Scientific Computing WS 2017/2018

Lecture 3

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Me

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  - Numerical solution of partial differential equations (PDEs)
  - Development, investigation, implementation of finite volume discretizations for nonlinear systems of PDEs
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  - Applications: electrochemistry, semiconductor physics, groundwater...
  - Software development:
    - WIAS code pdelib (http://pdelib.org)
    - Languages: C, C++, Python, Lua, Fortran
    - Visualization: OpenGL, VTK

Slide 2

Recap from last time

Scopes, Declaration, Initialization

- **All variables are typed and must be declared**
  - Declared variables "live" in scopes defined by braces `{ }`
  - Good practice: initialize variables along with declaration
  - "auto" is a great innovation in C++11 which is useful with complicated types which arise in template programming
    - type of *lvalue* (left hand side value) is detected from type of *rvalue* (value at the right hand side)

```
{
   int i=3;
   double x=15.0;
   auto y=33.0;
}
```

C++ : scalar data types

- Store character, integer and floating point values of various sizes
- Type sizes are the "usual ones" on 64bit systems

name	printf	bytes	bits	Minimum value	Maximum value
char	%c (%d)	1	8	-128	127
unsigned char	%c (%d)	1	8	0	255
short int	%d	2	16	-32768	32767
unsigned short int	%u	2	16	0	65535
int	%d	4	32	-2147483648	2147483647
unsigned int	%u	4	32	0	4294967295
long int	%ld	8	64	-9223372036854775808	9223372036854775807
unsigned long int	%lu	8	64	0	18446744073709551615
float	%e	4	32	1.175494e-38	3.402823e38
double	%e	8	64	2.225074e-308	1.797693e308
long double	%Le	16	128	3.362103e-4932	1.189731e4932
bool	%d	1	8	0	1

- The standard only guarantees that

  `sizeof(short ...) <= sizeof(...) <=sizeof(long ...)`
- E.g. on embedded systems sizes may be different
- Declaration and output (example)

```
#include <cstdio>
...
int i=3;
double x=15.0;
std::printf("i=%d, x=%e\n",i,x);
```

Arithmetic operators

- Assignment operator

```
a=b;
c=(a=b);
```

- Arithmetic operators `+`, `-`, `*`, `/`, modulo (%)
- Beware of precedence which (mostly) is like in math!
- If in doubt, use brackets, or look it up!

- Compund assignment: `+=`, `-=`, `*=`, `/=`, `%=`

```
x=x+a;
x+=a; // equivalent to =x+a
```

- Increment and decrement:
  `++`,`--`

```
y=x+1;
y=x++; // equivalent to y=x; x=x+1;
y=++x; // equivalent to x=x+1; y=x;
```

Functions

- Functions have to be *declared* and given names as other variables:

```
type name(type1 p1, type2 p2,...);
```

- `(...)` holds parameter list
  - each parameter has to be defined with its type
- `type` part of declaration describes type of return value
  - `void` for returning nothing

```
double multiply(double x, double y);
```

- Functions are *defined* by attaching a scope to the declaration
  - *Values of parameters are copied into the scope*

```
double multiply(double x, double y)
{
   return x*y;
}
```

- Functions are *called* by statements invoking the function with a particular set of parameters

```
{
    double s=3.0, t=9.0;
    double result=multiply(s,t);
    printf("s=%e, t=%e, s*t= %e\n",s,t,result); // s and t keep their values
}
```

Flow control: Statements and conditional statements

- Statements are individual expressions like declarations or instructions or sequences of statements enclosed in curly braces:

```
{ statement1; statement2; statement3; }
```

- Conditional execution: `if`

```
if (condition) statement;
if (condition) statement; else statement;
```

```
if (x>15)
{
    printf("error");
}
else
{
   x++;
}
```

Equivalent but less safe:

```
if (x>15)
    printf("error");
else
   x++;
```

Flow control: Simple loops

- While loop:
  `while (condition) statement;`

```
i=0;
while (i<9)
{
  printf("i=%d\n",i);
  i++;
}
```

