CS601: Software Development for Scientific Computing

Autumn 2022

Week8: Intermediate C++ (object orientation),
Motifs: N-body Problems

Course progress so far:

- Computational thinking
  - Data representation (IEEE 754)
  - System Architecture (cache hierarchy, pipelined logic)
  - Language considerations (C/C++ features)

- Patterns / Motifs in Scientific Computing
  - Dense matrix computations, Sparse matrix computations, FFT

- Tools
  - Git, make, overview of compiler tool chain.

Course in the next 7 weeks:

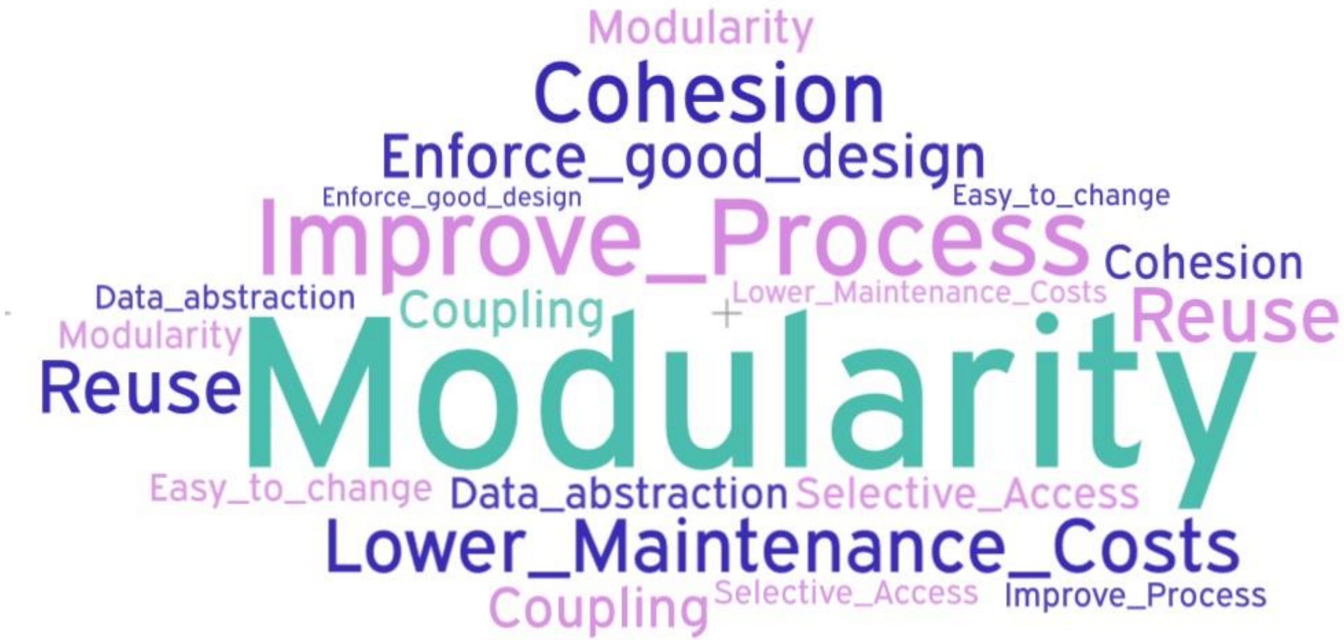
- Computational thinking
  - Data representation (IEEE 754, Object-oriented design)
  - System Architecture (cache hierarchy, pipelined logic)
  - Language considerations (C/C++ features Generic programming etc.)

- Patterns / Motifs in Scientific Computing
  - Dense matrix computations, Sparse matrix computations, FFT
  - N-body problems, Structured and Unstructured grids

- Tools
  - Git, make, overview of compiler tool chain.
  - Doxygen, gdb, valgrind, gprof

Recap: Object Orientation: Why?

