## C++ for Scientific Computing (2021)



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[^0]C++ is 'object-oriented'

- Modularity: All the data and methods of a particular object are held in one or two files - so can be worked on independently.
- Abstraction: The essential features and functionality are put in one place.
- Encapsulation: The implementation of an object is kept hidden from the caller (can be changed without breaking the interface).
- Extensibility: Code is easily re-used and extended.
- Polymorphism: The same code can be used for a variety of objects (or for different types of data).
- Inheritance: A powerful way to extend functionality.

Many lecture courses begin with these concepts. We'll cover the basics of programming without object orientation - and mention this on the way.

## Lecture 1 - The basics

General structure of a basic $\mathrm{C}++$ program

```
#include <header1>
#include <header2>
int main(int argc, char* argv[])
{
    line of code;
    // this is a comment, ignored by the compiler
    more code; // this is a comment as well
    /* Multi-line
    * comment
    */
    return 0;
}
```

This program prints the text "Hello World" to the screen

- iostream is a header file that is needed when using input and output
- std: :cout is a command that sends output to the console, i.e. the screen
- $\backslash \mathrm{n}$ is a formatting command that starts a new line
- All statements (lines of the program) inside the curly brackets end with a semicolon ;

Save this code as hello_world.cpp
Things to note

1. Header files are listed first. These are files that contain the functions needed for operations such as input, output and mathematical calculations
2. There is a section of code that starts "int main(int argc, char* $\operatorname{argv}[]$ )" (or "int main()" for brevity when command-line input is unimportant)
3. This section of code is followed by more code enclosed between curly brackets, $\{$ and \}
4. Comments may easily be inserted into the code
5. Lines of code that "do something" end with a semicolon ;
6. Just before the closing curly bracket at the end of the code is a statement return 0;

## A first $\mathrm{C}++$ program

```
#include <iostream>
int main(int argc, char* argv[])
{
    std::cout << "Hello World\n";
    return 0;
}
```


## Compiling the code

A key difference between Matlab and C++—before the code can be executed it must be compiled

When using the Gnu compiler of Unix/Cygwin this code can be compiled by saving the code and typing
g++ -Wall -0 -o hello_world hello_world.cpp
followed by return. This produces an executable called hello_world that can be executed by typing

## ./hello_world

Visual Studio can also be forced to compile on the command line (if you set the correct environment first):
cl /EHsc hello_world.cpp

Some example lines of code that add two integers and print the answer to screen are

```
int integer1, integer2, answer;
```

int integer1, integer2, answer;
integer1 = 5;
integer1 = 5;
integer2 = 10;
integer2 = 10;
answer = integer1 + integer2;
answer = integer1 + integer2;
std::cout << "The sum of " << integer1 << " and "
std::cout << "The sum of " << integer1 << " and "
<< integer2 << " is " << answer << "\n";

```
    << integer2 << " is " << answer << "\n";
```

Numerical variables

Before a variable is used the type of variable must be declared. For example if the variables $i$ and $j$ are integers and $a$ is a double precision floating point number the statements

```
int i, j;
double a;
```

must be included in the program before these variables are used.
It is advisable to use double rather than float in scientific computing applications

Some names, such as int, for, return may not be used as variable names because they are used by the language. These words are known as reserved words or keywords
see: example structure

## More on numerical variables

A variable may be initialised when defining the variable type, for example

```
int i = 5;
```

The line above is equivalent to declaring i to be of type int and assigning it the value 5 , in one step.

```
int i;
i = 5;
```

The details of the std: :cout statement will be explained later

When assigning values to floating point variables it is good programming practice to write numbers with decimal points, i.e.

```
double a = 5.0;
```

rather than
double $\mathrm{a}=5$;

If a quantity is a constant throughout the program it may be declared as such
const double density $=45.621$;

Some variable types and ranges in most 64 -bit operating system are given below. Note the ranges are operating system dependent

| Variable type | $\mathrm{C}++$ name | Range in 64 -bit |
| :--- | :--- | :--- |
| integer | short int | $-2^{15}$ to $2^{15}-1\left(\approx 10^{4}\right)$ |
| integer | int | $-2^{31}$ to $2^{31}-1\left(\approx 10^{9}\right)$ |
| integer | long int | $-2^{63}$ to $2^{63}-1\left(\approx 10^{19}\right)$ |
| unsigned integer | unsigned int | 0 to $2^{32}-1$ |
| floating point | float | $-3.4 \times 10^{38}$ to $3.4 \times 10^{38}$ |
| floating point | double | $-1.7 \times 10^{308}$ to $1.7 \times 10^{308}$ |
| floating point | long double | $-1.2 \times 10^{4932}$ to $1.2 \times 10^{4932}$ |

Note that long double is identical to double on an older 32-bit architecture

Note that the size of long int is identical to int 32 -bit architectures

There is a shorthand for some mathematical operations

| Longhand | Shorthand |  |
| :--- | :--- | :--- |
| $\mathrm{a}=\mathrm{a}+\mathrm{b} ;$ | $\mathrm{a}+=\mathrm{b} ;$ |  |
| $\mathrm{a}=\mathrm{a}-\mathrm{b} ;$ | $\mathrm{a}-=\mathrm{b} ;$ |  |
| $\mathrm{a}=\mathrm{a} * \mathrm{~b} ;$ | $\mathrm{a} *=\mathrm{b} ;$ |  |
| $\mathrm{a}=\mathrm{a} / \mathrm{b} ;$ | $\mathrm{a} /=\mathrm{b} ;$ |  |
| $\mathrm{a}=\mathrm{a}+1 ;$ | $\mathrm{a}++;$ | if a is an integer |
| $\mathrm{a}=\mathrm{a}-1 ;$ | $\mathrm{a}--;$ | if a is an integer |

```
float a, b;
double d, e;
a = 3.0;
b = (a * pow(a, 7.5) ) / 2.0;
d = 4.0;
e = 2.0 * sqrt(d);
```

pow $(x, y)$ gives the value of $x^{y}$.
sqrt (d) gives the square root of the variable $d$
When using mathematical functions such as pow, you should use the additional header file cmath and so you need the line of code

[^1]Division of an integer by another integer will almost certainly cause problems

An example is given in the following piece of code
int $i=5, j=2, k ;$
$k=i / j ;$
std: :cout $\ll k \ll " \backslash n " ;$

The variable k is an integer and so cannot store the true value, 2.5 Instead, it will store the value 2

Suppose an integer is divided by a variable of type double - or vice versa - and that the result returned is stored in a variable of type int, as shown in the code below.

The variable k in this code is unable to store the mathematically correct answer

```
double i = 5.0;
int j = 2, k;
k = i / j;
std::cout << k << "\n";
```

Only construct mathematical operations that are on elements of the same type

An integer can be converted to a different data type - see the next slide

Suppose an integer is divided by a variable of type double - or vice versa - and that the result returned is stored in a variable of type double, as shown in the code below.
The variable k in this code will contain the mathematically correct answer

```
double i = 5.0, k;
int j = 2;
k = i / j;
std::cout << k << "\n";
```

However, this is bad programming practice and should be avoided

```
double i = 5.0, k;
int j = 2;
k = i / ((double) (j));
std::cout << k << "\n";
```

In this example, ((double) ( j$)$ ) allows the variable j to behave as if it were a double variable.

## Modern $\mathrm{C}++$ aside: the auto type

Modern $\mathrm{C}++$ allows the type to be inferred if it is initialised to a value when it's declared.

```
auto i = 5.0;
auto j = 2;
```

This is useful when types are long (see Lecture 13).
But it is dangerous when we are using simple types such as int and double.

```
auto x = 20; // Compiler infers x as int
x += 2.5;
// Programmer might assume x is double
std::cout << "x = "<<x<<"\n"; // x = 22
```

${ }^{1+1}+$ To use modern $\mathrm{C}++$ features compile with $\mathrm{g}^{++}-$std=c++11

Elements of the array are accessed by placing the indices in separate square brackets, for example

```
array1[0] = 1;
array2[1][2] = 3.0;
```

Arrays can be initialised when they are declared, for example

```
double array1[3] = {0.0, 1.0, 2.0};
int array2[2][3] = { {1, 6, -4}, {2, 2, 2} };
```

Arrays (static allocation)
An array is known to mathematicians as a matrix or, in one dimension, a vector

If the size of the array is known in advance then it can be declared as follows

```
int i = 5, j = 4, array1[4];
double array2[3] [3]; //3 by 3 array
```

In contrast to Matlab and FORTRAN the indices of an array of length n start at 0 and end at $\mathrm{n}-1$

Either get used to the new index numbering, or define arrays to have one extra element

Note that the values of arrays may only be set using the curly bracket notation when they are declared-for example the code

```
int array[3] = {0, 1, 2};
```

is correct, but the code

```
int array[3];
array[3] = {0, 1, 2};
```

is not correct.
where the array array2 represents the matrix

$$
\left(\begin{array}{ccc}
1 & 6 & -4 \\
2 & 2 & 2
\end{array}\right)
$$

## Boolean variables

These variables take the values true or false, and are of use when using if conditionals and while loops

They are used as follows:

```
bool flag;
flag = true;
```


## Strings

A character is one letter or number, a string is an ordered collection of characters

For example, "C++" is a string consisting of the ordered list of characters "C", "+", and "+"

To use strings in C++ requires an extra header file as shown below

```
#include <iostream>
```

\#include <string>
int main()
\{
std::string city; // note the std::
city = "Oxford"; // note the double quotation marks
std::cout << city << "\n";
\}

## ASCII characters

ASCII characters are numbers, uppercase letters, lowercase letters and some other symbols
These characters may be represented using the data type char

```
#include <iostream>
int main()
{
    char letter;
    letter = 'a'; // note the single quotation marks
    std::cout << "The character is " << letter << "\n";
    return 0;
}
```

