

PY410 / 505  
Computational Physics 1

**Salvatore Rappoccio**

# Code

- Code is in `CompPhys/ReviewCpp/BasicExamples`

# Flow control : Iteration

# C++: Iteration

- It's a royal pain to count. Humans suck at it.
- Computers are really, really fantastic at it, though.
- Similarly, computers are great at doing the same thing over and over (and over and over and over and over and over and over)
- This is referred to as "iteration". C++ options:
  - "while" loop
  - "do while" loop
  - "for" loop
  - "goto" statements (never use them)

# C++: Iteration

- Most commonly used is probably “for” loops:

```
for ( initialization ; condition ; modification )  
    statement
```

- Initializes with “initialization”
- Executes “statement” until “condition” is met
- After each iteration, “modification” is performed

# C++: Iteration

- Example: “forloop.cc”:

```
#include <iostream>
int main(void){

    for ( unsigned int i = 0; i < 10; ++i) {
        std::cout << i << ", ";
    }
    std::cout << std::endl;
    return 0;
}
```

- compile and execute, and you get:

```
0, 1, 2, 3, 4, 5, 6, 7, 8, 9,
```

# C++: Iteration

- Can also nest them: “forloop\_nested.cc”:

```
#include <iostream>
int main(void){

    for ( unsigned int i = 0; i < 10; ++i) {
        for ( unsigned int j = i; j < 10; ++j ){
            std::cout << "(" << j << ", " << i << ")", ";
        }
        std::cout << std::endl;
    }
    return 0;
}
```

- Compile and run, what do you get?

# C++: Iteration

- Related concepts:
  - “continue” : automatically continue to the next iteration, don’t execute the rest
  - “break”: get out of the loop right away
  - Useful for termination abnormally and for error checking
- Things to be careful about:
  - Infinite loops : you didn’t give a correct termination condition
  - Incorrect initialization : your initialization was incomplete



# C++: Iteration

- Similar to “for” loops are “do, while” and “while” loops

```
do  
    statement  
while ( condition );
```

```
while ( condition )  
    statement
```

- Very similar, except the “do, while” loop ALWAYS executes the “statement” at least once, whereas “while” will only do it if the “condition” is met
- Use “break” and “continue” to get out, OR adjust the variables in “condition”

# C++: Iteration

- “while” and “for” loops can be made semantically identical (while syntactically different)

```
for ( initialization ; condition ; modification )  
    statement
```



```
initialization  
while ( condition ) {  
    statement  
    modification  
}
```

# C++: Iteration

- Example: “whileloop.cc”

```
#include <iostream>
int main(void){
    int i = 0;
    while( i < 5 ) {
        std::cout << i << ", ";
        ++i;
    }
    std::cout << std::endl;
    return 0;
}
```



# C++: Iteration

- How about using the “break” statement? “whileloop\_break.cc”

```
#include <iostream>
int main(void){
    int i = 0;
    std::cout << "Enter a number, negative number to quit" << std::endl;
    while( std::cin >> i ) {
        if ( i < 0 ) {
            std::cout << "Negative number entered, exiting." << std::endl;
            break;
        } else {
            std::cout << "You entered i=" << i << std::endl;
        }
    }
    return 0;
}
```

# C++: Iteration

- Another nice “either / or but not both” construct is the “conditional” operator “?”. Syntax is:

( *condition* )? *expression 1* : *expression 2*

- Fast way of saying :
  - if (condition) expression 1
  - else expression 2

# Scope

# C++: Scope

- Now in a position to talk about “scope”
- Scope is the lifetime of a variable, denoted by curly braces “{ }”
- A variable must be unique IN THE CURRENT SCOPE, but can be duplicated in DIFFERENT scopes
- Loops have different scopes because they are separated by {}
- So what does this give you? “scope.cc”

```
#include <iostream>
int main(void){
    unsigned int i = 1000;
    for( unsigned int i = 0; i < 10; ++i ) {
        std::cout << i << std::endl;
    }
    std::cout << "Outside the loop, i = " << i << std::endl;
    return 0;
}
```

