# Introduction to Programming and Computing for Scientists

Vytautas Vislavicius

Lund University

Lecture 5

Vytautas Vislavicius

**Programming for Scientists** 

Lecture 5 1 / 24

# Reminder: Hello, world!

```
#include <iostream> //Standard input/output library
int main() {
   std::cout << "Hello, world!" << std::endl;
   return 0;
}</pre>
```

- The main function is mandatory in every program.
- It returns an integer, where 0 means that the program execution finished successfully. Anything else indicates failure.
- iostream is the name of a library. It defines many objects and functions, like cout and endl, which print to the standard output.
- std:: denotes the namespace where cout and endl live. Different functions can share a name if they reside in different namespaces.

#### Control structures - if, else

```
if(condition) {
   statement;
}
else if(condition) {
   statement;
}
else {
   statement;
}
```

- if evaluates the condition. If it is true, the statement is executed.
- If it is false, the statement in the optional else clause is executed.
- if and else can be nested.

```
if(5 == 10) {
   std::cout << "This computer is insane" << std::endl;
}
else if(5 == 5) {
   std::cout << "Everything is fine" << std::endl;
}
else {
   std::cout << "This will never happen" << std::endl;
}</pre>
```

#### Control structures - for, while

```
for(initialization; condition; statement) {
   statement;
}
while(condition) {
   statement;
}
```

- The for and while loops execute statements while some condition is met. They are functionally equivalent.
- Use a for loop when you know how many iterations you want to do.
- Use a while loop when the number of iterations is unknown, for example if the stopping condition depends on user input.

```
for(int i = 0; i < 10; ++i) {
   std::cout << "i equals " << it<:endl;
}
bool keepGoing = true;
while(keepGoing) {
   std::cout << "Still going!" << std::endl;
   keepGoing = readUserInput(); //This magical function returns true or false
}</pre>
```

Control structures - continue, break

• The continue statement is used in loops to skip directly to the next iteration. It works in both for and while loops.

```
for(int i = 0; i < 10; +:1) {
    if(i == 5) continue; //5 won't be printed
    std::cout << "i equals " << i << std::end;
}</pre>
```

• The break statement is used to exit the loop entirely. It works in for and while loops as well as switch clauses (next slide).

```
while(true) {
   std::cout << "Still going!" << std::endl;
   if(readUserInput() != true) break;
}</pre>
```

#### Control structures - switch, do-while

• The switch clause can be used to replace many if statements.

```
switch(variable) {
   case 0:
   std::cout << "variable is 0" << std::endl;
   break;
   case 1:
   std::cout << "variable is 1" << std::endl;
   break;
   default:
   std::cout << "variable is neither 0 nor 1" << std::endl;
}</pre>
```

- The do-while loop works like a while loop, except the condition is checked at the end of the loop instead of the beginning.
- This guarantees that the statement will be executed at least once.

```
bool keepGoing = true;
do {
  std::cout << "Still going!" << std::endl;
  keepGoing = readUserInput(); //This magical function returns true or false
} while(keepGoing);
```

#### Namespaces

- A namespace is a place where variables, classes and functions live.
- They can share names as long as they live in different namespaces.
- Typing std:: in front of all standard functions soon gets tiresome. The using keyword allows them to be used without a qualifier.
- If you use an entire namespace, beware of collisions (e.g std::count exists).

```
#include <iostream> //For cout
using std::cout; //Now we don't have to type std::cout. Just cout will do.
using namespace std; //Like the above but for everything in the std namespace
namespace first {
    int a = 10;
    }
namespace second {
    int a = 20;
    }
int main() {
    cout << first::a << endl; //Will print 10
    cout << second::a << endl; //Will print 20
    first::a = 30;
    std::cout << first::a << std::endl; //Will print 30. Using std:: still works.
}</pre>
```

