### Intro to Efficient Programming

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HGS-HIRe power week
Limburg
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# Lecture I

# Introduction

#### Who we are

#### Mikolaj Krzewicki

- in ALICE since 2007
- ► ALICE High Level Trigger / ALICE O2
- Software validation
- ▶ TPC calibration
- Analysis (correlations and flow)

#### Patrick Huhn

- ▶ in ALICE since 2014
- ► PhD student since 2017
- Analysis (charged particle R<sub>AA</sub>)

#### Sandro Wenzel

- ➤ at CERN since 2012; in ALICE since 2015
- ▶ Detector Simulation
- Previous experience in various computing activities (PhD: Quantum Monte Carlo; The Blue Brain Project)

#### **Credits**

Material of this course building on previous courses given by Jens Wiechula, David Rohr, Matthias Richter and Jochen Klein.

# Outline / Goals of the week

Software development / computing in high energy physics is ubigous and essential knowledge. This week should help you to ...

- ▶ Be able to come up with efficient algorithms in C++ implementing software solutions to problems in (particle) physics.
- ▶ Be able to use ROOT as a library and to look into data using ROOT
- ▶ Be able to decompose problem into small pieces, structure code and work on software projects incrementally
- ▶ Understand tools and practices in the software development process
- ▶ Know about modern C++11 features and few optimization strategies
- Know about easy parallelism options and SIMD

#### Introduction

#### There are many aspects of efficiency

- Coding concepts
- Tools
- Fast development (prototyping)
- Fast code execution (optimization)
- ► Small memory imprint

- ► Code design
- Code flexibility / configurability
- **.**..

### Programme

#### What we want to cover:

- ▶ Modern C++ features and concepts (C++11, C++14, ...)
- ► Tools
- gcc
- ► (c)make
- ▶ git

- doxygen
- gdb
- profilers: valgrind, perf, ...

- Methods
  - object orientation, templates
  - libraries
- Algorithms
- Parallelisation
- SIMD vectorisation

# Outlook Programme 2

What we can't cover here but intend to do in part 2:

- ► GP-GPU
- ▶ Parallelization in more depth
- distributed computing and messaging
- **.**..

#### Course format

There will be some lectures but focus will be on practical side!

- Lot's of do-it yourself exercises/examples
- A real coding project touch typical high energy physics subject
- Possibility to do code reviews / interaction with lecturers

link to dynamic plan https://tinyurl.com/hgspw1

### A small project

- small groups (up to 5 people)
- work shall be carried out over the whole week, presentation of results on Friday (20+5), code reviews in between
- we want you to
  - use the tools
  - try the methods
  - test the algorithms

which are discussed during the meeting

- you should learn something
  - ⇒ try and understand what you are doing

# Computing I

▶ local servers (hostnames: power[1-4].power.week) personal user accounts: username: first letter of firstname + lastname, initial password: pwLimburg (reference environment, you can compare to your machine)

- Every groups gets assigned one server (please use it exclusively)
- separate network with WLAN access (or cable)
   SSID: power-week
   pw: efficient
- passwordless login often it is convenient to login usind ssh keys

```
ssh-keygen
ssh-copy-id <you-user-id>@power[1-4]
```

# Computing II

examples and slides are provided via git

```
git clone https://github.com/hgspowerweek/powerweek1/
cd powerweek1
git pull
```

do the last step before every session and you will get the latest examples and slides

- ► Slides are directly in this folder as pdfs
- Examples are in the folder examples

examples/bla

#### Lecture II

Introduction to code / document management using git – absolute basics

### Code repository

Why would you use a code repository?

- keep control over your changes
- keep a history of changes and go back to any previous state
- add logging messages to individual changes
- develop different topics in parallel
- keep a working version as a reference
- create releases for distribution of the code
- synchronize several developers

A code repository can serves as

- back-up solution
- communication medium
- team and product management tool

### git - the stupid content tracker

- Developed by Linus Torvalds and others in 2005 for the Linux kernel community
- ▶ Nobody knows what git stands for at least one does not get a real answer.
- Instead of beeing stupid see manpage it's a extremely powerful scalable, distributed revision control system.

