pip install ROOT Experiences making a complex multi-language package accessible for Python users

Vincenzo Eduardo Padulano<sup>1</sup>, Jonas Rembser<sup>1</sup>

[1] CERN, EP-SFT 21.10.2024, CHEP '24, Kraków, Poland





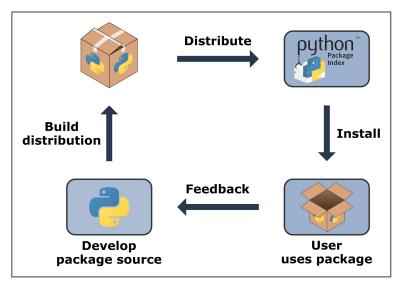
- Python packaging ecosystem
- ▶ pip install ROOT

# Python packaging ecosystem



### Python Packaging Authority (PyPA)

- Core working group for projects concerned with Python packaging
- Python packaging is a vast subject
  - <u>PyPA's overview</u>



Python Packages, 2023. Tomas Beuzen, Tiffany Timbers



# Python packaging

Three categories of distribution:

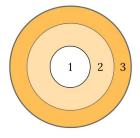
- Share one (or more) Python scripts
- sdist: source code installable via a backend
- wheel: binary compressed archive

"In fact, Python's package installer, pip, always prefers wheels because installation is always faster, so even pure-Python packages work better with wheels." PyPA. Overview of Python Packaging Packaging for Python tools and libraries

- 1. **.py** standalone modules
- 2. **sdist** Pure-Python packages
- 3. **wheel** Python packages

(With room to spare for static vs. dynamic linking)

PyPA. Overview of Python Packaging





## Python package build backends

### Generic

Support package building for many programming languages

Examples: <u>Anaconda</u>, <u>Spack</u>

Full flexibility in dependency management

Enable building complex software stacks in one environment

The same software provides package manager and build backend

### **Python-focused**

Specialised for building Python packages

Examples: setuptools, poetry, hatchling

Some emphasise integration with C, C++ code in the package

Examples: <u>scikit-build-core</u>, <u>py-build-cmake</u>, <u>meson-python</u>

Build backends are separate from the package manager (pip)

## pip install ROOT

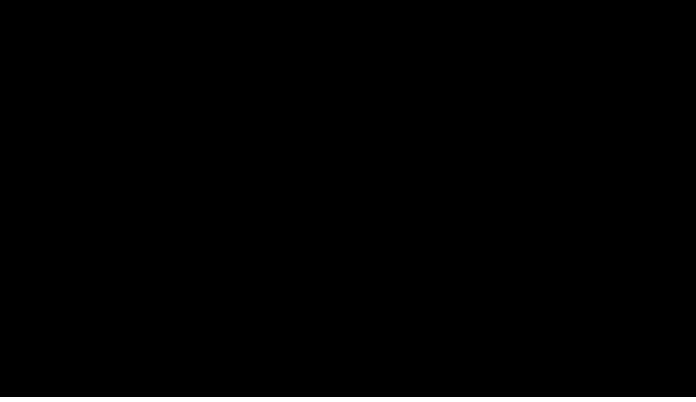


- ROOT: storage, I/O, processing, scientific analysis of structured data
- **EBs** data stored in **ROOT** format
- Many distribution channels
  - CVMFS, conda, system package managers (Linux, MacOS), official docker images, prebuilt binaries (Linux, MacOS, Windows), Snap.
- Missing distribution via pip
  - Makes the package more **easily obtainable** for Python users
  - Makes integration with downstream Python packages smoother