# C++: Scope

- This is the first instance of something having the same name but different scope
- You can declare variables to have GLOBAL scope or LOCAL scope
  - Global: all functions and all files can see it
    - Bad! Maximally violates principle of least privilege but sometimes has a use
  - Local: only defined within { }
    - Good! Principle of least privilege satisfied



# Special scopes: Functions

# C++: Functions

- Now we've seen how to execute BLOCKS of code
- What if we want to name those blocks?
  - That's a function
- We've already seen the first function ("main")
- What about others?
- Remember mathematical functions, like "squared"?

$$f(x) = x^2$$

- Literally: "input x, return x\*x"

# C++: Functions

- So we can generalize:



- Take inputs, do stuff, give output

# C++: Functions

- Lots of functions already defined (Example: cmath)
- <http://www.cplusplus.com/reference/cmath/>

## Trigonometric functions

<b>cos</b>	Compute cosine (function )
<b>sin</b>	Compute sine (function )
<b>tan</b>	Compute tangent (function )
<b>acos</b>	Compute arc cosine (function )
<b>asin</b>	Compute arc sine (function )
<b>atan</b>	Compute arc tangent (function )
<b>atan2</b>	Compute arc tangent with two parameters (function )

## Hyperbolic functions

<b>cosh</b>	Compute hyperbolic cosine (function )
<b>sinh</b>	Compute hyperbolic sine (function )
<b>tanh</b>	Compute hyperbolic tangent (function )
<b>acosh</b> <small>C++11</small>	Compute area hyperbolic cosine (function )
<b>asinh</b> <small>C++11</small>	Compute area hyperbolic sine (function )
<b>atanh</b> <small>C++11</small>	Compute area hyperbolic tangent (function )

## Exponential and logarithmic functions

<b>exp</b>	Compute exponential function (function )
<b>frexp</b>	Get significand and exponent (function )
<b>ldexp</b>	Generate value from significand and exponent (function )
<b>log</b>	Compute natural logarithm (function )
<b>log10</b>	Compute common logarithm (function )
<b>modf</b>	Break into fractional and integral parts (function )
<b>exp2</b> <small>C++11</small>	Compute binary exponential function (function )
<b>expm1</b> <small>C++11</small>	Compute exponential minus one (function )
<b>ilogb</b> <small>C++11</small>	Integer binary logarithm (function )
<b>log1p</b> <small>C++11</small>	Compute logarithm plus one (function )
<b>log2</b> <small>C++11</small>	Compute binary logarithm (function )
<b>logb</b> <small>C++11</small>	Compute floating-point base logarithm (function )
<b>scalbn</b> <small>C++11</small>	Scale significand using floating-point base exponent (function )
<b>scalbln</b> <small>C++11</small>	Scale significand using floating-point base exponent (long) (function )

## Power functions

<b>pow</b>	Raise to power (function )
<b>sqrt</b>	Compute square root (function )
<b>cbrt</b> <small>C++11</small>	Compute cubic root (function )
<b>hypot</b> <small>C++11</small>	Compute hypotenuse (function )

# C++: Functions

- Syntax is completely intuitive, so try “mathexamples.cc”
- Intuitive so I won't belabor:

```
#include <iostream>
#include <cmath>

int main(void) {
    float x = 0.5;

    std::cout << "sin(x)    = " << sin(x) << std::endl;
    std::cout << "tan(x)    = " << cos(x) << std::endl;
    std::cout << "cos(x)    = " << tan(x) << std::endl;
    std::cout << "log(x)     = " << log(x) << std::endl;
    std::cout << "log10(x)  = " << log10(x) << std::endl;

    return 0;
}
```

# C++: Functions

- Writing your own function:

*output type*   *function\_name* ( *arguments* ) {

*Function's body*

}

# C++: Functions

- Example: “xsquared.cc”  $x^2$

```
#include <iostream>
```

Function must be declared ahead of time

```
float xsquared( float x ) { return x*x; }
```

```
int main(void) {
```

```
    float x = 5.0;
```

Then you call it with parentheses: “bla(x)”

```
    std::cout << xsquared(x) << std::endl;
```

```
    return 0;
```

```
}
```