# I/O - Standard input and output

• We already know how to use std::cout to write to standard output. To read from standard input, use std::cin.

```
#include <iostream> //For cin and cout
int main() {
    int userInput = 0;
    std::cin >> userInput;
    std::cout << "The user provided " << userInput << std::endl;
    return 0;
}
```

• The read operation evaluates to true if successful. A common trick is to read many times by putting it in a while loop.

```
#include <iostream> //For cin and cout
int main() {
    int userInput = 0;
    int sum = 0;
    while(std::cin >> userInput) {
        sum += userInput;
        std::cout << "The sum of inputs is " << sum << std::endl;
    }
    return 0;
}
```

# I/O - Reading and writing files

• Reading and writing files is done using the ifstream and ofstream classes defined in the fstream library. The following program reads numbers from a file (input.txt) and prints the sum to another file (output.txt).

```
#include <iostream> //For cout
#include <fstream> //For ifstream and ofstream
int main() {
 std::ifstream inFile("input.txt"): //Name of the file to read from
 if(!inFile) {
    std::cout << "Error: could not read from file input.txt" << std::endl:
   return 1: //A nonzero return value indicates failure
 3
 double variable = 0.;
 double sum = 0.:
 while(inFile >> variable) { //Read numbers until we hit the end of file
    sum += variable:
 3
 inFile.close():
 std::ofstream outFile("output.txt");
 if(!outFile) {
    std::cout << "Error: could not write to file output.txt" << std::endl;</pre>
   return 1; //A nonzero return value indicates failure
 3
 outFile << sum << std::endl:
 outFile.close();
 return 0:
}
```

#### Containers. Arrays

• An array is a fixed-size sequential container used extensively in C.

```
#include <iostream> //For cout and cin
using namespace std;
int main() {
    const int length = 10; //The length must be known at compile time
    int arr[length]; //Thi array is fixed-size
    int input;
    int pos = 0; //An array doesn't know its own size or how many elements it contains
    while(cin >> input) {
        arr[pos] = input;
        if (pos == length) break; //Remember that the array can't grow, so this is our limit
        ++pos; //We have to keep track of the position
    }
    for(int i = 0; i < pos; ++i) cout << arr[i] << endl; //Easy to go out of range
    return 0;
}</pre>
```

- Try to avoid using arrays in C++. Use vectors instead (next slide). Comments to the code above contain possible pitfalls of using arrays.
- Arrays allocated on the heap are deleted with the delete[] operator.

#### Vectors

- A vector is a sequential container that can change size dynamically.
- It is a *template class*. The vector type must be defined at compile time.
- Vectors are fast at element access and insertion/removal at the end.

```
#include <iostream> //For cout and cin
#include <vector>
using namespace std;
int main() {
   vector<int> vec; //Create a vector with base type int
   int input;
   while(cin >> input) vec.push_back(input); //Store each input
   for(size_t i = 0; i < vec.size(); ++i) cout << vec.at(i) << endl; //Print them back
   return 0;
}</pre>
```

• Use at to access individual elements. It's also possible to use []. Try to avoid this! There is no bounds checking at run time. Your bugs will go unnoticed.

```
vector<int> vec; //Create an empty vector
cout << vec[3] << endl; //Index is out of bounds. Your program will happily print garbage
cout << vec.at(3) << endl; //Using at produces an error at run time, exposing your bug</pre>
```

### Strings

• A string is a sequence of characters, implemented by the string class.

```
#include <iostream> //For cout and cin
#include <string>
using namespace std;
int main() {
   string str("It's dangerous to go alone, take this!");
   size_t pos = str.find("take"); //Position in string where "take" is found
   cout << str.substr(0, 18) << str.substr(pos) << endl;
   return 0; //It's dangerous to take this!
}</pre>
```

