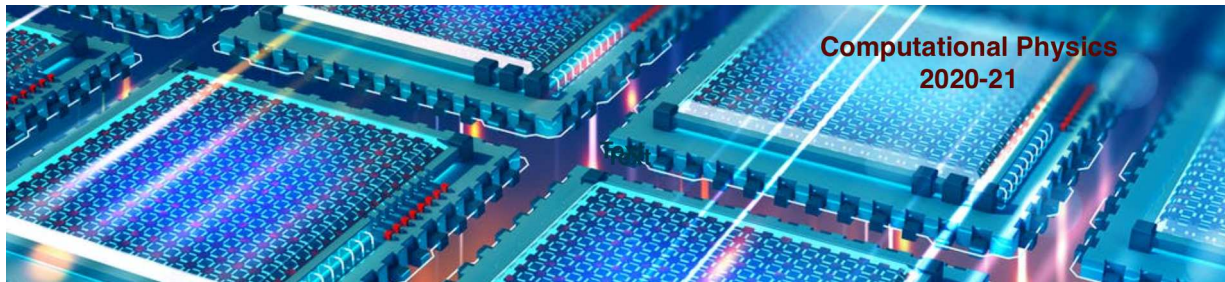




# Computational Physics

*numerical methods with C++ (and UNIX)*

**2020-21**



Fernando Barao

Instituto Superior Tecnico, Dep. Fisica  
email: fernando.barao@tecnico.ulisboa.pt

Computational Physics 2020-21 (Phys Dep IST, Lisbon)

Fernando Barao (1)



## Computational Physics

### **Classes and Objects**

**OOP programming**

Fernando Barao, Phys Department IST (Lisbon)

Computational Physics 2020-21 (Phys Dep IST, Lisbon)

Fernando Barao (2)



# C++ Classes and Objects

- ✓ In Object Oriented Programming (OOP) a group is a **class**, a class member is an **object** and a member function implements an **operation**
- ✓ Classes in OOP can be as simple as the set of numbers *int*, *float*, ...
- ✓ The member functions also called **methods** accomplish a broad range of tasks
  - **constructors**: default and parametered constructors
  - **accessor member methods**: query the objects
  - **mutator member methods**: operate and change the object
- ✓ Class members can be **public**, **private** or **protected**
  - public members can be accessed from the user program or user functions
  - private members can only be accessed from class members
  - protected: see inheritance



## C++ Classes and Objects (cont.)

- ✓ A member of a class is **private** by default
- ✓ Particular member functions are used to:
  - create and initialize objects - **constructors**
  - destroy objects - **destructors**
- ✓ The class declaration needs a semi-colon (;) at the end
- ✓ There can be functions, called **friends**, which **are not members of the class** but **have access to private and protected members** of the class