- Do-While loop: `do statement while (condition);`

Flow control: for loops

- This is the most important kind of loops for numerical methods.
  `for (initialization; condition; increase) statement;`
  1. initialization is executed. Generally, here, one declares a counter variable and sets it to some initial value. This is executed a single time, at the beginning of the loop.
  2. condition is checked. If it is true, the loop continues; otherwise, the loop ends, and statement is skipped, going directly to step 5.
  3. statement is executed. As usual, it can be either a single statement or a block enclosed in curly braces `{ }`
  4. increase is executed, and the loop gets back to step 2.
  5. The loop ends: execution continues at the next statement after it.
- All elements (initialization, condition, increase, statement) can be empty

```
for (int i=0;i<9;i++)   printf("i=%d\n",i); // same  as on previous slide
for(;;);  // completely valid, runs forever
```

Emulating modules

- File `mymodule.h` containing interface declarations

```
#ifndef MYMODULE_H // Handle multiple #include statements
#define MYMODULE_H
namespace mymodule
{
  void my_function(int i, double x);
}
#endif
```

- File `mymodule.cpp` containing function definitions

```
#include "mymodule.h"
namespace mymodule
{
  void my_function(int i, double x)
  {
    ...body of function definition...
  }
}
#endif
```

- File using `mymodule`:

```
#include "mymodule.h"
...
mymodule::my_function(3,15.0);
```

main

Now we are able to write a complete program in C++

- `main()`
  is the function called by the system when running the program.
  Everything else needs to be called from there.

Assume the follwing content of the file `run42.cxx`:

```
#include <cstdio>

int main()
{
   int i=4,j=2;
   int answer=10*i+j;
   printf("Hello world, the answer is %d!\n",answer);
   return 0;
}
```

Then the sequence of command line commands

```
$ g++ -o run42 run42.cxx
$ ./run42
```

gives the right answer to (almost) anything.

C/C++: the hard parts ...

Pointers. . .

. . . from xkcd

Addresses and pointers

- Objects are stored in memory, in order to find them they have an *address*
- We can determine the address of an object by the `&` operator
  - The result of this operation can be assigned to a variable called *pointer*
  - "pointer to type x" is another type denoted by `*x`
- Given an address (pointer) object we can refer to the content using the `*` operator

```
int i=15;  // i is an object
int *j= &i; // j is a pointer
int k=*j; // now, k=15
```

- The `nullptr` object can be assigned to a pointer in order to indicate that it points to "nothing"

```
int *p=nullptr;
```

Passing addresses to functions

- Instead of values, addresses can be passed to functions

```
void do_multiplication(double x, double y, double *result)
{
    *result=x*y;
}
...
double x=5,y=9;
double result=0;
do_multiplication(x,y,&result) // result now contains 45
```

Arrays

- Focusing on numerical methods for PDEs results in work with finite dimensional vectors which are represented as *arrays* - sequences of consecutively stored objects
- Stemming from C, in C++ array objects represent just the fixed amount of consecutive memory. No size info or whatsoever
- No bounds check
- First array index is always 0

```
double x[9]; // uninitialized array of 9 elements
double y[3]={1,2,3}; // initialized array of 3 elements
double z[]={1,2,3};  // Same
double z[]{1,2,3};   //Same
```

- Accessing arrays
  - [] is the array access operator in C++
  - Each element of an array has an index

```
double a=x[3];  // undefined value because x was not initialized
double b=y[12]; // undefined value because out of bounds
y[12]=19;       // may crash program ("segmentation fault"),
double c=z[0];  // Acces to first element in array, now c=1;
```

Arrays, pointers and pointer arithmetic

- Arrays are strongly linked to pointers
- Array object can be treated as pointer

```
double x[]={1,2,3,4};
double b=*x; // now x=1;
double *y=x+2; // y is a pointer to third value in arrax
double c=*y;   // now c=3
ptrdiff_t d=y-x; // We can also do differences between pointers
```

- Pointer arithmetic is valid only in memory regions belonging to the same array

Arrays and functions

- Arrays are passed by passing the pointer referring to its first element
- As they contain no length information, we need to pass that as well

```
void func_on_array1(double[] x, int len);
void func_on_array2(double* x, int len); // same
void func_on_array3(const double[] x, int len);//same, but prevent changing x
...
double x[]={3,4,5};
int len=sizeof(x)/sizeof(x[0]);
func_on_array1(x,len);
```

- Be careful with array return

```
double * some_func(void)
{
  double a[]={-1,-2,-3};
  return a; // illegal as with the end of scope, the life time of a is over
            // smart compilers at least warn
}
```

Arrays with length detected at runtime ?