- Improve costs
- Improve development process and
- Enforce good design



Header file (`myvec.h`)

```
#ifndef MYVEC_H
#define MYVEC_H



#endif
```

Header file (`myvec.h`)

- Declare the class

Class *declaration* opening scope

Keyword

Class name

Class *declaration* closing scope

```
#ifndef MYVEC_H
#define MYVEC_H
class MyVec{


};
#endif
```

Header file (`myvec.h`)

Declaring attributes

```
#ifndef MYVEC_H
#define MYVEC_H
class MyVec{
        //private attributes
        double* data;
        int vecLen;



};
#endif
```

Header file (`myvec.h`)

Specifying access control

Declaring operations

```
#ifndef MYVEC_H
#define MYVEC_H
class MyVec{
        //private attributes
        double* data;
        int vecLen;
public:
        MyVec(int len); //constructor
        ~MyVec(); //destructor

};
#endif
```

Defining the class (`myvec.h` and `myvec.cpp`)

```
#ifndef MYVEC_H
#define MYVEC_H
class MyVec{
	//private attributes
	double* data;
	int vecLen;
public:
	MyVec(int len); //constructor decl.
	~MyVec(); //destructor decl.

};
#endif
```

```
#include"myvec.h"
//defining the constructor
MyVec::MyVec(int len) {
	vecLen=len;
	data=new double[vecLen];
}

//defining the destructor
MyVec::~MyVec() {
	delete [] data;
}
```

Scope resolution operator
Constructor: no return type.
Destructor: no parameters, no return type.

Defining the class (`myvec.h` and `myvec.cpp`)

```cpp
#ifndef MYVEC_H
#define MYVEC_H
class MyVec{
        //private attributes
        double* data;
        int vecLen;
public:
        MyVec(int len); //constructor decl.
        ~MyVec(); //destructor decl.
        int GetVecLen(); //member function


};
#endif
~
~
```

```cpp
#include"myvec.h"
//defining the constructor
MyVec::MyVec(int len) {
        vecLen=len;
        data=new double[vecLen];
}

//defining the destructor
MyVec::~MyVec() {
        delete [] data;
}

//defining GetVecLen member function
int MyVec::GetVecLen() {
        return vecLen;
}
```

Using an object

```
#include<iostream>
#include"myvec.h"
using namespace std;
int main() {
        MyVec v(10); //calls the constructor and passes the argument 10
        int size=v.GetVecLen(); //calls the member function
        cout<<"size of MyVec is: "<<size<<" elements"<<endl;
}
```

Recap: Polymorphism and Destructors

- declare base class destructors as `virtual` if using base class in a polymorphic way

```
file Fruit.h
#include<string>

class Fruit {
protected:
       string commonName;
public:
       Fruit(string name);
       virtual string GetName();
       virtual ~Fruit();
};
```

```
...
Fruit* item1 = new Mango("Mango",
"Alphonso");
...
delete item1; //calls Mango::~Mango()
first and then Fruit::~Fruit()
```

Exercise

- https://forms.gle/xzd83oioSmdyTBn86

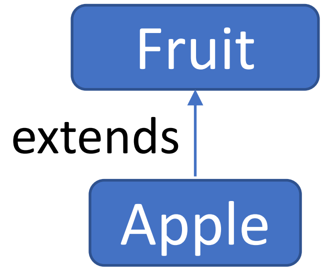
Recap: Abstract base classes

- A class can have a `virtual` method without a definition – *pure virtual functions*
- E.g

```
class Fruit {
protected:
    string commonName;
    float weight;
    float energyPerUnitWeight; //in kCals / 100g
public:
    Fruit(string name, float weight);
    virtual string GetName();
    virtual ~Fruit();
    virtual void Energy() = 0;
};
```

Energy is ‘pure’ – no implementation

Recap: Defining pure virtual function

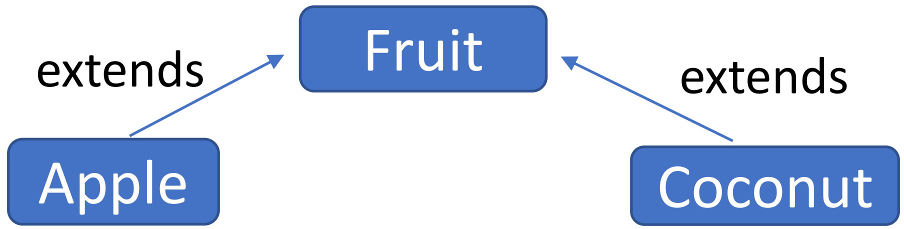



```
class Apple : public Fruit {
    vector<pair<string, float> > constituents;
public:
    Apple(string name, float weight);
    virtual ~Apple();
    . . .
    void Energy() {
    energyPerUnitWeight = ComputeEnergy(weight, constituents);
    }
};
```

Pure virtual method defined in derived class.