In contrast to other versioning systems (CVS, subversion),

- git allows to use the full functionality of a code repository locally
- can be distributed
- does not require a central server, but can be used with a server

### git commands in a nutshell

#### **Basic operations:**

- ▶ git init
- ▶ git clone
- git add add something to staging area
- git commit commit staging area to local reposity
- pit checkout <commit> retrieve certain state

#### **Getting information**

- ▶ git log show commit history
- ▶ git status
- git diff show differences
   (between commits)

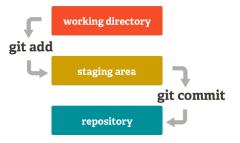
#### **Advanced commands**

- ▶ git stash
- git push publish repo somewhere else (some URL)
- git pull sync/get changes from somwhere else (some URL)
- git rebase/merge integrate someone elses changes; change history

# git - the stupid content tracker

How is a git repository structured:

- ▶ local copy (tree) those are your files.
- staging area (intermediate store) changes (diffs) staged for commit.
- local repository full repository containing all changes to all branches. Everybody has a full copy, there is no concept of a central repository you still may declare some repository the central one.



### git - One time (identity) setup

- git config Configure git or query configuration
- ► Some essential setup: Give yourself a git identity:

```
git config --global user.name "Foo Bar"
git config --global user.email foo.bar@cern.ch
```

- ▶ git config -1 will show you the whole configuration including your identity
- ► configuration is stored in a file \${HOME}/gitconfig which can also be edited

# git - Creating and cloning repositories

#### Creating an initial repository:

```
mkdir -p ~/src/project
cd ~/src/project
git init
Initialized empty Git repository in ~/src/project/.git
```

#### Cloning a repository:

```
git clone power1:/data/PowerWeek
Cloning into 'PowerWeek'...
Password:
remote: Counting objects: 6, done.
remote: Compressing objects: 100% (4/4), done.
remote: Total 6 (delta 1), reused 0 (delta 0)
Receiving objects: 100% (6/6), done.
Resolving deltas: 100% (1/1), done.
Checking connectivity... done
```

### git - status of the local repository

#### Command: git status

```
richterm@power1 ~ git status
# On branch master
# Changes not staged for commit:
   (use "qit add <file>..." to update what will be committed)
   (use "qit checkout -- <file>..." to discard changes in working directory)
       modified: twoparticle.C
# Untracked files:
    (use "git add <file>..." to include in what will be committed)
    result.root
       twoparticle C.d
       twoparticle_C.so
no changes added to commit (use "git add" and/or "git commit -a")
```

- ▶ information about the current branch
- ▶ files which are staged for commit
- tracked files whith local changes
- untracked files (can be masked by .gitignore)

# git - committing



#### Step 1: git add mark changes to be committed

```
richterm@power1 ~/src/example_01 $ git add twoparticle.C
richterm@power1 ~/src/example_01 $ git status
# On branch master
# Changes to be committed:
# (use "git reset HEAD <file>..." to unstage)
#
# modified: twoparticle.C
#
# Untracked files:
# (use "git add <file>..." to include in what will be committed)
#
# result.root
# twoparticle_C.d
# twoparticle_C.so
```

# git - committing



#### Step 2: git commit changes

```
richterm@power1 ~/src/example_01 git commit -m "initial version of particle class"
[master a56e827] initial version of particle class
```

#### Now it is locally committed, check the log

```
richterm@power1 ~/src/example_01 git log
commit a56e8270fd6f3c99d4cdbcdb0e45f287e1c71711
```

Author: Matthias Richter <richterm@power1.power.week>

Date: Tue Nov 26 11:51:09 2013 +0100

initial version of particle class

 ${\tt commit \ ea2c328e7ac3e21c5546480dad1a55af4a0f5e35}$ 

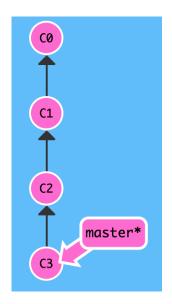
Author: Jochen Klein <jochen.klein@cern.ch>

Date: Mon Nov 25 13:51:12 2013 +0100

- initial commit of example

# git commits; git checkout

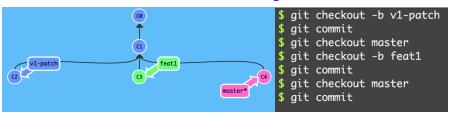
- git organizes commits in a connected tree of nodes; A git commit adds a new node
- each node consists of
  - ► The actual changeset/diff to files
  - Metadata (author, ...)
  - A commit message
  - A SHA-256 hash digest This hash uniquely identifies the precise node and all its history!
- one can checkout specific nodes by using git checkout <commit-sha>
- pointer to last node of main development line - is typically called master



#### The commit tree and branches

The git commit structure can be a tree. Pointers to leave nodes are called branches.