- A C-string is a NULL terminated array of characters used extensively in C.
- Using C-strings are unwelcome for the same reasons as for arrays. Use string class instead.
- To get the C-string representation of a string, use the c\_str() function.

```
char cString[10] = "Test"; //Contains 5 characters including the terminating \0
const char* cStringPtr = "Test"; //Pointer to string literal, can't be modified
string cppString("Test"); //Using cppString.c_str() returns const char*
```

# Command line parameters

```
#include <iostream> //For cout
int main(int argc, char* argv[]) {
   std::cout << "Received " << argc << " parameters:" << std::endl;
   for(int i = 0; i < argc; ++i) {
      std::cout << argv[i] << std::endl;
   }
   return 0;
}</pre>
```

- You can pass parameters to a program via command line. They arrive as C-strings contained within an array.
- The first parameter is always the name of the program. Let's say, for the sake of example, that it's called 'commandLineParams'.
- Here is what it would look like if built and run from a terminal.

```
$ g++ -o commandLineParams commandLineParams.cpp
$ ./commandLineParams abc 123 -bla --bla
Received 5 parameters
./commandLineParams
abc
123
-bla
--bla
```

### The stack and the heap

- The memory available for a program to use (at least as far as we're concerned) is made up of two areas The stack and the heap.
- The stack is a small (megabytes), fixed size chunk of memory for local variables. All examples so far have used only the stack.
- When a variable on the stack falls out of scope, it is deallocated. You don't have to worry about memory management with the stack.
- The stack is small, so it overflows if you put too many things on it. But don't worry This typically only happens due to bugs (e.g an infinite loop).



<

#### The stack and the heap

- The heap is a large pool of memory that can grow dynamically.
- To put a variable on the heap, create it with the new operator. This operator returns a *pointer* through which the variable is accessed.
- A pointer is really just an integer. The number corresponds to a memory address. The pointer *points* to that memory.
- Variables on the heap are never deallocated automatically. The memory must be freed manually using the delete operator.
- The pointer itself is on the stack and is deallocated automatically.





Programming for Scientists

#### Pointers and references

- A pointer can point anywhere in memory, both the stack and the heap.
- To declare that a variable is a pointer, put an asterisk (\*) after its type.
- To get the memory address of a variable, use the reference operator (&).
- If you have a pointer and you want the value that the pointer points to, use the dereference operator (\*). That's right - The asterisk has two uses!



• To access members of a class via pointer, use the arrow (->) operator.



#### Pass by value, reference or pointer

- When calling a function, you are really passing *copies* of all the arguments.
- If you want to change the passed values, you must use references or pointers.

```
int x = 1;
int y = 2;
void swapByValue(x, y); //This will NOT swap the values!
void swapByReference(x, y); //This will work. Using references is recommended.
void swapByPointer(&x, &y); //This will work, but don't use pointers unless necessary.
```

```
void swapByValue(int a, int b) { //a and b are copies of x and y
    int temp = a; //Whatever we do here has no effect on the original x and y
    a = b;
    b = temp;
}
```

```
void swapByReference(int& a, int& b) { //a and b are references to x and y
    int temp = a; //For all intents and purposes, they ARE x and y
    a = b;
    b = temp;
}
```

```
void swapByPointer(int* a, int* b) { //a and b are pointers to x and y
    int temp = *a; //Not safe - What if they are NULL pointers? Use references instead.
    *a = *b;
    *b = temp;
}
```

# Writing a C++ class

- A class is a container for data and functions. This simple class stores coordinates. It has two member variables; an x and a y coordinate.
- You can create many coords, e.g (2,5) and (1,1). They have the same type but different internal states. An instance of the class is called an *object*.
- The constructor creates new objects. The destructor cleans up when an object is destroyed. We'll talk more about these important functions later.

```
class coords { //Here I declare a class of type "coords"
    public:
    coords(int xCoord, int yCoord); //Constructor. Call to create an instance of the class.
    "coords(); //Destructor. Gets called when an instance of the class is destroyed.
    int x; //The only two member variables are the x and y coordinates
    int y;
    private: //This class has no private members
    };
coords::coords(int xCoord, int yCoord) { //Simply store the user supplied coordinates
    x = xCoord;
    y = yCoord;
    }
    coords::"coords() { //There are no special tasks to perform when destroying a set of coordinates
    }
}
```

