Introduction to Scientific Programming with C++

Session 2: More data types

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Arrays

Definition

array a series of elements of the same type occupying a contiguous block of memory.

Format for declaring an array is:

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type name[num_elements];
```

Where `type` is any valid data type and `num_elements` is a constant positive integer.

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Format for declaring an array is:

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type name[num_elements];
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Where `type` is any valid data type and `num_elements` is a constant positive integer. Some examples:

```
unsigned int lotteryNumbers[7];

double planetMasses[8];

const unsigned int numParticles = 128;
double xPositions[numParticles];
double yPositions[numParticles];
```

Last example shows how we can use constant variable as array size.

Initialising arrays

When declaring an array it can be initialised as follows:

```
unsigned int lotteryNumbers[7] = {16, 3, 28, 9, 24, 10, 8}
```

the size can be left out, in which case the number of values given is used:

```
unsigned int lotteryNumbers[] = {16, 3, 28, 9, 24, 10, 8}
```

Accessing elements

To access an element of an array the format is:

```
name[index]
```

Warning!

In C++ array numbering starts at 0! This is a huge source of confusion especially if you're used to a programming language like Fortran where arrays start at 1.

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For example, to read the 3^{rd} lottery number use:

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unsigned int third = lotteryNumbers[2];
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For example, to read the 3rd lottery number use:

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unsigned int third = lotteryNumbers[2];
```

To write the 3rd lottery number use:

```
lotteryNumber[2] = 23;
```

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For example, to read the 3^{rd} lottery number use:

```
unsigned int third = lotteryNumbers[2];
```

To write the 3^{rd} lottery number use:

```
lotteryNumber[2] = 23;
```

You can also access the elements using a variable:

```
for(int i = 0; i < 7; ++i)
   std::cout << lotteryNumbers[i] << " ";
```

Accessing elements

Array index out of bounds

Warning!

Be careful not to access elements past the end of an array. Consider:

```
const unsigned int numPlanets = 8;
double masses[numPlanets];
for(int i = 0; i <= numPlanets; ++i)
  masses[i] = random();
```

Seems ok, but wait. The last iteration will try to set `masses[8]` which is past the end of the array!

Multidimensional arrays

Because with only two friends 1D is sooo boring

Think of multidimensional arrays as being "arrays of arrays". An example:

```
const unsigned int numParticles = 10;
double positions[numParticles][3];  // positions x,y,z
double masses[numParticles];
double centreOfMass[3] = {0.0, 0.0, 0.0};

// Populate arrays with random masses and positions

for(int i = 0; i < numParticles; ++i)
{
  for(int dim = 0; dim < 3; ++dim)
  {
    centreOfMass[dim] += masses[i] * positions[i][dim] /
      numParticles;
  }
}

std::cout << "Centre of mass: " << centreOfMass[0] << " "
```

../code/2_more_data_types/lectures/centre_of_mass.cpp

Multidimensional arrays

Why stop at two

In theory you can have as many array dimensions as you want. For example a 3D array of ising spins could be represented as:

```
bool isingSpins[nX][nY][nZ];
```

In practice you have to worry about how much memory your array needs!

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In theory you can have as many array dimensions as you want. For example a 3D array of ising spins could be represented as:

```
bool isingSpins[nX][nY][nZ];
```

In practice you have to worry about how much memory your array needs! If you want to find out use:

```
std::cout << "Need: " << sizeof(bool) * nX * nY * nZ <<
  " bytes";
```

std::array

Like c-style arrays but safer and easier to use

```
std::array<double,5> myArray={2.3, 4.2, 7.5, 8.2, 9.1};
```

These arrays are just as fast, have built in protection and are easier to manipulate. They protect against code such as this:

```
double SingleValue = myArray[8];
```

Accessing elements outside a C-style array is dangerous.
To use them the following header file must be included

```
#include<array>
```

You may also need to compile with the option –std=+11 for g++.

Strings

A string of characters, used to store text.

```cpp
std::string message = "Physics rocks!";
```

Strings use the c-style char arrays internally but are much easier to use. To use strings make sure to use the following include:

```cpp
#include <string>  // At the top of your file
```

String variables

All strung out

So what can we do with strings?