- The master branch is the main development line
- Other branches typically used for feature development in isolation (Feat1) or for releasing a certain stable version and patches (v1-patch)
- branches are started with git commit -b NewFeature on the currently checked out commit
- ▶ one can switch between branches with git checkout branchname



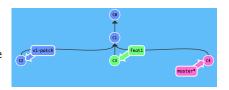
# Short intro to merging and rebasing

- merging/rebasing : operations on the tree to bring together 2 branches
- used to integrate commits from one branch into the other
- for example when feature is fully developed

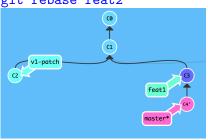
#### git merge feat1



- tree (old commits) stays intact
- merge creates adds a special commit



#### git rebase feat2



- branches are linearized
- no new commit; but old commits rewritten

### git - branching summary

- ▶ A branch means launching a separate line of development within a software project.
- ► A branch allows development to continue in multiple directions simultaneously
- ▶ Branches can be merged later on in the development cycle

#### Reasons for using branches:

- represent an individual customer release
- encapsulate a development phase, e.g prototype, beta, stable
- isolate the development of a single feature or research into a particularly complex bug
- represent the work of an individual contributor

### git - looking at the difference

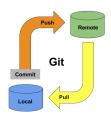
#### Command: git diff

```
richterm@power1 ~/src/example_01 git diff twoparticle.C
diff --git a/twoparticle.C b/twoparticle.C
index fdca6ac..77d77c5 100644
--- a/twoparticle.C
+++ b/twoparticle.C
00 - 1,7 + 1,7 00
// a simple macro with surprises for the purpose of training usage of valgrind
 // include header files for the porpose of compilation
-#ifndef CINT
+#if !defined(__CINT__) || defined(__MAKECINT__)
 #include "TParticle.h."
 #include "TSustem.h"
 #include "TH1.h"
```

- shows local differences in tracked files.
- without arguments: for all tracked files
- can be used to show differences between revisions

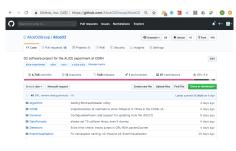
# Distributed gits: push and pull

- A git repository can exist at various locations (or in multiple copies) at the same time (it's distributed); one speaks of local and remote repositories.
- the authorative version of a git repository is often hosted on some web server (remote)
  - if you cloned from the remote it is called 'origin'
  - otherwise you can declare a remote repo with git remote add foo URL
- Users syncronize local and remote repositories via git pull and git push commands.
  - git pull [-rebase] foo get all remote changes and apply locally
  - git push foo publish your own changes to the remote



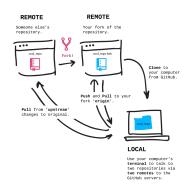
# Github/Gitlab/Bitbucket

- many open source projects host git on platforms like Github, Gitlab or Bitbucket
- free git server and infrastructure
- collaborative code reviews
- integrations with other services
  - task tracking
  - continuous integration (CI) automatic testing of new code and accepting only if good
  - documentation



# Github/Gitlab/Bitbucket - workflow

- ► A typical workflow on those platforms uses 3 repositories
  - the authorative repo (remote)
  - ▶ a fork (a user copy remote)
  - the local user repository
- Changes are integrated via push to fork and pull requests to real repo



### git - Further reading

We found the following nice looking pages ... but there are tons other really

- https://rogerdudler.github.io/git-guide/index.de.html
- https://try.github.io/ resources to learn git;
- https://www.atlassian.com/git/tutorials
- https://www.edureka.co/blog/git-tutorial/
- ▶ git help

#### git - stash

You are in the middle of developing and get a request to fix something or update your clone

⇒ stash allows to save your current status

```
> git pull
# ... pull fails due to merge conflicts ...
> git stash save
> git pull
> git stash pop
```