# Writing a C++ class

- Let's improve the coords class. We want the ability to change an existing coordinate. We also want the ability to work in a polar coordinate system.
- At this point we should divide the code into a header file (.h) for the class declaration and a source file (.cpp) for the implementation.
- The constructor now accepts a third argument isPolar. If it is not provided explicitly, false is used. This is called a default argument.

```
#ifndef BETTERCOORDS_H //This macro ensures that the .h file is only read once
#define BETTERCOORDS_H //It's fine if you don't understand how this works in detail
class betterCoords {
 public:
 betterCoords(double firstCoord, double secondCoord, bool isPolar = false);
 ~betterCoords() {}:
 void setCartesian(double xCoord, double yCoord); //Set coordinates in cartesian space
 void setPolar(double rCoord, double phiCoord); //Set coordinates in polar space
 double x: //Cartesian coords
 double y;
 double r: //Polar coords
 double phi:
 private:
 void transformToCartesian(): //Helper functions to transform between coordinate systems
 void transformToPolar():
1:
#endif //This ends the ifndef macro
```

Vytautas Vislavicius

# Writing a C++ class

```
#include "betterCoords.h" //Include the class declaration
#include <cmath> //For sqrt, sin, cos and atan2
using namespace std;
betterCoords::betterCoords(double firstCoord, double secondCoord, bool isPolar) {
 if(isPolar) setPolar(firstCoord, secondCoord); //The user supplied polar coordinates
 else setCartesian(firstCoord, secondCoord); //The user supplied cartesian coordinates
}
void betterCoords::setCartesian(double xCoord, double yCoord) {
 x = xCoord: //Set cartesian coordinates
 y = yCoord;
 transformToPolar(); //Then calculate the equivalent polar coordinates
}
void betterCoords::setPolar(double rCoord, double phiCoord) {
 r = rCoord: //Set polar coordinates
 phi = phiCoord:
 transformToCartesian(); //Then calculate the equivalent cartesian coordinates
3
void betterCoords::transformToCartesian() {
 x = r * cos(phi);
 y = r*sin(phi);
}
void betterCoords::transformToPolar() {
 r = sqrt(x*x + y*y);
 phi = atan2(x, y);
3
```

#### Constructors and Destructors

 Constructors are called to create new instances of a class. They should initialize all member variables of the class. In general they accept arguments.



- A constructor that takes no arguments is called a *default* constructor.
- Always write one. It is often invoked automatically, e.g vector<coords>(5).

```
coords::coords() {
    x = 0; //Choose a reasonable default value
    y = 0;
}
coords myCoords(); //Will be (0,0)
```

• To create copies of other objects, write a *copy* constructor.

```
coords::coords(coords& toCopy) {
    x = toCopy.x; //Copy values from the other object
    y = toCopy.y;
}
coords myCoords(existingCoords); //Initialize as copy of existingCoords
coords myCoords = existingCoords; //These two lines are equivalent
```

Vytautas Vislavicius

#### Constructors and Destructors

- A class must have a non-copy constructor. If you do not write one, the compiler automatically generates a default constructor with an empty body.
- A class must have a copy constructor. If you do not write one, the compiler generates one that performs a member-wise copy (aka a *shallow* copy).
- Consider this line class. Note that it stores *pointers* to coordinates.