Initialise

```
std::string firstName = "Bjarne";
std::string lastName("Stroustrup"); // Equivalent to above
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Concatenate (add two or more together)

```
std::string fullName = firstName + " " + lastName;
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Notice ability to mix string variables and literals (i.e. things in quotes).

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std::string fullName = firstName + " " + lastName;
```

Notice ability to mix string variables and literals (i.e. things in quotes).

Read from user

```
std::cout << "Enter first name: "
std::cin >> firstName;
```

Pointers

Pointers are low level C-stlye code that can be error prone and difficult to use. In modern C++ they can usually be avoided.

Every variable lives at a memory address. A pointer is a special data type that stores such an addresses.

Pointer declaration

To declare a pointer the format is:

```
type * name;
```

This tells the compiler that `name` is a pointer that points to the address of a variable of type `type`. Got it?

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Some examples:

```
int * pointerToInt;
std::string * pointerToString;
```

Using pointers

Pointer initialisation

To set pointers we can use the reference operator: & (read "address of").

```
int upSpins = 10;
int * spinsPointer = &upSpins;
```

line 2 tells the compiler to:

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So what's in a pointer?

```
std::cout << "Address is: "
  << spinsPointer
  << "\n";
```

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So what's in a pointer?

```
std::cout << "Address is: "
  << spinsPointer
  << "\n";
```

Output: `Address is: 0x00CBF748`
This is how C++ prints memory addresses.

Using pointers

Reading the value

To access, use the the dereference operator: $*$ (read "value pointed by").

```
std::cout << "Value is: "
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std::cout << "Value is: "
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Output: `Value is: 10`

Setting the value

To set the value pointed to by a pointer also use dereference operator:

```
*spinsPointer = 20;
std::cout << "New upSpins: "
  << upSpins
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To access, use the the dereference operator: * (read "value pointed by").

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Output: `New upSpins:  20`

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Output: `Value is:  10`

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*spinsPointer = 20;
std::cout << "New upSpins: "
  << upSpins
```

Output: `New upSpins:  20`

Assigning pointers

Later on we may want to assign the pointer to point to a different value:

```
int downSpins = 7;
spinsPointer = &downSpins;
std::cout << "Down spins : "
  << *spinsPointer;
```

Using pointers

Reading the value

To access, use the the dereference operator: $*$ (read "value pointed by").

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std::cout << "Value is: "
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Pointers

Pointers can be very dangerous they have literally cost lives!

Warning!

C++ pointers can be dangerous! Consider:

```
int * upSpinsPointer;
std::cout << *upSpinsPointer;
```

I've asked for the value pointed by `upSpinsPointer`. But what's it pointing to? It could be a valid address or garbage.

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Do

Set pointers to the special value `0` upon declaration which indicates that it is not pointing to a valid memory address:

```
int * upSpinsPointer = 0;
```

This is called a null pointer. The program will crash immediately if you try to dereference it and you will find out straight away what went wrong.

Dynamic memory

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```
unsigned int spinChainLength;
std::cout << "Enter spin chain length: ";
std::cin >> spinChainLength;
bool spinChain[spinChainLength]; // ERROR!
```

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But we can only create arrays of known, *constant*, size!

Solution: dynamic memory.

`new` and `new[]` operators

To allocate dynamic memory the format is:

```
  pointer = new type;                 // single variable
  pointer = new type[num_elements]; // array
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`new` and `new[]` operators

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  pointer = new type;                // single variable
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```

Let's try again:

```
bool * spinChain = new bool[spinChainLength]; // Good
```

Dynamic memory

Don't forget to clean up

`delete` and `delete[]` operators

To free dynamic memory the format is:

```
delete pointer;   // single variable
delete[] pointer; // array
```

Make sure you use the correct version, otherwise bad things *will* happen.

Dynamic memory

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Don’t

Forget the free your memory once you’re done with it. Otherwise it will leak and you won’t get it back until your program ends!

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Don't

Forget the free your memory once you're done with it. Otherwise it will leak and you won't get it back until your program ends!

Do

Set the pointer to 0 after the memory has been freed:

```
delete[] spinChain;
spinChain = 0;
```

std::vector

Dynamic arrays made easy, all the memory allocation with new[] and delete[] is done for you.

```
std::vector<double> myVector;
```

Elements can easily be added on the fly using push_back().

```
myVector.push_back(2.3);
myVector.push_back(3.3);
myVector.push_back(5.6);
```

The elements can be accessed as normal with [] or myVector.at() if you want to use a more modern syntax.