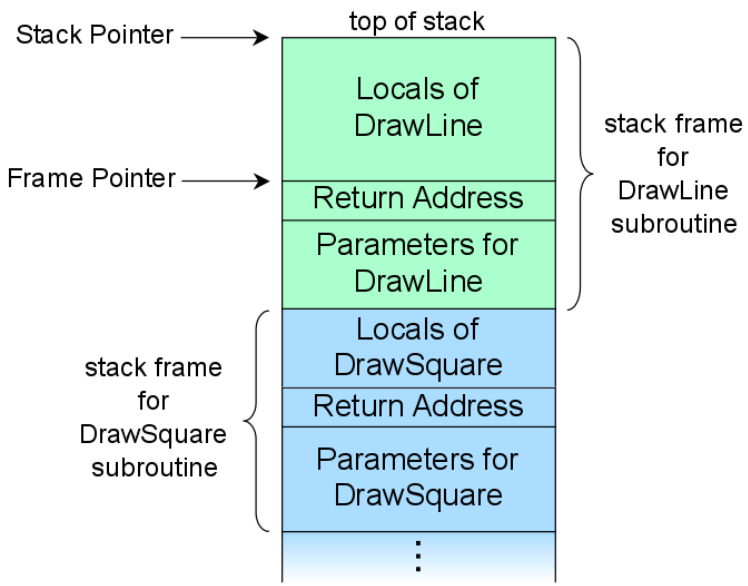
- This one is illegal (not part of C++ standard), though often compilers accept it

```
void another_func(int n)
{
    int b[n];
}
```

- Even in main() this will be illegal.
- How to work on problems where size information is obtained only during runtime, e.g. user input ?

Memory: stack

- pre-allocated memory where `main()` and all functions called from there put their data.
  - Any time a function is called, the current position in the instruction stream is stored in the stack as the return address, and the called function is allowed to work with the memory space after that




```
void DrawLine(double x0, double y0, double x1, double y1)
{
  paint ...
}

void DrawSquare(double x0,double y0, double a)
{
  DrawLine(x0,y0,x0+a,y0);
  DrawLine(x0+a,y0,x0+a,y0+a);
  DrawLine(x0+a,y0+a,x0,y0+a);
  DrawLine(x0,y0+a,x0,y0);
}
```

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Stack space is scarce

- Variables declared in `{}` blocks get placed on the stack
- All previous examples had their data on the stack, even large arrays
- Stack space should be considered scarce
- Stack size for a program is fixed, set by the system
- On UNIX, use `ulimit -s` to check/set stack size default

Memory: heap

- Chunks from free system memory can be reserved – "allocated" – on demand in order to provide memory space for objects
- The operator `new` reserves the memory and returns an address which can be assigned to a pointer variable
- The operator `delete` (`delete[]` for arrays) releases this memory and makes it available for other processes
- Compared to declarations on the stack, these operations are expensive
- Use cases:
  - Problem sizes unknown at compile time
  - Large amounts of data
  - . . . so, yes, we will need this. . .

```
double *x= new double(5); // allocate space for a double, initialize it with 5
double *y=new double[5];  // allocate space of five doubles, uninitialized
x[3]=1;                   // Segmentation fault
y[3]=1;                   // Perfect...
delete x;                 // Choose the right delete!
delete[] y;               // Choose the right delete!
```

Multidimensional Arrays

- Multidimensional arrays are useful for storing matrices, tensors, arrays of coordinate vectors etc.
- It is easy to declare a multidimensional array on the stack when the size the array is known at compile time

```
double x[5][6];

for (int i=0;i<5;i++)
   for (int j=0;j<6;j++)
      x[i][j]=0;
```

- Determining array dimensions from function parameters may work with some compilers, but are not backed by the standard
- One option to have 2D arrays with arbitrary, run-time defined dimensions is to allocate a an array of pointers to double, and to use `new` to allocate each (!) row
  ... this leads to nowhere ...