Tip: automated builders and IDEs

- Possibly start with an editor and a command-line compiler
- As projects get larger you need something to keep track of the compilation for you
- Make is a good dependency-checker: time-stamps determine what is re-made (Lecture 7). CMake is useful for configuration.
- SCons is a more sophisticated tool (written in Python). MD5 hashes are used to decide what needs to be re-made.
- Integrated development environments: Visual Studio (Windows), Borland (Windows), Xcode (OSX), Kdevelop (KDE) and Eclipse (multi-platform) either use Make/SCons or their own dependency checkers
- An IDE will help you to write code by cross-referencing between your files, saving your work and offering a debugger


## Lecture 2 - Flow of control

The if statement
Suppose you want to execute two statements if the condition $p>q$ is met
This is achieved using the following code

```
if (p > q)
{
    statement1;
    statement2;
}
```

Note the indentation of the block between $\{$ and $\}$. This makes it clear which statements are executed in the block

Third example - more than one condition

```
if (p == 0)
{
    statement1;
}
else if (p < 0)
{
    statement2;
    statement3;
}
else
{
    // p > 0
    statement4;
}
```

If only one statement is to be executed curly brackets aren't strictly necessary
For example, the following code will execute statement1 if the condition $\mathrm{p}>\mathrm{q}$ is met

```
if (p > q)
    statement1;
```

but this is poor software engineering practice
Instead, write this code as

```
if (p > q)
{
    statement1;
```

\}

The use of curly brackets makes it clear which statement(s) are to be executed

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Fourth example - nested if statements

```
if (p < q)
{
    if (x >= y)
    {
        statement1;
        }
}
```

Fifth example - more than one condition

```
if (p < q || x < y)
{
    statement1;
}
```

statement1 is executed if and only if one or both of $\mathrm{p}<\mathrm{q}$ and $\mathrm{x}<$ y is true - i.e. $\|$ is the logical OR operator

Relational and logical operators

| relation | operator |  |
| :--- | :--- | :--- |
| equal to | $==$ | (note that it isn't " $="$ ") |
| not equal to | $>$ |  |
| greater than | $<$ |  |
| less than | $>=$ |  |
| greater than or equal to | $>=$ |  |
| less than or equal to | $<$ |  |

Boolean variables may be used in if statements as follows

```
bool flag1 = true, flag2 = false;
```

bool flag1 = true, flag2 = false;
if (flag1)
if (flag1)
{
{
std::cout << "Does print something" << "\n";
std::cout << "Does print something" << "\n";
}
if (flag2)
if (flag2)
{
{
std::cout << "Doesn't print anything" << "\n";
std::cout << "Doesn't print anything" << "\n";
}
if (!flag2)
if (!flag2)
{
{
std::cout << "Does print something" << "\n";
std::cout << "Does print something" << "\n";
}
}
{

```
    {
```

for loops
The following loop executes the statements inside the loop 10 times.
Note that i must have been declared as an integer earlier in the code

```
for (i=0; i<10; i++)
{
    statement1;
    statement2;
}
```

Alternatively, the integer i may be declared inside the loop:

```
for (int i=0; i<10; i++)
{
    statement1;
    statement2;
}
```

The output from the section of code on the previous slide is

| $i=0$ | $j=5$ |
| :--- | :--- |
| $i=0$ | $j=4$ |
| $i=0$ | $j=3$ |
| $i=0$ | $j=2$ |
| $i=0$ | $j=1$ |
| $i=1$ | $j=5$ |
| $i=1$ | $j=4$ |
| $i=1$ | $j=3$ |
| $i=1$ | $j=2$ |
| $i=2$ | $j=5$ |
| $i=2$ | $j=4$ |
| $i=2$ | $j=3$ |
| $i=3$ | $j=5$ |
| $i=3$ | $j=4$ |
| $i=4$ | $j=5$ |

for loops can be nested and run over variable indices. The output from the following section of code is given on the next slide

```
for (int i=0; i<5; i++)
{
    for (int j=5; j>i; j--)
    {
        std::cout << "i = " << i << " j = " << j << "\n";
    }
}
```

Use of assert statements for debugging
assert statements can be used in code to confirm something you expect to be true

For example, you may wish to confirm that a number you are about to take the square root of is non-negative

If the condition is not met, the code aborts giving an error message that explains what went wrong

To use assert statements you must use the header file cassert

An example of the use of assert statements is given on the next slide

```
#include <iostream>
#include <cassert>
#include <cmath>
int main()
{
    double a;
    std::cout << "Enter a non-negative number\n";
    std::cin >> a;
    assert(a >= 0.0);
    std::cout << "The square root of a is " << sqrt(a) << "\n";
    return 0;
}
```


## Lecture 3 - Input and output

Console output
Console output may be achieved by using std: : cout
We have already seen that the statement
std::cout << "Hello World $\backslash n$ ";
prints the text "Hello World" to the screen, followed by a newline The statements

```
int x = 1, y = 2;
std::cout << "x = " << x << " and y = " << y << "\n";
```

If the code on the previous slide is compiled and run, and the user enters " -5 " at the prompt, the code will be terminated and the following error message given:

```
msqrt:: msqrt.cpp:10: int main(): Assertion 'a >= 0.0' failed
```

This error message tells us to look at line 10 in program. cpp, where the assertion in quotes failed the test

Note that any spaces required in the output must be included within quotation marks
Some useful formatting commands are

| Command | Symbol |
| :--- | :--- |
| newline | $\backslash \mathrm{n}$ |
| tab | $\backslash \mathrm{t}$ |
| , | $\backslash$ |
| $"$ | $\backslash "$ |
| $?$ | $\backslash ?$ |
| $($ bell $)$ | $\backslash \mathrm{a}$ |

give output to the screen

[^2]Sometimes, for example if the computer is busy doing a large volume of computation, the program may not print the output to the screen immediately. If immediate output is desirable then use std::cout.flush() after any std::cout commands

```
std::cout << "Hello World\n";
```

std: :cout.flush();

Keyboard input for strings is slightly different. An example is given below

```
#include <iostream>
#include <string>
int main()
{
    std::string name;
    std::cout << "Enter your name and then hit RETURN\n";
    std::getline(std::cin, name);
    std::cout << "Your name is " << name << "\n";
    return 0;
}
```

Keyboard input
Keyboard input for numbers and characters is achieved using std::cin

The following statements prompts someone to enter their PIN

```
int pin;
std::cout << "Enter your PIN, then hit RETURN\n";
std::cin >> pin;
```

cin may be used to ask for more than one input at a time

## int accountno, pin;

std::cout << "Enter your account number then hit RETURN,\n"; std::cout << "and then your PIN followed by RETURN\n"; std::cin >> accountno >> pin;

## Redirecting output

Instead of printing the output to screen, you may want to write the output to file. Suppose the executable is called my_prog. The screen output may be redirected to the file output by the command

## ./my_prog > output

When output has been redirected, you may prefer to print errors to screen. This can be done using std::cerr

```
std::cerr << "Error - division by zero\n";
```

When output is redirected to the file output, the errors printed using std: :cerr are not printed to file, only to the screen

## Writing to file

When writing to file, an additional header function fstream is needed. It can be a good idea to include these header files whether or not they are needed:

```
#include <iostream>
#include <fstream>
#include <string>
#include <cmath>
```

The file output.dat may be opened using the statement
std::ofstream out("output.dat");

We can then write to this file in a similar manner as writing to the screen, with the exception that cout is replaced by out

Reading from file
Very similar to writing to file
Suppose the file numbers. dat (in my home directory) has 5 rows and 3 columns of numbers. This file can be read using the following code

```
double x, y, z;
std::ifstream input("/home/joe/numbers.dat");
assert(input.is_open());
for (int i=0; i<5; i++)
{
    input >> x >> y >> z;
    // ... do something with x, y, z ...
}
input.close();
```

There are a number of formatting options provided by $\mathrm{C}++$ The following prints data in scientific format

```
```

\#include <iostream>

```
```

\#include <iostream>
\#include <fstream>
\#include <fstream>
int main()
int main()
{
{
double x = -1.0, y = 45.3275893627129, z = 0.00000001;
double x = -1.0, y = 45.3275893627129, z = 0.00000001;
std::ofstream out("output.dat");
std::ofstream out("output.dat");
assert(out.is_open());
assert(out.is_open());
out.setf(std::ios::scientific|std::ios::showpos);
out.setf(std::ios::scientific|std::ios::showpos);
out << x << " " << y << " " << z << "\n";
out << x << " " << y << " " << z << "\n";
out.close();
out.close();
return 0;

```
```

    return 0;
    ```
```

\}

It doesn't matter if we don't know how long the file is - we can read data until we reach the end of the file

Using the example on the previous slide where the file numbers.dat has an unknown number of rows and 3 columns we may use the following code

```
double x, y, z;
std::ifstream input("/home/joe/numbers.dat");
assert(input.is_open());
while (!input.eof())
{
    input >> x >> y >> z;
}
input.close();
```

input.eof() is a Boolean variable that contains "true" if the end of file has been reached and "false" otherwise. (See exercises.)

Reading from command-line arguments
Command-line arguments (or flags) are read from the user of your program via the "argument count" and "argument values" parameters of main.
Here's some example code that reads from the command-line

```
#include <iostream>
int main(int argc, char* argv[])
{
    for (int i=0; i<argc; i++)
    {
        std::cout<<"argv "<<i<<" is "<<argv[i]<<"\n";
    }
}
```

Tip: version control

- Big IDEs like Xcode and Visual Studio do this for you (in the same disk space)
- Modern version control systems like Subversion, Git and Mercurial let you work on a code-base concurrently
- There are many places that will host your project for you:
- Bitbucket (Git and Mercurial)
- GitHub (Git)
- GitLab (Git)
- Unfuddle (Subversion and Git)
- Eclipse has a Subversion and Git plug-ins (Subclipse \& eGit)
- GitHub and Trac offer repository, bug-control and Wiki

Here's that code in action