# git - checking logs revisited

tig; gitk; etc

#### **Exercises**

- Create a git repo; Do some add-commit cycles
- Play with branching merging:
  - locally
    - ▶ as an interactive game https://learngitbranching.js.org/
- ► Get familiar with github by forking or cloning the PowerWeek github repo https://github.com/hgspowerweek/powerweek1.
  - Look around
  - Contribute to the documentation of F.A.Q. section

### Lecture III

# Code compilation

#### What is GCC

- Originally 'only' GNU C Compiler
- ▶ Release in March 1987 as the first **free** ANSI C optimizing compiler
- ▶ C++ support was added in December of that year
- ▶ Now, many other languages are supported as well, e.g. Objective-C, Objective-C++, Fortran (gfortran), Java (gcj), ...
- ► In addition, many different CPU architectures supported, e.g. Intel, ARM, Alpha, PowerPC, ...
- Today GCC stands for GNU Compiler Collection

#### Compilers

A compiler translates the human readable code into machine executable code

The main compilers of the GCC suite we are interested in are the GNU C and C++ compilers: gcc and g++

Brian Gough http://www.network-theory.co.uk/docs/gccintro/

```
#include <iostream>
int main()
{
   std::cout << "hello world" << std::endl;
   return 0;
}
The hello world example above (hello_world.cpp) can be compiled using
   g++ -Wall hello_world.cpp -o hello_world
-o specifies the name of the executable (default it is a.out)</pre>
```

recommended to use

To run the program simply type

```
/hello world
```

Try it!

```
#include <iostream>
int main()
{
   std::cout << "hello world" << std::endl;
   return 0;
}</pre>
```

The hello world example above (hello\_world.cpp) can be compiled using g++ -Wall hello\_world.cpp -o hello\_world

- gri waii heiio\_woiiu.cpp o heiio\_woiiu
- specifies the name of the executable (default it is a.out)
- -Wall turns on most commonly used compiler warning o **highly**

#### recommended to use

To run the program simply type

```
/hollo world
```

Try it!

```
#include <iostream>
int main()
{
   std::cout << "hello world" << std::endl;
   return 0;
}</pre>
```

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- -o specifies the name of the executable (default it is a.out)
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#### recommended to use

To run the program simply type

```
./hello_world
```

Try it



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#include <iostream>
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}</pre>
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To run the program simply type

```
./hello_world
```

Try it!

# Splitting code

Often it is useful to split the code into separate logical files

- Enhances readability and maintenance
- Enables to compile code parts independently
  - Saves compilation time, not all code needs to be recompiled if somethings changes
- ► Allows to compile code using the functionality of other code without knowing the actual implementation

We split the hello\_world example into three files:

- ► main.cpp
- ▶ hello\_fn.h
- ► hello\_fn.cpp

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We split the hello\_world example into three files:

- main.cpp
- ▶ hello\_fn.h
- ▶ hello\_fn.cpp

## Splitting code - example

#### main.cpp

```
#include "hello_fn.h"
int main()
  hello("world");
  return 0;
hello fn.h
void hello(const char* to);
hello_fn.cpp
#include <iostream>
void hello(const char* to)
  // function to print hello to someone on the command line
  std::cout << "Hello " << to << std::endl;
}
```

## Splitting code - header files

- Separate the declaration of classes / functions from the actual implementation
- ▶ The declaration is given in the header file ending on .h
- ► When using external code in an own class, during compilation only the declaration is needed
- ► A declaration should not be included several times (compilation time), this is handled by a pre-compiler directive (header guard)

```
#ifndef MYCODE_H
#define MYCODE_H
void myfunction(int x, float y);
#endif
```

# Compile multiple source files

#### To compile the code run

```
g++ -Wall main.cpp hello_fn.cpp -o hello_world
```

 $\Rightarrow$  Try it!

Not won too much, still all code is compiled all the time

- compile parts of the code into separate object files
- ▶ *link* the *object files* to the executable

## Compile multiple source files

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Not won too much, still all code is compiled all the time

- compile parts of the code into separate object files
- ▶ link the object files to the executable

# Creating object files

We create one *object file* per input file:

```
g++ -Wall -c main.cpp hello_fn.cpp
```

- -c tells the compiler to create an object
- object files are machine code, but not yet executable

Produces the object files main.o and hello\_fn.o

```
This can also be run separately for each file
g++ -Wall -c main.cpp
g++ -Wall -c hello_fn.cpp
```

⇒ Try it

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This can also be run separately for each file

```
g++ -Wall -c main.cpp
g++ -Wall -c hello_fn.cpp
```

 $\Rightarrow$  Try it!

