Scientific Computing for Physicists (PHY1610H)

Ramses van Zon   Marcelo Ponce

Winter 2021

Course Topics

This course aims at making you a more productive and efficient computational scientist.

It will cover best practices in scientific computing and programming skills, optimization and a bit of parallel programming.

There are three main themes in this course:

1. Scientific Software Development
2. Numerical Tools for Physical Scientists
3. High Performance Scientific Computing

Instructors

Your instructors are High-Performance Computing Analysts from SciNet:

Ramses van Zon and Marcelo Ponce

The TA for this course is Kamil Krawczyk. He'll be helping with the grading of the assignments.

What is SciNet?

SciNet is UofT's supercomputer centre, which hosts and supports Canada's fastest supercomputer for use by academic researchers.

We also do a lot of other teaching (Bash, Python, R, Fortran, C++, GPU programming, databases, machine learning, parallel programming, visualization, . . .)

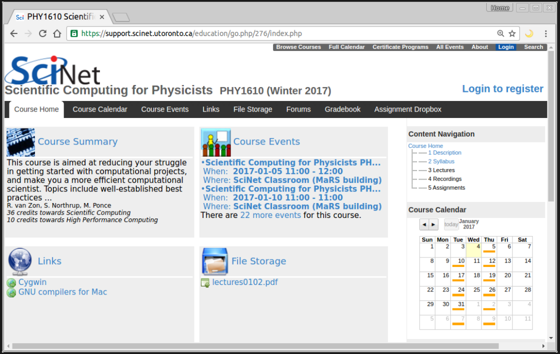
Course website

https://courses.scinet.utoronto.ca/545

- Lectures (+Recordings)
- Assignments
- Forum
- . . .

Near-weekly assignments given on Thursdays, posted on the site.

To be able to submit homework and get course emails, you to be able to login to the site (use your SciNet account if you have one).



Scientific Computing for Physicists PHY1610 (Winter 2017)

Course Summary

This course is aimed at reducing your struggle in getting started with computational projects, and make you a more efficient computational scientist. Topics include well-established best practices ...
R. van Zon, S. Northrup, M. Ponce
36 credits towards Scientific Computing
10 credits towards High Performance Computing

Course Events

- Scientific Computing for Physicists PH...
  When: 2017-01-05 11:00 - 12:00
  Where: SciNet Classroom (MaRS building)
- Scientific Computing for Physicists PH...
  When: 2017-01-10 11:00 - 11:00
  Where: SciNet Classroom (MaRS building)

There are 22 more events for this course.

Links

- Cygwin
- GNU compilers for Mac

File Storage

- lectures0102.pdf

Content Navigation

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- 3 Lectures
- 4 Recordings
- 5 Assignments

Course Calendar

today January 2017

Sun	Mon	Tue	Wed	Thu	Fri	Sat
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30	31	1	2	3	4
5	6	7	8	9	10	11

If you are going to take the course for (physics) credit, make sure you are sign up for the course in ACORN.

Accounts, assignments, . . .

- You'll have access to SciNet's teaching cluster using a temporary student account, or your SciNet-enabled Compute Canada account.

  ```
  ssh USERNAME@teach.scinet.utoronto.ca
  ```

- If you do not have a Compute Canada account:
  - Your login name on the education site is something that starts with `tmp_...`
  - Your USERNAME for the Teach cluster is different from that, it will be of the form `phy1610student...`

    You can receive this USERNAME for the Teach cluster during the first office hours tomorrow at 2 pm.

- Initially, you can choose to do the homework assignments on your own computer, provided it has a unix-like environment with the g++ compiler, make, and git.

  Assignments are marked on how they can be compiled and run on the Teach cluster.

- Get a CC/SciNet account, if you want to keep working on SciNet after the course.
  See www.scinet.utoronto.ca/getting-a-scinet-account

Grading scheme

- **Near-weekly programming assignments** posted on the website.
- These assignments are **due the next week.**
- Each student should submit their own work.
- The average of the assignments will make up your grade.
- All sets of homework need to be handed in for a passing grade.

Penalty policy

- Homework may be submitted up to 1 week after the due date, at a penalty of 5 points per day, out of the 100 points per homework.

  Deviations of this rule will only be considered, on a case-by-case basis, in exceptional circumstances (i.e., not “I was busy’ ’).
- If, due to exceptional circumstances, an assignment was missed, a make-up assignment on a topic of the instructors’ choice can be given at the end of the course.