```
$ ./show_args
argv O is ./show_args
$ ./show_args one two
argv O is ./show_args
argv 1 is one
argv 2 is two
```

Note that the first element of the values argv [0] is always the name of program itself.
argv is an array of strings. If you want to interpret an argument as an integer then you will need atoi.

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## Chaste



Timeline

## 2904410: Today

- 12:32 Changeset [8788] by jmpf@comlab.ox.ac.uk

Fix falling nighly Streeter wtr 18736 (moved sinquare patch of evicardial

- 09:44 Changeset [8787] by james. southern@uk. Fuilitsu.com.


## 0410: Yesterday


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- $14: 25$ Changeset [8785] by jonc@comlab.ox.ac.uk

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- 12:34 Changeset [8784] by jonc@comlab.ox.ac.uk $\begin{aligned} & \text { \#1204- use Filefinder to simplif Testcardiacsimulationarchiver. hpe. }\end{aligned}$
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## Lecture 4 - Pointers and arrays

## Pointers

A variable's address in the computer's memory is called a pointer

If a variable has been declared by

```
int total_sum
```

then the address of total_sum is given by \&total_sum
\&total_sum takes a constant value, because the address of total_sum in the computer's memory was allocated when it was declared.
\&total_sum is therefore known as a constant pointer

The contents of the memory that a pointer $p_{\text {_ }} \mathrm{x}$ points to is given by *p_x, for example

```
double y, z; // y, z store double precision numbers
double* p_x; // p_x stores the address
    // of a double precision number
z = 3.0;
p_x = &z; // p_x stores the address of z
y = *p_x + 1.0; // *p_x is the contents of the memory p_x,
    // i.e. the value z
```

Note here that * p_x means two different things, depending on where it is

Variable pointers may be declared as follows

```
double* p_x;
int* p_i;
```

$p_{\_} x$ is a variable pointer to a variable of type double, $p_{-} i$ is a variable pointer to an integer
Note that spacing can vary: double* p_x and double *p_x are equivalent, but the first is clearer.

If p_x and p-y are both to be declared as pointers this is done by
double *p_x, *p_y;
In the declaration
int *p_i, j;
$p_{-} i$ is a pointer to an integer, and $j$ is an integer. It is generally clearer to declare each new pointer on a separate line.

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A variable pointer cannot be used until first having been assigned a valid address, for example the following portion of code is incorrect

```
double* p_x; // p_x can store the address of a double
    // precision number - haven't said which
    // address yet
*p_x = 1.0; // trying to store the value 1.0 in an unspecified // memory location
```

because an address must first be assigned to $p_{-} x$ before a value is stored in that address

One way of assigning a valid address is to use the operator new

```
double* p_x; // p_x can store the address of a double
    // precision number
p_x = new double; // assigns an address to p_x
*p_x = 1.0; // stores 1.0 in memory with
    // address p_x
delete p_x; // relinquish memory
```


## Dynamic allocation of memory for arrays

Pointers can be used to allocate memory dynamically for arrays Dynamic allocation of memory has several advantages

1. The size of the array doesn't need to be known at compile time
2. The size of the array may be changed while the program is running
3. If a large array is only needed for a small section of the code, memory can be allocated for the array when it is needed and de-allocated when it isn't
4. Efficient handling of irregularly sized arrays

Memory can be allocated using the new operator, and de-allocated using the delete operator

Pointers should be used with care. Consider the following example:

```
double y;
double* p_x;
y = 3.0;
p_x = &y;
std::cout << "y = " << y << "\n";
*p_x = 1.0; // This changes the value of y
std::cout << "y = " << y << "\n";
```

The first time y is printed it takes the value 3: the second time y is printed it takes the value 1 .

The line between the cout statements has altered the value of $y$, possibly unintentionally
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To create a one-dimensional array of double precision numbers of length 10 called x we use the following section of code

```
double* x;
x = new double [10];
```

The array then may be used as if it had been created by using the declaration

```
double x[10];
```

The memory allocated to x may be de-allocated by the command

## delete [] x ;

Always be sure to free any memory allocated-a code can very quickly use all available memory otherwise

In the dynamic allocation of the array allocated using the pointer x on the previous slide, x is the address of the first element of the array: this can be tested by using the code

```
std::cout << x << "\n";
std::cout << &x[0] << "\n";
```

A is a pointer to a pointer:

- A[i] contains the address of A[i] [0]
- A contains the address of the pointer A [0]

A is therefore an array of pointers

To create a two-dimensional array of double precision numbers with 5 rows and 3 columns called A we use the following section of code

```
double** A;
A = new double* [5];
for (i=0; i<5; i++)
{
    A[i] = new double[3];
}
```

The array then may be used as if it had been created by using the declaration

```
double A[5][3];
```

The memory allocated to A may be de-allocated by the code

```
for (i=0; i<5; i++)
{
    delete[] A[i];
}
delete[] A;
```

Always be sure to delete any memory dynamically allocated, particularly memory allocated inside loops - if not you will run out of memory

## Irregularly sized arrays

Suppose we want to define a lower triangular matrix A of integers with 10,000 rows and 10,000 columns

This may be done by the following declaration

## int A [10000] [10000];

but this wastes a considerable amount of memory saving the super-diagonal elements which are all 0

Instead, we may allocate the memory dynamically using the code on the following slide

Modern C++ compilers allow the user to create new memory which doesn't need to be deleted explicitly.

```
int main()
{
    std::shared_ptr<int> p_x(new int);
    std::cout<<"p_x use count: "<<p_x.use_count()<<"\n";
    *p_x = 5; // 'de-reference' to alter contents
    std::shared_ptr<int> p_y = p_x;
}
```

A "number of uses" of the pointer maintained at run-time.
When this drops to zero, then the memory is automatically deleted.

## Tip: memory leak detection

```
```

double x[10];

```
```

double x[10];
for (int i=0; i<10; i++){
for (int i=0; i<10; i++){
x[i]=i;
x[i]=i;
}
}
int total=0;
int total=0;
for (int i=0; i<=10; i++)//Equality is wrong
for (int i=0; i<=10; i++)//Equality is wrong
{
{
total += x[i];
total += x[i];
}
}
std::cout<<"Total is "<<total<<"\n";

```
```

std::cout<<"Total is "<<total<<"\n";

```
```

```
int** A;
```

int** A;
A = new int* [10000];
A = new int* [10000];
for (i=0; i<10000; i++)
for (i=0; i<10000; i++)
{
{
A[i] = new int[i+1];
A[i] = new int[i+1];
}

```
```

jmpf@userpc30:~\$ ./Leak
Total is 45
jmpf@userpc30:~\$ valgrind --leak-check=yes ./Leak
==15050== Memcheck, a memory error detector.
==15050== Use of uninitialised value of size 4
==15050== at 0x40B8D21:(within/usr/lib/libstdc++.so.6.0.10)
==15050==
Total is 45
==15050==
==15050== ERROR SUMMARY: 6 errors from 4 contexts (suppressed: 17 from 1)

```

The same name may be used for a variable both inside the block (local variable) and outside the block (global variable)

This is bad programming practice, as it can lead to confusion
```

{
int i = 5;
std::cout << i << "\n";
{
int i = 10;
std::cout << i << "\n"; // local value of i is 10
// variable i with value 5 is not accessible
}
std::cout << i << "\n"; // value of i is 5

```
\}

\section*{Lecture 5 - Blocks, functions and references}

\section*{Blocks}

A block is a piece of code between curly brackets
A variable, when declared, may be used throughout that block
```

{
int i;
i = 5; // OK
{
int j;
i = 10; // OK
j = 10; // OK
}
j = 5; // incorrect - j not declared here

```
\}

\section*{Functions}

The code on the next slide is an example containing a function that multiplies two double precision floating point numbers
Note the function prototype that is the second line of code
The function prototype tells the compiler about function's return value and parameters
The variable names x and y in the prototype are ignored by the compiler and don't have to be included. But including them can clarify the program
```

\#include <iostream>
double multiply(double x, double y); // function prototype
int main()
{
double a = 1.0, b = 2.0, z;
z = multiply(a, b);
std::cout << a <<" times "<< b <<" equals "<< z <<"\n";
return 0;
}
double multiply(double x, double y)
{
return x * y
}

```
```

\#include <iostream>
void output(int score, int passMark);
int main()
{
int score = 29, pass_mark = 30;
output(score, pass_mark);
return 0;
}
void output(int score, int passMark)
{
if (score >= passMark)
std::cout << "Pass - congratulations!\n";
else
std::cout << "Fail - better luck next time\n";
}

```

A function may also return no value, and be declared as void An example of a void function is shown on the next slide

The pass mark for an exam is 30 marks. This function prints out a message informing a candidate whether or not they have passed the exam

Note the poor software engineering practice on the previous slide curly brackets should have been used with the if statements

Any variables that are used in the function must be declared as in the main program
For example
```

double mult5(double x)
{
double y = 5.0;
return x * y
}

```

Under most conditions a function can only change the value of a variable inside the function, and not in the main program

This is because the code makes a copy of the variable sent to a function, and sends this copy to the function

On return from the function changes in this copied variable have no effect on the original variable

One exception to a function being unable to change the value of a variable outside a function is when an array - either dynamically allocated or not - is sent to a function

For example the following code does alter the value of x [0]
```

double x[10];
x[0] = 2.0;
someeffect(x);
std::cout << x[0] << "\n"; // will print out 3.0
void someeffect(double x[10])
{
x[0] += 1.0;
}

```

For example the following function has no effect on the variable x outside the function
```

```
x = 2.0;
```

```
x = 2.0;
noeffect(x);
noeffect(x);
std::cout << x << "\n"; // will print out 2.0
std::cout << x << "\n"; // will print out 2.0
void noeffect(double x)
void noeffect(double x)
{
{
    // x takes the value 2.0 here
    // x takes the value 2.0 here
    x += 1.0;
    x += 1.0;
    // x takes the value 3.0 here
```

    // x takes the value 3.0 here
    ```
}
```

One method of allowing a function to change the value of a variable is to send the address of the variable to the function

```
#include <iostream>
void add(double x, double y, double* pz);
int main()
{
    double a = 1.0, b = 2.0, z;
    add(a, b, &z);
    std::cout << a <<" plus "<< b <<" equals "<< z <<"\n";
    return 0;
}
void add(double x, double y, double* pz)
{
    *pz = x + y;
}
```

On the previous slide, the variables $a$ and $b$ are sent to the function-these values cannot be changed by the function

We also send the address of $z$ to the function-we therefore cannot change the address of $z$, but we can change the contents of pz

The contents of pz are changed in the function using the line of code

$$
\text { *pz }=x+y ;
$$

Suppose a is a vector whose size is allocated dynamically, and b is a matrix whose size is allocated dynamically. These arrays may be sent to the functions as follows. The prototype is

```
void example(int* a, int** b);
```

an example function is

```
void example(int* a, int** b)
{
    b[0][0] = a[1];
}
```

and this function may be called with the following statement

```
example(a, b);
```

for suitably declared a and b

Arrays whose sizes are allocated at compile time may be sent to functions as follows. There should be a prototype, for example

```
void example(int a[8], int b[3] [3]);
```

and function

```
void example(int a [8], int b[3] [3])
{
    b[0] [0] = a[1];
}
```

This function may then be called with the following statement

```
int x[8], y[3] [3];
example(x, y);
```


## References

Another way of allowing a function to change the value of a variable outside the function is to use references
These are much easier to use: all that has to be done is the inclusion of the symbol \& before the variable name in the declaration of the function and the prototype.