## Linking objects to an executable

Now the objects can be *linked* together to the executable:

```
g++ main.o hello_fn.o -o hello_world
```

#### NOTE:

The code is already compiled  $\rightarrow$  You don't need warning options

```
\Rightarrow Try it!
```

- ightharpoonup Modify something in one of the files (e.g. world ightarrow moon in main.cpp)
- ► Recompile only main.cpp
- ▶ Link all files to one executable

#### $\Rightarrow$ Try it

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The code is already compiled  $\rightarrow$  You don't need warning options

 $\Rightarrow$  Try it!

- ightharpoonup Modify something in one of the files (e.g. world ightarrow moon in main.cpp)
- Recompile only main.cpp
- Link all files to one executable
- $\Rightarrow$  Try it!

#### Makefiles

- ► The steps mentioned above can be automatized using the make system
- ▶ Define dependencies (e.g. the executable can only be built if all objects files are available)
- Only compiles code which changed

#### Documentation:

https://www.gnu.org/software/make/manual/make.html

# Makefiles - An example

```
CXX = /usr/bin/g++
CXXFLAGS = -Wall -Wextra -Wshodow -Wconversion -Wshadow -g
I.DFI.AGS =
OB.J
       = hello_fn.o main.o
split: $(OBJ)
        $(CXX) -o $0 $(OBJ) $(LDFLAGS)
main.o: main.cpp hello_fn.h
        (CXX) - 0 = 0 - c < (CXXFLAGS)
%.o: %.cpp %.h
         $(CXX) $(CXXFLAGS) -c $< -o $0
clean:
        @rm -f ${OBJ} split
```

#### Makefiles - Primer

Makefiles consist of rules that tell the make system what to do. A rule has the form:

```
target ...: prerequisites ...
<tab> recipe
<tab> ...
<tab> ...
```

target is usually an output file name, prerequisites can be other targets or e.g. file names

NOTE: A recipe MUST be started with a < tab >

When the make command is called, it looks for a file called *Makefile* or *makefile* in the present directory and processes the first target (*default target*).

#### Makefiles - Primer

A few important automatic variables are defined in the make system:

- ▶ \$@ The target name
- ▶ \$< The first prerequisite
- ▶ \$^ The names of all the prerequisites, with spaces between them

For more see https://www.gnu.org/software/make/manual/make.html#Automatic-Variables

 $\Rightarrow$  Try it!

#### CMake - introduction

- treatment of dependencies and automatic re-compilation covered by Makefiles and make
- manual maintenance of Makefiles can become tedious and error-prone
- configuration for specific setup of SDK and external dependencies covered by autotools suite or CMake

#### CMake - introduction

CMake is an open-source, cross-platform family of tools designed to build, test and package software.

- universal (toolchain agnostic) description of build flow in CMakeLists.txt
- automated creation of Makefiles depending on configuration options environment found
- automatic re-evaluation when needed
- possibly add testing and packaging steps

here: CMake with Makefiles

## typical build layout

- separate build into different directories:
  - source: no generated files
  - build: generated files, object files, libraries, executables possibly more than one with different build options
  - ▶ install: final files only
- ▶ test stage
- delivering/deploying stage

## a minimal CMake project

```
cmake_minimum_required(VERSION 3.9)
project(MyPowerProject CXX)
add_executable(testExe test.cc)
```

- always specify minimum version of CMake (depending on the features you use)
- declare project and language used
- add targets (here just one executable)

#### example project:

```
examples/cmake_simple
```

#### a CMake run

```
cd <build directory>
cmake <source directory>
make -j$(nproc)
```

bu

#### happens in phases:

- configuration: evaluation of CMakeLists.txt files, additional options, toolchain probing
- generation: generation of build files (depending on selected generator)
- compilation: actual build using Makefiles

#### **libraries**

```
add_library(power power.cc)
add_executable(main main.cc)
target_link_libraries(main power)
```

- ▶ add target for library and source files needed to build it
- ► link executable against library
- ▶ include directories are propagated to the targets using the library