Base class attribute

Recap: Defining pure virtual function




```
class Coconut : public Fruit {
    vector<pair<string, float> > constituents;
public:
    Coconut(string name, float weight);
    virtual ~Coconut();
    . . .
    void Energy() {
    float effWeight = GetEdibleContentWeight();
    energyPerUnitWeight = ComputeEnergy(effWeight, constituents);
    }
};
```

Computation is different from that of Apple’s method

Recap: Abstract base classes..

- Cannot create objects from abstract base classes. But may need constructors. Why?

```
Fruit item1; //not allowed. Fruit::Energy() is pure virtual
```

- Can create pointers to abstract base classes and use them in polymorphic way

```
Fruit* item1 = new Apple(“Apple”, 0.24);
cout<<item1->Energy()<<“Kcals per 100 g”<<endl;
```

- Often used to create *interfaces*

Recap: Friend functions

- Can access `private` and `protected` members

```
class Coconut {
    vector<pair<string, float> > constituents;
public:
    ...
    friend float ComputeEnergy(float wt, Coconut* c);
};

float ComputeEnergy(float weight, Coconut* c) {
//get a set of items, for each item, get its weight and
//energy_per_g. multiply both. Sum the product of all items...
//read from c->constituents to get the set of items.
}
```

The non-member function `ComputeEnergy` can access private attribute `constituent` of Coconut class

Exercise

- https://forms.gle/JwVF8zSj9Trp4qLx5

Operator overloading

- How can we assign one object to another?

```
Apple a1("Apple", 1.2); //constructor Apple::Apple(string, float)
                        //is invoked
Apple a2; //constructor Apple::Apple() is invoked.

a2=a1 //a1 is assigned to a2. assignment operator invoked

Apple& Apple::operator=(const Apple& rhs){
    commonName = rhs.commonName;
    weight = rhs.weight;
    energyPerUnitWeight = rhs.energyPerUnitWeight;
    constituents = rhs.constituents;
    return *this;
    }
```

Called Copy Assignment Operator

Operator overloading []

```cpp
#ifndef MYVEC_H
#define MYVEC_H
class MyVec{
        //private attributes
        double* data;
        int vecLen;
public:
        MyVec(int len); //constructor decl.
        ~MyVec(); //destructor decl.
        int GetVecLen(); //member function
        double& operator[](int index);


};

#endif
```

```cpp
        delete [] data;
}

//defining GetVecLen member function
int MyVec::GetVecLen() {
        return vecLen;
}

double& MyVec::operator[](int index) {
        return data[index];
}
```

Operator overloading - usage

```
#include<iostream>
#include"myvec.h"
using namespace std;
int main() {
        MyVec v(10); //calls the constructor MyVec::MyVec(int) and passes the argument 10
        int size=v.GetVecLen(); //calls the member function
        cout<<"size of MyVec is: "<<size<<" elements"<<endl;
        cout<<"Setting first element to 100"<<endl;
        v[0]=100;
        cout<<"Fetching first element value: "<< v[0] << endl;
}
```

Copying Objects

```
Apple a1("Apple_red", 0.2);

Apple a2 = a1; //calls copy constructor

Apple::Apple(const Apple& rhs) {
            commonName = rhs.commonName;
            weight = rhs.weight;
            energyPerUnitWeight = rhs.energyPerUnitWeight;
    }
```

Copy constructor – another example

```
#include<iostream>
#include"myvec.h"
using namespace std;
int main() {
        MyVec v(10); //calls the constructor MyVec::MyVec(int) and passes the argument 1
        int size=v.GetVecLen(); //calls the member function
        cout<<"size of MyVec is: "<<size<<" elements"<<endl;
        cout<<"Setting first element to 100"<<endl;
        v[0]=100;
        cout<<"Fetching first element value: "<< v[0] << endl;
        MyVec v2=v; //calls the copy constructor
        cout<<"v2's first element: "<<v2[0]<<endl;
}
```

