Programming and Data Analysis for Scientists

C++ Workshop 1

The shell and C++

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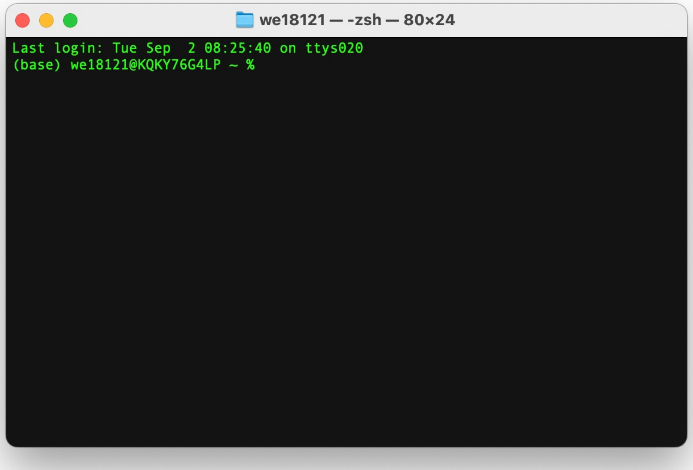
The shell and C++

The purpose of this workshop is to introduce the C++ programming language. The *learning objectives* are:

- Learn some basic shell command line instructions
- Appreciate the advantages and uses of C++
- Understand what compilation of C++ code means
- Compile, run and post-process data from a simple C++ computation

Using the **shell** terminal

Back in the 1970’s a *terminal* was a physical device for logging into a mainframe. These days it refers to a minimal text input and output graphical application emulating this device.



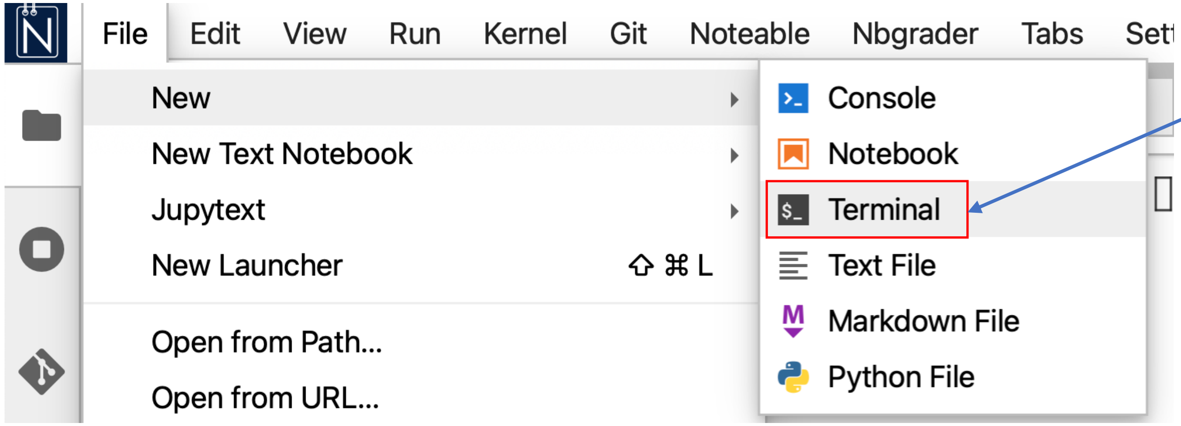
```
Last login: Tue Sep  2 08:25:40 on ttys020
(base) we18121@KQKY76G4LP ~ %
```

The *shell* is a command-line interpreter program. You type commands into the terminal, which sends them to the shell (like `Bash` or `Zsh`) for execution and the return results are displayed back in the terminal window.

While primitive in appearance the shell is extremely powerful. Any interactions with a high-performance computing facility will be via a shell.

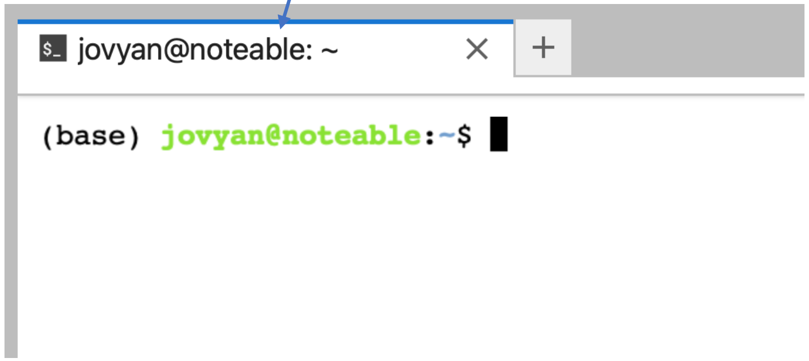
Start a shell on *Noteable*

You are already familiar with the ***Noteable*** server for running your Python Jupyter lab. The same resource can be used here. Start up Jupyter server …



Create Terminal session

It appears as a new tab in the Jupyter lab in your browser

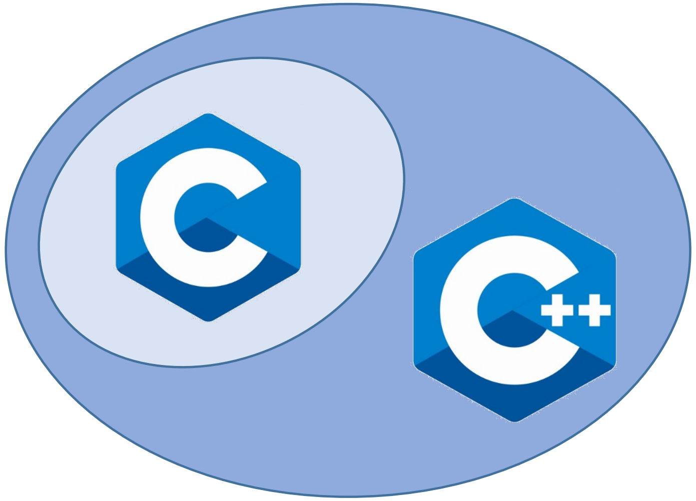


```
(base) jovyan@noteable:~$ 
```

We can run shell commands here that will be executed on the Noteable server.

