OOP for Scientific Computing Notes - SoSe 24

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Preface

This is a Quarto book.

To learn more about Quarto books visit https://quarto.org/docs/books.

Part I

CMake Tutorial

Notes from the official CMake Tutorial link

1 Step 1

- Introduce CMake basic syntax, commands, and variables.
- Do three exercises and create a simple project.

1.1 Exercise 1

- Most basic CMake project is an executable built from a **single file**. Only `CMakeLists.txt` with **three** components is required. This is our **goal** with this exercise.

> ℹ Note
>
> Stylistically lower case commands are preffered in CMake

1.1.1 The Three Basic Commands

1. Any project's top most `CMakeLists.txt` must start by specifying a minimum CMake version using using the `cmake_minimum_required()` command.
2. Afterwards we use the `project()` command to set the **project name**.
3. Finally we use the `add_executable()` to make CMake create an executable using the specified source code files

1.1.2 Getting Started

We will build the following c++ file that computes the square root of a number:

- We complete the initial 3 TODOS of the `CMakeLists.txt`:

Listing 1.1 `tutorial.cxx`

```
// A simple program that computes the square root of a number
#include <cmath>
#include <cstdlib> // TODO 5: Remove this line
#include <iostream>
#include <string>

// TODO 11: Include TutorialConfig.h

int main(int argc, char* argv[])
{
  if (argc < 2) {
    // TODO 12: Create a print statement using Tutorial_VERSION_MAJOR
    //          and Tutorial_VERSION_MINOR
    std::cout << "Usage: " << argv[0] << " number" << std::endl;
    return 1;
  }

  // convert input to double
  // TODO 4: Replace atof(argv[1]) with std::stod(argv[1])
  const double inputValue = atof(argv[1]);

  // calculate square root
  const double outputValue = sqrt(inputValue);
  std::cout << "The square root of " << inputValue << " is " << outputValue
            << std::endl;
  return 0;
}
```

1.1.3 Build and Run

1. create a build directory:

   ```
   mkdir build
   ```

2. change into the build directory and build with `cmake`:

   ```
   cd build
   cmake ../
   ```

3. Actually compile/link the project with

Listing 1.2 `CMakelists.txt`

```
# TODO 1: Set the minimum required version of CMake to be 3.10
cmake_minimum_required(VERSION 3.10)

# TODO 2: Create a project named Tutorial
project(Tutorial)

# TODO 7: Set the project version number as 1.0 in the above project command

# TODO 6: Set the variable CMAKE_CXX_STANDARD to 11
#         and the variable CMAKE_CXX_STANDARD_REQUIRED to True

# TODO 8: Use configure_file to configure and copy TutorialConfig.h.in to
#         TutorialConfig.h

# TODO 3: Add an executable called Tutorial to the project
# Hint: Be sure to specify the source file as tutorial.cxx
add_executable(Tutorial tutorial.cxx)

# TODO 9: Use target_include_directories to include ${PROJECT_BINARY_DIR}
```

```
cmake --build .
```

Now an executable `Tutorial` has been created and can be run with

```
./Tutorial 3.0
```

with the output

```
The square root of 3 is 1.73205
```

All good!

1.2 Exercise 2

- CMake has some special variables that have meanig to CMake when set by project
- Many of these variables start with `CMAKE_`. Two of these special variables:

- CMAKE_CXX_STANDARD
    - CMAKE_CXX_STANDARD_REQUIRED
- These two together may be used to specify the C++ standard needed to build the project
- **Goal**: Add a feature that requires C++11 and utilize above two variables. TODO4 - TODO6

1.2.1 Getting Started

- TODO 4 & 5 - adding C++11 code to the source `tutorial.cxx`:

Listing 1.3 `tutorial.cxx`

```
// A simple program that computes the square root of a number
#include <cmath>
//#include <cstdlib> // TODO 5: Remove this line
#include <iostream>
#include <string>

// TODO 11: Include TutorialConfig.h

int main(int argc, char* argv[])
{
  if (argc < 2) {
    // TODO 12: Create a print statement using Tutorial_VERSION_MAJOR
    //          and Tutorial_VERSION_MINOR
    std::cout << "Usage: " << argv[0] << " number" << std::endl;
    return 1;
  }

  // convert input to double
  // TODO 4: Replace atof(argv[1]) with std::stod(argv[1])
  const double inputValue = std::stod(argv[1]);

  // calculate square root
  const double outputValue = sqrt(inputValue);
  std::cout << "The square root of " << inputValue << " is " << outputValue
            << std::endl;
  return 0;
}
```