#### • A shallow copy copies the pointers rather than what they point to.

```
line::line(line& toCopy) { //This is a shallow copy
start = toCopy.start;
stop = toCopy.start;
}
line::line(line& toCopy) { //After a deep copy, line and toCopy are independent
start = new betterCoords(toCopy.start->x, toCopy.start->y);
stop = new betterCoords(toCopy.stop->x, toCopy.stop->y);
}
```

### Constructors and Destructors

- The destructor is automatically called when an object is destroyed.
- It should delete objects on the heap and perform any other cleanup tasks.
- The compiler generates an empty destructor if you don't write one yourself.

```
line::Tine() {
  if(start) { //Safeguard against deleting NULL pointers
    delete start; //This destroys the object pointed to by start
    start = 0; //Not necessary here but good practice in more complicated cases
    j
    if(stop) {
        delete stop;
        stop = 0;
    }
}
```

- Once all pointers to a heap allocated variable are lost, it can't be deleted.
- This is called a *memory leak*. Here's a good rule of thumb:
- Every call to new should be matched by exactly one call to delete.

```
#include <stdlib.h> /* atof */
#include <unistd.h> /* usleep */
using namespace std;
int main(int argc, char* argv[]) {
    Vytautas Vislavicius Programming for Scientists Lecture 5 23 / 24
```

#### Next Lecture

- Inheritance
- Polymorphism
- The const keyword
- Type Casting
- Operator overloading
- Templates

# Lists, Pairs

- A list is a container with fast element insertion and removal.
- Unlike vectors, elements in a list have no absolute position. Use an iterator to loop through them. Iterators act similarly to pointers.

```
#include <iostream> //For cout and cin
#include <list>
using namespace std;
int main() {
    list<int> lst, //List with base type int
    lst.push_back(10); //Insert some elements, then iterate over the list and print them
    lst.push_back(15);
    for(list<int>::iterator it = lst.begin(); it != lst.end(); ++it) cout << *it << endl;
    return 0;
}</pre>
```

• A pair is a simple container that stores two values.

```
#include <iostream> //For cout and cin
#include <utility> //For pair
using namespace std;
int main() {
    pair<int, double> p(5, 3.14); //A pair of int and double
    cout << "The pair is " << p.first ", " << p.second << endl;
    return 0;
}</pre>
```

#### Sets

- A set is a container that stores unique objects. If a set already contains a certain element, adding that element again does nothing. Sets are ordered.
- Adding/removing elements takes logarithmic time, which is relatively slow.
- Searching also takes logarithmic time This is as fast as a search can get!

```
#include <iostream> //For cout and cin
#include <set>
using namespace std;
int main() {
   set<int> s; //Set with base type int
   s.insert(7); //Add some elements. The order in which they are added doesn't matter.
   s.insert(1);
   s.insert(5);
   for(set<int>:iterator it = s.begin(); it != s.end(); ++it) { //Traverse with iterator
        cout << *it << endl; //Prints 1, 5, 7
   }
   if(s.count(8)) cout << "The set contains the number 8" << endl; //Search in the set
   return 0;
}</pre>
```

#### Maps

• A map is an associative container that stores key/value pairs. A key can not be inserted twice, but the value of an existing key can be changed.

```
#include <iostream> //For cout and cin
#include <string>
#include <map>
#include <utility> //For make pair
using namespace std;
int main() {
 map<string, int> pBook; //Map associating strings to ints. It's a phone book!
 pBook.insert(make_pair("Reginald", 123)); //Pairs can be inserted in various ways
 pBook.insert(pair<string, int>("Marmaduke", 456));
 pBook["Bobby Floyd"] = 789:
 map<string, int>::iterator it = pBook.find("Bruce Lee"); //How to search a map
 if(it != pBook.end()) cout << it->first << "has number " << it->second << end]:
 pBook["Reginald"] = pBook["Jim Bob"]; //Beware of using [] - Jim Bob is now in the book
 for(map<string, int>::iterator it2 = pBook.begin(): it2 != pBook.end(): ++it2) {
    cout << it2->first << " - " << it2->second << endl: //Print everyone in the book
 3
 return 0:
}
```

Bobby Floyd - 789 Jim Bob - 0 Marmaduke - 456 Reginald - 0