What are C and C++?

C is a procedural programming language developed in 1972. It is a light-weight mid to low-level language developed for systems programming.



C++ is a superset of C first developed in 1985 to enhance it to include object orientated formalism.

C++ uses C syntax along with many new extensions. It continues to be updated and evolve.

Elegant base syntax of C is the *lingua franca* of modern programming. Not only C++, but Java, C#, as well as Python inherited many key features from it.

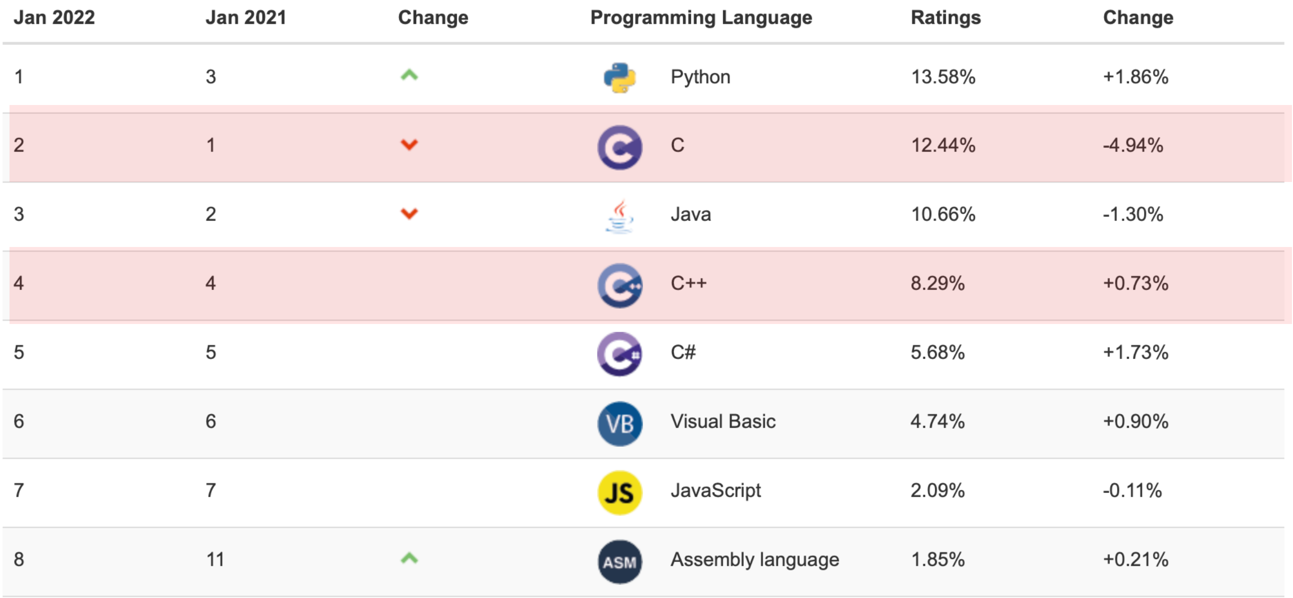
Why bother to learn C++ in 2025?

Legacy, maturity and ecosystem. It has been around for over 40 years. Unix, Mac OS, Linux, Windows, Google's Android OS are all written and continue to be developed in C++. Most problems have a C++ solution already written.

Since it is compiled it is **fast**! Most new computationally intensive applications like machine learning, scientific computing, virtual machines, device drivers, high-frequency trading, video games … are all written in C++.

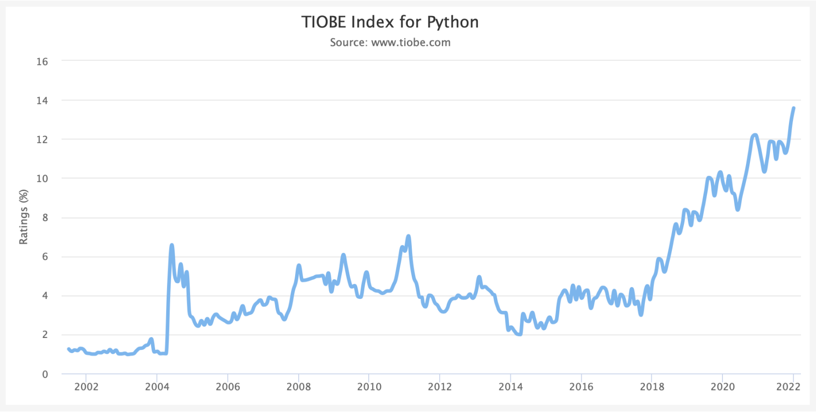
Since it is compiled it can be **small**! For embedded devices powering the IoT memory and processing is limited (due to power consumption and physical size) so their firmware is almost always written in C++.

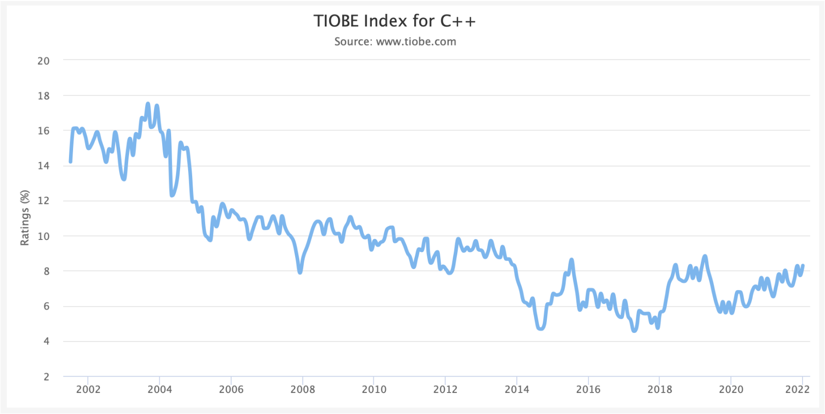
How popular are C and C++ currently?