Zoom, lectures, office hours, email, . . .

Zoom lectures

Lectures takes place via Zoom.

You will need to click on the Zoom link from the course website, then enter the meeting password.

You'll be put in the waiting room until the host lets you in.

Lectures are recorded and posted on the site afterwards (often towards the end of the day).

Office hours

For the duration of the course, Zoom office hours will be on

- Wednesdays from 2:00 pm to 3:00 pm, and
- Fridays from 12 noon to 1 pm.

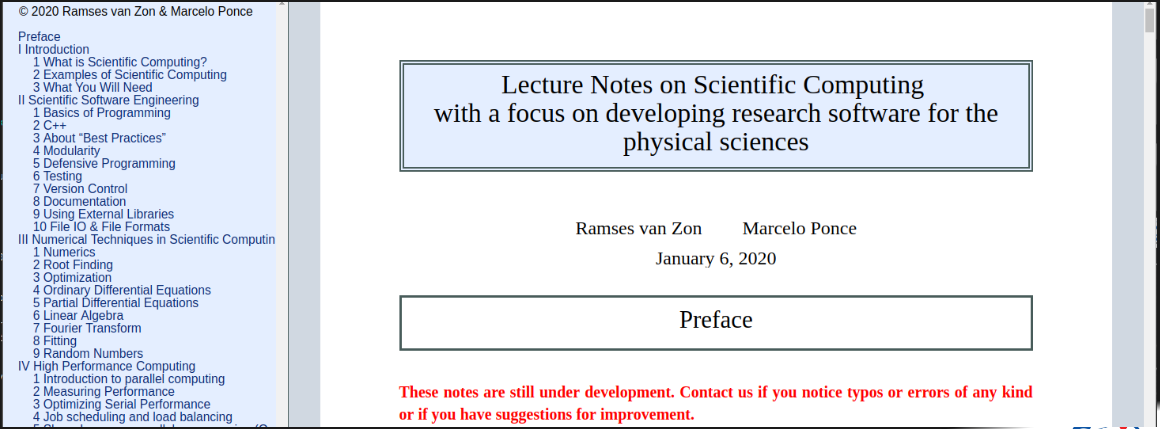
Questions/comments/concerns/etc. about the course?

For questions regarding the course, use the forum on the course website or use the email courses@scinet.utoronto.ca.

Course lecture notes

For further reading, you might like the lecture notes of last year's course:

https://support.scinet.utoronto.ca/materials/sclecturenotes.html



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Lecture Notes on Scientific Computing
with a focus on developing research software for the physical sciences

Ramses van Zon   Marcelo Ponce

January 6, 2020

Preface

These notes are still under development. Contact us if you notice typos or errors of any kind or if you have suggestions for improvement.

Course Outline

1) Scientific Software Development

- C++ intro
- Modular programming
- Building software with make
- Arrays and object
- Version control with git
- Unit testing
- I/O

2) Numerical Tools for Physicists

- Using libraries
- Ordinary differential equations
- Partial differental equations and lin. algebra
- Fast Fourier transforms
- Random numbers and Monte Carlo
- Molecular Dynamics

3) High Performance Computing

- Profiling tools
- Intro to parallel computing
- Batch processing
- Shared memory programming
- Distributed parallel programming

Section 1

Scientific Software Development

Programming

- We program to have the computer perform a number of similar computations or data manipulations.
- A program specifies the actions that the computer should take, as well as (restrictions on) the order in which they should be taken.
- Each action will have a net effect on the program's "state".
- There is limited set of predefined actions, in terms of which we must express all other actions: that is programming.

Programming

- A common pattern of actions to achieve a specific net effect (*computation*) is an **algorithm**.
- A **function**, **procedure**, or **subroutine** is a specification of actions that can be used as a newly defined action.
- A **program** is a function that can be executed.
- Programs may accept some external data as **input** and produce data as **output**.

Program State

- Program state is stored in memory.
- At least part of the state is made up of the program's **variables**.
- Variables are values that are assigned to a **variable name**.
- This variable name is associated with a portion of **memory** that holds the variable's value.

Control structures

- Some actions could be done conditionally on the state of the program and external input.
- **Conditional control structures** perform a different actions depending on whether a certain assertion of the state of the system is true.
- Repetition of a set of actions: **loops**.