TODO 6 - set the aforementioned variables:

- `set(CMAKE_CXX_STANDARD 11)`
- `set(CMAKE_CXX_STANDARD_REQUIRED True)`

Listing 1.4 `CMakelists.txt`

```
# TODO 1: Set the minimum required version of CMake to be 3.10
cmake_minimum_required(VERSION 3.10)

# TODO 2: Create a project named Tutorial
project(Tutorial)

# TODO 7: Set the project version number as 1.0 in the above project command

# TODO 6: Set the variable CMAKE_CXX_STANDARD to 11
#         and the variable CMAKE_CXX_STANDARD_REQUIRED to True
set(CMAKE_CXX_STANDARD 11)
set(CMAKE_CXX_STANDARD_REQUIRED True)


# TODO 8: Use configure_file to configure and copy TutorialConfig.h.in to
#         TutorialConfig.h

# TODO 3: Add an executable called Tutorial to the project
# Hint: Be sure to specify the source file as tutorial.cxx
add_executable(Tutorial tutorial.cxx)

# TODO 9: Use target_include_directories to include ${PROJECT_BINARY_DIR}
```

1.2.2 Build and Run

We already created a build directory adn ran `cmake ../` in the previous exercise, which created the project configurations. We don't need to redo this steps, instead we simply rebuild the project:

```
cd build
cmake --build .
```

We run the executable

```
./Tutorial 10
```

to obtain:

```
The square root of 10 is 3.16228
```

1.3 Exercise 3

Sometimes it is useful to have a variable that is defined in `CMakelists.txt` file also be available in source code. In our case we will define the **version number** in `CMakelists.txt` and make it available in a header file.

We can accomplished this with a **configured header file**, where there are two variables that can be replaced marked with `@VAR@`. We use `configure_file()` command to copy the contents of the configured header file to a standard header file, where the `@VAR@` variables are automatically replaced by CMake.

We include this header file generated by CMake in our source code and use the variables defined therein.

We could edit these variables directly in the source code, but using `CMake` avoids duplication and creates a single source of truth.

Goal: Define and report the project's version number. TODOS: 7 - 12.

1.3.1 Getting Started

First we define the version number with `project()` command:

```
project(
  Tutorial
  VERSION 1.0
)
```

Now CMake automatically sets in the background two variables:

- `Tutorial_VERION_MAJOR` as 1
- `Tutorial_VERION_MINOR` as 0

since we defined the VERSION as 1.0.

Now we can utilize these variables in a `TutorialConfig.h.in` file that we will use as an input to CMake to generate a `TutorialConfig.h`.

We create `TutorialConfig.h.in` an add following two lines

Listing 1.5 `TutorialConfig.h.in`

```
//File: TutorialConfig.h.in
#define Tutorial_VERSION_MAJOR @Tutorial_VERSION_MAJOR@
#define Tutorial_VERSION_MINOR @Tutorial_VERSION_MINOR@
:::
```

Note that we access the CMake variables that were previously automatically set by the `project()` command via the `@VAR@` syntax.

Next we instruct CMake to generate a `TutorialConfig.h` from `TutorialConfig.h.in` with the `configure_file()` command:

```
configure_file(TutorialConfig.h.in TutorialConfig.h)
```

The generated header file will be written into the **project binary directory**. In our case it is simply `build/` directory.

We must add this directory to the list of paths that CMake searches for include files with the `target_include_directories()` command:

```
target_include_directories(
  Tutorial
  PUBLIC "${PROJECT_BINARY_DIR}"
)
```

Finally we modify `tutorial.cxx` to include the generated header file:

```
#include "TutorialConfig.h"
```

and include the print directives that utilize the variables from the header file:

```
  if (argc < 2) {
    // TODO 12: Create a print statement using Tutorial_VERSION_MAJOR
    //          and Tutorial_VERSION_MINOR
    std::cout << argv[0] << " Version " << Tutorial_VERSION_MAJOR << "."
                                        << Tutorial_VERSION_MINOR << std::endl;
    std::cout << "Usage: " << argv[0] << " number" << std::endl;
    return 1;
  }
```

1.3.2 Build & Run

Again we only need to rebuild:

```
cd build
cmake --build .
```

If we run `Tutorial` with wrong argument list we get the Version number and the usage message:

```
./Tutorial
```

Output:

```
./Tutorial Version 1.0
Usage: ./Tutorial number
```

The end!