Jan 2022	Jan 2021	Change	Programming Language	Ratings	Change
1	3	▲	Python	13.58%	+1.86%
2	1	▼	C	12.44%	-4.94%
3	2	▼	Java	10.66%	-1.30%
4	4		C++	8.29%	+0.73%
5	5		C#	5.68%	+1.73%
6	6		Visual Basic	4.74%	+0.90%
7	7		JavaScript	2.09%	-0.11%
8	11	▲	Assembly language	1.85%	+0.21%

C and C++ still **very** well used.

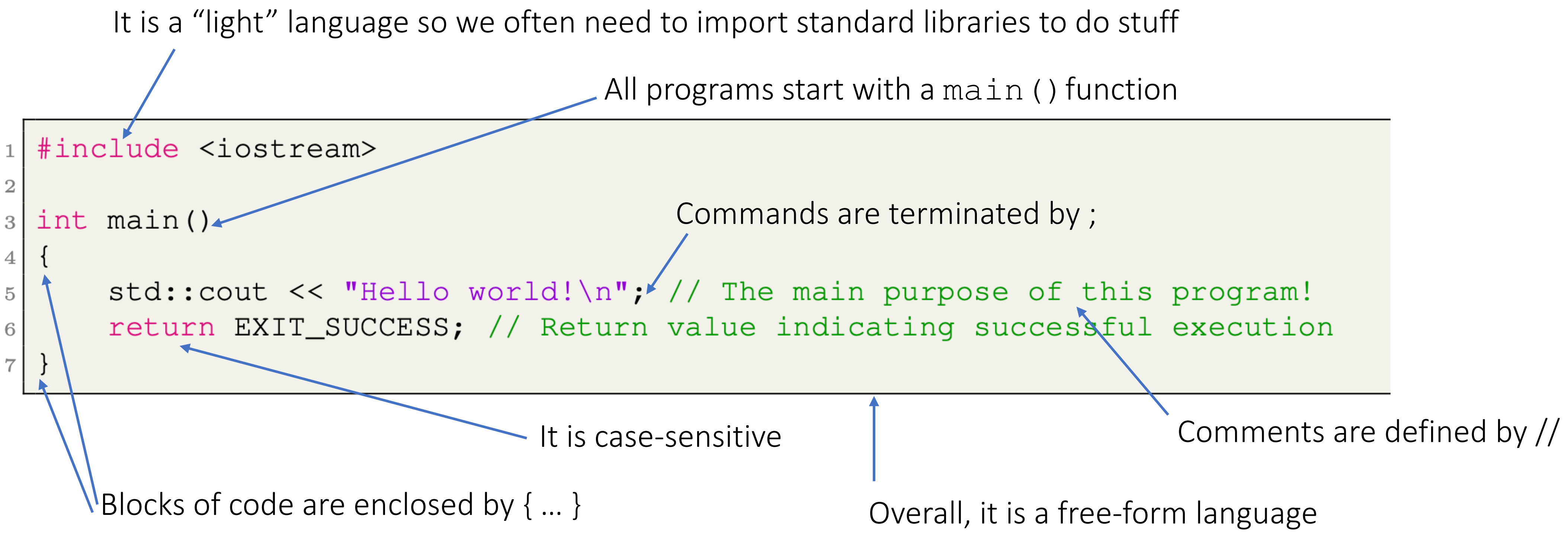




Source: tiobe.com

Anatomy of a C++ program

Take the customary first program anyone writes `hello.cpp`. We can highlight a number of essential features about C++ code:



It is a “light” language so we often need to import standard libraries to do stuff

All programs start with a `main()` function

Commands are terminated by ;

```cpp
#include <iostream>

int main()
{
    std::cout << "Hello world!\n"; // The main purpose of this program!
    return EXIT_SUCCESS; // Return value indicating successful execution
}
```

It is case-sensitive

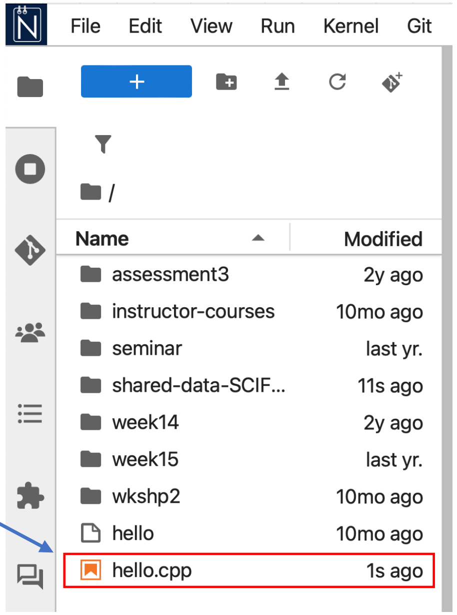
Comments are defined by //

Blocks of code are enclosed by { … }

Overall, it is a free-form language

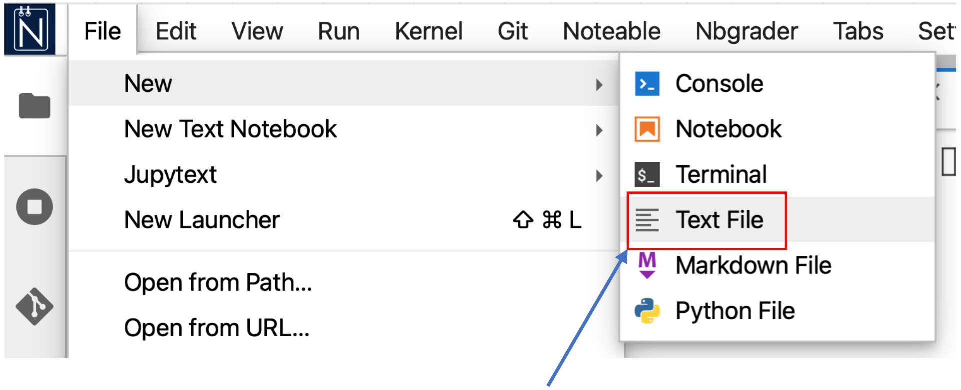
Using *Noteable* for C++ code

C++ source files are just plain text files with a .cpp extension. We can open or create a file in Noteable and use the built-in code editor …