Some ideas were taken from:

“A Short Introduction to the Art of Programming’ ’ (E. W. Dijkstra, 1971)

Why C++?

Advantages

- High performance
- Low-level programming
- Ubiquitous and standardized
- Useful libraries
- Modular design

Disadvantages

- Labour intensive, error prone
- High-level programming up to you
- Non-interactive
- Things like graphics can be hard
- Beware of performance pitfalls

For e.g. Python, many advantages and disadvantages are reversed.

Note: You can program poorly and inefficiently in any language.

Section 2

C++ Introduction

C++ Introduction

- C and C++ are **compiled** languages: their basic 'actions' are to be compiled into a set of basic 'native' instructions that the processor can execute.
- C was designed for (unix) system programming.
- C has a very small base.
- Most functionality is in (standard) libraries.
- C++ is almost a superset of C.
- For definiteness sake, let's say we use the **C++14** standard.

C++ Introduction: Basic C++ program

```cpp
// hw.cpp - prints "Hello world."
#include <iostream>
#include <string>
int main()  // this is the main function which is called when the app is run
{  // braces delimit a code block
   std::string message = "Hello world."; // a variable
   std::cout << message                  // prints to console out
             << std::endl;               // end of line
   return 0;
   // return value to the shell
}
```

Command-line shell compilation:

```
$ ssh rzon@teach.scinet.utoronto.ca
$ module load gcc
$ nano hw.cpp
$ g++ -std=c++14 -o hw hw.cpp
$ ./hw
Hello world.
$ echo $?
0
```

Need to brush up on your Linux/supercomputer skills?

Intro to Niagara

Wednesday January 13, 2021, 10:00 am - 11:30 am

This is a class of approximately 60-90 minutes to introduce SciNet and the supercomputer Niagara, and teach you how to use Niagara.

Niagara is SciNet's largest supercomputer, but its setup is very similar to that of the Teach cluster, so this may still be very useful for you.

https://courses.scinet.utoronto.ca/556

Intro to the Linux Shell

Wednesday January 20, 2021, 10:00 am - 1:00 pm

Learn the basics of how to use the unix shell in two hours. Very useful for new users of SciNet that have little or no experience with unix or linux.

https://courses.scinet.utoronto.ca/568

Super-short intro to the shell

There is a prompt, e.g. `"rzon@teach:~>"` after which you can type in commmands.

Any command you type at the prompt is read by a 'shell interpreter'. The teach cluster uses the 'bash' shell.

You are always "in" a current directory/folder in the file system tree. Your default directory, called your "home" directory, is where you start.

You can change to a directory with `cd DIRNAME`

`~` is a shorthand for that home directory.

`.` is a shorthand for the current directory

`..` is a shorthand for the parent directory.

Commands are either:

- built-in, or
- provided by executables in standard locations (encoded in the so called PATH variable), or
- executables of which the path is specified

Examples:
List the files in the curent directory with `ls`.
If the current directory contains an executable 'first', execute it with the command `./first`.
Connect to a different computer with `ssh`.

After a command, you can optionally have more words, called the "arguments" of the command. What those arguments do, depends on the command.

Tips

Getting a terminal shell

For windows, get MobaXterm or use the Linux Subsystem for Windows.
It comes with ssh, so you can connect to teach using the ssh command.
For Mac and Linux, find your terminal application. It should also already come with the ssh command.

Editing code

Text-based editing of (code) files in the shell can be done using different applications.

- 'vi' is ubiquitous but not loved by all.
- 'emacs' is often available, and has a GUI form as well.
- 'nano' is a beginner friendly editor because all the possible actions are visible on the screen.
- Advanced: 'sshfs' can be used to make the files on the Teach cluster available on your local machine, then you can use your favorite local editor.

C++ Intro: Basic syntax aspects

```
// hw.cpp - prints "Hello world."
#include <iostream>
#include <string>
int main()  // this is the main function which ...
{  // braces delimit a code block
   std::string message = "Hello world."; // a v...
   std::cout << message                  // pri...
             << std::endl;               // end...
   return 0;
   // return value to the shell
}
```

- Other C++ files can be included with the `#include` directive.
- Each executable statement or declaration ends with a semicolon.
- Curly braces delimit a code block.
- When declaring a variable or function to be of a certain type, the type is specified before the variable or function name.
- The value to be given back by a function is specified by the `return` statement, which exits the function.
- Comments can be added using the double slashes //.