friend functions are declared on the private or public sector of the class

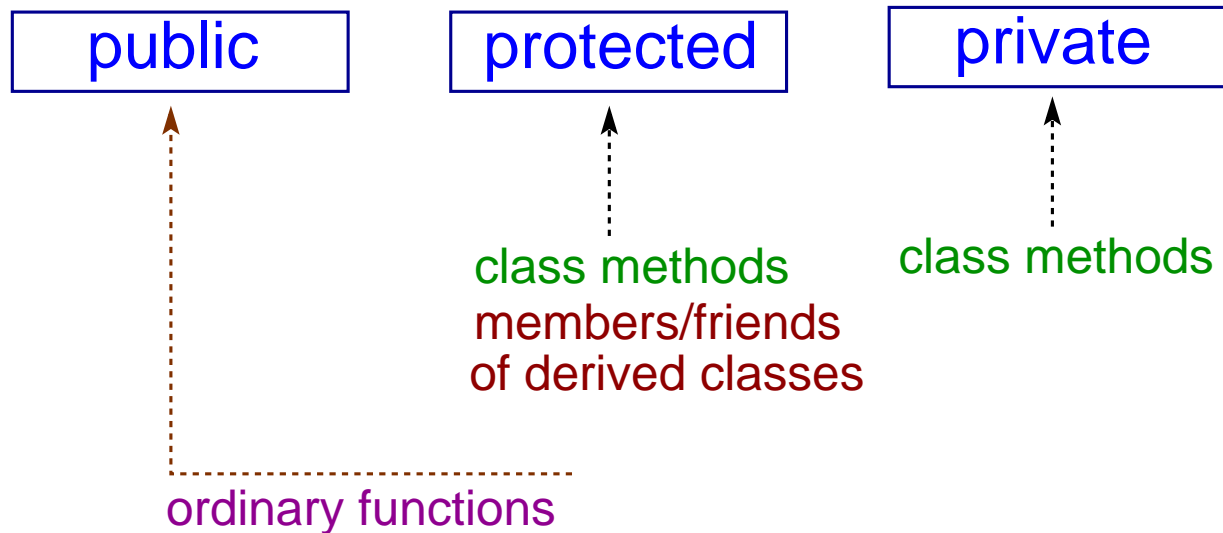
```
friend double function();
```

- ✓ Member functions **inline** need to be defined (coded) inside class declaration code (why? compiler needs to know it...cannot be in a library!)
- ✓ The **struct** data type in C++, is a class with all members **public**



# accessing members

## kind of members in a class: access



# OOP programming

- ✓ A very simple class defining an object *point*
- ✓ *point class* contains two data fields of type *double*: *x* and *y* to store the *x* and *y* coordinates of the point object
- ✓ **This is not Object Oriented Programming!** In OOP we would like the user to think about the **point** as an object, never dealing directly with its data members!

**point class**

```

class point {
public:
    double x; //X coordinate
    double y; //Y coordinate
};
  
```

**main.C**

```

point P;
P.x = 10.;
P.y = 2.;
  
```

- ✓ The class shall have methods to access the data members (now private)

**point class**

```

class point {
public:
    double X() const {return x;} // method to access the value of the x coordinate
    double Y() const {return y;} // method to access the value of the Y coordinate
private: //could not be explicitly written (by default they are private)
    double x; //X coordinate
    double y; //Y coordinate
};
  
```

- ✓ *const* declaration implies that a compilation error arises if there is a trial to change the point object being called



# Building an object: constructor

- ✓ For building an object we simply write:

**building point**

```
point P;
```

- ✓ this declaration makes the C++ compiler to call the **default constructor** of the object that allocates the required memory for the data members of the class and init them

**default constructor**

```
class point {
public:
    point() { //default constructor
        x = 0.; y=0.; //init data
    }
};
```

- ✓ If no constructor is written, then the C++ compiler invokes its own default constructor and the data members are initialized with random numbers  
**write always your own constructor!**

- ✓ Build a more sophisticated constructor able to initialize the data members and work also as default constructor

**we just set default values in the arguments!**

**constructor**

```
class point {
public:
    point(double fx=0, double fy=0) {
        x = fx; y=fy; //init data
    }
};
```

- ✓ In the operation above, **1)** memory was allocated for data members that were filled with random values and **2)** members were initialized

**this can be done more efficiently with the initialization list**

**constructor with initialization list**

```
class point {
public:
    point(double fx=0, double fy=0) : x(fx), y(fy) {}
};
```



# Building an object: example

## point (2D) class header

```
1  #ifndef __point__
2  #define __point__
3
4  class point {
5  public:
6
7      // constructor, destructor
8      point(float x=0., float y=0.);
9      ~point(); // destructor
10
11     // other
12     void Dump() const;
13
14 private:
15     // point coordinates
16     float* coo;
17 };
18 #endif
```

## main program

```
1  #include "point.h"
2
3  int main() {
4      printf("____ constructor\n" );
5      point P;
6      point P(0.25, 3.1);
7      printf("____ ending\n" );
8  }
```

## output

```
____ constructor
[point::point(float, float)] constructor...
[void point::Dump() const] (0x7ffee48bd460) 0.000000 0.000000
[point::point(float, float)] constructor...
[void point::Dump() const] (0x7ffee48bd448) 0.234000 1.093000

____ ending
[point::~~point()] destructor... (0x7ffee48bd448)
[point::~~point()] destructor... (0x7ffee48bd460)
```