Intermediate Summary

- This was mostly all (besides structs) of the C subset of C++
  - Most "old" C libraries and code written in previous versions of C++ are mostly compatible to modern C++
- Many "classical" programs use the `(int size, double * data)` style of passing data, especially in numerics
  - UMFPACK, Pardiso direct solvers
  - PetsC library for distributed linear algebra
  - triangle, tetgen mesh generators
  - ...
- On this level it is possible to call Fortran programs from C++
  - BLAS vector operations
  - LAPACK dense matrix linear algebra
  - ARPACK eigenvalue computations
  - ...
- Understanding these interfaces is the main reason to know about plain C pointers and arrays
- Modern C++ has easier to handle and safer ways to do these things, so they should be avoided as much as possible in new programs

C++: classes

Classes and members

- Classes are data types which collect different kinds of data, and methods to work on them.

```
class class_name
{
  private:
    private_member1;
    private_member2;
    ...
  public:
    public_member1;
    public_member2;
    ...
};
```

- If not declared otherwise, all members are private
- `struct` is the same as `class` but by default all members are public
- Accessing members of a class object:

```
class_name x;
x.public_member1=...
```

- Accessing members of a pointer to class object:

```
class_name *x;
(*x).public_member1=...
x->public_member1=...
```

Example class

- Define a class `vector` which holds data and length information and thus is more comfortable than plain arrays

```
class vector
{
  private:
      double *data;
  public:
       int size;
      double get_value( int i) {return data[i];};
      void set_value( int i, double value); {data[i]=value;};
};

...

{
  vector v;
  v.data=new double(5);  // would work if data would be public
  v.size=5;
  v.set_value(3,5);

  b=v.get_value(3); // now, b=5
  v.size=6;  // size changed, but not the length of the data array...
             // and who is responsible for delete[] at the end of scope ?
}
```

Constructors and Destructors

```
class vector
{ private:
      double *data=nullptr;
      int size=0;
  public:
      int get_size(){ return size;};
      double get_value( int i ) { return data[i]; };
      void set_value( int i, double value ) { data[i]=value; };
      Vector( int new_size ) { data = new double[new_size];
                               size=new_size; };
      ~Vector() { delete [] data; };
};
...
{ vector v(5);
  for (int i=0;i<5;i++) v.set_value(i,0.0);
  v.set_value(3,5);
  b=v.get_value(3); // now, b=5
  v.size=6;  // Size is now private and can not be set;
  vector w(5);
  for (int i=0;i<5;i++) w.set_value(i,v.get_value(i));
  // Destructors automatically called at end of scope.
}
```

- Constructors are declared as `classname(...)`
- Destructors are declared as `~classname()`

Interlude: References

- C style access to objects is direct or via pointers
- C++ adds another option - references
  - References essentially are alias names for already existing variables
  - Must always be initialized
  - Can be used in function parameters and in return values
  - No pointer arithmetics with them
- Declaration of reference

```
double a=10.0;
double &b=a;

b=15; // a=15 now as well
```

- Reference as function parameter: no copying of data!

```
void do_multiplication(double x, double y, double &result)
{
    result=x*y;
}
...
double x=5,y=9;
double result=0;
do_multiplication(x,y,result) // result now contains 45
```

Vector class again

- We can define () and [] operators!

```
class vector
{
  private:
      double *data=nullptr;
      int size=0;
  public:
      int get_size( return size);
      double & operator()(int i) { return data[i]; };
      double & operator[](int i) { return data[i]; };
      vector( int new_size) { data = new double[new_size];
                              size=new_size;}
      ~vector() { delete [] data;}
};
...
{
  vector v(5);
  for (int i=0;i<5;i++) v[i]=0.0;
  v[3]=5;
  b=v[3]; // now, b=5
  vector w(5);
  for (int i=0;i<5;i++) w(i)=v(i);
}
```

Matrix class

- We can define `(i,j)` but not `[i,j]`

```
class matrix
{ private:
      double *data=nullptr;
      int size=0;  int nrows=0;
      int ncols=0;
  public:
      int get_nrows( return nrows);
      int get_ncols( return ncols);
      double & operator()(int i,int j) { return data[i*nrow+j]);
      matrix( int new_rows,new_cols)
      { nrows=new_rows; ncols=new_cols;
        size=nrows*ncols;
        data = new double[size];
      }
      ~matrix() { delete [] data;}
};
...
{
  matrix m(3,3);
  for (int i=0;i<3;i++)
    for (int j=0;j<3;j++)
        m(i,j)=0.0;
}
```