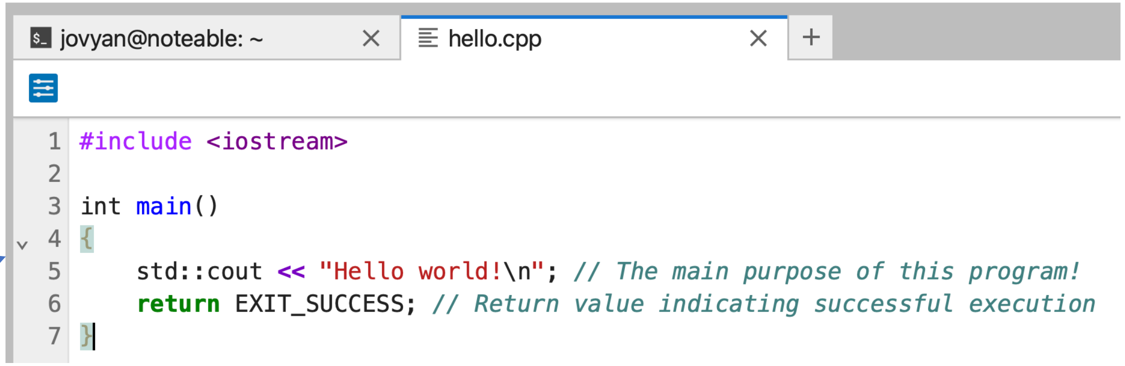


Name	Modified
assessment3	2y ago
instructor-courses	10mo ago
seminar	last yr.
shared-data-SCIF…	11s ago
week14	2y ago
week15	last yr.
wkshp2	10mo ago
hello	10mo ago
hello.cpp	1s ago

Open existing file in cloud filesystem



Create a new text file opening the editor



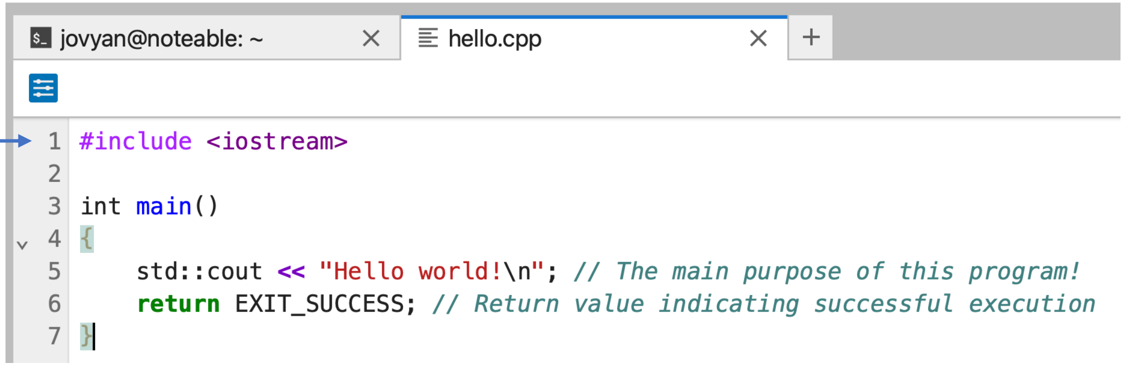
```
#include <iostream>

int main()
{
    std::cout << "Hello world!\n"; // The main purpose of this program!
    return EXIT_SUCCESS; // Return value indicating successful execution
}
```

New or existing file is opened as a new tab

Running C++ code on *Noteable*

When editing a .cpp file C++ language syntax highlighting will automatically switch on. If you created a new text file then rename it <something>.cpp, and then highlighting will turn on:

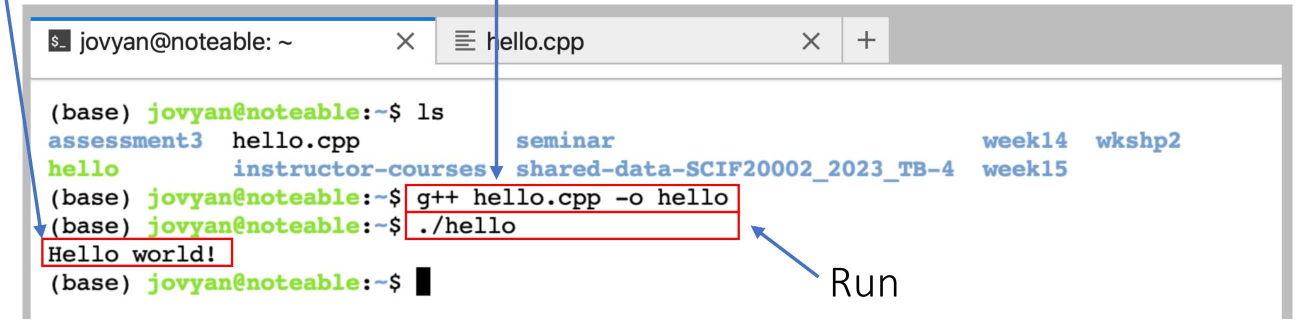
Language recognition



```cpp
#include <iostream>

int main()
{
    std::cout << "Hello world!\n"; // The main purpose of this program!
    return EXIT_SUCCESS; // Return value indicating successful execution
}
```

Output

Compile

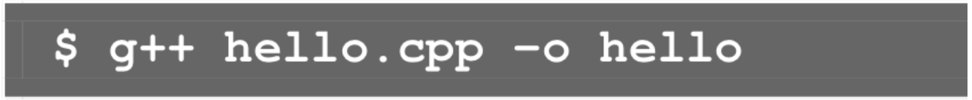


```
(base) jovyan@noteable:~$ ls
assessment3  hello.cpp           seminar                          week14  wkshp2
hello        instructor-courses  shared-data-SCIF20002_2023_TB-4  week15
(base) jovyan@noteable:~$ g++ hello.cpp -o hello
(base) jovyan@noteable:~$ ./hello
Hello world!
(base) jovyan@noteable:~$ 
```