C++ Summary

These are the elements of C++ we'll be using in this class:

- Variables
- Functions
- Function arguments by value and by reference
- Loops
- Pointers
- Dynamically allocated arrays
- Conditionals
- Objects[1]
- Templates[1]
- Libraries
- Namespaces
- IO and file streams
- Compiling and linking

[1] only using these, you will not be required to write these (though you may).

C++ Overview: Variables

- Variables are named pieces of data stored in the computers memory.
- In C/C++ variables have a particular type, and are defined as having a particular type.
- The data stored in a variable can be manipulated (e.g. through assignment, addition, . . .).
- E.g. the same name cannot be used to refer to both an integer and a string, and a string cannot be stored in a variable that has been declared as an integer.

C++ Overview: Variable definition

```
type name [=value];
```

Here, type may be a:

- floating point type:

  `float, double, long double, std::complex<float>, ...`

- integer type:

  `[unsigned] short, int, long, long long`

- character or string of characters:

  `char, char*, std::string`

- boolean: `bool`

- array, pointer, class, structure, enumerated type, union

Examples:

```
int a;
int b;
a = 4;
b = a + 2;
```

```
float f = 4.0f;
double d = 4.0;
d += f;
```

```
char* str = "Hello There!";
```

```
bool itis2018 = false;
```

The type can be proceeded by `const` to make it immutable.

Non-initialized variables are not 0, but have random values!

C++ Overview: Functions

Function = a piece of code that can be reused.

A function has:

1. a name
2. a set of arguments of specific type
3. and returns a value of some specfic type

These three properties are called the function's signature.

- To write a piece of code that uses ("calls") the functions, we only need to know its signature or interface;

  To make the signature known, one has to place a function declaration before the piece of code that is to use the function.

- The actual code (function definition) can be in a different file or in a library.

C++ Overview: Functions, an example

```cpp
// funcexample.cpp

// external function prototypes:
#include <cmath>

// function prototype:
double arithmetic_mean(double a, double b);

// main function to call when program starts:
int main()
{
    double x = 16.3;
    double y = 102.4;
    return arithmetic_mean(x,y);
}

// function definition:
double arithmetic_mean(double a, double b)
{
    return sqrt(a*b);
}
```

```
$ ssh USERNAME@teach.scinet.utoronto.ca

$ module load gcc

$ g++ -std=c++14 -o funcexample funcexample.cpp

$ ./funcexample
$ echo $?
40
```

C++ Overview: Functions

- Function declaration (prototype/signature/interface)

```
returntype name(argument-spec);
```

  `argument-spec` = comma separated list of variable definitions

- Function definition (code/implementation)

```
returntype name(argument-spec) {
    statements
    return expression-of-type-returntype ;
}
```

  Functions which do not return anything have to be declared with a `returntype` of `void`.
  Functions which have a non-void return type must have a `return` statement (except main).

- Function call

```
var = name(argument-list);
f(name(argument-list));
name(argument-list);
```

  `argument-list` = comma separated list of values

C++ Overview: Pass by value or by reference

Passing function arguments by value

```
// passval.cpp
void inc(int i)
{
    i = i+1;
}

int main()
{
    int j = 10;
    inc(j);
    return j;
}
```

```
$ g++ -std=c++14 -o passval passval.cpp
$ ./passval
$ echo $?
10
$
```

- `j` is set to 10.
- `j` is passed to `inc`,
- where it is copied into a variable called `i`.
- `i` is increased by one,
- but the original `j` is not changed.

C++ Overview: Pass by value or by reference

Passing function arguments by reference

```
// passref.cpp
void inc(int &i)
{
    i = i+1;
}

int main()
{
    int j = 10;
    inc(j);
    return j;
}
```

```
$ g++ -std=c++14 -o passref passref.cpp
$ ./passref
$ echo $?
11
$
```

- `j` is set to 10.
- `j` is passed to `inc`,
- where it referred to as `i` (but it's still `j`).
- `i` is increased by one,
- because `i` is just an alias for `j`, `j` reflects this change.