For example, see the code on the next slide

```
#include <iostream>
void add(double x, double y, double& rz);
int main()
{
    double x = 1.0, y = 2.0, z;
    add(x, y, z);
    std::cout << x <<" plus "<< y <<" equals "<< z <<"\n";
    return 0;
}
void add(double x, double y, double& rz)
{
    rz = x + y
}
```

If the variables were localised within loops this would not happen-for example the code below is equivalent to that on the previous slide, but the compiler would flag the bug

```
double a[10] [10], b [10];
for (int i=0; i<10; i++)
{
    for (int j=0; j<10; j++)
    {
        a[i][j] = 1.0;
    }
}
for (int i=0; i<10; i++)
{
    b[j] = 10.0; // j is not defined here
```

\}

Tip: use local variables
Consider the following piece of code

```
int i, j;
double a[10][10], b[10];
for (i=0; i<10; i++)
{
    for (j=0; j<10; j++)
    {
        a[i][j] = 1.0;
    }
}
for (i=0; i<10; i++)
{
    b[j] = 10.0; // bug: should read b[i] = 10.0
}
```

This bug will not be picked up by the compiler

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## Lecture 6 - Functions and modules

Default values for function parameters
It is possible to allow a function to be called without specifying all the parameters needed

Default parameters will be used for the other parameters
These parameters should be declared in the function prototype
The arguments with default parameters must be the last parameters in the parameter list
This should be used with care: it is easy to forget that default parameters exist

For example, a solver may be written

```
void solver(double x, double epsilon, int maxiter)
{
}
```

The function prototype may be written

```
void solver(double x, double epsilon = 0.0001, int maxiter = 100);
```

This solver may be called using any of the following

```
solver(x, 0.01, 10000)
solver(x, 0.01); // default value used for maxiter
solver(x); // default value used for epsilon and maxiter
```


## Modules

A module is a collection of functions that performs a given task
An example of a module is a collection of functions that comprise a linear solver for solving the $n$ by $n$ matrix equation $A \mathbf{x}=\mathbf{b}$
Every module has an interface - this may be thought of as a list of variables that contains (i) those that must be input to the module, and (ii) those that are output by the module

The module may then be used as a "black box", provided the interface is known

Using the example of the linear solver, this module may take form shown on the next slide
void SolveLinearSys (double** A, double* $x$, double* $b$, int $n$ ) \{
//...lines of code;
// a line of code that uses SolveFunc1;
// a line of code that uses SolveFunc2;
\}
void SolveFunc1(...)
\{
-•
\}
void SolveFunc2(...)
\{
\}

Modules are useful for code re-use, and for fast code development by programmers with no understanding of the operations that a module performs

Consider the linear solver example.

- Numerical analysts use linear solvers in almost every code they write. A module allows them to re-use this code rather than write a new linear solver each time.
- Other scientists with little mathematical expertise may have to solve a linear system. A module allows them to do so without learning how

But the use of modules may cause problems

Suppose you want to solve the $m$ by $m$ matrix equation $P u=v$ using the module on the previous slide
After including the module in your code all you have to do is include the line of code

## SolveLinearSys(P, u, v, m);

There is no need to understand the code used by this module.
All that is required is to understand the interface, i.e. the ordered list of variables in the line of code above

## Problems that may arise when using modules

Suppose the linear solver that has been written has been based on the GMRES solver

This solver requires the calculation of the scalar product between two vectors
A function would therefore be written to calculate the scalar product of two vectors of a given length

This function may be used by another module of the code, for example an ODE solver

Suppose whoever was programming the ODE solver decided to change the inputs to the scalar product function. This would inadvertently cause the linear solver to stop functioning correctly
The linear solver module could then not be treated as a black box

## More problems

Suppose matrices are stored in an array as in a previous lecture
When a function is written to multiply two matrices, the arrays and the sizes of the arrays must be sent to this function

There is no way of checking that the size is correct
It would be more useful to have a new data type called "matrix" that contained both the size and the entries of the array-i.e. all the information is stored within one object

## Lecture 7 - An introduction to classes

As an example we will develop a class of books
Each book will have the following attributes:

- an author;
- a title;
- a format;
- a price;
- a year of publication; and
- a publisher.

We will begin by writing a class with these attributes, and then develop the class further

Encapsulation using classes
The shortcomings of modules described on the previous two slides for solving the linear system $A \mathbf{x}=\mathbf{b}$ could be overcome if we could write code in such a way that the variables $A, \mathbf{x}$ and $\mathbf{b}$ could be processed by a "module" that:

1. contains all the functions needed to solve the system;
2. can not be accessed by any other part of the program except through the interface; and
3. can not itself access any other part of the program
4. consistently handles data as well as functions

This is possible, through the use of classes
The specifications described above are known as encapsulation

```
#include <string>
class Book
{
public:
    std::string author, title, publisher, format;
    int price; //Given in pence
    int yearOfPublication;
};
```

Don't worry about the term public - that will be explained later Note the semicolon after the curly bracket at the end of the class

Save the code on the previous slide as Book.hpp
The class can then be used using the code on the following slide

Recall that we want to write functions that are associated only with the class

We will write a function CalculateEuroPrice that takes a floating point number (Euros to the pound) as input and returns the price of the book in Euro cents

We define the function inside the file Book.hpp
The body of the function is written inside another file Book.cpp
The files Book.hpp and Book. cpp are shown on the next two slides
Technically a function on an object is known as a method of the object

```
#include <iostream>
#include "Book.hpp"
int main()
{
    Book fave_book;
    fave_book.author = "Lewis Carroll";
    fave_book.title = "Alice's adventures in Wonderland";
    fave_book.publisher = "Macmillan";
    fave_book.price = 199;
    fave_book.format = "hardback";
    fave_book.yearOfPublication = 1865;
    std::cout << "Year of publication of "
            << fave_book.title << " is "
            << fave_book.yearOfPublication << "\n";
    return 0;
```

\}

## Book.hpp

```
#include <string>
class Book
{
public:
    std::string author, title, publisher, format;
    int price; //Given in pence
    int yearOfPublication;
    int CalculateEuroPrice(double rate);
};
```

Book.cpp

```
#include <cmath> // For ceil
#include "Book.hpp"
int Book::CalculateEuroPrice(double rate)
{
    double euro_price = price*rate;
    // Round up to nearest cent
    return ((int) ceil(euro_price));
```

\}

Loosely speaking, a list of variables and functions is included in the .hpp file, and the functions are included in the .cpp file
use_book.cpp

```
#include <iostream>
#include "Book.hpp"
int main()
{
    Book fave_book;
    fave_book.author = "Lewis Carroll";
    fave_book.title = "Alice's adventures in Wonderland";
    fave_book.price = 199;
    fave_book.format = "hardback";
    std::cout << "Price in Euro cents = "
                << fave_book.CalculateEuroPrice(1.13)<<"\n";
    return 0;
}
```

On the previous slide note that the function written is associated with the class Book through the statement

```
int Book::CalculateEuroPrice(double rate)
```

This function may used outside the class by using statements such as std::cout << fave_book. CalculateEuroPrice(1.13)<<"\n";

Some example code is given on the next slide

## Compiling multiple files

Before we can compile the file use_book. cpp on the previous slide we first need to compile the Book class. This is done by using the -c option when compiling:
g++ -Wall -0 -c Book.cpp

This produces an object file Book.o. We can now compile use_book.cpp by typing

```
g++ -Wall -O -o use_book use_book.cpp Book.o
```

The code may be run as before by typing

## Using a Makefile

Suppose a code UseClasses.cpp uses two classes: Class1 and Class2 It is easy to forget to compile the files Class1.cpp and Class2.cpp each time they are modified

Also, you only need to compile classes that have been changed since they were last compiled

Makefiles are a very efficient solution to these problems

When using a makefile, the line
UseClasses : Class1.o Class2.o UseClasses.cpp
means that the executable UseClasses depends on the files
Class1.o, Class2.o and UseClasses.cpp

In turn, the line
Class1.o : Class1.cpp Class1.hpp
means that the object file Class1.o depends on the files Class1.cpp and Class1.hpp

The file Class1.cpp will only be compiled if Class1.cpp or Class1.hpp have changed since the last time Class1.o was created

When "make" is invoked without a target, it will attempt to build the first target in the Makefile

Save the following code as Makefile

```
all : UseClasses
Class1.o : Class1.cpp Class1.hpp
    g++ -c -O Class1.cpp
Class2.o : Class2.cpp Class2.hpp
    g++ -c -0 Class2.cpp
UseClasses : Class1.o Class2.o UseClasses.cpp
    g++ -0 -o UseClasses Class1.o Class2.o UseClasses.cpp
```

The executable UseClasses may be created by typing "make UseClasses"