- Not necessary to define the copy constructor. Compiler defines one for us.

```cpp
#include<iostream>
#include"myvec.h"
using namespace std;
int main() {
        MyVec v(10); //calls the constructor MyVec::MyVec(int) and passes the argument 10
        int size=v.GetVecLen(); //calls the member function
        cout<<"size of MyVec is: "<<size<<" elements"<<endl;
        cout<<"Setting first element to 100"<<endl;
        v[0]=100;
        cout<<"Fetching first element value: "<< v[0] << endl;
        MyVec v2=v; //calls the copy constructor
        cout<<"v2's first element: "<<v2[0]<<endl;
}
```

```
size of MyVec is: 10 elements
Setting first element to 100
Fetching first element value: 100
v2's first element: 100
free(): double free detected in tcache 2
Aborted
```

```cpp
#include<iostream>
#include"myvec.h"
using namespace std;
int main() {
	MyVec v(10); //calls the constructor MyVec::MyVec(int) and passes the argument 10
	int size=v.GetVecLen(); //calls the member function
	cout<<"size of MyVec is: "<<size<<" elements"<<endl;
	cout<<"Setting first element to 100"<<endl;
	v[0]=100;
	cout<<"Fetching first element value: "<< v[0] << endl;
	MyVec v2=v; //calls the copy constructor
	cout<<"v2's first element: "<<v2[0]<<endl;
}
```

```
size of MyVec is: 10 elements
Setting first element to 100
v2's first element: 100
free(): double free detected in tcache 2
Aborted
```

If you don't define a copy constructor, in some cases, e.g., for class MyVec, the program aborts. *Why in this case?*

const and references

```cpp
#ifndef MYVEC_H
#define MYVEC_H
class MyVec{
	//private attributes
	double* data;
	int vecLen;
public:
	MyVec(int len); //constructor decl.
	MyVec(const MyVec& rhs); //copy constructor
	int GetVecLen() const; //member function
	double& operator[](int index) const;
	~MyVec(); //destructor decl.


};
```

```cpp
}

MyVec::MyVec(const MyVec& rhs) {
	vecLen=rhs.GetVecLen();
	data=new double[vecLen];
	for(int i=0;i<vecLen;i++) {
		data[i] = rhs[i];
	}
}

//defining GetVecLen member function
int MyVec::GetVecLen() const {
	return vecLen;
}

double& MyVec::operator[](int index) const {
	return data[index];
}
```

```
#ifndef MYVEC_H
#define MYVEC_H
class MyVec{
        //private attributes
        double* data;
        int vecLen;
public:
        MyVec(int len); //constructor decl.
        MyVec(const MyVec& rhs); //copy cons
tructor
        int GetVecLen() const; //member func
tion
        double& operator[](int index) const;
        ~MyVec(); //destructor decl.


};
```

```
}

MyVec::MyVec(const MyVec& rhs) {
        vecLen=rhs.GetVecLen();
        data=new double[vecLen];
        for(int i=0;i<vecLen;i++) {
                data[i] = rhs[i];
        }
}

//defining GetVecLen member function
int MyVec::GetVecLen() const {
        return vecLen;
}

double& MyVec::operator[](int index) const {
        return data[index];
```

Define the copy constructor. Now you need to make changes to other methods (const) as well.

```
Setting first element to 100
Fetching first element value: 100
v2's first element: 100
```

Const and References - Summary

- Allow for compiler optimizations
  - pass-by-reference: allows for passing large objects to a function call
- Tell us immediately (by looking at the interface) that a parameter is read-only

Detour: References and Const

- We saw reference variables earlier (week 2)
  - Closely related to pointers:
  - Directly *name* another object of the *same* type.
  - Recall:
    - A pointer is defined using the * (dereference operator) symbol.
    - A reference is defined using the & (address of operator) symbol. Furthermore, unlike in pointer definitions, a reference must be defined/initialized with the object that it names *(cannot be changed later)*.