2 Step 2

- In step 1 we learned how to create a simple project with a single `.cxx` file and a single executable
- In step 2 we learn:
  - how to create and use a **library**,
  - how to make the use of the library optional

2.1 Exercise 1 - Creating a Library

Goal: Add and use a library

To add a library with CMake, use the `add_library()` command and specify the source files that make up the library.

Instead of placing all source files in a single directory, we can **organize** our project with one or more subdirectories. Here we create a subdirectory specifically for our library.

To this subdirectory we add another `CMakeLists.txt` file and source files.

In the top level `CMakeLists.txt` file, use the `add_subdirectory()` command to add the subdirectory to the build.

The library is connected to the executable target with

- `target_include_directories()`
- `target_link_libraries()`

2.1.1 Getting Started

We add a library that contains own implementation for computing square root of a number. The executable can then optionally use this library instead of the standard square root function.

The libary is put into a subdirectory `MathFunctions`. This directory already contains:

- header files:

  - `mysqrt.h`
  - `MathFunctions.h`

- their respective source files:

  - `mysqrt.cxx` contains custom implementation of square root function
  - `MathFunctions.cxx` contains a wrapper around `sqrt` function from `msqrt.cxx` in order to hide implementation details.

- TODO: 1 - 6

  1. Creating a library target
  2. Making use of the new library target
  3. Linking the new library target to the executable target
  4. Specifying library's header location
  5. Using the library
  6. Replacing `sqrt` with the wrapper function `mathfunctions::sqrt`

In the `CMakeLists.txt` file in the `MathFunctions` directoyr, we craete a library target called `MathFunctions` with `add_library()`.

2.1.1.1 TODO 1 - Creating a Library Target

In the `CMakeLists.txt` in the `MathFunctions` directory, we create a library target called `MathFunctions` with `add_library()`:

Listing 2.1 `MathFunctions/CMakeLists.txt`

```
# TODO 1: Add a library called MathFunctions with sources MathFunctions.cxx
add_library(MathFunctions MathFunctions.cxx mysqrt.cxx)
```

The source files of the library are passed as arguments.

2.1.1.2 TODO 2 - Making use of the new Library

To make use of the new library we add an `add_subdirectory()` in the **top-level** `CMakeLists.txt`:

Listing 2.2 `CMakeLists.txt`

```
add_subdirectory(MathFunctions)
```

2.1.1.3 TODO 3 - Linking the new Library Target to the Executable Target

We link the new library target to the executable target with `target_link_libraries()`

Listing 2.3 `CMakeLists.txt`

```
target_link_libraries(Tutorial PUBLIC MathFunctions)
```

2.1.1.4 TODO 4 - Specifying Library's Header File Location

Modify the existing `target_include_directories()` to add the `MathFunctions` subdirectory as an include directory so that the `MathFunctions.h` header file can be found:

Listing 2.4 `CMakeLists.txt`

```
# TODO 4: Add MathFunctions to Tutorial's target_include_directories()
# Hint: ${PROJECT_SOURCE_DIR} is a path to the project source. AKA This folder!

# add the binary tree to the search path for include files
# so that we will find TutorialConfig.h
target_include_directories(Tutorial PUBLIC
                           "${PROJECT_BINARY_DIR}"
                           "${PROJECT_BINARY_DIR}/MathFunctions"
                           )
```

2.1.1.5 TODO 5 & 6- Using the Library

We use the library by including `MathFunctions.h` in `tutorial.cxx`:

Listing 2.5 `tutorial.cxx`

```
// TODO 5: Include MathFunctions.h
#include "MathFunctions/MathFunctions.h"
```

Replace `sqrt` with the wrapper function `mathfunctions::sqrt`:

Listing 2.6 `tutorial.cxx`

```
// TODO 6: Replace sqrt with mathfunctions::sqrt

// calculate square root
// const double outputValue = sqrt(inputValue);
const double outputValue = mathfunctions::sqrt(inputValue);
```

2.2 Exercise 2 - Adding an Option

In this exercise we add an option in the `MathFunctions` library to allow developers to select either the custom or the built-in implementation using the `option()` command

Goal: Add an option to build without `MathFunctions`

2.2.1 Getting Started

We will create a variable `USE_MYMATH` using `option()` in `MathFunctions/CMakeLists.txt` There we use that option to pass a **compile time definition** to the `MathFunctions` library.

Then, update `MathFunctions.cxx` to redirect compilation based on `USE_MYMATH`.