Inheritance

- Classes in C++ can be extended, creating new classes which retain characteristics of the base class.
- The *derived class* inherits the members of the *base class*, on top of which it can add its own members.

```
class vector2d
{  private:
    double *data;
    int nrow, ncol;
    int size;
  public:
    double & operator(int i, int j);
    vector2d(int nrow, ncol);
    ~vector2d();
}
class matrix: public vector2d
{ public:
    apply(const vector1d & u, vector1d &v);
    solve(vector1d &u, const vector1d &rhs);
}
```

- All operations which can be performed with instances of `vector2d` can be performed with instances of `matrix` as well
- In addition, `matrix` has methods for linear system solution and matrix-vector multiplication

C++: Generic programming

Generic programming: templates

- Templates allow to write code where a data type is a parameter
- We want do be able to have vectors of any basic data type.
- We do not want to write new code for each type

```
template <typename T>
class vector
{
  private:
      T *data=nullptr;
      int size=0;
  public:
      int get_size( return size);
      T & operator[](int i) { return data[i]; };
      vector( int new_size) { data = new T[new_size];
                              size = new_size;};
      ~vector() { delete [] data;};
};
...
{
  vector<double> v(5);
  vector<int> iv(3);
}
```

C++ template libray

- The standard template library (STL) became part of the C++11 standard
- Whenever you can, use the classes available from there
- For one-dimensional data, std::vector is appropriate
- For two-dimensional data, things become more complicated
  - There is no reasonable matrix class
    - std::vector< std::vector> is possible but has to allocate each matrix row and is inefficient
  - it is hard to create a std::vector from already existing data

Smart pointers

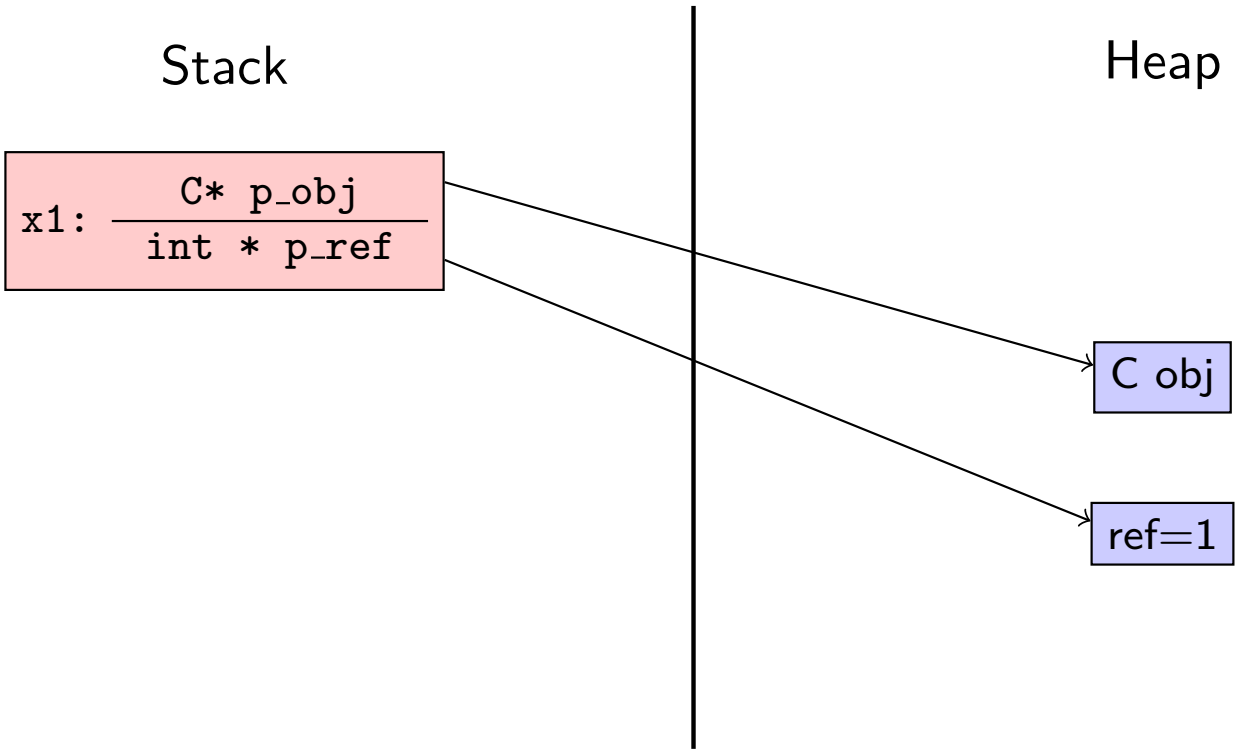
. . . with a little help from Timo Streckenbach from WIAS who introduced smart pointers into our simulation code.