References

```
int n=10;
int &re=n; //re must be initialized
int* ptr; //ptr need not be initialized here
ptr=&n //ptr now initialized (now pointing to n)
int x=20;
ptr=&x; //ptr now pointing to x
re=x; //is illegal. Cannot change what re names.
printf("%p %p\n",&re, &n); // re and n are naming the
same box in memory. Hence, they have the same address.
```

Quick tour: `const`

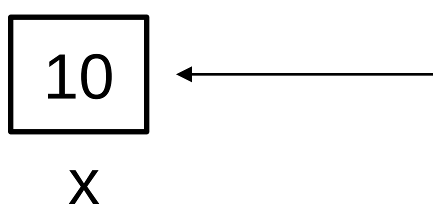
- A type qualifier
- The type is a constant (cannot be modified).
- `const` is the keyword
- Example:

```
const int x=10; //equivalent to: int const x=10;

//x is a constant integer. Hence, cannot be modified.
```

In what memory segment does x gets stored?

Const Properties

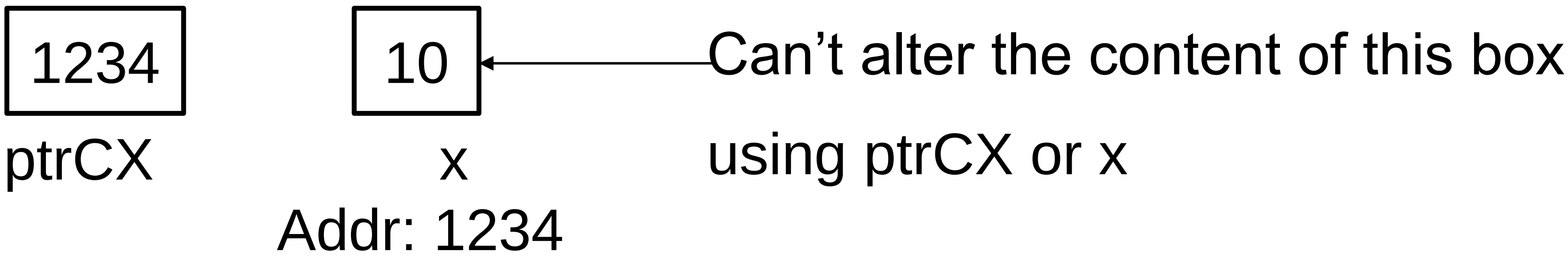
- Needs to be initialized at the time of definition
- Can’t modify after definition
- `const int x=10;`
  `x=20; //compiler would throw an error`
- `int const x=10;`
  `x=10; //can’t even assign the same value`
- `int const y; //uninitialized const variable y. Useless.`



Can’t alter the content of this box

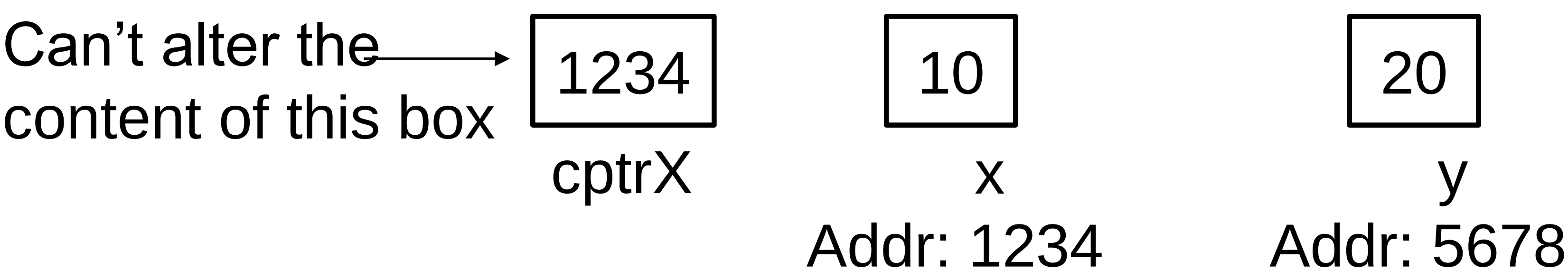
Const Example1 (error)

```
/*ptrCX is a pointer to a constant integer. So,
can’t modify what ptrCX points to.*/

const int* ptrCX; //or equivalently:
int const* ptrCX;


int const x=10;
ptrCX = &x;
*ptrCX = 20; //Error
```



