# PY410 / 505 Computational Physics 1

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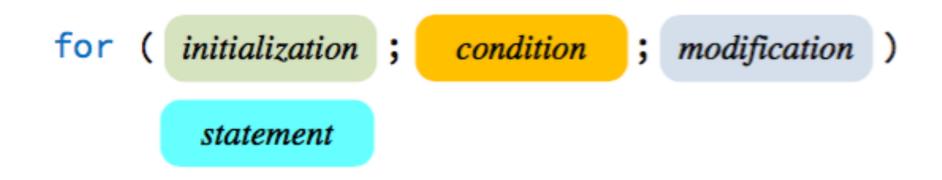
#### Code

Code is in CompPhys/ReviewCpp/BasicExamples

#### Flow control : 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 andoverandoverandover)
- This is referred to as "iteration". C++ options:
  - -"while" loop
  - -"do while" loop
  - -"for" loop
  - -"goto" statements (never use them)

Most commonly used is probably "for" loops:



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

• 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;
}</pre>
```

compile and execute, and you get:
0, 1, 2, 3, 4, 5, 6, 7, 8, 9,

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;
}</pre>
```

Compile and run, what do you get?

- 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

• Similar to "for" loops are "do, while" and "while" loops



- 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"

 "while" and "for" loops can be made semantically identical (while syntactically different)

for	(	initialization	ı ;		cond	lition	;	modification	)
		statement							
			initi	aliz	zation				
			whi	le	(	conditie	on	) {	
					stat	ement			
					modi	fication	2		
			}						

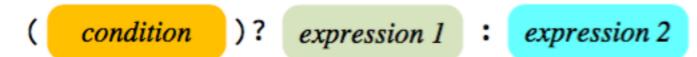
#### • Example: "whileloop.cc"

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

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;</pre>
  while( std::cin >> i ) {
    if ( i < 0 ) {
      std::cout << "Negative number entered, exiting." << std::endl;</pre>
      break;
    } else {
      std::cout << "You entered i=" << i << std::endl;</pre>
    }
  }
  return 0;
}
```

• Another nice "either / or but not both" construct is the "conditional" operator "?". Syntax is:



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



### 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;
}</pre>
```

#### 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

- 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"

• So we can generalize:

• Take inputs, do stuff, give output

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

#### **Trigonometric functions**

cos Compute cosine (function )				
sin Compute sine (function )				
tan Compute tangent (function )				
acos Compute arc cosine (function ) Exponential and logarithmic functions	onential and logarithmic functions			
asin Compute arc sine (function ) exp Compute exponential function (function )				
atan Compute arc tangent (function ) frexp Get significand and exponent (function )				
atan2 Compute arc tangent with two parameters (function ) Idexp Generate value from significand and exponent	(function )			
log Compute natural logarithm (function )				
Hyperbolic functions logarithm (function )				
cosh         Compute hyperbolic cosine (function )         modf         Break into fractional and integral parts (function)	on )			
sinh Compute hyperbolic sine (function )	Compute binary exponential function (function ) Compute exponential minus one (function )			
tanh Compute hyperbolic tangent (function )				
acosh [[++1]] Compute area hyperbolic cosine (function )				
asinh [***]     Compute area hyperbolic sine (function )				
log1p \cdots Compute logarithm plus one (function )	Compute logarithm plus one (function )			
atanh 📖 Compute area hyperbolic tangent (function ) log2 💷 Compute binary logarithm (function )				
logb 🚥 Compute floating-point base logarithm (function	n )			
scalbn 🚥 Scale significand using floating-point base exp	onent (function )			

#### Power functions

scalbin 🚥

pow	Raise to power (function )
sqrt	Compute square root (function )
cbrt C++II	Compute cubic root (function )
hypot 🚥	Compute hypotenuse (function )

Scale significand using floating-point base exponent (long) (function )

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

#include <iostream>
#include <cmath>

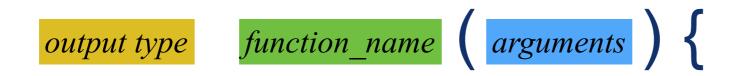
```
int main(void) {
  float x = 0.5;
```

```
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;</pre>
```

