
- Evaluate to either true (non-zero int) or false (zero).

Logical Operators

Getting Started

```
> y is x greater than y?
x >= y is x greater than or equal to y?
x < y is x less than y?
x \le y is x less than or equal to y?
x == y is x equal to y?
x != y is x different to y?
```



Using == Safely

Getting Started

The danger of the easily-made typo:

if
$$(x = 3)$$
 {Statement;}

is it will always return true and execute the statement, it will also overwrite x with 3. This is not only undesirable as it is will not be testing the desired expression, but it is valid code so will not always throw an error - making debugging very tricky.

if
$$(3 == x) \{ Statement; \}$$



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```
if (x = 3) {Statement;}
```

is it will always return true and execute the statement, it will also overwrite x with 3. This is not only undesirable as it is will not be testing the desired expression, but it is valid code so will not always throw an error - making debugging very tricky.

A Preventative Measure

If the variables x and 3 were to be swapped, such as:

```
if (3 == x) \{ Statement; \}
```

Then if = was used rather than == it would cause an error as a value cannot be assigned to 3, but it keeps the expression logically equivalent. Getting into the habit of using the variables this way round can save hours of debugging!



Compound Logical Expressions

Getting Started

We can create compound logical expressions using the following operators:

- || is a *logical or.* 1e1 || 1e2 returns false if both 1e1 and 1e2 are false and true otherwise.
- && is a *logical and*. le1 && le2 returns true if and only if both le1 and le2 are true.
- ! is a *logical not*. !le1 returns the opposite of le1.

Here are two identical examples:

- \bullet (x < 100) && (x%2 == 0)
- (x < 100) && !(x%2)

Control Statements

Executes block(s) of code depending on the evaluation of a logical expression.

```
Simple if
            if (logical expression) { statements; }
if, else if, else
   if (logical expression)
       { statements; }
   else if (logical expression)
       { statements; }
   else if (logical expression)
       { statements; }
   else
       { statements; }
```

Flow Control - while

A while loop is used to repeatedly execute code as long as a logical expression is true.

Structure

```
while (logical expression)
{ statements ;}
```

 If logical expression is false, then the statements are never executed.

Flow Control - do {} while ()

We place the *logical expression* after the *statements* giving us:

Structure

```
do { statements: }
while (logical expression)
```

The statements are executed at least once.

```
do while or while?
```

Generally I prefer while over do while, as it forces me to initialise variables properly.

Flow Control - for loop

```
for ( start expression ;
    logical expression ;
    step expression)
    { statements ; }
```

Print out ten numbers:

```
for (x=0; x < 10; x = x + 1)
printf("x = %d\n", x);
```

Keep looping indefinitely (printing out dots)

```
for (;;) printf(".");
```

Flow Control - switch - case

We can selectively execute code based on a value, using the following:

```
switch (integer_statement) {
case integer_value1: statements1; break;
case integer_value2: statements2; break;
case integer_value3:
case integer_value4: statements3; break;
default: statements4; break;}
```

- Execution starts at either one of the case's or at default.
- Execution stops at the end } or at break.
- case, default and break are optional.



Some Loop Control Features

Getting Started

Execution of code inside a loop (do, while, for) can be manipulated by the following statements.

break;

Break out of the current loop. Any statements in the loop following the break are ignored and the loop condition automatically evaluates to false, ending the loop.

continue;

Jump to the end of the current loop (effectively ignoring everything below the continue statement. Whether or not the loop continues executing depends on the loop condition.



As seen in the examples, the printf function can be used to print out variables. The function *prototype* takes the form:

```
int printf(char * formatString, ...)
```



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```
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```

formatString

The first argument of printf is the format string, this specifies how many variables need printing out, how they are to be printed, and in what order.



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```
int printf(char * formatString, ...)
```

This is C shorthand for *variable number of arguments*.



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```
int printf(char * formatString, ...)
```

Return value: int

printf returns the number of characters printed.



3 H / 3 L / 3 E / 3 E /

printf - declared in <stdio.h>

We call printf as follows:

```
printf(formatString, var1, var2, ..., varN);
where.
```

formatString

The format string tells printf how many variables need printing. A format string can contain format specifiers, these tell printf exactly how to print out each variable, some examples:

```
"%6d"
         print out an integer (6 characters wide).
```

print out a floating point number. "%a"

We call printf as follows:

```
printf(formatString, var1, var2, ..., varN);
```

where.

formatString

The format string tells printf how many variables need printing. A format string can contain format specifiers, these tell printf exactly how to print out each variable, some examples:

```
"%6d" print out an integer (6 characters wide).
```

"%q" print out a floating point number.

```
var1, ...
```

printf accepts a variable list of arguments, which can be of different type. Care must be taken to match formatString with the variables.



- The backslash \ character in C has a special meaning, it is known as the *escape character*.
- We combine the escape character with other characters, to form an escape sequence, here are some examples:

printf

scanf() - Reading Data from Standard Input

For two variables A and B, both of type double, we use:

```
scanf("%lf %lf", &A, &B);
```

where the % represent format specifiers

Format Specifiers

Consist of a %, a numerical width specification and a field code

• and the & represents the *address* of the variable in memory. This is known as a *pointer reference operator*.



scanf () - Reading Data from Standard Input

For two variables A and B, both of type double, we use:

```
scanf("%lf %lf", &A, &B);
```

where the % represent format specifiers

Format Specifiers

Consist of a %, a numerical width specification and a field code:

```
float (general form)
d
   int
                              lf double (fixed form)
   unsigned int
   float (fixed form)
                              le double (exponential form)
   float (exponential form)
                              lg
                                   double (general form)
```

• and the & represents the address of the variable in memory. This is known as a *pointer reference operator*.



- Functions in C can return only one value.
- Sometimes we want more than one value to change.
- If we tell scanf where the variables are in memory, scanf can change them itself.

The ability to manipulate memory directly is what makes C so powerful (and potentially dangerous).

scanf

Pointers

A *pointer* is a variable that stores a memory location, they are declared as follows:

& - Pointer reference operator

Returns the memory address (pointer to) of a variable.

$$ptrA = &A$$
 // $ptrA$ points to A



Pointers

A *pointer* is a variable that stores a memory location, they are declared as follows:

& - Pointer reference operator

Returns the memory address (pointer to) of a variable.

Pointer de-reference operator

Converts a memory address to a variable:

```
* ptrA = 1.234; // A is now 1.234
```



Summary

Getting Started

- C is a cross-platform, compiled language which can produce results much guicker than other methods/languages.
- We use an IDE to write source, compile, link and debug our C programs.
- The basic structure of a C program has been demonstrated.
- There are two categories of number in C: integers and floating point numbers.
- We have seen how logic and statements can control the flow of a program.
- printf and scanf will write and read from the console respectively.