C++ Operators

Arithmetic	
a+b	Add a and b
a-b	Subtract a and b
a*b	Multiply a and b
a/b	Divide a and b
a%b	Remainder of a over b

Assignment

a=b	Assign a expression b to the variable b
a+=b	Add b to a (result stored in a)
a-=b	Substract b from a (result stored in a)
a*=b	Multiply a with b (result stored in a)
a/=b	Divide a by b (result stored in a)
a++	Increase value of a by one

Logic

a==b	a equals b
a!=b	a does not equal b
!a	a is not true (also: `not a`)
a&&b	both a and b are true (also: `a and b`)
a||b	either a or b is true (also: `a or b`)

Logic/Numeric

a<b	is a less than b
a>b	is a greater than b
a<=b	is a less then or equal to b
a>=b	is a greater than or equal to b

What is 1/4?

`1/4 = 0`

Why?

- In 1/4 both operands, i.e., 1 and 4, are integers.
- Hence, the result of $1/4$ is the integer part of the division, which is 0.
- Generally, literal expressions, such as `"Hi"`, `0`, `1.2e-4`, `2.4f`, `0xff`, `true` have types, just as variables do.
- The result-type of an operator depends on the types of the operands.

Fix: Convert between types. In C/C++ this is called **casting**.

Casting one numeric type into another

Treat the type as a function.

Example:

```cpp
// 1over4.cpp
#include <iostream>

int main()
{
    int   a = 1;
    int   b = 4;
    int   c = a/b;
    float d = float(a)/float(b);

    std::cout << c << " "
              << d << " "
              << int(d) << std::endl;
}
```

```
$ g++ -std=c++14 1over4.cpp -o 1over4

$ ./1over4
0 0.25 0
```

Note: the 'proper' C++ way to do casting is to use `static_cast<TYPE>(value)` *or* `reinterpret_cast<TYPE>(value)`.

Automatic Casting

If an expression expects a variable or literal of a certain type, but it receives another, C++ may be able to convert it automatically. E.g.

```
1.0/4
```

is equal to

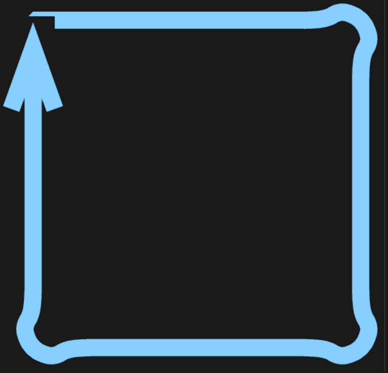
```
1.0/4.0
```

The expression may be a function call too, so that in this example:

```
int unchanged(int i)
{
   return i;
}
int main()
{
   return unchanged(2.3);
}
```

the argument 2.3 gets converted to an int first, and then passed to the function `unchanged`, so the returned value is 2.

C++ Overview: Loops



- In scientific computing, we often want to do the same thing for all points on a grid, or for every piece of experimental data, etc.
- If the grid points or data points are numbers, this means we consecutively want to consider the first point, do something with it, then the second point, do something with it, etc., until we run out of points.
- That's called a loop, because the same 'do something' is executed again and again for different cases.

C++ Overview: Loops

Two forms:

- for loop

```
for (initialization ; condition ; increment){
    statements
}
```

- while loop

```
while (condition) {
    statements
}
```

You can use the break statement to exit the loop.

For-loop example:

```
// count.cpp

#include <iostream>

int main()
{
    for (int i=1; i<=10; i++) {
        std::cout << i << " ";
    }
    std::cout << std::endl;
}
```

```
$ g++ -std=c++14 -o count count.cpp
$ ./count
1 2 3 4 5 6 7 8 9 10
```

Advanced: third loop form

There's actually a third form of `for`, called a range-based for:

```
for (type var: iterable-object-or-expression ) {
  statements
}
```

Example:

```cpp
// rangebasedfor.cpp

#include <iostream>

int main()
{
    for (int i: { 1,2,3,4,5,6,7,8,9,10 } ) {
        std::cout << i << " ";
    }
    std::cout << std::endl;
}
```

```
$ g++ -std=c++14 -o rangebasedfor rangebasedfor.cpp
$ ./rangebasedfor
1 2 3 4 5 6 7 8 9 10
$
```

C++ Overview: Pointers

- Pointers are memory addresses of variables.
- For each type of variable `type`, there is a pointer type `type*` that can hold an address of such a variable.
- Null pointer, denoted by `nullptr`, points to nowhere.
- Pointers are good for:
  - Arrays
  - Dynamic memory allocation
  - Linked lists, binary trees, . . .
  - Calling C library functions