## Setting variables

We can use functions to set variables - this allows us to check that the values assigned are sensible. For example

```
void Book::SetYearOfPublication(int year)
{
    assert ((year > 1440) && (year < 2025));
    yearOfPublication = year;
}
```


## Access privileges

An instance of a class is known as an object. For example in the previous slide fav_book is an object of the class

Variables and functions associated with a class - for example yearOfPublication and CalculateEuroPrice - are known as class members and methods

There are three degrees of access to class members

- private - these class members are only accessible to other class members, unless friend is used
- public - these class members are accessible to everyone
- protected - these class members are accessible to other class members and to derived classes

First we add the function definition to the file Book.hpp as we did with the function CalculateEuroPrice:

## void SetYearOfPublication(int year);

Then we add the function on the previous slide to the file Book.cpp This allows us to set the variable using statements such as
fave_book.SetYearOfPublication(1865);

Now we have written a function to set the variable
yearOfPublication that checks that it takes an appropriate value, it seems sensible only to allow ourselves to assign a value to this variable through this function

We now need to think about access privileges

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To make the variable yearOfPublication only accessible from outside the class through the function SetYearOfPublication we make yearOfPublication a private class member

To highlight that it is now private we might also modify the name from yearOfPublication to mYearOfPublication:

```
class Book
{
private:
    int mYearOfPublication;
public:
    std::string author, title, publisher, format;
    int price;
...
```

The reserved words private and public may be used as often as desired. For example the following is acceptable code

```
class Book
{
public:
    std::string author, title, publisher, format;
private:
    int mYearOfPublication;
public:
    int price;
...
```


## Lecture 8 - More on classes

Constructors and Destructors
Each time an object of the class of books is created the program calls a function that allocates space in memory for all the variables used This function is called a constructor and is automatically generated This default constructor can be overridden if desired - for example in our class we may want to set all the string variables to "unspecified" when a new object is created

This function has the same name as the class, takes no arguments, has no return type and must be public
The default for variables in a class is private
For example, in the following code the variables author, title, publisher, format are actually private

```
class Book
{
    std::string author, title, publisher, format;
private:
    int mYearOfPublication;
public:
    int price;
...
```

But now we can't access the variable mYearOfPublication outside the class. We need to write a public class member to access this variable

```
int Book::GetYearOfPublication()
{
return mYearOfPublication;
}
```

and this function may be used in the main code as follows

```
std::cout << "Year of publication of "
    << fave book.title << " is "
    << fave_book.GetYearOfPublication() << "\n";
```

It is good software engineering practice to access as many variables as possible in this way

An overridden default constructor function is included in the class shown below

```
class Book
{
private:
    int mYearOfPublication;
public:
    Book();
```

and the function is written

```
Book: :Book()
{
    author = "unspecified"; title = "unspecified";
    publisher = "unspecified"; format = "unspecified";
}
```

Other constructors
Other constructors may be written.
For example you can write a constructor that initialises the title of a new Book object

This allows code to be written such as
Book recent_book("The explorer");

The constructor must be added to the list of class members in the file Book.hpp:

Book(std::string bookTitle);

Copy constructors
Another constructor that is automatically generated is a copy constructor

The line of code
Book fave_book_copy(fave_book);
will create another object fav_book_copy with variables initialised to those of fav_book

This constructor may also be overridden in the same way as for the default constructor

The constructor is then written as

```
Book::Book(std::string bookTitle)
{
    title = bookTitle;
}
```

This code is added to the file Book. cpp

## Destructors

When an object leaves scope it is destroyed
A destructor is automatically created that deletes the variables associated with that object

Destructors can also be overridden - there will be an example later

Use of pointers to classes

An instance of a class can be sent to a function in the same way as data types such as double, int, etc.

This is shown in the example code on the next slide

Note on the previous slide that as the function SomeFunction was called without the argument fav_book being a pointer,
SomeFunction is unable to change any of the members of fav_book outside the body of the function

If you do want to change members of fav_book outside the body of the function, the function should be written to accept a pointer or a reference to fav_book.

Code for sending a pointer to fav_book into a function is shown on the next slide

```
#include "Book.hpp"
void SomeFunction(Book* pBook);
int main()
{
    Book fave_book;
    //...
    SomeFunction(&fave_book);
    return 0;
}
void SomeFunction(Book* pBook)
{
    // Uplift price by one pound
    (*pBook).price += 100;
}
```

Tip: coding standards
If you stick to a coding standard, then you're more likely to know what's what. For example,

- Proper indentation (with spaces rather than tabs)
- Braces (\{\}) on a line of their own
- Pointer names begin with ' p ' (p_return_result)
- Locally declared names have underscores
- Names are meaningful (local_index)
- Method names arguments are in camel-case (firstDimension)
- Method names are in camel-case with verbs (GetSize())
- Class data is camel-case with ' m ' to denote private (mSize)
- Lots of descriptive comments
- Avoid floating point comparisons, cut-and-paste...

The line of code on the previous slide

## (*pBook).price += 100

is a little clumsy. An equivalent statement is

## pBook->price += 100

```
An example from code I work with
void VentilationProblem::SetDynamicResistance(bool dynamicResistance)
{
    mDynamicResistance = dynamicResistance;
}
void VentilationProblem::SetPressureAtBoundaryNode(const Node<3>& rNode, double pressure)
{
    if (rNode.IsBoundaryNode() == false)
    {
        // Handle error ...
    }
    assert(mFluxGivenAtInflow == false);
    // Store the requirement in a map for the direct solver
    mPressureCondition[rNode.GetIndex()] = pressure;
}
double VentilationProblem::GetFluxAtOutflow()
{
    return mFlux[mOutletNodeIndex];
```

3

## Lecture 9 - Inheritance and derived classes

Suppose we are running a bookshop and want to write a class of electronic e-books

An electronic book is a book, and so each object in this new class is also an object in the class of books
It has two special features: the format is "electronic" and it has an additional class member that contains a private URL
The "is a" relationship allows us to derive the class of e-books (Ebook) from the class of books (Book)
Each object in the class of e-books inherits many properties from the class of books

Inheritance allows us to re-use code
Book is the base class and Ebook is the derived class

The word "public" in the first line of code on the previous slide has the effect that

- public members of Book are public members of Ebook
- protected members of Book are protected members of Ebook
- private members of Book are hidden from Ebook

These access privileges may be changed by using protected or private
In practice public inheritance is far more common the protected or private inheritance

The header file for the class of electronic books, Ebook.hpp may be written

```
#include <string>
#include "Book.hpp"
class Ebook: public Book
{
public:
    Ebook();
    std::string hiddenUrl;
};
```

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The file Ebook.cpp that contains the functions (methods) of the class is given by

```
#include "Ebook.hpp"
Ebook::Ebook()
: Book()
{
    format = "electronic";
}
```

This constructor sets the format of all members of the class of electronic books to "electronic"

Example code using this class is on the next slide
Note that we can still use the functions and variables of the class
Book when using an object of type Ebook

The code - which may be written on one line - on the previous slide

```
Ebook::Ebook()
```

: Book()
indicates which constructor in the class Book we want to call when creating an object of the class Ebook

```
#include <iostream>
#include "Book.hpp"
#include "Ebook.hpp"
int main()
{
    Ebook reading("The skull beneath the skin");
    reading.author = "P D James";
    std::cout << "The author is " << reading.author << "\n";
    std::cout << "The title is " << reading.title << "\n";
    std::cout << "The format is " << reading.format << "\n";
    reading.hiddenUrl = "http://ebook.example.com/ex-book";
    std::cout << "The URL is " << reading.hiddenUrl << "\n";
    return 0;
}
```

To re-use the constructor of the class Book that required a string as input we would have

```
Ebook::Ebook(std::string bookTitle)
    : Book(bookTitle)
{
    format = "electronic";
}
```

in the file Ebook. cpp
The following constructor is declared in the file Ebook.hpp
Ebook(std::string bookTitle);
and the original constructor

```
Book(std::string bookTitle)
```

was declared in the file Book.hpp

C ++ for Scientific Computing (2021)
It doesn't matter if we include header files such as iostream, string, etc. more than once

But we should not include files such as Book.hpp more than once This can be occur inadvertently: on the code on the previous slide we include the file Book.hpp.

The same header file is included in the file Ebook.hpp
We are therefore including the file Book.hpp twice - this can cause problems

To avoid this code being included twice we adapt our header functions to be of the form shown on the next slide

## example.hpp

```
#ifndef EXAMPLEDEF__ // if variable EXAMPLEDEF__
                    // not defined then execute lines of
                    // code until #endif statement
#define EXAMPLEDEF__ // define the variable EXAMPLEDEF__.
            // Ensures that this code is only
            // compiled once, no matter how
            // many times it is included
class example
{
    lines of code // body of header file
};
#endif // need one of these for every #ifndef statement
```

Suppose the hotel has negotiated special rates for individuals from particular organisations. The function that computes the total bill will be different for these clients

This can be handled with if statements, but this can get messy. A more practical solution is to use virtual functions where the function used to compute the total bill does different things for different derived classes before returning the value of the total bill

This is known as run-time polymorphism
The function should be defined as virtual in the base class as shown on the next slide

The class Guest has header file Guest. hpp

```
#ifndef GUEST_-
#define GUEST_-
#include <string>
class Guest
{
public:
    std::string name, roomType, arrivalDate;
    int numberOfNights;
    double minibarBill, telephoneBill;
    virtual double CalculateBill();
};
#endif
```

Suppose the hotel have negotiated a deal with a company that reduces the room rate to $£ 45$ for the first night and $£ 40$ for subsequent nights that a guest stays in the hotel

The header file for our derived class SpecialGuest.hpp is

```
#ifndef SPECIALGUEST__
#define SPECIALGUEST_-
#include "Guest.hpp"
class SpecialGuest : public Guest
{
public:
    double CalculateBill();
};
#endif
```

The file Guest.cpp is

```
#include "Guest.hpp"
double Guest::CalculateBill()
{
    double room_bill, total;
    room_bill = numberOfNights * 50.0;
    total = room_bill + minibarBill + telephoneBill;
    return total;
```