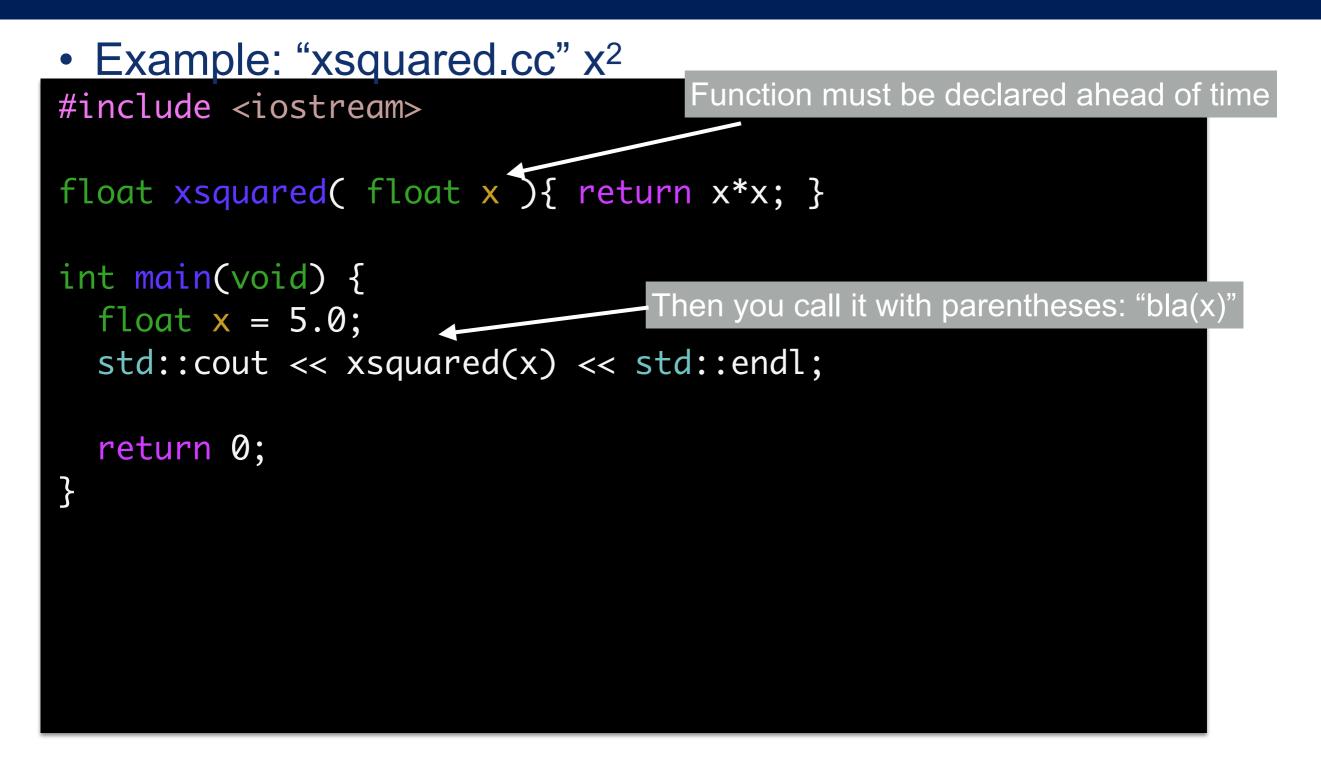
return 0;

}

• Writing your own function:







- 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

- 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 :)

• 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;
}</pre>
```

- 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;
}</pre>
```

- Can call functions within functions
- Can call YOUR OWN function within functions (recursion)
- Example: Fibonacci sequence "fibo.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) << ", ";</pre>
  }
 std::cout << std::endl;</pre>
  return 0;
```

- C++ has a nice feature in OVERLOADING functions
  - -Example: if you want x<sup>2</sup>, 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

#### 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;</pre>
```

#### return 0;

- 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:

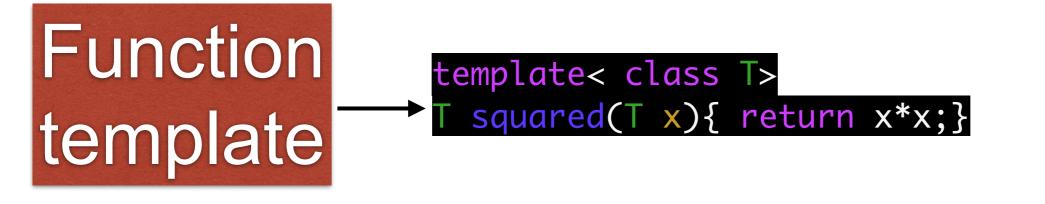
template< class T>
T squared(T x){ return x\*x;}

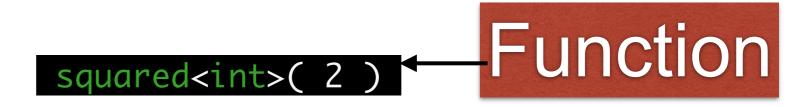
This is NOT A FUNCTION. This is a TEMPLATE for a function.

#### C++: Function Template









## 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