Definition:

```
type* name ;
```

Assignment (“address-of”):

```
name = &variable-of-type ;
```

Deferencing (“content-at”):

```
variable-of-type = *name ;
```

Example:

```
int main()
{
    int  a = 5;  // a equal to 5
    int* b = &a; // b points to a
    *b = 7;      // *b is equivalent to a
    return a;    // so this returns 7
}
```

*Note: These are so-called **raw pointers**, in contrast with smart pointers that are in the C++ standard library.*

C++ Overview: Automatic arrays

```
type name [ number ];
```

(square brackets are not indicating an optional part here, but are part of the syntax)

- `name` is equivalent to a pointer to the first element.
- Access to elements: `name[i]`.
- C/C++ arrays are zero-based.
- They're dangerous.

C++ Overview: Automatic arrays, example

```cpp
// autoarr.cpp

#include <iostream>

int main()
{
    int a[6] = { 2,3,4,6,8,2 } ;
    int sum = 0;
    for (int i=0;i<6;i++) {
        sum += a[i];
    }
    std::cout << sum << std::endl;
}
```

```
$ g++ -std=c++14 -o autoarr autoarr.cpp
$ ./autoarr
25
$
```

What's so dangerous about automatic arrays?

- C standard only says at least one automatic array of at least 65535 bytes can be used.
- In practice, limit is set by compiler and OS.
- Compiler will not warn about the limit; the program will just crash.

C++ Overview: Automatic arrays, example

```cpp
// autoarr1e8.cpp

#include <iostream>

int main()
{
    int a[100000000] = { 2,3,4,6,8,2 } ;
    int sum = 0;
    for (int i=0;i<100000000;i++) {
        sum += a[i];
    }
    std::cout << sum << std::endl;
}
```

```
$ g++ -std=c++14 -o autoarr autoarr.cpp
$ ./autoarr
25
$
```

```
$ g++ -std=c++14 -o autoarr1e8 autoarr1e8.cpp
$ ./autoarr1e8
Segmentation fault (core dumped)
$
```

What's so dangerous about automatic arrays?

- C standard only says at least one automatic array of at least 65535 bytes can be used.
- In practice, limit is set by compiler and OS.
- Compiler will not warn about the limit; the program will just crash.

C++ Overview: Dynamically allocated array

Dynamically allocated arrays are defined as a pointer to memory:

```
type* name ;
```

Allocated using the keyword new :

```
name = new type [ number ];
```

(the square brackets are part of the syntax)

Deallocated by a function call:

```
delete [] name ;
```

- Usage of these arrays is the same as for automatic arrays.
- Can access all available memory.
- Can control when memory is given back.
- Must deallocate, or you'll have a memory leak.

Array allocation - Improved version

```
// dynarr.cpp

#include <iostream>

int main()
{
    int* a = new int[6] { 2,3,4,6,8,2 };
    int sum=0;
    for (int i=0;i<6;i++) {
        sum += a[i];
    }
    std::cout << sum << std::endl;
    delete[] a;
}
```

```
$ g++ -std=c++14 -o dynarr dynarr.cpp
$ ./dynarr
25
$
```

Multidimensional arrays, you ask?

Unfortunately, no fully dynamic multi-dimensional version of the `new` keyword exists C++.

More about multi-dimensional arrays and other data structures in a later class.

Dynamic allocation of single variables

One can also dynamically allocate a single variable:

```
int main() {
    double* v = new double;
    *v = 4.2;
    std::cout << *v << std::endl;
    delete v;
}
```

Note the absence of `[]` in the delete statement.

You might use this in more dynamic data structures.

Note: this is where smart pointers like a `unique_ptr` *or* `shared_ptr` *is useful.*

```
#include <memory>
int main() {
    std::unique_ptr<double> v = std::make_unique<double>();
    *v = 4.2;
    std::cout << *v << std::endl;
    // no delete necessary
}
```

Arrays as function arguments

Array expressions and pointers are equivalent. Consider e.g. a function to print an array of integers:

```
void printarr(int size, int x[])
{
    for (int i=0; i<size; i++) {
        std::cout << x[i] << " ";
    }
    std::cout << std::endl;
}
```

We would call this function with an automatic array as follows:

```
int main() {
    int numbers[4] = {1,2,3,4};
    printarr(4, numbers);
}
```

Here, the size of the array has to be explicitly given to the function as its first argument.