- Automatic book-keeping of pointers to objects in memory.
- Instead of the meory addres of an object aka. pointer, a structure is passed around *by value* which holds the memory address and a pointer to a *reference count* object.
- It delegates the member access operator `->` and the address resolution operator `*` to the pointer it contains.
- Each assignment of a smart pointer increases this reference count.
- Each destructor invocation from a copy of the smart pointer structure decreases the reference count.
- If the reference count reaches zero, the memory is freed.
- `std::shared_ptr` is part of the C++11 standard

Smart pointer schematic

(this is one possibe way to implement it)

```
class C;
```

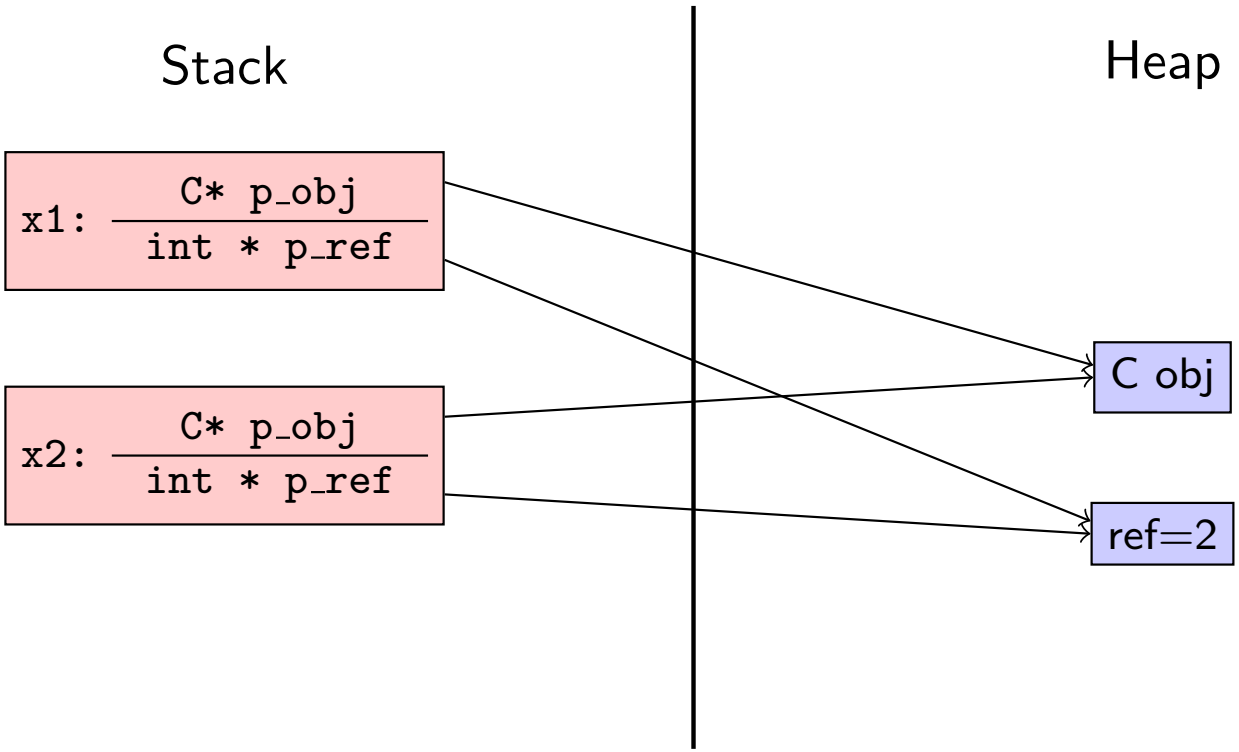



```
std::shared_ptr<C> x1= std::make_shared<C>();
```