Run

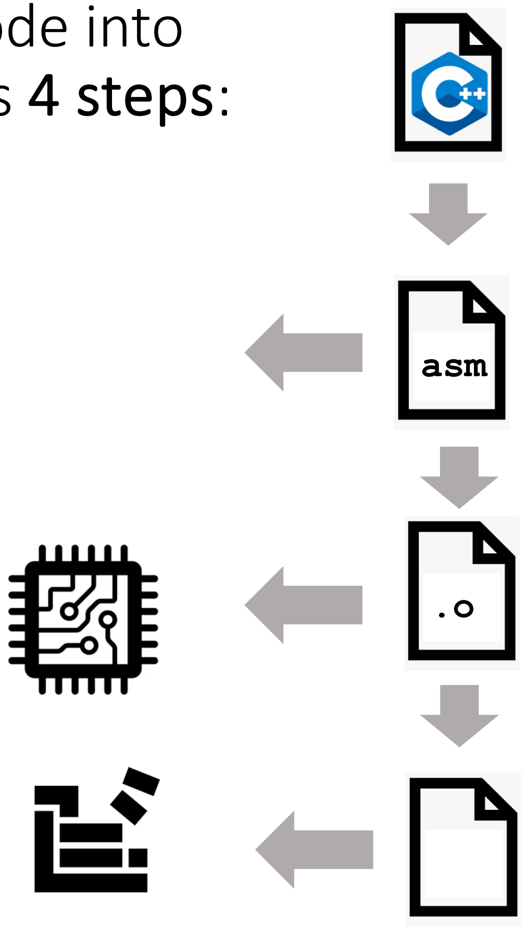
Switch to shell tab to compile and run in terminal

What is compilation?



```
$ g++ hello.cpp -o hello
```

The process of converting source code into binary machine code. It typically has **4 steps**:

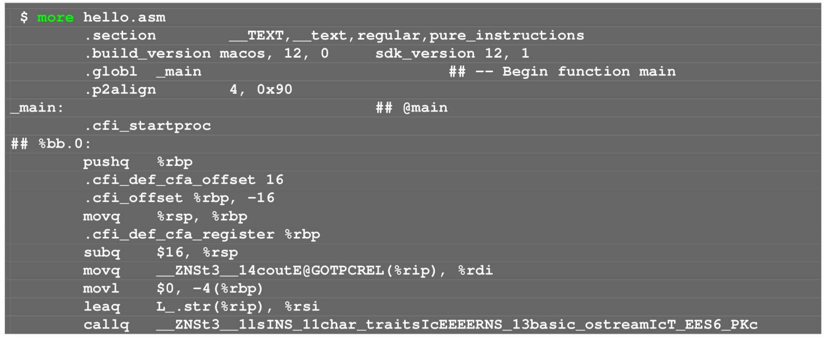


Preprocessing

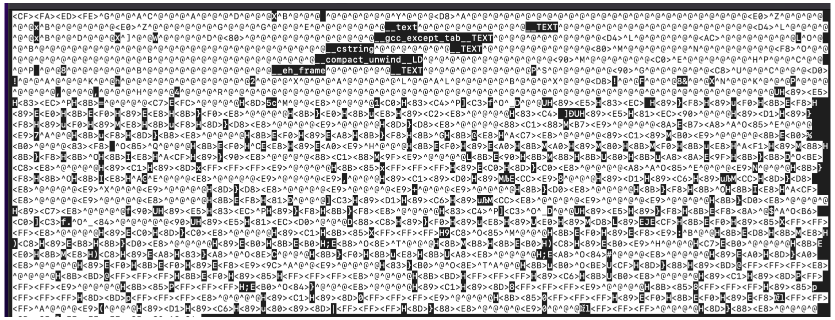
Compilation

Assembly

Linking



```
$ more hello.asm
        .section        __TEXT,__text,regular,pure_instructions
        .build_version macos, 12, 0     sdk_version 12, 1
        .globl  _main                           ## -- Begin function main
        .p2align        4, 0x90
_main:                                  ## @main
        .cfi_startproc
## %bb.0:
        pushq   %rbp
        .cfi_def_cfa_offset 16
        .cfi_offset %rbp, -16
        movq    %rsp, %rbp
        .cfi_def_cfa_register %rbp
        subq    $16, %rsp
        movq    __ZNSt3__14coutE@GOTPCREL(%rip), %rdi
        movl    $0, -4(%rbp)
        leaq    L_.str(%rip), %rsi
        callq   __ZNSt3__1lsINS_11char_traitsIcEEEERNS_13basic_ostreamIcT_EES6_PKc
```



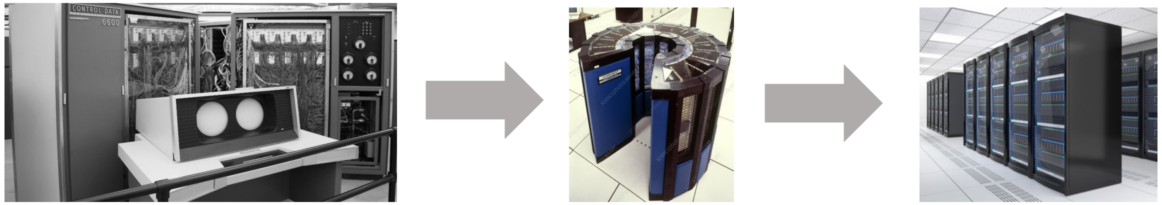
What is HPC?

A “supercomputer” is a specially optimized computer that achieves high performance in floating-point operations (FLOPS) central to scientific calculations.