This is because the array variable `numbers`, which used as an expression for the seconds argument, is converted to a pointer to the first element of the array.

From this pointer, there is no way to deduce how big the array was.

Command Line Arguments

Linux commands can be followed by arguments.

To get their value in a C++ program, we need change from `int main()` to

```
int main(int argc, char* argv[])
{
        ....
}
```

where:

- `argc` is the number of arguments, where the command itself counts as an argument as well
- `argv` is an array of character string, with the first string, `argv[0]` equal to the command

Note this is precisely how we just saw that an array needs to be passed to a function.

All arguments are strings. To convert them to integers or floats, use functions like `atoi` and `atof`, e.g. `int n = atoi(argv[1]);` stores the integer value of the first command line argument into the variable `n`.

Command Line Arguments Example

```
#include <iostream>
int main(int argc, char* argv[]) {
    for (int i=0; i<argc; i++) {
        std::cout << argv[i] << std::endl;
    }
}
```

```
$ g++ -std=c++14 -o printargs printargs.cpp
$ ./printargs Hello There!
./printargs
Hello
There!
$
```

C++ Overview: Conditionals

```
if (condition) {
    statements
} else if (othercondition) {
    statements
} else {
    statements
}
```

Example:

```
int main(int argc, char* argv[]) {
    int  n = atoi(argv[1]);
    if ( n <= 20 ) {
        int* a = new int[n];
        for (int i=0; i<n; i++) {
            a[i] = i+1;
        }
        printarr(n,a);
        delete[] a;
    } else {
      std::cout << "Number given is too large\n";
    }
}
```

```
$ g++ -std=c++14 -o ifm ifm.cpp
$ ./ifm 20
0 1 4 9 16 25 36 49 64 81 100
121 144 169 196 225 256 289
324 361
```

Change `n = 20` to `n = 2000000000`:

```
$ ./ifm 2000000000
Number given is too large
$
```

C++ Overview: Exceptions

```
try {
    statements
}
catch (type varname) {
    statements
}
```

```
int main() {
    int  n = 20;
    int* a;
    try {
        a = new int[n];
    }
    catch (std::bad_alloc b) {
        std::cout << "Error in main" << std::endl;
        return 1;
    }
    for (int i=0; i<n; i++) {
        a[i] = i+1;
    }
    printarr(n,a);
    delete[] a;
}
```

```
$ g++ -std=c++14 -o ifm ifm.cpp
$ ./ifm
0 1 4 9 16 25 36 49 64 81 100
121 144 169 196 225 256 289
324 361
```

Change `n = 20` to `n = 2000000000`:

```
$ g++ -std=c++14 -o ifm ifm.cpp
$ ./ifm
Error in main
$
```

C++ Overview: Objects

Classes are a generalization of types.
Objects are a generalization of variables.

Syntax similar to variable declarations

```
classname objectname;
classname objectname(arguments);
classname objectname{arguments};
```

Differences between classes and regular types

- Object declarations can have arguments, supplied to construct the object.
- An object has members (fields) and member functions (methods), accessed using the "." notation.

```
object.field
object.method(arguments)
```

- You can create your own classes (though this isn't required for your course work).

C++ Overview: Classes and objects

Example of a member function/method

```
#include <string>
std::string s("Hello");
int stringlen = s.size();
```

Example of a member/field

```
#include <utility>
std::pair<int,float> p(1, 0.314e01);
int    int_of_pair   = p.first;
float  float_of_pair = p.second;
```

What are those angular brackets with types in between them?

C++ Overview: Templates

Templates

- Some algorithms and classes depend on a type. E.g. an list of doubles, a list of ints, . . .

  These objects can often be implemented with the same code, except for a change in type.
- Using generic programming, one can write this code once, with one or more type parameters.
- In C++, generic programming uses templates.
- Type parameters appear in between angular brackets <> instead of parenthesis.
- Many templated functions and classes are in the standard library, which we'll use.