Smart pointer schematic

(this is one possibe way to implement it)

```
class C;
```

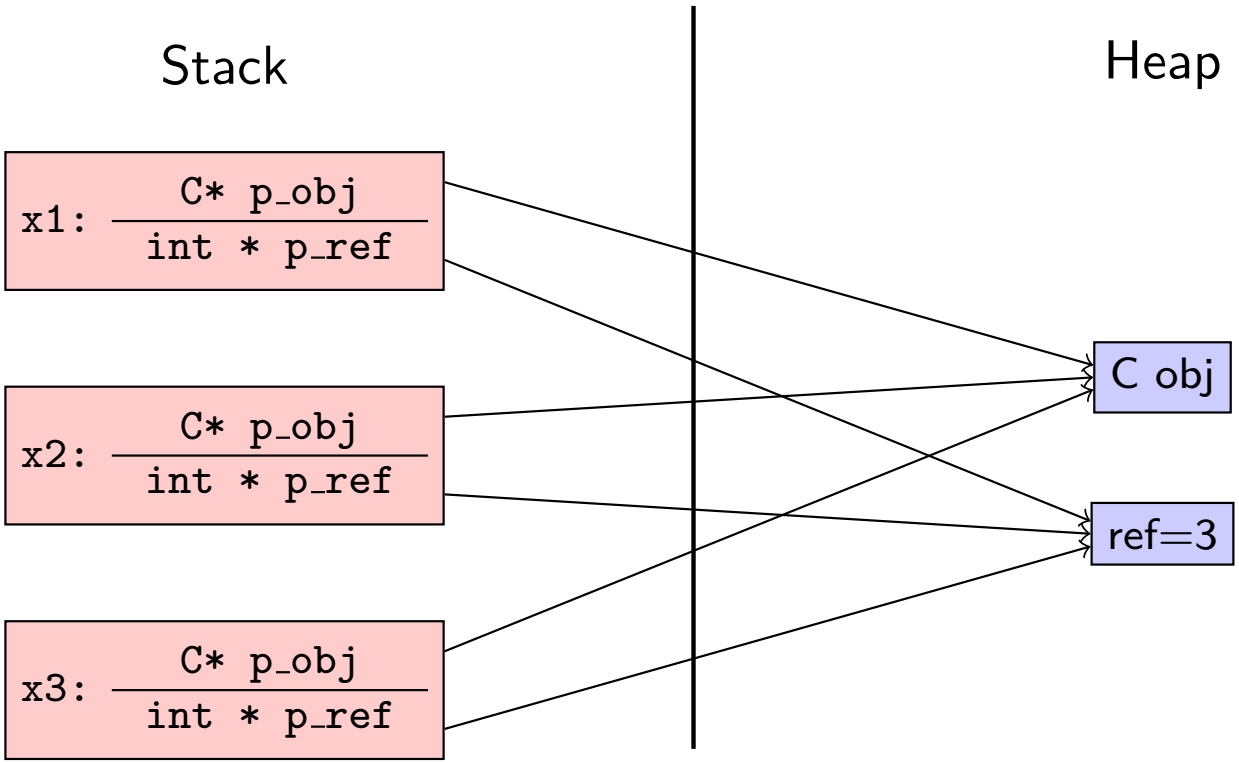



```
std::shared_ptr<C> x1= std::make_shared<C>();
std::shared_ptr<C> x2= x1;
```

Smart pointer schematic

(this is one possibe way to implement it)

```
class C;
```




```
std::shared_ptr<C> x1= std::make_shared<C>();
std::shared_ptr<C> x2= x1;
std::shared_ptr<C> x3= x1;
```

Smart pointers vs. *-pointers

- When writing code using smart pointers, write

```
#include <memory>
class R;
std::shared_ptr<R> ReturnObjectOfClassR(void);
void PassObjectOfClassR(std::shared_ptr<R> pR);
...
{  auto pR=std::make_shared<R>();
   PassObjectOfClassR(pR)
   // Smart pointer object is deleted at end of scope and frees memory
}
```

instead of

```
class R;
R* ReturnObjectOfClassR(void);
void PassObjectOfClassR(R* o);
...
{  R* pR=new R;
   PassObjectOfClassR(pR);
   delete pR; // never forget this here!!!
}
```

Smart pointer advantages vs. *-pointers

- “Forget” about memory deallocation
- Automatic book-keeping in situations when members of several different objects point to the same allocated memory
- Proper reference counting when working together with other libraries