### Seeing it in action

### Working ROOT installation with pip (1.5x video speedup)





#### pip install ROOT -i https://root-experimental-python-wheels.web.cern.ch

```
$:docker run --rm -it python /bin/bash
root@6f40406ea5f2:/# python -m venv myenv
root@6f40406ea5f2:/# source myenv/bin/activate
(myenv) root@6f40406ea5f2:/# pip install ROOT -i https://root-experimental-python-wheels.w
eb.cern.ch
Looking in indexes: https://root-experimental-python-wheels.web.cern.ch
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Installing collected packages: ROOT
Successfully installed ROOT-0.1a6
(myenv) root@6f40406ea5f2:/# python
Python 3.13.0 (main, Oct 8 2024, 00:06:32) [GCC 12.2.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import ROOT
>>> df = ROOT.RDataFrame(10)
>>> df.Count().GetValue()
10
```





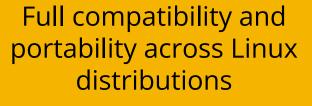
- ROOT is published as a wheel
  - One wheel per supported Python version (3.8+)
  - For now, only support all Linux distributions (x86\_64)
- The build backend (for now) is setuptools
- The wheels are built using two excellent tools
  - <u>cibuildwheel</u>
  - <u>manylinux</u> container image

**SETUPTOOLS** 

## The ROOT wheels

### cibuildwheel

- CI job orchestration
- Automatic process to build wheel
- Includes options to run tests
- manylinux
  - Portable Linux build distributions (<u>PEP513</u>)
  - Defines a minimal image with core set of dependencies (like conda)
    - glibc + few others
  - ROOT wheel complies with manylinux\_2\_28\_x86\_64 (PEP600)





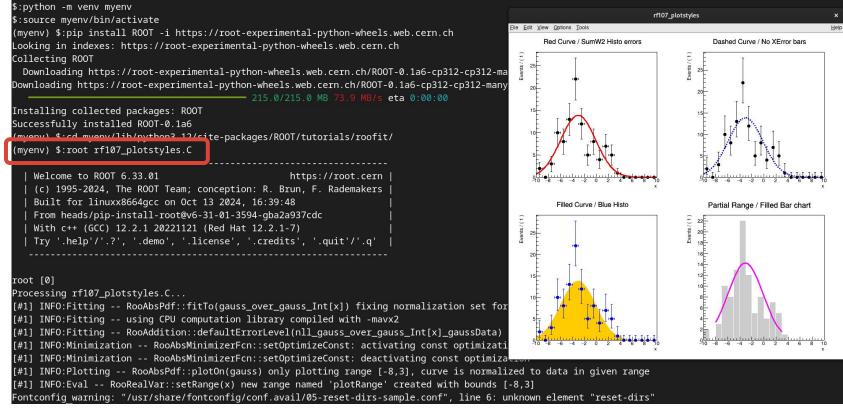
# Wheel work in progress

- WIP at <u>https://github.com/root-project/root/pull/16669</u>
- Few important ingredients
  - Proper management of RPATH variable aligned with "standard" Python venv directory layout
  - Similarly, install ROOT modules and libraries where they are expected
- Introducing changes that benefit the whole ROOT build system
- Currently provide only few components, to try things out
  - cling, Core libraries, I/O, RDataFrame, RooFit
- Showcase CLI executables with root



### ROOT cli executables

### As a first showcase, provide the root executable





### A more complete example

### Analysis grand challenge benchmark with CMS OpenData



### A more complete example

### Analysis grand challenge benchmark with CMS OpenData

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- Scientific packages often have non-trivial dependencies
- For this purpose, ROOT benefits a lot from conda
- pip build backends do not support external dependencies
  - This is a known and discussed limitation (<u>PEP725</u>, <u>1</u>, <u>2</u>, <u>3</u>)
- What to do in the meanwhile?