C++ Overview: Class Templates

Usage

To create an object from a template class called `tc`:

```
tc<type> object(arguments);
```

Examples:

```
std::complex<float> z;     // single precision complex number
std::vector<int> i(20);    // array of 20 integers
rarray<float,2> x(20,20);  // 2d array of 20x20 floats (using the rarray library)
```

C++ Overview: Libraries

Usage

- Put an include line in the source code, e.g.

```
#include <iostream>
#include <mpi.h>
```

- Include the libraries at link time using `-l[libname]`. Implicit for the standard libraries.

Common standard libraries (Standard Template Library)

- string: character strings
- iostream: input/output, e.g., cin and cout
- fstream: file input/output, e.g., ifstream and ofstream
- containers: vector, complex, list, map, . . .
- algorithm: sort, find, min, max, . . .
- cmath: special functions (inherited from C), e.g. sqrt
- cstdlib, cstring, cassert, . . . : C header files

Example: sort an array

```
#include <iostream>
#include <algorithm>

int main()
{
    int* a = new int[6] { 2,3,4,6,8,2 };
    std::sort(&a[0], &a[6]);
    for (int i=0;i<6;i++) {
        std::cout << a[i] << std::endl;
    }
    delete[] a;
}
```

- The `algorithm` library contains a template function to sort containers.
- You give it the pointers (or iterators) to the beginning and to the end.
- The 'end' here is one further than the last element (this should sound familiar if you know Python's list slicing).

C++ Overview: Namespaces

- Variables and function, as well as variable types, have names.
- In larger projects, you could have variable types of the same name.
- To avoid such name clashes, one can use namespaces
- One usually puts all functions, types, ... of a module in a namespace:

```
namespace modname {
...
}
```

  (namespace is the keyword, modname is an identifier of your choosing)

- Effectively prefixes all of ... with `modname::`

  Example:

```
std::cout << "Hello, world" << std::endl;
```

- Many standard functions/types are in namespace std.

C++ Overview: Scope

Variables do not live forever, they have well-defined scopes in which they exist. These are the rules:

If you define a variable inside a code block, it exists only until the your code hits the closing curly brace (}) that correspond to the opening curly brace ({) that started the block. This is its local scope.

The variable will only be known in that code block and its subblocks.

If you call a function from a code block, variable from that block will not be known in the body of the function.

It is possible to define variables outside of any code block; these are global variables. Avoid those.

When a variable goes out of scope, the memory associated with it is returned to the system, except for memory that was dynamically allocated.

When that variable is an object, a special member function of it called the destructor is called. This gives objects that dynamically allocate memory the opportunity to delete that memory.

C++ Overview: IO Streams

In C++, stream object are responsible for I/O.
You can output an object obj to a stream str simply by

```
str << obj
```

while you can read an object obj from a stream str simply by

```
str >> obj
```

The stream will encode these object in ascii format, provided a proper operator is defined (true for the standard c++ types).

Standard streams

- `std::cout` For output to the screen (buffered)
- `std::cin` For input from the keyboard
- `std::cerr` For error messages (by default to the screen too)

These are defined in the header file `iostream`.

C++ Overview: IO Streams Example

```
#include <iostream>
int main() {
    std::cout << "Print a number: " << std::endl;
    int i;
    std::cin >> i;
    std::cout << "Twice that is: " << 2*i << std::endl;
}
```

C++ Overview: File Streams

- Classes for file IO are defined in the header `fstream`.
- The ofstream class is for output to a file.
- The ifstream class is for input from a file.
- You have to declare an object of these classes first.
- Then you can use the streaming operators << and >> .
- Use member functions read / write to read/write binary.

C++ Overview: File Streams Examples

```
#include <fstream>
int main() {
    std::ofstream fout("out.txt");
    int x = 4;
    float y = 1.5;
    fout << x << " " << y << std::endl;
    fout.close();
}
```

```
#include <fstream>
#include <iostream>
int main() {
    std::ifstream fin("out.txt");
    int x;
    float y;
    fin >> x >> y;
    fin.close();
    std::cout << "x=" << x << " y=" << y <<std::endl;
}
```

C++ Summary

These are the elements of C++ we'll be using in this class:

- Variables
- Functions
- Function arguments by value and by reference
- Loops
- Pointers
- Dynamically allocated arrays
- Conditionals
- Objects[1]
- Templates[1]
- Libraries
- Namespaces
- IO and file streams
- Compiling and linking

[1] only using these, you will not be required to write these (though you may).

Some online resource that may help you out:

- learncpp.com
- cplusplus.com