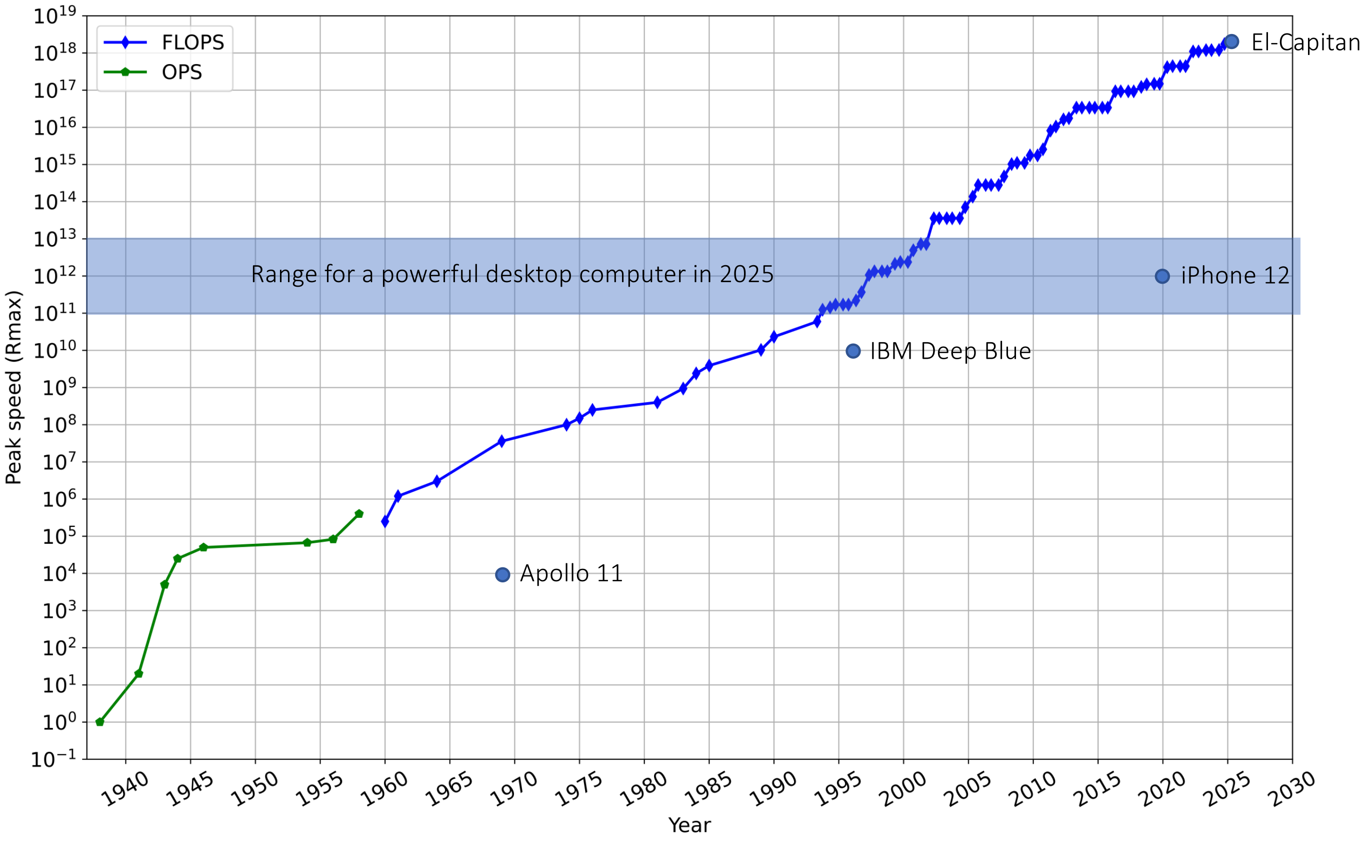
From the 1990’s onwards supercomputers evolved from being a dedicated single machine to being built from 10,000’s of networked “off-the-shelf” machines allowing for massive parallelization.

Since 2017 all the top 500 supercomputers run a Linux-based OS.

What is HPC?



Currently (2025) the most powerful supercomputers can do in excess of 10^{18} FLOPS distributed over millions of CPU cores.



