Introduction to C++

Outline

- 1. Introduction
- Basic Syntax
 Control Flow

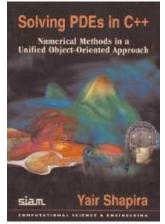
Slides/Exercices:

git clone https://qithub.com/MolSSI-Education/introductory-cpp

Part I Introduction

Why Learn C++?

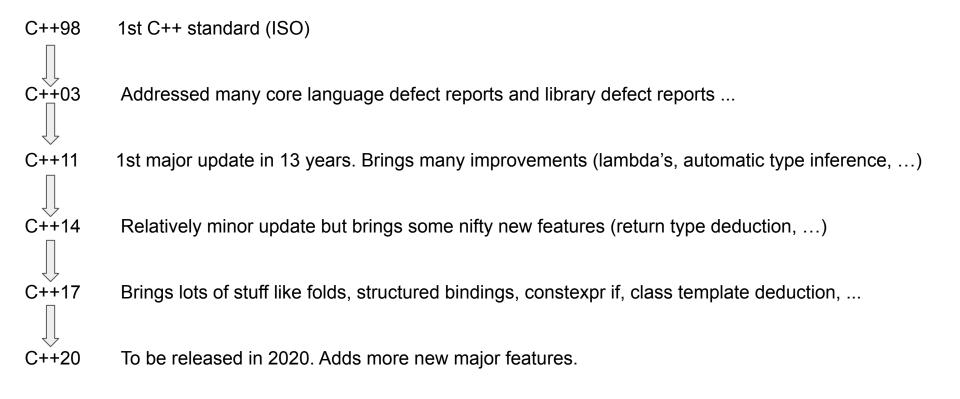
- Popular: lots of scientific code written in C++
- Powerful: fast, flexible, portable, scalable
- Multi-paradigm: procedural, functional, object-oriented, generic programming
- Wide support from vendors (LLVM, Microsoft, Intel, Oracle, IBM, Free Software Foundation, ...)



What is C++?

- Object-oriented language developed in 1979 (Bjarne Stroustrup, Bell Labs)
- Considered to be the "successor" to C (procedural language). Most (<u>but not all</u>!) C features
 are a subset of C++.
- Complex language but its features are designed to be zero-cost, i.e. if your program doesn't use a feature, it won't slow it down.
- Very few people know all of the standard. You can use what you are comfortable with and learn as you go along.

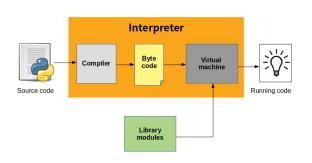
Evolution of C++

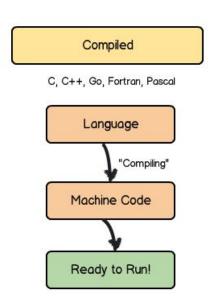


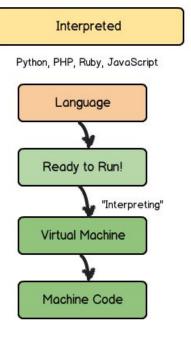
Programming Language Implementation

High-level programming languages are translated to machine code via one of the following methods:

- 1 Compilation
- 2 Interpretation
- 3 Complex combination of both







Example 1: Hello World

cd Part-I/Ex1

Method 1:

Compilation & linking: g++ main.cc

Execution: ./a.out

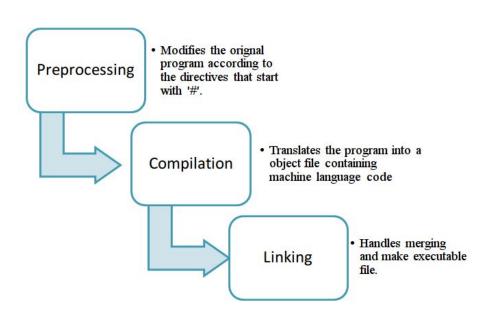
Method 2:

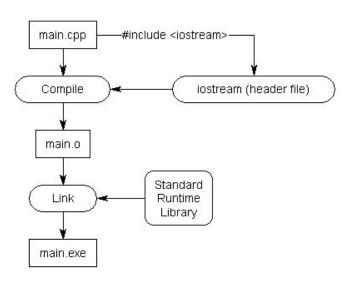
Compilation: g++ main.cc -c

Linking: **g++ main.o**

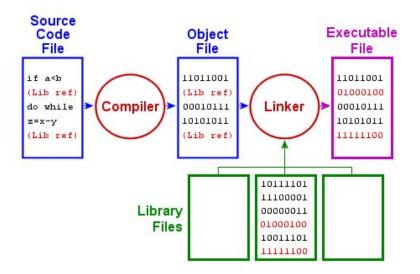
Execution: ./a.out

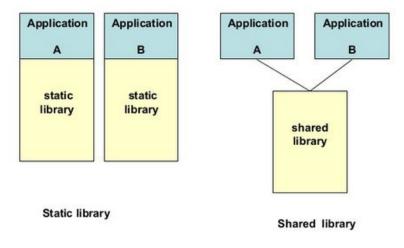
Compilation & Linking





Libraries & Executables





Example 2: Library Linking

cd ../Ex2

Static library compilation:

g++ library.cc -c ar rv libname.a library.o

Executable compilation & linking:

g++ main.cc -lname.a -L.

Dynamic vs Static Typing

Static typing:

double variable; variable type declared

✓ variable = 1.0;

x string variable = "Ben"; variable cannot change type

- Easier to read
- References resolved during compile time
- Faster execution

Dynamic typing:

variable = 1.0; variable type not declared

✓ variable = "Ben"; variable can change type

- Harder to read
- References resolved during runtime
- Slower execution

Fundamental Data Types

Category	Туре	Contents
<u>Integral</u>	char	Type char is an integral type that usually contains members of the basic execution character set.
	bool	Type bool is an integral type that can have one of the two values true or false. Its size is unspecified.
	int	Type int is an integral type that is larger than or equal to the size of type short int, and shorter than or equal to the size of type long.
Floating point	float	Type float is the smallest floating point type.
	double	Type double is a floating point type that is larger than or equal to type float, but shorter than or equal to the size of type long double.

Example 3: BMI Calculator

cd ../Ex3

1 file to edit:

□ **bmi.cc**: entry point ("main" function)

Compilation:

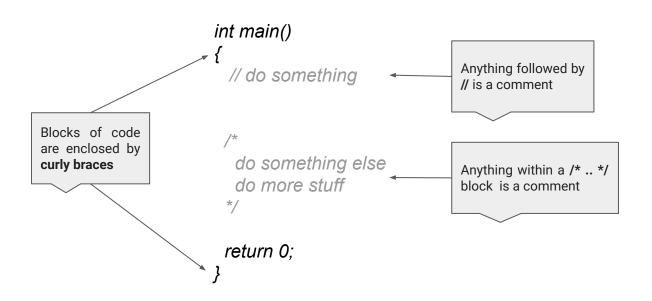
g++ main.cc -o bmi.out

Run:

./bmi.out

Part II Basic Syntax

Program Structure



C++ vs Python: Syntax

C++ for loop:

```
for (int i = 0; i < 10; i++)
{
// do something
// do something else
}

Blocks of code
are enclosed by
curly braces
```

Python for loop:

```
for i in range(10):

# do something

# do something else

Blocks of code
are denoted by
whitespace
```

C++ vs Python: Scope

C++ function

```
#include <iostream>
void foo(bool isPositive)
                                               expression
                                           followed by a
                                           semicolon is a
      int variable; -
                                           statement
      if(isPositive)
             variable = 1;
      else
             variable = -1;
      std::cout << "variable = " << variable:
    Variables must be declared before they can be used
```

Python function

```
def foo(isPositive):
    # no need to declare variable

if(isPositive):
    variable = 1
    else:
    variable = -1

print("variable =", variable)
```

Exercise 1: Scope

cd ../../Part-II/Ex1

Fix the logical bug to get result = 448.

1 file to edit:

☐ main.cc: entry point ("main" function)

Compilation:

g++ main.cc print_int.cc -o print_int.a

Run:

./print_int.a

Identifiers

A C++ identifier is a name used to identify a variable, function, class, module, or any other user-defined item. An identifier starts with a letter A to Z or a to z or an underscore (_) followed by zero or more letters, underscores, and digits (0 to 9).

An identifier cannot be a reserved keyword.