Different strategies can be adopted:

- Bundling external dependency in library (<u>quite common</u>)
- Load libraries from other pip-installable dependencies (e.g. xrootd, tbb) (<u>challenging</u>)
- Expect the dependency in the system, fail graciously otherwise
  - Inviting the user to follow installation instructions



#### Without

#### >>> import ROOT

ERROR in cling::CIFactory::createCI(): cannot extract standard library include paths! Invoking:

LC\_ALL=C c++ -xc++ -E -v /dev/null 2>&1 | sed -n -e '/^.include/,\${' -e '/^ V.\*++/p' -e '}' Results was:

With exit code 0

input\_line\_1:1:10: fatal error: 'new' file not found #include <new>

Warning in cling::IncrementalParser::CheckABlCompatibility(): Failed to extract C++ standard library version. input\_line\_4:36:10: fatal error: 'cassert' file not found

#include <cassert>

~~~~~~

input\_line\_9:1:10: error: 'iostream' file not found with <angled> include; use "quotes" instead #include <iostream>

^~~~~~~

#### "iostream"

IncrementalExecutor::executeFunction: symbol '\_ZN5cling7runtime6gClingE' unresolved while linking [cling interface function]!

You are probably missing the definition of cling::runtime::gCling

Maybe you need to load the corresponding shared library?

IncrementalExecutor::executeFunction: symbol '\_ZN5cling7runtime6gClingE' unresolved while linking [cling interface function]!

You are probably missing the definition of cling::runtime::gCling

Maybe you need to load the corresponding shared library?

IncrementalExecutor::executeFunction: symbol '\_ZN5cling7runtime6gClingE' unresolved while linking [cling interface function]!

You are probably missing the definition of cling::runtime::gCling

Maybe you need to load the corresponding shared library?

IncrementalExecutor::executeFunction: symbol '\_ZN5cling7runtime6gClingE' unresolved while linking [cling interface function]!

You are probably missing the definition of cling::runtime::gCling Maybe you need to load the corresponding shared library? \*\*\* Break \*\*\* segmentation violation Generating stack trace...

#### `docker run <u>python:3.12-slim</u>` (~45MB)

#### With

#### >>> import ROOT

Traceback (most recent call last): File "/myenv/lib/python3.12/site-packages/ROOT/\_\_init\_\_.py", line 22, in <module> subprocess.run(cmd, env=env, check=True, File "/usr/local/lib/python3.12/subprocess.py", line 548, in run

with Popen(\*popenargs, \*\*kwargs) as process:

File "/usr/local/lib/python3.12/subprocess.py", line 1026, in \_\_init\_\_ self.\_execute\_child(args, executable, preexec\_fn, close\_fds, File "/usr/local/lib/python3.12/subprocess.py", line 1955, in \_execute\_child raise child\_exception\_type(errno\_num, err\_msg, err\_filename) FileNotFoundError: [Errno 2] No such file or directory: 'c++'

The above exception was the direct cause of the following exception:

Traceback (most recent call last): File "<stdin>", line 1, in <module> File "/myenv/lib/python3.12/site-packages/ROOT/\_\_init\_\_.py", line 30, in <module> raise ImportError(textwrap.fill(msg. width=80)) from e

ImportError: Could not find a C++ compiler when importing ROOT. Make sure a C++ compiler as well as the C++ standard libraries are installed. For example, run `[apt,dnf] install g++` or follow similar instructions for your distribution. For more info, visit https://root.cern/install/dependencies

# Conclusions and outlook



## Conclusions and outlook

pip install ROOT -i https://root-experimental-python-wheels.web.cern.ch

- Demonstrated **ROOT** installation via **pip**
- Experimental wheels are provided
  - Installable and working on **any Linux distribution** (x86\_64)
  - Featuring some ROOT components to try out
- Drastically lowered obtainability barrier for Python users
- Next steps:
  - Run ROOT's **test suite** with **pip** builds as part of ROOT CI
  - Try more **flexible** build **backends** scikit-build-core?
  - Split in **smaller wheels**, e.g. root-core, root-rdf, root-roofit
  - Make the **pip** installation **robust**, **towards** a first **beta version**



## Conclusions and outlook

pip install ROOT -i https://root-experimental-python-wheels.web.cern.ch

Want to know more? Eager to try it out? Do you have suggestions for improvements? Would you like to contribute? Meet me around CHEP! And feel free to contact me at vincenzo.eduardo.padulano@cern.ch And of course also send us feedback <u>on the forum</u>!