Lastly, we prevent `mysqrt.cxx` from being compiled when `USE_MYMATH` is on by making it its own library inside of the `USE_MYMATH` block of `MathFunctions/CMakeLists.txt`

TODOS: 7 - 14:

7. Add an option to `MathFunctions/CMakeLists.txt`
8. Make building and linking our library with `mysqrt` function conditional using this new option
9. Add the corresponding changes to the source code `MathFunctions/MathFunctions.cxx`
10. Including `mysqrt.h` if the optional varible is defined.
11. Including `cmath` as well
12. Ommitting unneccesary usage/build of `mysqrt.cxx` if the custom option is off.
13. Link `SqrtLibrary` onto `MathFunctions` when the optional variable is enabled.
14. We remove `mysqrt.cxx` from `MathFunctions` library source list because it will be pulled when `SqrtLibrary` is enabled.

2.2.1.1 TODO 7 - Adding an Option

We add an option to `MathFunctions/CMakeLists.txt`. This will be displayed in the `cmake-gui` and `ccmake` with a default value of `ON`.

Listing 2.7 `MathFunctions/CMakeLists.txt`

```
# TODO 7: Create a variable USE_MYMATH using option and set default to ON
option(USE_MYMATH "Use custom math implementation" ON)
```

2.2.1.2 TODO 8 - Make Building and Linking the Library Conditional

Make building and linking our library with `mysqrt` function conditional using this new option.

Create an `if()` statement which checks the value of `USE_MATH`. Inside the `if()` put the `target_compile_definitions()` command with the compile definition `USE_MYMATH`:

Listing 2.8 `MathFunctions/CMakeLists.txt`

```
# TODO 8: If USE_MYMATH is ON, use target_compile_definitions to pass
# USE_MYMATH as a precompiled definition to our source files
if(USE_MYMATH)
    target_compile_definitions(MathFunctions PRIVATE "USE_MYMATH")
endif()
```

Now when `USE_MYMATH` is `ON`, the compile definition `USE_MYMATH` will be set. We can then use this compile definitnion to enable or disable sections of our source code.

2.2.1.3 TODO 9 - Adding the Changes to the Source Code

We add the corresponding changes to the source code. In `MathFunctions.cxx` we use `USE_MYMATH` to control which square root function is used:

Listing 2.9 `MathFunctions/MathFunctions.cxx`

```
  // TODO 9: If USE_MYMATH is defined, use detail::mysqrt.
  // Otherwise, use std::sqrt.
  #ifdef USE_MYMATH
    return detail::mysqrt(x);
  #else
    return std::sqrt(x);
  #endif
```

2.2.1.4 TODO 10 - Including `mysqrt.h` Conditionally

Next, we need to include `mysqrt.h` if `USE_MYMATH` is defined.

Listing 2.10 `MathFunctions/MathFunctions.cxx`

```
// TODO 10: Wrap the mysqrt include in a precompiled ifdef based on USE_MYMATH
#ifdef USE_MYMATH
  #include "mysqrt.h"
#endif
```

2.2.1.5 TODO 11 - Including `cmath`

Now since we use `std::sqrt()` (see TODO 9), we must include `cmath`:

Listing 2.11 `MathFunctions/MathFunctions.cxx`

```
// TODO 11: include cmath
#include <cmath>
```

2.2.1.6 TODO 12 & 13 - Omitting Compilation of `mysqrt.cxx` if Option is off

At this piont, even if `USE_MYMATH` is off, `mysqrt.cxx` would not be used but **still compiled** because `MathFunctions` target has `mysqrt.cxx` listed under sources.

We can fix this in various ways:

1. use `target_sources()` to add `mysqrt.cxx` rom within the `USE_MYMATH` block.
2. create an additional library within the `USE_MYMATH` block which is responsible for compiling `mysqrt.cxx`.

We will go with the second option.