# C++: Functions

- In C++, you must DECLARE a function ahead of time
- However, you can DEFINE it whenever you want
  - Declare: Shows the types.
  - Define: the actual code of the function

- declaration:

```
float xsquared( float );
```

- definition:

```
float xsquared( float x ){ return x*x; }
```

- Can be the same, but need not be
  - For complicated functions, usually don't define them ahead of time, just declare them



# C++: Functions

- Return values:
  - Can only return ONE VALUE
  - Python can do many, but not C++
- Important programming practice: returning a number “by value” as in a function makes THREE COPIES of the return type
  - Fine for built-in types
  - Terrible, horrible, no good, bad for big classes
  - C++0x and later have “move” semantics (more on that later) that makes 1.5 copies instead of three :)

# C++: Functions

- Can also specify a DEFAULT value for function inputs:

```
#include <iostream>

int squared( int i = 0 ) { return i*i;}

int main(void)
{
    std::cout << squared() << std::endl;    // Returns 0
    std::cout << squared(2) << std::endl;    // Returns 4
    return 0;
}
```

# C++: Functions

- What about SCOPE of variables? “funcscope.cc”
  - Global scope: variable available to ALL functions
  - Local scope: variable available to THIS function only
  - static: variable available to THIS function, but value is kept after scope ends (useful for counting)

```
#include <iostream>
unsigned int i = 1000;
int duh( void ) {
    static unsigned int count = 0;
    unsigned int i = 2;
    std::cout << "for the " << count << "th time, i = " << i << std::endl;
    ++count;
    return i;
}

int main(void){
    for ( unsigned int i = 10; i < 20; ++i ) {
        std::cout << "i = " << i << ", duh() = " << duh() << ", global i = " << ::i << std::endl;
    }
    return 0;
}
```

# C++: Functions

- Can call functions within functions
- Can call YOUR OWN function within functions (recursion)
- Example: Fibonacci sequence “fibonacci.cc”:

```
#include <iostream>

int fibonacci(int n) {
    if (n <= 0)
        return 0;
    else if (n == 1)
        return 1;
    else
        return fibonacci(n - 2) + fibonacci(n - 1);
}

int main(void)
{
    for ( unsigned int i = 0; i < 10; ++i ) {
        std::cout << fibonacci(i) << ", ";
    }
    std::cout << std::endl;

    return 0;
}
```

# C++: Functions

- C++ has a nice feature in OVERLOADING functions
  - Example: if you want  $x^2$ , what do you need?
    - Input as int
    - Input as float
    - Input as double
    - Input as unsigned int
    - Input as short
    - Input as unsigned long
    - ...
- But you probably want them all to be called the same thing (xsquared)
- You can define multiple functions with different ARGUMENT TYPES
  - Caveat: Cannot differ only by return type

# C++: Functions

- Looks like this: “xsquared\_types.cc”

```
include <iostream>

int squared(int x){ return x*x;}
float squared(float x){ return x*x;}
double squared(double x){ return x*x;}
long squared( long x) { return x*x;}

int main(void)
{
    int i = 5;
    long j = 10;
    float x = 0.5;
    double y = 1.5;

    std::cout << squared(i) << std::endl;
    std::cout << squared(j) << std::endl;
    std::cout << squared(x) << std::endl;
    std::cout << squared(y) << std::endl;

    return 0;
}
```

# C++: Functions

- Isn't it annoying to write that over and over? And if I try a new type, I have to recompile? What a pain.
- If only there were some way to fix this...

# Function templates



# C++: Function Templates

- Do I have a DEAL for YOU!
- You can create a “function template” instead of a function
- This tells you HOW to create a function if you are GIVEN the types
- Syntax is a bit weird:

```
template< class T>  
T squared(T x){ return x*x;}
```

This is NOT A FUNCTION.  
This is a TEMPLATE for a function.

# C++: Function Template

Cookie  
template



Cookie

Function  
template

```
template< class T>  
T squared(T x){ return x*x;}
```

```
squared<int>( 2 )
```

Function

# C++: Function Templates

- Functions : Compiled, exist in memory
- Function templates: NOT compiled, must be given a type
- EACH type gets a SEPARATE function in memory, on demand
- More on templates later