In order to use vectors you must include the following header.

```
#include<vector>
```

References

More safe than keeping your money in a Swiss bank account

A reference is similar to a pointer only more limited, and more safe.

Reference declaration and initialisation

To declare a reference and initialise it the format is:

```
type & name = variable_name;
```

This tells the compiler that name is a reference to an existing variable called `variable_name` which is of type `type`. References *cannot* be uninitialised!

Example:

```
int upSpins = 10;
int & spinsReference = upSpins;
int & downSpins; // Error: cannot be uninitialised
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```

Using references

Once a reference is declared it can be used almost exactly as if it were an ordinary variable.

Pointers vs. references

Practical comparison

```
#include <iostream>

int main()
{
  int upSpins = 10;
  int downSpins = 7;
  int * spinsPointer = &upSpins;

  std::cout << "Address is: "
    << spinsPointer
    << "\n";

  std::cout << "Value is: "
    << *spinsPointer
    << "\n";

  *spinsPointer = 20;
  std::cout << "New upSpins: "
    << upSpins
    << "\n";

  spinsPointer = &downSpins;
  std::cout << "Down spins : "
    << *spinsPointer;

  return 0;
}
```

```
#include <iostream>

int main()
{
  int upSpins = 10;
  int downSpins = 7;
  int & spinsReference = upSpins;

//  std::cout << "Address is: "
//    << spinsReference
//    << "\n";

  std::cout << "Value is: "
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    << "\n";

  spinsReference = 20;
  std::cout << "New upSpins: "
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    << "\n";

//  spinsReference = downSpins;
//  std::cout << "Down spins : "
//    << spinsReference;

  return 0;
}
```

Changing variable value in a function

Consider:

```
void runningSum(int sum, int value)
{
  sum += value;
}
int main()
{
  int sum = 0;
  for(int i = 1; i < 100; ++i)
    runningSum(sum, i);

  std::cout << "Sum is: "
    << sum << "\n";
}
```

Output: `Sum is:  0`

But wait. What's happened? `sum` is still 0[1].

[1] Although our program fails to calculate this sum, legend has it that Gauss produced the correct answer within seconds when asked during a primary school lesson.

Changing variable value in a function

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  std::cout << "Sum is: "
    << sum << "\n";
}
```

Output: `Sum is: 0`

But wait. What's happened? `sum` is still 0[1].

Problem is that `runningSum` got a *copy* of the value in `sum` at the time it was called.

[1] Although our program fails to calculate this sum, legend has it that Gauss produced the correct answer within seconds when asked during a primary school lesson.

Passing using pointers

Let's try again but this time using a pointer:

```
void runningSum(int * sum, int
    value)
{
  *sum += value;
}
int main()
{
  int sum = 0;
  for(int i = 1; i <= 100; ++i)
    runningSum(&sum, i);

  std::cout << "Sum is: "
    << sum << "\n";
}
```

Output: `Sum is: 5050`

Passing using references

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```
void runningSum(int & sum, int
    value)
{
  sum += value;
}
int main()
{
  int sum = 0;
  for(int i = 1; i <= 100; ++i)
    runningSum(sum, i);

  std::cout << "Sum is: "
    << sum << "\n";
}
```

Output: `Sum is:  5050`

Passing by value, pointer and reference

What's the difference?

So we have three ways to pass parameters:

```
/*1.*/ void runningSum(int sum, int value);  // by value
/*2.*/ void runningSum(int * sum, int value);// by pointer
/*3.*/ void runningSum(int & sum, int value);// by reference
```

Imagine you're the function and I'm passing you an Edward Hopper[2] painting I keep on my living room wall:

[2] Nighthawks to be exact (http://en.wikipedia.org/wiki/Nighthawks)

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1. I make an exact duplicate and give it to you. Any changes you make to yours don't affect mine.

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1. I make an exact duplicate and give it to you. Any changes you make to yours don't affect mine.
2. I give you my address and you can view and change the painting by visiting (dereferencing) my address.
3. I create a second painting that is quantum entangled with mine. Any changes you make to yours affect mine instantly.

[2] Nighthawks to be exact (`http://en.wikipedia.org/wiki/Nighthawks`)