## using lists

```
set(SOURCES s1.cc s2.cc s3.cc)
add_library(s ${SOURCES})

set(EXECUTABLES e1 e2 e3)
foreach(EXE ${EXECUTABLES})
add_executable(${EXE} ${EXE}.cc)
target_link_libraries(${EXE} power)
endforeach()
```

- define lists that can be reused
- avoid overly repetitive code

## **ROOT** integration

```
find_package(ROOT)
include(${ROOT_USE_FILE})
if(ROOT_FOUND)

message(STATUS "Using ROOT: ${ROOT_VERSION} <${ROOT_CONFIG}>")
target_compile_definitions(power PUBLIC "-DUSE_ROOT")
target_include_directories(power PRIVATE ${ROOT_INCLUDE_DIRS})
target_include_directories(power PRIVATE .)
ROOT_GENERATE_DICTIONARY(G__Power ${CMAKE_CURRENT_SOURCE_DIR}/power.h LINKDEF Lintarget_sources(power PRIVATE power_rooted.cc G__Power)
target_link_libraries(power ROOT::Core ROOT::Gui ROOT::Tree)
endif(ROOT_FOUND)
```

ROOT comes with additional tools to build dictionaries

## warnings and errors

```
message("something important")
message(STATUS "just a status message")
message(WARNING "something's fishy here")
message(ERROR "this is plain wrong")
message(FATAL_ERROR "this is too wrong, I rather die ...")
```

 use messages to check on your build, don't be blind on what is happening

#### language options

```
set(CMAKE_CXX_STANDARD 14)
set(CMAKE_CXX_STANDARD_REQUIRED ON)
message(STATUS "Using C++${CMAKE_CXX_STANDARD}")
enable_language(CUDA)
```

- compiler-agnostic settings of language standard
   N.B.: you can also request specific language features
- enabling of additional programming languages

### build types and compiler options

```
set(CMAKE_CXX_FLAGS_DEBUG "-00 -ggdb -DDEBUG -D__DEBUG")
set(CMAKE_CXX_FLAGS_RELWITHDEBINFO "${CMAKE_CXX_FLAGS_RELEASE} -ggdb")
set(CMAKE_CXX_FLAGS_RELEASE "-03 -march=native -ftree-vectorize -ffast-math -DNODED
message(STATUS "Using CXX flags for ${CMAKE_BUILD_TYPE}: ${CMAKE_CXX_FLAGS_${CMAKE_CXX_FLAGS_$}$
```

- compiler options/flags are controlled by build types
- can be changed separately for different build types
- don't put target-specific stuff here

```
cmake -DCMAKE_BUILD_TYPE=DEBUG <source dir>
```

# default build type

```
# by default build optimized code with debug symbols
if(NOT CMAKE_BUILD_TYPE AND NOT CMAKE_CONFIGURATION_TYPES)
set(CMAKE_BUILD_TYPE RELWITHDEBINFO)
endif()

set(CMAKE_ALLOWED_BUILD_TYPES DEBUG RELEASE RELWITHDEBINFO)
if(NOT CMAKE_BUILD_TYPE IN_LIST CMAKE_ALLOWED_BUILD_TYPES)
   message(FATAL_ERROR "Invalid build type ${CMAKE_BUILD_TYPE}}. Use one of: ${CMAKE_endif()}
```

explicit control over default build type

#### install

```
install(TARGETS main power
  LIBRARY DESTINATION lib
  RUNTIME DESTINATION bin
)
```

- ▶ this should install only the final build products
- ▶ try and adhere to conventions about installation paths

#### some more involved stuff

- nested projects
- tests

## nested projects

```
add_subdirectory(sub1)
add_subdirectory(sub2)
```

- include sub-projects in sub-directories, hierarchical layout
- sub-directories can contain project, this allows to build the sub-project independently
- different directories:
  - CMAKE\_SOURCE\_DIRECTORY: directory from which cmake was run
  - CMAKE\_PROJECT\_SOURCE\_DIRECTORY: (sub-)project directory
  - CMAKE\_CURRENT\_SOURCE\_DIRECTORY: current directory in source tree

#### **CTest**

you can add tests which can be run programatically

```
enable_testing()
add_test(NAME MyPowerTest COMMAND echo done)
ctest
```

#### summary

- surely not an extensive coverage of CMake, but it should get you started
- extensive documentation on project pages
   but not always good explanation of the underlying concepts