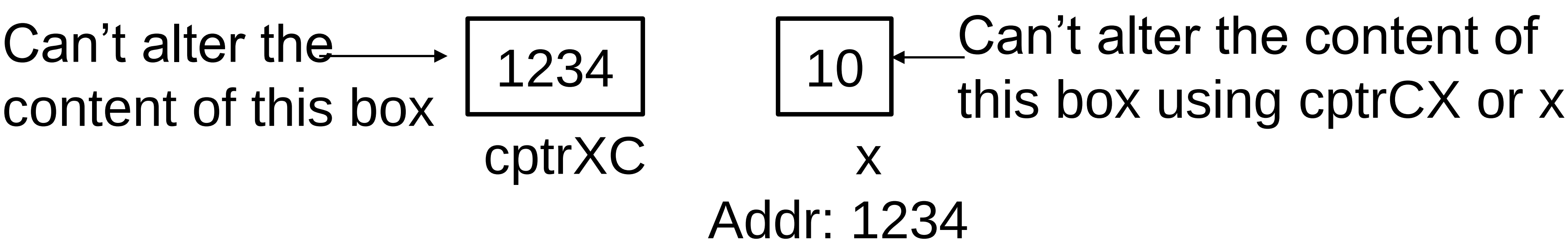
Const Example2 (error)

```
/*cptrX is a constant pointer to an integer. So, can’t
point to anything else after initialized.*/
int x=10, y=20;
int *const cptrX=&x;
cptrX = &y; //Error
```



Const Example3 (error)

```
/*cptrXC is a constant pointer to a constant integer. So,
can't point to anything else after initialized. Also,
can't modify what cptrXC points to.*/

const int x=10, y=20;
const int *const cptrXC=&x;
int const *const cptrXC2=&x; //equivalent to prev. defn.
cptrXC = &y; //Error
*cptrXC = 40; //Error
```



Const Example4 (warning)

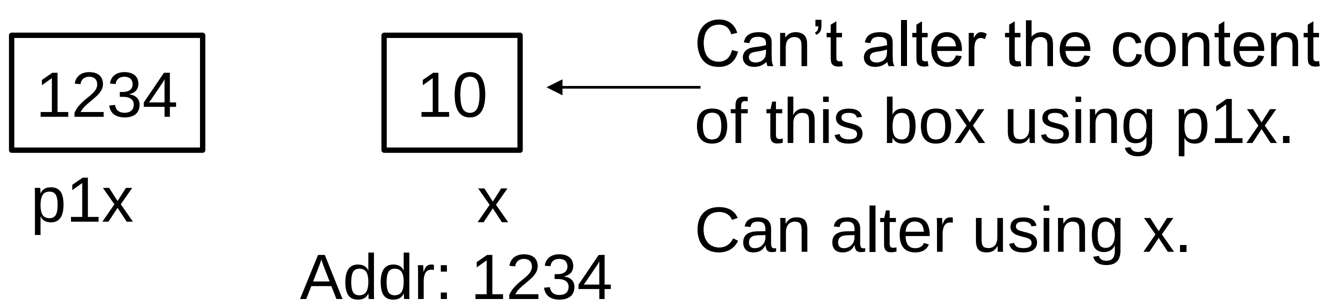
```
/*p2x is a pointer to an integer. So, we can use p2x to
alter the contents of the memory location that it points
to. However, the memory location contains read-only data -
cannot be altered. */

const int x=10;
const int *p1x=&x;
int *p2x=&x; //warning
*p2x = 20; //goes through. Might crash depending on memory
location accessed
```

1234	1234	10
p2x	p1x	x Addr: 1234

Can't alter the content of this box using p1x or x. Can alter using p2x.