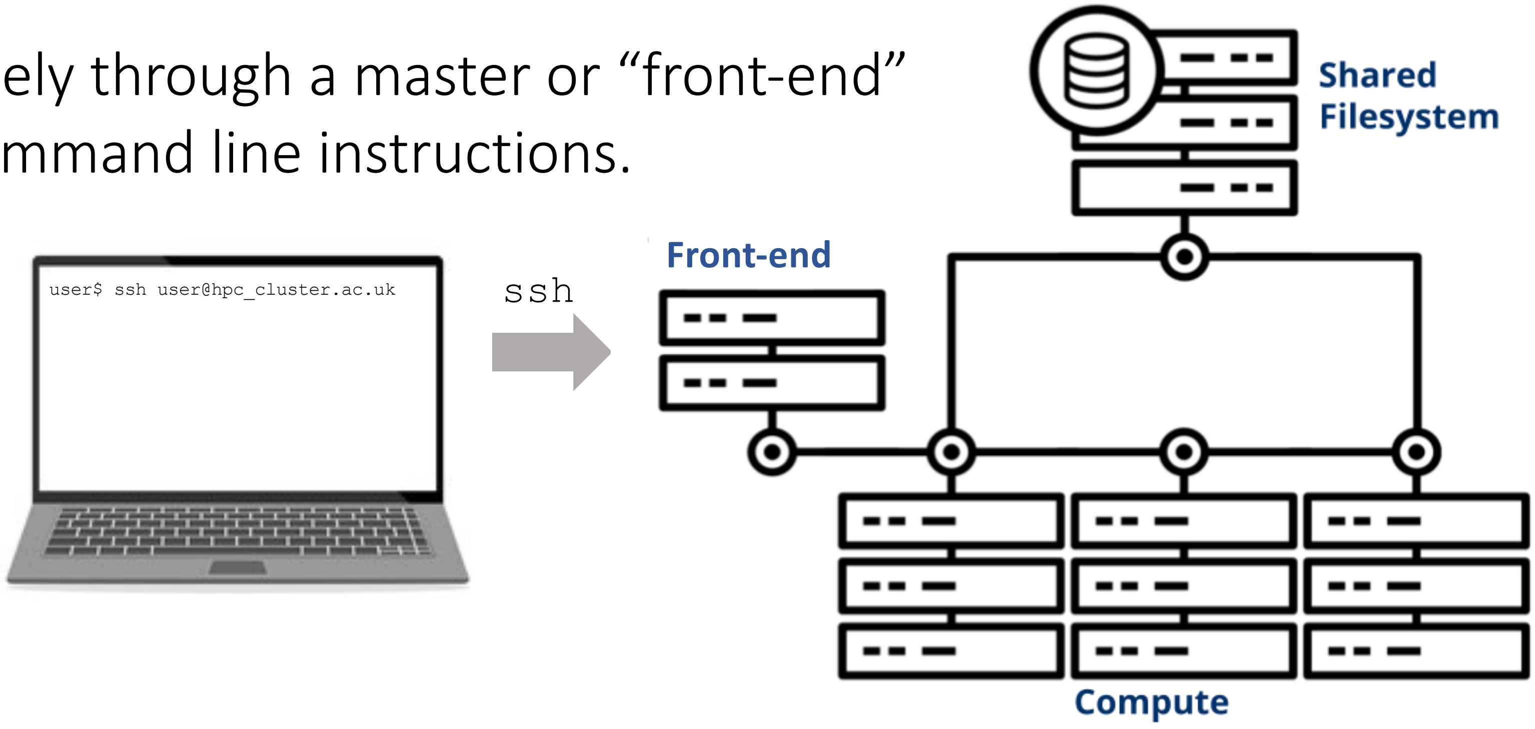
Source: Wikipedia/wiki/Supercomputer

Anatomy of a HPC cluster

Modern HPC cluster comprise many high-powered compute nodes connected via a superfast internal network.

It is accessed remotely through a master or “front-end” node via **ssh** and command line instructions.

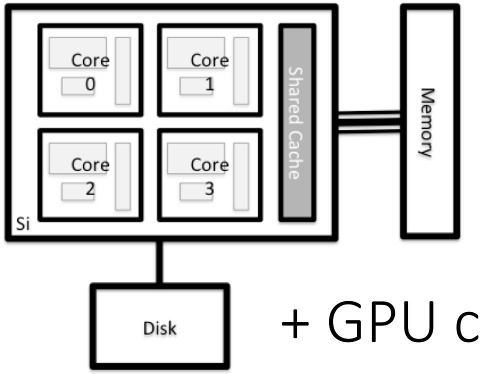
Code and data are stored on a shared filesystem.



```
user$ ssh user@hpc_cluster.ac.uk
```

HPC compute nodes

A “compute node” in a HPC cluster is individually a very high-powered (often dual multicore (12-24) processors) large memory (4-10GB per core) computer packaged compactly as a **rack-mounted** server blade:



Compute node

+ GPU cards

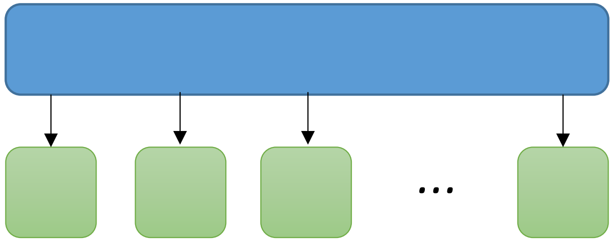
Server rack

Air-conditioned room

Why do we need HPC?

→ See lecture in Week 15

HPC enables complex scientific calculations that are **impossible** or **infeasibly slow** on a standalone computer. Two cases arise:

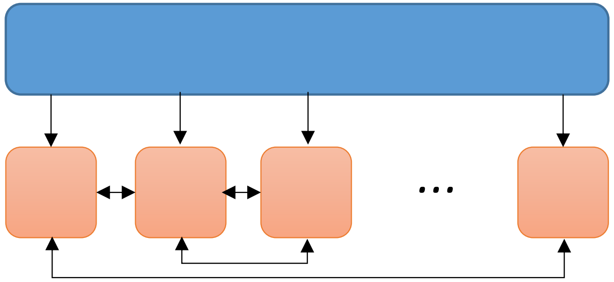


- *“Embarrassingly parallelizable problems”*
  Naturally divides into many independent tasks whose computation requires no communication between them.