\}

The file SpecialGuest.cpp is

```
#include "SpecialGuest.hpp"
double SpecialGuest::CalculateBill()
{
    double room_bill, total;
    room_bill = (numberOfNights - 1) * 40.0 + 45.0;
    total = room_bill + minibarBill;
    return total;
}
```

Example use of the class SpecialGuest is

```
#include <iostream>
#include "Guest.hpp"
#include "SpecialGuest.hpp"
int main()
{
    SpecialGuest harry;
    harry.numberOfNights = 2;
    harry.minibarBill = 30.99;
    std::cout << "Harry's bill = "
            << harry.CalculateBill() << "\n";
    return 0;
}
```

Example of polymorphism in action. (Imagine an array of pointers to Guests.)

```
Guest* p_gu1 = new Guest;
Guest* p_gu2 = new Guest;
Guest* p_gu3 = new SpecialGuest; //Pointer of different type
//Set the three guests identically
p_gu1->numberOfNights = 3;
p_gu2->numberOfNights = 3;
p_gu3->numberOfNights = 3;
std::cout << "Bill 1 = " << p_gu1->CalculateBill() << "\n";
std::cout << "Bill 2 = " << p_gu2->CalculateBill() << "\n";
std::cout << "Bill 3 = " << p_gu3->CalculateBill() << "\n";
// The last one gets a smaller bill
```

Note that declaring the function CalculateBill() as virtual in the class Guest does not require that this function must be redefined in derived classes - instead it gives us the option to redefine it

If the function wasn't redefined then objects of the class SpecialGuest would use the function CalculateBill() defined in the class Guest

Note that the function CalculateBill() could have been declared as virtual in the class SpecialGuest
This would allow any class derived from SpecialGuest to redefine the function CalculateBill() if desired

When using derived classes, the destructor for the base class should always be a virtual function

C++ for Scientific Computing (2021)
Tip: plugging C++ into Matlab
You may need to interface C++ with Matlab (or with Gnu Octave)

- to get the speed of compiled code in a critical place
- to use an external library written in C++

This is possible with a Matlab executable file (Mex)
In the simplest case the $\mathrm{C}++$ code is a single file containing a function called mexFunction with a specific signature

The function mexFunction takes points to arrays for output and input
This is compiled with mex (a wrapper compiler to g++) and a .mex file is produced
The .mex file is treated like a .m file by Matlab

An example file myFunc.cpp

```
#include "mex.h"
#include <iostream>
void
mexFunction(int nlhs, mxArray* plhs[], int nrhs,
    const mxArray* prhs[])
{
    mxArray* v = mxCreateDoubleMatrix(1, 1, mxREAL);
    double* data = mxGetPr(v);
    *data = 3.142;
    std::cout<<"Num args = "<<nrhs<<" \n";
    plhs[0] = v;
}
```


## Lecture 10 - A class of vectors

We will design a class of vectors in such a way that:

1. objects of this class behave like a new data type; and
2. code similar in style to MATLAB may be written using objects of this class.

We will define operations on and between objects of the class of vectors, and between these objects and data types such as int and double

We want to be able to write code such as

$$
\begin{array}{ll}
\text { Vector } u(3), ~ v(3) ; & / / \text { vectors of length } 3 \\
\text { Matrix } A(3,3) ; & / / \text { matrix of size } 3 \text { by } 3
\end{array} \quad \begin{aligned}
& \text { v }=\mathrm{A} * \mathrm{u} ; \\
& \mathrm{u}=\operatorname{gmres}(\mathrm{A}, \mathrm{v}) ;
\end{aligned}
$$



Constructors for vectors
We want the declaration

```
Vector u(3);
```

to have the following effect:

- The compiler allocates memory for an array of three double precision floating point numbers and initialises these numbers to zero
- We can access the elements of $u$
- We can access the size of u

The code on the next two slides achieves these goals

## The following file should be saved as Vector .hpp

```
#ifndef VECTOR__
#define VECTOR_
// a simple class of vectors
class Vector
{
public:
    // member variables
    double* data; // data stored in vector
    int size; // size of vector
    // construct vector of given length
    Vector(int sizeVal);
};
#endif
```


## An example of use of the class of vectors:

```
#include <iostream>
#include "Vector.hpp"
int main()
{
    Vector u(3), v(3);
    std::cout << u.size << "\n";
    u.data[0] = v.data[1] = 5.0
    std::cout << u.data[0] + v.data[1] << "\n";
    return 0;
}
```

The size of $u$ is accessed by $u$.size
Element $n$ of $u$ is accessed by $u$.data[n]

The following file should be saved as Vector.cpp

```
#include "Vector.hpp"
// constructor that creates vector of given size with
// double precision entries all initially set to zero
Vector::Vector(int sizeVal)
{
    data = new double[sizeVal];
    size = sizeVal;
    for (int i=0; i<size; i++)
    {
        data[i] = 0.0;
    }
}
```

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## Default constructor (no longer exists)

The default constructor is not appropriate when declaring a vector: we need to know the length of the vector in advance
Because we have given an alternative constructor, and have not overridden the default constructor, the compiler automatically revokes the default constructor

The code

```
Vector a_vector
```

will now give a compiler error.

## Copy constructors

When using the copy constructor generated by the compiler statements such as

Vector w(u);
will not have the desired effect.
The length of the vector will be correctly set
However, instead of setting the elements of w equal to the elements of u , the pointer to the first element of w will be set to the pointer to the first element of $u$

This has the effect that the computer will attempt to store both $u$ and w in the same memory space, which will obviously lead to errors

The copy constructor may then be written

```
Vector::Vector(const Vector& rOther)
{
    size = rOther.size;
    data = new double[size];
    for (int i=O; i<rOther.size; i++)
    {
        data[i] = rOther.data[i];
    }
}
```

and should be included in the file Vector.cpp

Statements such as

## Vector $\mathrm{w}(\mathrm{u})$;

are not commonly used in Matlab, there is little need for this constructor

However, if the compiler generated copy constructor is not overridden there may be errors
The copy constructor may as well be written. First the constructor must be added to the list of public members in the file Vector. hpp

```
Vector(const Vector& rOther);
```

Note the use of const Vector\& rOther on the previous slide
The function could have been prototyped by

## Vector (Vector otherVec)

The argument of the function would then not be a reference variable.
A copy of this variable would be made for use in the constructor function. If the vector is big this will slow down the program

Using a reference variable allows us to use the same variable in the function

The qualifier const in the prototype ensures that this reference variable cannot be altered inside the function

## Destructors

Recall that a destructor function is automatically generated and is called when a variable is destroyed, i.e. goes out of scope
We want our destructor to do more than this: we want it to free the memory that was allocated to the vector

We therefore need to override the default destructor
First the destructor must be included in the file Vector.hpp
~Vector();

The destructor should then be added to the file Vector.cpp

```
Vector:: ~Vector()
{
    delete[] data;
```

\}

## Functions

Recall that functions (methods) may be defined on classes
For example, the method norm ( p ), the $p$-norm of $u$
We will assign p the default value 2
Add the following line of code into the list of public members of the class Vector
double norm(int $\mathrm{p}=2$ ) const;
together with the function given on the following slide. The const keyword after the method informs the compiler that there should be no changes to the class. The norm of a Vector may be calculated using statements such as

```
x = u.norm();
y = v.norm(1);
```

Destructors are called automatically

A further advantage of writing classes of vectors and matrices is that a destructor will automatically be called when a vector or matrix goes out of scope - this ensures that memory allocated to these objects is automatically deleted.

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```
double Vector::norm(int p) const
{
    double temp, sum, norm_val;
    sum = 0.0;
    for (int i=0; i<size; i++)
    {
        temp = fabs(data[i]); // floating point absolute value
        sum += pow(temp, p);
    }
    norm_val = pow(sum, 1.0/((double)p) );
    return norm_val;
```

\}

External function versus member method

We have written a function that calculates the $p$-norm a vector u using statements such as
dp = u.norm();

This notation is clumsy - we would rather write statements similar to those that we would use in Matlab such as

## $\mathrm{dp}=\operatorname{norm}(\mathrm{u})$;

This can be done, but at the expense of compromising on good software engineering principles

Tip: documenting code
In the norm method on a previous slide, it is not obvious what is happening, even though there are only a few lines of code

Comments should be added to the code to aid anyone reading the code

For example a description of the function should be given first

```
// Function to calculate the p-norm of a vector
```

// See 'An Introduction to Numerical Analysis'" by
// Endre Suli and David Mayers, page 60, for definition
// of the p-norm of a vector
double Vector::norm(int p) const
\{
...
\}

The function norm is declared as a friend in the file Vector.hpp
friend double norm(Vector vec, int p);

Declaring a function as a friend of a class allows this function to access the private members of the class

The function norm is now no longer encapsulated within the class of vectors, and so must be prototyped in Vector.hpp:
double norm(Vector vec, int p);
and is now written
double norm(Vector vec, int p)
\{
\}
see: another example of friend

C++ for Scientific Computing (2021)

Explain what is happening in the loop
// Loop over all elements of vector to calculate the // sum required for the p-norm
sum $=0.0$;
for (int i=0; i<size; i++)
\{
temp = fabs(data[i]);
sum += pow(temp, p);
\}

Documenting code is an art rather than a science
A few tips:
Describe what part of the problem the code is solving. Don't describe the code. For example, don't include documentation such as

```
// Loop over values of p going from 0 to n-1
for (p=0; p<n; p++)
```

Using lots of empty lines can make the code look more readable

## Lecture 11 - Operator overloading

We want to write code such as
$\mathrm{w}=\mathrm{u}+\mathrm{v}$;
where $\mathrm{u}, \mathrm{v}$, w are defined to be objects of the class Vector
We have to define within the class what is meant by the operators + and $=$ in this context

This can be achieved by overloading the + operator and the $=$ operator for the class of vectors

First we will restrict access to the data in the vector class

If you want to emphasise something you can simulate underlining, for example

```
// Very important comment
// ----------------------
```

Alternatively, can emphasise something by putting it in a box:

```
// ****************************************************
// ****************************************************
// ** **
// ** Function to calculate p-norm of vector **
// ** **
// ****************************************************
// *************************************************
```

We may overload the ( ) operator in order to access elements of an array in the same way as Matlab and FORTRAN

This allows us to assign indices from 1 to n inclusive for an array of length n , instead of 0 to $\mathrm{n}-1$ as when using conventional $\mathrm{C}++$

We will worry about error checking ( $0 \leq i \leq$ size) later
The function required to do this is

```
double& Vector::operator()(int i)
{
    return data[i-1]; // (NB we should check that i is in range)
}
```

and the following line must be included in the file Vector.hpp double\& operator()(int i);

We can now access the first element of $u$ by writing $u(1)$, instead of the clumsy notation u.data[0]

Note the appearance of the symbol \& on the previous slide
This indicates that the operator returns a reference
This allows us to use terms such as $u(1)$ on the left hand side of expressions such as $u(1)=2.0$

We can also overload the square brackets operator with

```
double& operator[](int i);
```

(This is an exercise)
see: accessing elements of an array

The function length is given below

```
int length(const Vector& rVec)
{
    return rVec.mSize;
}
```

Binary operators
To write code such as

$$
\mathrm{w}=\mathrm{u}+\mathrm{v} ;
$$

then the lines

```
Vector& operator=(const Vector& rVec);
friend Vector operator+(const Vector& rVec1, const Vector& rVec2);
```

should be added within the class description in the file Vector.hpp, and then the following two functions should be included in the file Vector.cpp
}

```
```

Vector operator+(const Vector\& rVec1,

```
Vector operator+(const Vector& rVec1,
                const Vector& rVec2)
                const Vector& rVec2)
{
{
    // (We should check that the sizes match)
    // (We should check that the sizes match)
    Vector result(rVec1.mSize);
    Vector result(rVec1.mSize);
    for (int i=0; i<rVec1.mSize; i++)
    for (int i=0; i<rVec1.mSize; i++)
    {
    {
        result.mData[i] = rVec1.mData[i] + rVec2.mData[i];
        result.mData[i] = rVec1.mData[i] + rVec2.mData[i];
    }
    }
    return result
```

    return result
    ```
```

Vector\& Vector::operator=(const Vector\& rVec)
{
// (We should check that the sizes match)
for (int i=0; i<rVec.mSize; i++)
{
mData[i] = rVec.mData[i];
}
return *this;

```
\}
this is a pointer to the object
*this is the contents of the object that the pointer points at

It is essential that a destructor and copy constructor have been written before the code on the previous slide is used

A vector result is declared within the function-this will go out of scope at the end of the function (but its content will be copied)

If the destructor or copy constructor are not written correctly this may cause problems

The binary operators - and * can be overloaded in a similar way as to \(+\)

When overloading * we first have to define what \(u\) * v means for a vector, i.e. do we mean the scalar product or the vector product?

We can also also overload * to define multiplication between an array of double precision numbers and a double precision number

For example, if a is a double precision floating point variable, and \(u\) is an array of double precision floating point numbers we can define what is meant by the operator \(*\) in the case \(a * u\)

\section*{Binary operators without 'friend'}

In overloading operator+ we have used an external friend function rather than a local method because it feels natural to be adding two objects.
```

Vector operator+(const Vector\& rVec1,
const Vector\& rVec2)
{
Vector result(rVec1.mSize);
for (int i=0; i<rVec1.mSize; i++)
{
result.mData[i] = rVec1.mData[i] + rVec2.mData[i];
}
return result;
}

```
```

Vector operator*(double a, const Vector\& rVec)
{
Vector result(rVec.mSize);
for (int i=0; i<rVec.mSize; i++)
{
result.mData[i] = a * rVec.mData[i];
}
return result;
}

```
after the following line has been included into the file Vector.hpp
friend Vector operator*(double a, const Vector\& rVec);

However, it is more efficient to write a binary operator as a member of a class.
```

Vector Vector::operator+(const Vector\& rOther)
{
Vector result(mSize);
for (int i=0; i<mSize; i++)
{
result.mData[i] = mData[i] + rOther.mData[i];
}
return result

```
\}

Both operators would be instantiated as \(\mathrm{a}=\mathrm{b}+\mathrm{c}\), but in the case of the second style, it would be run as an internal method of b. (mSize evaluates to b's mSize.)

\section*{Unary operators}

The unary operators - and + may also be overloaded in a similar manner to binary operators: add the line
friend Vector operator-(const Vector\& rVec);
to the list of public members of Vector in the file Vector.hpp, and add the function on the following slide to the file Vector.cpp

\section*{Overloading the output operator}

C++ does not know how to print out a vector, unless you tell it how.
(If you print a pointer, then a memory address will be printed.)
Overload the << operator in the hpp file:
```

class Vector
{
private:
int mSize;
double* x;
public:
Vector(int);
...
friend std::ostream\&
operator<<(std::ostream\& output, const Vector\& rVec);
};

```

The implementation might look like this:
```

// std::cout << "a_vector = " << a_vector << "\n";
// appears as: a_vector = (10, 20)
std::ostream\& operator<<
(std::ostream\& output, const Vector\& rVec)
{
output << "(";
for (int i=0; i<rVec.mSize; i++){
output << rVec.mData[i];
if (i != rVec.mSize-1)
output << ", ";
else
output << ")";
}
return output; // for multiple << operators.

```
\}

Tip: step-through debuggers
- Visual Studio and Borland Delphi etc. have their own integrated step-through debuggers
- Eclipse offers a debugging plug-in which by default links to Gnu's gdb debugger, but supplies a user interface over the top
- Other graphical front-ends to gdb exist. I like ddd.
- Note: Executable files suitable for debugging need to be compiled with -g (debug) rather than -0 (optimized).

\section*{Lecture 12 - Exceptions}

Suppose we have lines of code that read
```

bigger_vector = a_vector;
smaller_vector = a_vector;

```
where smaller_vector, a_vector and bigger_vector are vectors that have been declared as having 1, 2 and 3 elements respectively.

The assignment operator is expecting that the size of its input vector (on the right-hand side) matches the object which it is assigning to.
There are clearly errors here - the current implementation will attempt to add too much data into smaller_vector.
What should the program do when the sizes do not match?
\begin{tabular}{|c|c|c|}
\hline \multicolumn{3}{|l|}{} \\
\hline \multicolumn{3}{|l|}{Elie Edat Miew Erogam Commends siats scurce Data} \\
\hline 0. * (a-vector. \(\mathrm{moata)}\) ) & &  \\
\hline \multicolumn{3}{|l|}{Locals} \\
\hline \multicolumn{3}{|l|}{} \\
\hline  & \(\frac{\mathrm{R}}{\text { Run }}\) & \\
\hline  & \multirow[t]{2}{*}{} & \\
\hline & & \\
\hline & Uniil frinh & \\
\hline & & \\
\hline  & Lp Down & \\
\hline \% \#ncluad <iostrean> & \({ }^{\text {Lindo }}\) Edt & \\
\hline \multicolumn{3}{|l|}{int manc)} \\
\hline \multicolumn{3}{|l|}{\multirow[t]{2}{*}{//This would produce a conpiler warning (there is no default constructor)
// Vector badly_formed;}} \\
\hline & & \\
\hline \multicolumn{3}{|l|}{} \\
\hline \multicolumn{3}{|l|}{\[
\text { - vector ( } 12=10.0
\]} \\
\hline \multicolumn{3}{|l|}{\multirow[t]{2}{*}{//Show that friends and methods can be used to do the same thing assert ( a_vector. norm() \(==\) norm(a_vector));}} \\
\hline & & \\
\hline \multicolumn{3}{|l|}{std: : cout << "a_vector = " << a_vector << "nn";} \\
\hline \multicolumn{3}{|l|}{\multirow[t]{2}{*}{\begin{tabular}{l}
Vector bigger-vector (3); \\
std: :cout <<" "The following produces a warningখn"
\end{tabular}}} \\
\hline & & \\
\hline \multicolumn{3}{|l|}{\multirow[t]{2}{*}{\begin{tabular}{l}
(gdb) break use_vectors.cpp:1 \\
Ereakpoint 1 at \(0 \times 400 e c c:\) file use_vectors.cpp, \(11 n e 14\). (gdb) run
\end{tabular}}} \\
\hline & & \\
\hline \multicolumn{3}{|l|}{\multirow[t]{3}{*}{\begin{tabular}{l}
 \\
gabe graph display jnfo 10cals \\
(gab)
\end{tabular}}} \\
\hline & & \\
\hline & & \\
\hline
\end{tabular}

The answer is - "It depends".
It's good to have a hierarchy of errors
Level 1 If the error can be fixed safely, then fix it. If need be, warn the user.

Level 2 If the error could be caused by user input then throw exception up to calling code, since the calling code should have enough context to fix the problem.

Level 3 If the error should not happen under normal circumstances then trip an assertion.

Exceptions are a compromise between carrying on regardless and stopping completely.

Exceptions require use of the keywords try, throw and catch try tells the code to execute some statements
throw identifies an error
catch attempts to fix the error

The file Exception.hpp may be written
```

\#ifndef EXCEPTION_
\#define EXCEPTION_-
\#include <string>
class Exception
{
public:
std::string problem, summary;
Exception(std::string sum, std::string prob);
void DebugPrint();
};
\#endif

```

We will use the example of assigning to a vector of the wrong length using the overloaded \(=\) operator for vectors

When assigning to a longer vector we will treat it as a Level 1 error pad the extra entries with zeroes and warn the user. When assigning to a shorter vector we will treat it as a Level 2 error and throw an exception, because data would be lost otherwise.

When an error occurs we want the code to "throw" two pieces of information
1. A summary
2. A description of the error

We will write a class Exception to store these two pieces of information, and with the ability to print this information when required

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```

\#include "Exception.hpp"
Exception::Exception(std::string sum, std::string prob)
{
problem = prob;
summary = sum;
}
void Exception::DebugPrint()
{
std::cerr << "** Exception ("<<summary<<") **\n";
std::cerr << "Problem: " << problem << "\n\n";
}