**notice reverse order of objects  
destruction wrt creation**



# Building an object: copy constructor

- ✓ For building an object we can also use another object

## building points

```
point P(3.,5.);
point Q(P); //creating Q=(3,5)
point T=P; //creating T=(3,5)
```

- ✓ we used the **copy constructor** that made a new object by copying the data members of the object that is passed
- ✓ if no **copy constructor** is defined in the class block declaration, then the compiler invokes its **default copy constructor**
- ✓ the **copy constructor** is invoked every time an object is passed to a function by value

## copy constructor

```
point(const point& p):x(p.x),
                    y(p.y){};
```

In C++ we can define a **reference** to an existing variable

## reference

```
point P;
point& q=P; //reference
```

**q** is not an independent **point** object but a reference-to-point-object **P**

No copy constructor is used! -> which means time saving

## returning reference to object

```
const point& point::GetObject() {
    //this=pointer to current object
    return *this; //de-reference this pointer
}
```

```
point P;
point q = P.GetObject();
```



# Default copying: example

## point (2D) class header

```
1  #ifndef __point__
2  #define __point__
3
4  class point {
5  public:
6      // constructor, destructor
7      point(float x=0., float y=0.);
8      point(const point&) = default;
9      ~point() = default; //destructor
10
11     // What is a good destructor?
12     // something that shall erase
13     // allocated memory
14     // => delete [] coo
15
16  private:
17     // point coordinates
18     float* coo;
19 };
```

## main program

```
1  #include "point.h"
2  int main() {
3      point A(0.25,3.1);
4      point B(A);
5      B.Dump();
6      point C = A;
7      C.Dump();
8  }
```

## output

```
[pointS::pointS(float, float)] constructor...
[void pointS::Dump() const] 0.234000 1.093000
obj pointer=0x7ffee298d460 | C-array pointer=0x7fd557c058a0
[void pointS::Dump() const] 0.234000 1.093000
obj pointer=0x7ffee298d458 | C-array pointer=0x7fd557c058a0
[void pointS::Dump() const] 0.234000 1.093000
obj pointer=0x7ffee298d450 | C-array pointer=0x7fd557c058a0
_____ ending
```

1. Is default copy constructor correct?  
**NO! Object not replicated!!!**
2. Is default destructor correct?  
**NO! MEMORY LEAKAGE!!!!**



## copy assignment: operator=

- ✓ To assign the value of an existing object **Q** to existing point objects **T** and **V** an **assignment operator (=)** must be defined

### object assignment

```
point Q, T, V(5.,3.);
Q = T = V; //assignment is similar to do: T.operator=(V);
```

- ✓ Above, the assignment operator shall assign the value of the **V** object to the **current object T**, but also **return a reference to it** (no need to implicit call copy constructor)

### copy assignment declaration

```
const point& operator=(const point& p);
```

### copy assignment implementation

```
const point& operator=(const point& p) {
    //check if address of the current object (this) is the same of the argument
    if (this != &p) {
        x=p.x;
        y=p.y;
    }
    return *this; //return object reference
}
```



## move semantics

**move semantics** is a concept introduced by C++11 revision that allows the compiler to replace **copy concept** by **move concept**: a temporary object (i.e., that will disappear) is moved to an addressable object

- ✓ **lvalues**: (left hand side value) its address is recoverable (& operator)

### lvalues

```
float x = 10.; // x has a memory address recoverable, so it's an lvalue
              // 10. is an rvalue
float *px = &x; // address of x (x can be changed)
}
```

- ✓ **rvalues**: (right hand side value) temporary object as for instance a variable returned by value on a function

### rvalues

```
float x = 10.; // x has a memory address recoverable, so it's an lvalue
float y = (x+1.); // (x+1) is an rvalue
string('text'); // temporary object
```

- ✓ **rvalues references**: reference to r value variable (&& operator)

**moving a large object (i.e., vampirize it)** is much more code efficient than **allocate memory + copy**



# move constructor

- ✓ Content of a **source object** is transferred to a **destination object**; the source loses its content. this happens to *unnamed objects*, objects that are temporary by nature and thus haven't yet a name!
- ✓ the **move constructor** is called when an object is initialized on construction using an unnamed temporary