Acceptable identifiers:

- **⊒** John
- **⊒** john
- **⊒** _temp
- **→** Pi22
- ☐ foo_123



<u>Unacceptable identifiers:</u>

- □ @John
- **□** \$john
- → -temp
- **□** 22Pi
- **□** double



Some Reserved Words

asm	else	new	this
auto	enum	operator	throw
bool	explicit	private	true
break	export	protected	try
case	extern	public	typedef
catch	false	register	typeid
char	float	reinterpret_cast	typename
class	for	return	union
const	friend	short	unsigned
const_cast	goto	signed	using
continue	if	sizeof	virtual
default	inline	static	void
delete	int	static_cast	volatile
do	long	struct	wchar_t
double	mutable	switch	while
dynamic_cast	namespace	template	

C++ Files

Function "foo" declaration

```
// my_file.h
#ifndef MY_FILE_H // include guard
#define MY_FILE_H

void foo(int);
#endif
```

Function "foo" definition

```
// my_file.cc
#include "my_file.h"
#include <iostream>

void foo(int integer)
{
    std::cout << integer << std::endl;
}</pre>
```

Exercise 2: Declaration vs Definition

cd ../Ex2

3 files to edit:

- → main.cc: entry point ("main" function)
- print_int.cc: user-defined function definition
- print_int.h: user-defined function declaration

Compilation:

g++ main.cc print_int.cc -o print_int.a

Run:

./print_int.a

```
<<: insertion operator
e.g. cout << "hello world!";</pre>
```

```
>>: extraction operator e.g. cin >> input;
```

Namespaces

```
namespace

// members such as functions &
// classes go here

// Unnamed namespaces are typically used to shield global data

// members such as functions &
// classes go here
}
```

```
namespace nameSpaceB
{
    namespace subNameSpace
    {
        // memberB
    }
```

```
namespace nameSpaceA
{
    // memberA
}
```

e.g.
nameSpace::memberA
nameSpaceB::subNameSpace::memberB

This provides accessibility similar to that of Python modules e.g. module.memberA

module.submodule.memberB



Members accessible via the **scope**

operator ::



C++ Files

Function "foo" declaration

```
// my_file.h
#ifndef MY_FILE_H // include guard
#define MY_FILE_H

namespace name
{
    void foo(int);
}
```

Function "foo" definition

```
// my_file.cc
#include "my_file.h"
#include <iostream>

void name::foo(int integer)
{
    std::cout << integer << std::endl;
}</pre>
```

Exercise 3: Namespaces

cd ../Ex3

1 file to edit:

- ☐ main.cc: entry point ("main" function)
- □ **print_int.cc**: define user-defined functions

Compilation:

g++ main.cc print_int.cc -o print_int.a

Run:

./print_int.a

```
namespace some_name
{
    Members
}
```

Part III Control Flow

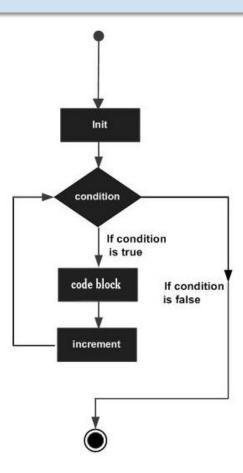
If Statements

```
if (expression)
     // statement
else
     // statement
```

```
if (expression)
{
     // statement1
     // statement2
     // ...
}
else
{
     // statement1
     // statement2
     // ...
}
```

For Loop

```
for (initialization; condition; increment)
      // statement
for (initialization; condition; increment)
      // statement1
      // statement2
     // ...
```



For Loop: Example

value of a: 19

```
#include <iostream>

int main ()
{
    // for loop execution
    for( int a = 10; a < 20; a = a + 1 )
        std::cout << "value of a: " << a << std::endl;

return 0;
}

value of a: 10
value of a: 12
value of a: 13
value of a: 14
value of a: 15
value of a: 16
value of a: 17
value of a: 18</pre>
```

Range-based For Loop

```
#include <iostream>
                                                                               value of a: 10
                                                                               value of a: 11
int main ()
                                                                                value of a: 12
                                                                               value of a: 13
  int array[] = {10, 11, 12, 13, 14, 15, 16, 17, 18, 19};
                                                                               value of a: 14
                                                                                value of a: 15
  // Range-based for loop execution
                                                                                value of a: 16
  for( int a: array )
                                                                               value of a: 17
      std::cout << "value of a: " << a << std::endl;</pre>
                                                                               value of a: 18
                                                                               value of a: 19
  return 0;
```

Exercise 1: Recursive Factorial

cd ../../Part-III/Ex1

1 file to edit:

■ main.cc: entry point ("main" function)

Compilation:

g++ main.cc -o factorial.a

Run:

./factorial.a

Factorials:

$$N! = N(N-1)(N-2)...(1)$$

 $0! = 1$

No custom header files!