```

Here's the new assignment operator (2 slides)
```

Vector\& Vector::operator=(const Vector\& rVec)
{
// if rhs vector is too long then throw
// if rhs vector is too short, assume missing entries are 0
if (rVec.mSize == mSize)
{
for (int i=O; i<mSize; i++)
mData[i] = rVec.mData[i];
}
else if (rVec.mSize > mSize)
{
throw Exception("length mismatch",
"vector assignment operator - vectors have different lengths");
}

```

We may now test the exception written in our overloaded assignment operator for vectors
```

Vector smaller_vector(1);
Vector a_vector(2);
Vector bigger_vector(3);
//This produces a warning
bigger_vector = a_vector;
//This produces an exception
try
{
smaller_vector = a_vector;
}
catch (Exception\& err)
{
err.DebugPrint();
}

```
\}
```

else //if (rVec.mSize < mSize)

```
else //if (rVec.mSize < mSize)
{
{
    for (int i=0; i<rVec.mSize; i++)
    for (int i=0; i<rVec.mSize; i++)
        mData[i] = rVec.mData[i];
        mData[i] = rVec.mData[i];
    for (int i=rVec.mSize; i<mSize; i++)
    for (int i=rVec.mSize; i<mSize; i++)
        mData[i] = 0.0;
        mData[i] = 0.0;
    std::cout << "vector assignment - copied vector too short";
    std::cout << "vector assignment - copied vector too short";
    std::cout << " and has been extended with zeroes\n";
    std::cout << " and has been extended with zeroes\n";
}
}
    return *this;
```

    return *this;
    ```

\section*{Tip: test first}
- Test driven development means that you always start with the code for a test (not the code itself)
- Choose the simplest piece of functionality which you want to implement first
- Make a test before you make the implementation (it won't compile and it won't pass)
- Write the missing functionality until the test passes
- Always check that all tests pass as you add new functionality (then you know as soon as the program gives different behaviour)

An example from my own code (with CxxTest)
void TestPatientData() throw (Exception)
\{ problem.SetOutflowPressure (0.0)
problem.SetConstantInflowPressures(50.0);
TetrahedralMesh<1, 3>\& r_mesh=problem.rGetMesh();
TS_ASSERT_EQUALS(r_mesh.GetNumNodes(), 56379u);
TS_ASSERT_EQUALS (r_mesh. GetNumElements(), 56378u);
problem.SetDynamicResistance(false);
problem.Solve();
std::vector<double> flux, pressure;
problem.GetSolutionAsFluxesAndPressures(flux, pressure)
double top_radius \(=\) r_mesh.GetNode(0)->rGetNodeAttributes() [0];
TS_ASSERT_DELTA(top_radius, 8.0517, 1e-4); //mm
double top_reynolds_number \(=\) fabs ( \(2.0 *\) problem.GetDensity() \(*\) flux[0]
/ (problem.GetViscosity() * M_PI * top_radius) );
// Poiseuille
TS_ASSERT_DELTA(problem.GetFluxAtOutflow(), -7.975182e6, 1.0);
TS_ASSERT_DELTA(top_reynolds_number, 49591, 1.0);
//...

Each new instance of the function requires the code to re-compiled for that particular value
}
```

```
```

template <class T>

```
```

template <class T>
T GetMin (T a, T b) {
T GetMin (T a, T b) {
if (a<b){
if (a<b){
return a;
return a;
}
}
return b; // When a>=b
return b; // When a>=b
main(){
main(){
std::cout << GetMin<int>(10,-2) << "\n";
std::cout << GetMin<int>(10,-2) << "\n";
double ans=GetMin<double>(22.0/7.0, M_PI);

```
    double ans=GetMin<double>(22.0/7.0, M_PI);
```

\}

Use the template keyword to produce as many functions as may be required

## Lecture 13 - Templates and the STL

- Templates introduce compile-time polymorphism: generics
- They are used where the same code may need to repeated for
small numbers of different values or for different types
}
}

```
```

mesh_3d.SolvePoisson();

```
mesh_3d.SolvePoisson();
mesh_2d.Create();
mesh_2d.Create();
double GetMin(double a, double b)
double GetMin(double a, double b)
{
{
    if (a<b){return a;} return b;
    if (a<b){return a;} return b;
int GetMin(int a, int b)
int GetMin(int a, int b)
{
{
if (a<b){return a;} return b;
```

if (a<b){return a;} return b;

```
```

template<unsigned DIM>
class TemplatedVector
{
double mData[DIM]; // Static size (fixed at compile-time)
public:
double\& operator[](int pos){
assert(pos<DIM); return(mData[pos]);
}
};
int main()
{
TemplatedVector<5> a;
a[0]=10; a[1]=11;
std::cout<<a[0]+a[1]<<"\n";
a[5]=0; //Trips assertion
}
;

```
2 C
3 \{

\section*{The Standard Template Library (STL)}

This is a set of commonly used patterns which can be re-used for different types of objects
- Containers. e.g. random access vectors, linked lists
- Algorithms. e.g. sorting
- Iterators
- Special containers e.g. Queues and maps
- The vector template class provides a form of dynamic array that expands at the end as necessary to accommodate additional elements
- It is declared with std::vector<type>
- It contains methods like bool empty(), push_back(value), int size(), int capacity(), reserve(int)
- The implementation is responsible for doing the memory management for you
- If you grow a vector dynamically, then STL may make a new larger space for it and move it. Therefore, it's not good to store the addresses of vector elements elsewhere.
- Insertions/deletions at the end of the vector are fast
- Insertions/deletions at the front will take linear time
- std: : deque has fast insertions at front or back
- The map template class provides the machinery to make a mathematical map
- This lets us recall the value to which a particular key maps, rapidly
- The internal organisation of a map relies on the ability to compare the values of keys
- Many plain data types (int, double) have obvious comparison functions. std::string types can be compared lexicographically.
- For more complicated keys, you need to write and add a definition of the 'less than' operator
- There are also set (like map with just the keys), bag (like set, but with multiple copies of the same element) and multimap (allowing the same key to be mapped to many things)
```

std::map<std::string, int> Phonebook;
Phonebook["Joe"] = 83511;
Phonebook["Sandy"] = 15208;
Phonebook["Sam"] = 10666;
std::cout << "Phonebook[Joe]=" << Phonebook["Joe"] << "\n\n";
std::cout << "Map size: " << Phonebook.size() << "\n";
for( std::map[std::string,int](std::string,int)::iterator
ii=Phonebook.begin(); ii!=Phonebook.end(); ii++)
{
std::cout << (*ii).first << ": " << (*ii).second << "\n";
}
assert(Phonebook.count("Laura") == 0);

```

Thus we get key comparison (two-dimensional point comparison) for use in a set
```

int main()
{
std::set<Point2d> points;
Point2d origin(0,0);
points.insert(origin);
points.insert(Point2d(0,1));
points.insert(Point2d(1,0));
points.insert(Point2d(0,0)); //No different from origin
std::cout<<points.size()<<"\n";
std::cout<<points.count(Point2d(0,0))<<"\n";
}

```
```

class Point2d
{
int x, y;
public:
Point2d(int xval, int yval)
{
x=xval; y=yval;
}
bool operator<(const Point2d\& rOther) const
{
if (x < rOther.x) return true;
if (x > rOther.x) return false;
return (y < rOther.y); //Returns false if y>=rOther.y
}
};

```

Comparison can be used for sorting
```

\#include <algorithm>
std::vector<int> squares_mod_10;
for (int i=0; i<10; i++){
squares_mod_10.push_back( rand() % 10 );
}
// e.g. 3 6 7 5 3 5 6 2 9 1
sort(squares_mod_10.begin(), squares_mod_10.end());
for (int i=0; i< squares_mod_10.size(); i++){
std::cout<<squares_mod_10[i]<<" ";
}
std::cout<<"\n"
// e.g. 1 2 3 3 5 5 6 6 7 9

```

Modern C++ aside: enriched features in the STL

Modern \(\mathrm{C}++\) contains many useful features which have been added to the STL:
- a more accessible array container
- easier initialisation of containers
- easier iteration over containers
```

```
std::vector<int> nums = {0, 1, 2};
```

```
std::vector<int> nums = {0, 1, 2};
// Use a reference to alter the members
// Use a reference to alter the members
for (int& r_num : nums) r_num++
for (int& r_num : nums) r_num++
// More compact form
// More compact form
for (auto n:nums) std::cout<<n<<"\n";
```

```
for (auto n:nums) std::cout<<n<<"\n";
```

```

\section*{©} To use modern C++ features compile with g++ -std=c++11

\section*{Tip: re-use of robust libraries}

If you write it yourself then you understand it better. However, it's not likely to be correct first time and it's not likely to be the optimal solution. Using code that has had decades of effort put into it is better, even if the learning curve is steeper.
- Standard Template Library for extensible vectors, sorting searching, indexing and mappings
- Boost for simple added functionality such as serialisation and small matrices
- PETSc for large-scale, robust and sparse linear algebra
- MPI for distributed-memory parallelism
- ...
- STL may look heavy-weight at first, since you have to put lots of lists of things into angle-brackets
- Some of the use of iterators (e.g. set union) look very clumsy
- STL concentrates on frequently used design patterns and it's good to know the patterns (even if you don't use the library)
- STL functionality is highly-optimised by compiler writers to give complexity assurances and a low memory-footprint

\section*{The end - Useful tips}

Software carpentry: You can increase your programming productivity (in terms of speed and of correctness) by using available tools
The "tips" you have seen apply to all languages (not just to C++)
- Automated builders and IDEs
- Version control
- Memory leak detection
- Coding standards
- Documenting code
- Step-through debuggers
- Test first
- Re-use of robust libraries

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[^0]:    from material by Joe Pitt-Francis \& Jonathan Whiteley

[^1]:    \#include <cmath>

[^2]:    $\mathrm{x}=1$ and $\mathrm{y}=2$