## using move constructor

```
point P = fn(); // move constructor called, fn() returns an object point
point P = point(); // move assignment called
point A; point P = A; // copy constructor called
```

## point class with move constructor

```
1 class point {
2     double *x, *y;
3 public:
4     // constructor
5     point (double fx=0., double fy=0.) {
6         x = new double(fx); //init to zero
7         y = new double(fy);
8     }
9     // destructor
10    ~point() {delete x; delete y;}
11    (...)
```

```
1 class point {
2     double *x, *y;
3 public:
4     (...)
5     // move constructor
6     // memory already allocated is moved
7     point (point&& P) : x(P.x), y(P.y) {
8         P.x = nullptr;
9         P.y=nullptr;
10    }
11 };
```



# move assignment

## move assignment

```
1 class point {
2     double *x, *y;
3 public:
4
5     // constructor: initialize members though init list (fastest way)
6     point (double fx=0., double fy=0.) : x(new double(fx)), y(new double(fy)) {;}
7
8     // destructor
9     ~point() {delete x; delete y;}
10
11    // move assignment (memory already allocated is moved)
12    point& operator= (point&& P) {
13        delete x;
14        delete y;
15        x = P.x;
16        y = P.y;
17        P.x = nullptr;
18        P.y = nullptr;
19        return *this;
20    }
21 };
```





## class special member functions

- ✓ There are some class member functions that can be **implicitly defined** under certain conditions!

default constructor	<code>C::C()</code>	if no other constructors
destructor	<code>C::~~C()</code>	if no destructor
copy constructor	<code>C::C(const C&amp;)</code>	if no move constructor and no move assignment
copy assignment	<code>C&amp; operator= (const C&amp;)</code>	if no move constructor and no move assignment
move constructor	<code>C::C (C&amp;&amp;)</code>	if no destructor, no copy constructor and no copy nor move assignment
move assignment	<code>C&amp; operator= (C&amp;&amp;)</code>	if no destructor, no copy constructor and no copy nor move assignment



## C++ Operators overloading

- ✓ commonly overloaded operators on user-defined classes

<b>assignment operator</b>	<code>=</code>
<b>binary arithmetic operators</b>	<code>+</code> <code>-</code> <code>*</code>
<b>compound assignment operators</b>	<code>+=</code> <code>-=</code> <code>*=</code>
<b>comparison operators</b>	<code>==</code> <code>!=</code>
<b>unary operators</b>	<code>++</code> <code>--</code> <code>-</code> <code>!</code>





## Adding two objects

```

1 point P(1.,2.);
2 point Q(3.,1.);
3 point T = P + Q; // P is the current object
4                 // Q is the argument
5                 // similar to: point T = P.operator+(Q);

```

### binary operator +

```

// adds two points
point point::operator+(const point& A) {
    return point(x+A.x , y+A.y);
    // in case we had pointers on private members
    return point(*x+*(A.x), *y+*(A.y));
}

```

Note that cannot be returned a reference to the object because it is a local *point* object (it disappears when function ends)!



## C++ compound assignment operators

- ✓ Compound assignment operators are destructive operators; they update or replace the values on left-hand side of the assignment  
they apply to the current object and update it

```

1 point P(1.,2.);
2 point Q(3.,1.);
3 Q += P; // Q = P + Q

```

### += operator

```

// adds a point to the current point
const point& point::operator+=(const point& p) {
    x += p.x;
    y += p.y;
    return *this;
}

```



## C++ unary operators

- ✓ they apply to the current object modifying or not their values

```
1 point P(1.,2.);
2 point Q = -P; // P.operator-() && copy constructor
3
4 point E;
5 E = -P; // P.operator-() && copy assignment
```

### unary operator -

```
const point& point::operator-() {
    x = -x;
    y = -y;
    return *this;
}
```



## C++ comparison operators

```
1 point P(1.,2.);
2 point Q = P;
3 if (Q==P) {
4     cout << "similar points!" << endl;
5 }
```

### comparison operator ==

```
bool point::operator==(const point& A) {
    if (*x == *(A.x) && *y == *(A.y)) return true;
}
```

91-1

91-2