Exercise 2: Iterative Factorial

cd ../Ex2

1 file to edit:

□ main.cc: entry point ("main" function)

Compilation:

g++ main.cc -o factorial.a

Run:

./factorial.a

Factorials:

No custom header files!

Extras

Documentation: Doxygen

```
/* @brief C++ implementation of Fortran BLAS daxypy
Computes the equation ys[i] <- xs[i] * alpha + beta

@note Function with C-linkage.

@param[in] n Array size. Size of xs and ys
@param[in] xs Input array xs
@param[in, out] ys Output array ys
@param[in] alpha Linear coefficient
@return Void

*/
```

Function Documentation

C++ implementation of Fotran BLAS daxypy
Computes the equation ys[i] <- xs[i] * alpha + beta.

Note

Function with C-linkage.

Parameters

```
    [in] n Array size. Size of xs and ys
    [in] xs Input array xs
    [in,out] ys Output array ys
    [in] alpha Linear coefficient Void
```

Testing Frameworks

CMake has support for adding tests to a project:

```
enable_testing()
```

This adds another build target, which is test for Makefile generators, or RUN_TESTS for integrated development environments (like Visual Studio).

From that point on, you can use the add test command to add tests to the project:

```
add_test(testname Exename arg1 arg2 ...)
```

Or, in its longer form:

```
add_test(NAME <name> [CONFIGURATIONS [Debug|Release|...]]
    [WORKING_DIRECTORY dir]
    COMMAND <command> [arg1 [arg2 ...]])
```

Once you have built the project, you can execute all tests via

```
make test
```

with Makefile generators, or by rebuilding the RUN_TESTS target in your IDE. Internally this runs CTest to actually perform the testing; you could just as well execute

```
ctest
```

in the binary directory of your build.

In some projects you will want to set "_POSTFIX properties on executables that will be executed for testing, e.g. to make executables compiled with debug information distinguishable ("-debug"). Note that the shorthand version of add_test does not automatically append these postfixes to the commands it calls for the test target, i.e. your test will want to call "" but the executable is "-debug", resulting in an error message. Use the long version of the add_test() in this case, which adds the appropriate _POSTFIX to the command name.

For more information, check the CMake Documentation or run:

```
cmake --help-command enable_testing
cmake --help-command add_test
cmake --help-property "<CONFIG>_POSTFIX"
cmake --help-command set_property
```

ctest



```
TEST CASE("Test positives", "[classic]")
      SECTION("Test all up to 10") {
        REQUIRE(fizzbuzz(1) == "1");
         REOUIRE(fizzbuzz(2) == "2");
         REOUIRE(fizzbuzz(3) == "fizz"):
         REQUIRE(fizzbuzz(4) == "4");
         REQUIRE(fizzbuzz(5) == "buzz");
         REQUIRE(fizzbuzz(6) == "fizz");
        REOUIRE(fizzbuzz(7) == "7");
10
         REOUIRE(fizzbuzz(8) == "8");
        REQUIRE(fizzbuzz(9) == "fizz");
13
         REQUIRE(fizzbuzz(10) == "buzz");
14
16
      SECTION("Test all multiples of 3 only up to 100") {
         for (int i = 3: i <= 100: i+=3) {
18
            if (i % 5) REQUIRE(fizzbuzz(i) == "fizz");
20
      SECTION("Test all multiples of 5 only up to 100") {
        for (int i = 5; i \le 100; i += 5) {
            if (i % 3) REQUIRE(fizzbuzz(i) == "buzz");
24
26
28
      SECTION("Test all multiples of 3 and 5 up to 100") {
        for (int i = 15; i <= 100; i += 15) {
29
            REQUIRE(fizzbuzz(i) == "fizzbuzz");
30
32
```

References

BOOKS

A Tour of C++ (2nd Edition) (C++ In-Depth Series)

Bjarne Stroustrup

Effective Modern C++: 42 Specific Ways to Improve Your Use of C++11 and C++14

Scott Meyers

C++ Primer Plus (6th Edition) (Developer's Library)

Stephen Prata

C++ Coding Standards: 101 Rules, Guidelines, and Best

Practices

Herb Sutter

WEBSITES

https://isocpp.org/get-started

http://www.learncpp.com

http://www.cplusplus.com/doc/tutorial

http://cppreference.com

The definitive reference on the C++ standard library

Questions?

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Thankyou