First we create an additional library from within `USE_MYMATH` called `SqrtLibrary` that has sources `mysqrt.cxx`:

Next, we link `SqrtLibrary` onto `MathFunctions` when `USE_MYMATH` is enabled:

Listing 2.12 `MathFunctions/CMakeLists.txt`

```
if(USE_MYMATH)
    target_compile_definitions(MathFunctions PRIVATE "USE_MYMATH")
    # TODO 12: When USE_MYMATH is ON, add a library for SqrtLibrary with
    # source mysqrt.cxx
    add_library(SqrtLibrary STATIC
                mysqrt.cxx)
endif()
```

Listing 2.13 `MathFunctions/CMakeLists.txt`

```
if(USE_MYMATH)
    target_compile_definitions(MathFunctions PRIVATE "USE_MYMATH")
    # TODO 12: When USE_MYMATH is ON, add a library for SqrtLibrary with
    # source mysqrt.cxx
    add_library(SqrtLibrary STATIC
                mysqrt.cxx)
    # TODO 13: When USE_MYMATH is ON, link SqrtLibrary to the MathFunctions Library
    target_link_libraries(MathFunctions PRIVATE SqrtLibrary)
endif()
```

2.2.1.7 TODO 14 - Removing `mysqrt.cxx` from Library Source

Finally, we can remove `mysqrt.cxx` from our `MathFunctions` library source list because it will be pulled when `SqrtLibrary` is included.

Listing 2.14 `MathFunctions/CMakeLists.txt`

```
add_library(MathFunctions MathFunctions.cxx)
```

With these changes, the `mysqrt` function is now completely optional to whoever is building and using `MathFunctions` library. Users can toggle `USE_MYMATH` to this end.

2.2.2 Building & Running

Part II

Basic Concepts of C++

- variables and types
- pointers and references
- control structures
- functions and templates
- classes and inheritance
- namespaces and structure

3 Variables, Temporaries, Literals

3.1 Variables

3.2 Temporaries

3.3 Literals

4 Data Types

4.1 Introducing New Types

4.1.1 Enum

```
enum Color = {RED, BLUE, GREEN}
```

4.1.2 Struct

...

4.2 Const-Correctness

Marks something that can't be modified.

```
include <iostream>

int main(int argc, char const *argv[])
{
    int n = 5;
    const int j = 4;
    const int &k = n; //k can't be modified, equivalently n can't be modified over k
    n++; //but this changes n and indirectly k (because k references n)


    const int *p1 = &n; // modifiable pointer to const int
    int const *p2 = &n; // same thing
    int *const p3 = &n; // constant pointer to modifiable int

    // p1 = &j -- ok
    // *p1 = 3 -- not ok!
    // p3 = &j -- not ok
```

```
    // *p3 = 10 -- ok

    std::cout << "n: " << n << std::endl
              << "j: " << j << std::endl
              << "p1: " << p1 << std::endl
              << "p2: " << p2 << std::endl
              << "p3: " << p3 << std::endl;


    return 0;
}
```

5 Indirection

5.1 Pointers

```
include <iostream>

int main(int argc, char const *argv[])
{
    int i = 5;
    int *p1 = &i;
    int *p2 = new int;

    std::cout << "i: " << i << std::endl
              << "*p1: " << *p1 << std::endl
              << "p1: " << p1 << std::endl
              << "&p1: " << &p1 << std::endl
              << "p2: " << p2 << std::endl
              << "*p2: " << *p2 << std::endl;
    delete p2;
    return 0;
}
```

output:

```
i: 5
*p1: 5
p1: 0x7fff8d568184
&p1: 0x7fff8d568188
p2: 0x55c014358eb0
*p2: 0
```

- release memory with `delete`.
- deleting too early -> bugs, too late -> memory leaks

5.2 References

References are **aliases for an existing entity**. k

```
include <iostream>

int main(int argc, const char** argv) {

    int a = 4;
    std::cout << "a: " << a <<std::endl;
    int &b = a;
    b = 5;
    std::cout << "a: " << a << std::endl
              << "b: " << b << std::endl;

    return 0;
}
```

output:

```
a: 4
a: 5
b: 5
```

5.3 Rvalue (double) References

Two uses:

- **range-based** `for` loops
- **move semantics**

lvalue references refer to entities, rvalue references refer to literals.

6 Control Flow

6.1 If

```
include <iostream>

int main(int argc, char const *argv[])
{
    int i;
    std::cin >> i;

    if (i % 2 == 0) std::cout << i << " is even" << std::endl;
    else std::cout << i << " is odd" << std::endl;
    return 0;
}
```

6.2 Switch

```
include <iostream>

enum Color {RED, BLUE, GREEN};

int main(int argc, char const *argv[])
{
    int i;
    Color c = RED;

    std::cin >> i;

    switch(i) {
        case 0:
            c = RED;
            break;
```

```
        case 1 :
            c = BLUE;
            break;
        case 2 :
            c = GREEN;
            break;
        default :
            std::cout << "error: invalid color" << std::endl;
    }

    std::cout << c << std::endl;

    return 0;
}
```