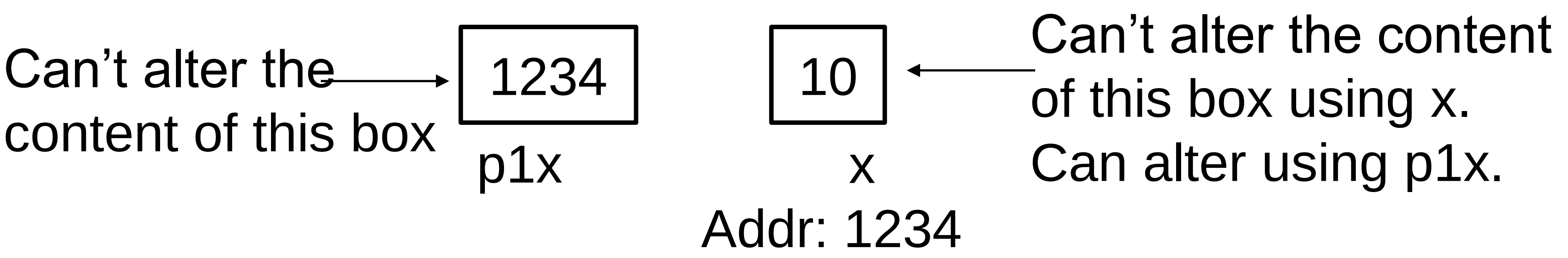
Const Example5 (no warning, no error)

```
/*p1x is a pointer to a constant integer. So, we can't use
p1x to alter the content of the memory location that it
points to. However, the memory location it points to can
be altered (through some other means e.g. using x)*/

int x=10;
const int *p1x=&x;
```



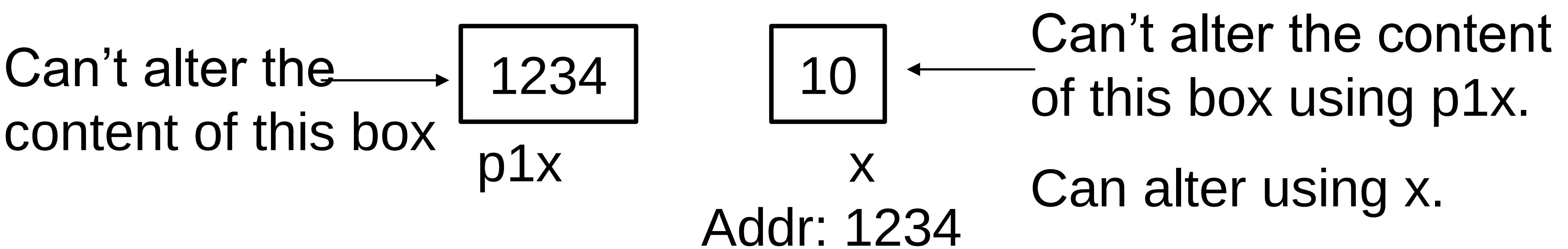
Const Example6 (warning)

```
/*p1x is a constant pointer to an integer. So, we can use
p1x to alter the contents of the memory location that it
points to (and we can’t let p1x point to something else
other than x). However, the memory location contains read-
only data - cannot be altered. */

const int x=10;
int *const p1x=&x;//warning
*p1x = 20; //goes through. Might crash depending on memory
location accessed
```



Const Example7 (no warning, no error)

```
/*p1x is a constant pointer to a constant integer. So, we
can't use p1x to alter the content of the memory location
that it points to. However, the memory location it points
to can be altered (through some other means e.g. using
x)*/

int x=10;
const int *const p1x=&x;
```



Templating Functions

- Provide a recipe for generating multiple versions of the function based on the data type of the data on which the function operates

Function Templates - Goal

```
double scprod(int len,
              double* vec1,
              double* vec2)
{
     double result;
     //compute result
     //return result
}
```

```
int scprod(int len,
              int* vec1,
              int* vec2)
{
     int result;
     //compute result
     //return result
}
```

How can you avoid multiple implementations of the same functionality but with different types?

Function Templates – Implementation and Invocation

```
template<typename T>
double scprod(int len,
         T* vec1,
         T* vec2)
{
    T result;
    //compute result
    //return result
}
```

Add this template definition in .h file! why .h and not .cpp?

Called template parameter. Can choose any name other than T. the keyword ‘typename’ can be replaced with ‘class’

```
int main() {
//define vec1-vec4
scprod<double>(10,vec1, vec2); //explicit instantiation
scprod<int>(100,vec3,vec4); //explicit instantiation
scprod(100, vec3,vec4); //implicit instantiation
```