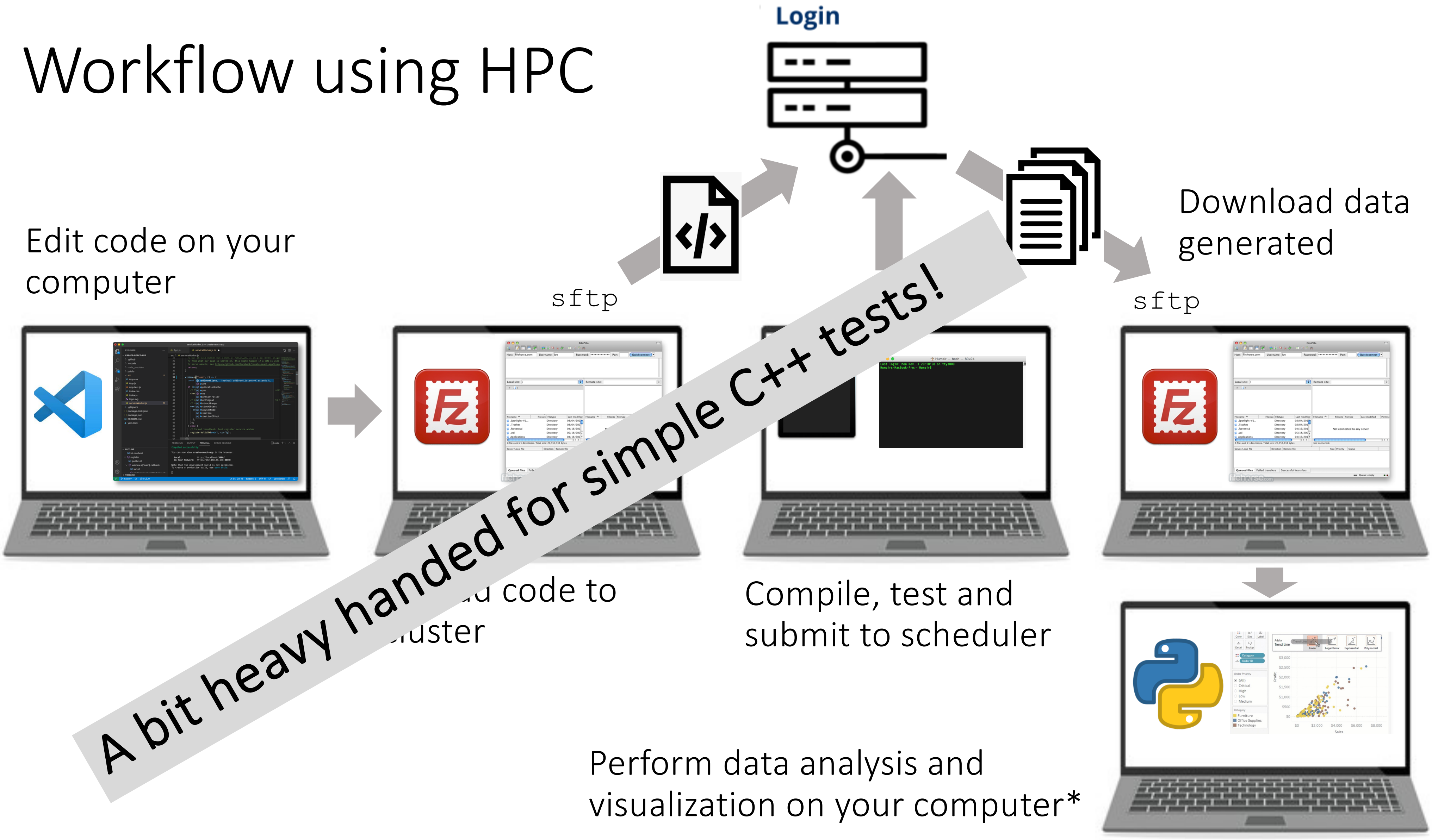
Example: *Monte Carlo sampling*

- *“Complex parallelization problems”*
  Only divides into many dependent tasks whose computation requires substantial communication between them.

Example: *High-resolution fluid dynamics*



Workflow using HPC



Edit code on your computer

d code to
luster

Compile, test and submit to scheduler

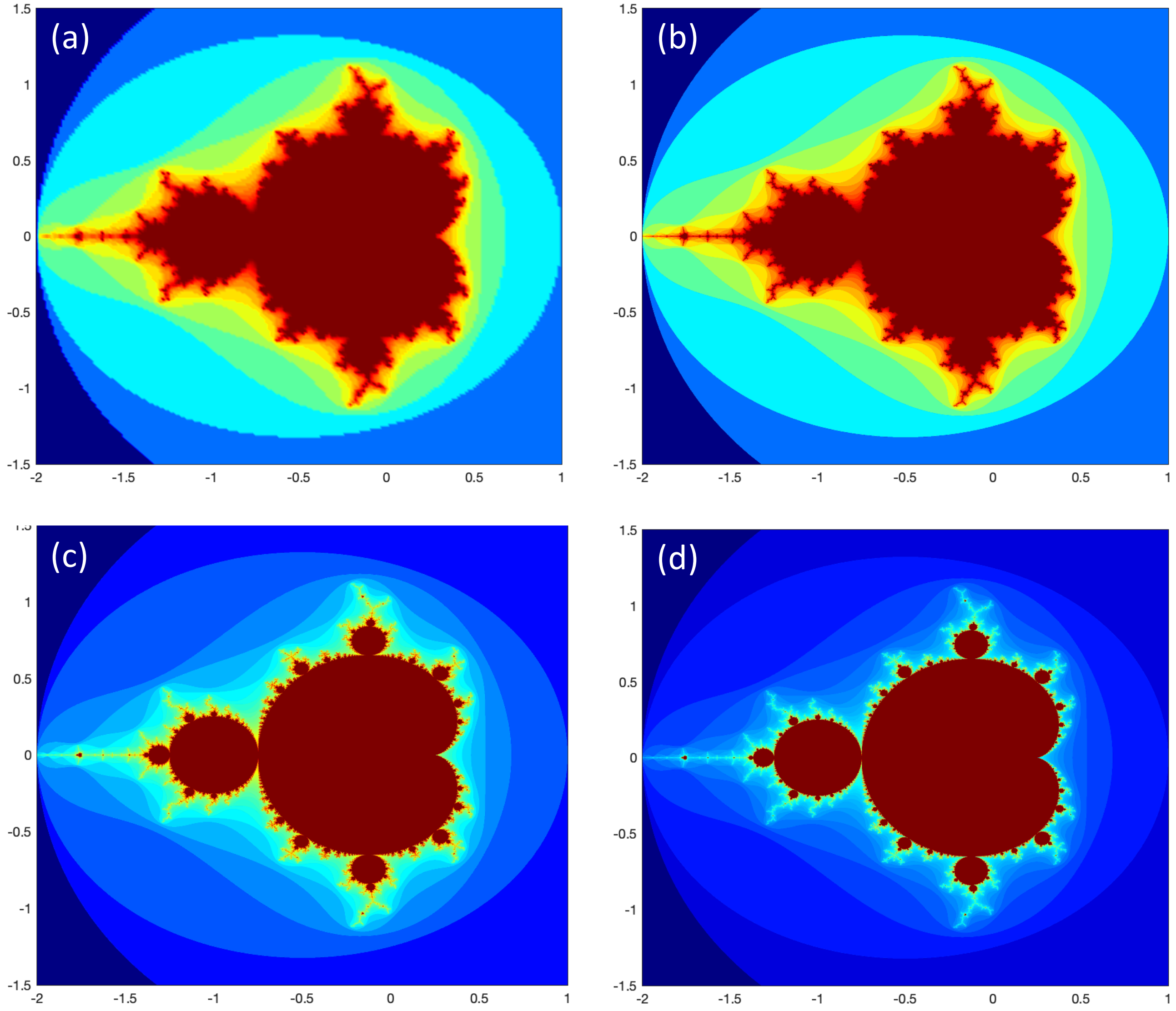
Download data generated

Perform data analysis and visualization on your computer*

A bit heavy handed for simple C++ tests!

Neat example:

You are given C++ code that can compute the well-known Mandelbrot set fractal. The main tasks of this workshop will be to compile it, run it and then post-process the output data to generate a plot similar to these …


(a)
(b)
(c)
(d)
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-1.5
-1
-0.5
0
0.5
1