Everything* you didn't know you needed

*blatant marketing nonsense

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CoDaS-HEP school 2022

Slides available as 🗘 open source, contributions welcome.

11/2/2022

Git & starting new projects

Pre-commit hooks &



Run small checks *before* you commit

- !? Problem: How can I stop myself from committing low-quality code?
- Solution:
 - git hooks allow you to run scripts that are triggered by certain actions
 - a pre-commit hook is triggered every time yourun `git commit`
 - in principle you can set them up yourself by placing scripts into `.git/hooks`

Making it practical:

- The pre-commit framework is a python package that makes configuring precommit hooks easy!
- All hooks are configured with a single `.pre-commit-config.yaml` file
- Few-clicks GitHub integration available: precommit.ci
- **Setting** it up:
 - 1. `pipx install pre-commit`
 - 2. 'cd <your repo>'
 - 3. `touch .pre-commit-config.yaml`
 - 4. `pre-commit install`
 - 5. Profit 🎉

Pre-commit hooks &

A config that will always be useful. Optional pre-commit.ci CI service.

```
repos:
     - repo: https://github.com/pre-commit/pre-commit-hooks
       rev: 'v4.3.0'
      hooks:
      - id: check-added-large-files
      - id: check-case-conflict
      - id: check-merge-conflict
       id: detect-private-key
       - id: end-of-file-fixer
 9
10
       - id: trailing-whitespace
11
12
     - repo: https://github.com/codespell-project/codespell # the spell checker with ~0 false positives
13
       rev: 'v2.1.0'
14
      hooks:
     - id: codespell
15
16
         # args: ["-I", "codespell.txt"] # Optional to add exceptions
17
18
     ci:
19
         autoupdate_schedule: monthly # default is weekly
```

Pre-commit hooks for python!

```
repo: https://github.com/psf/black # Reformat code without compromises!
         rev: '22.6.0'
         hooks:

    id: black

        # or, if you also work with Jupyter notebooks
        # - id: black-jupyter
        repo: https://github.com/PyCQA/flake8 # Simple static checks
         rev: '5.0.1'
         hooks:
10
         id: flake8
11
             additional_dependencies: ['flake8-bugbear']
12
         repo: https://github.com/pre-commit/mirrors-mypy # Check typing (slightly more advanced)
13
        rev: 'v0.971'
         hooks:
14
         - id: mypy
15
16
        repo: https://qithub.com/asottile/pyupgrade # Automatically upgrade old Python syntax
17
         rev: 'v2.37.2'
18
         hooks:
         id: pyupgrade
19
20
             args: [--py37-plus]
```

■ Try it out: Go here for a quick step-by-step tutorial

Cookiecutter

- !? Problem: Setting up e.g., a python package with unit testing/CI/CD, pre-commits, license, packaging information, etc., is a lot of "scaffolding" to be added.
- **Solution:** Creating templates
- Making it practical: cookiecutter is a command line utility for project templates

Examples:

- scikit-hep project template: All the features,
 all the best-practices
- my personal python template: Fewer options, easier to read (I think;))
- Pro-tip: cruft is a cookiecutter extension that allows to propagate updates to the template back to the projects that use it

Trying it out:

```
pipx install cookiecutter

# alternative: cruft https://...

cookiecutter https://github.com/scikit-hep/cookie/

# e.g., select project type = setuptools

# for the "traditional" way to set up your python

# package
```

SSH & Terminal Kung-fu

SSH Config

- !? Problem: Typing long servernames and potentially tunnelling can be tiresome
- **Solution:** Create configuration in `~/.ssh/config`. You can even add pattern matching!

```
# Server I want to connect to
Host tiger*
Hostname tiger.princeton.edu
User k15675

# Tunnel that I might use sometimes
Host tigressgateway
Hostname tigressgateway.princeton.edu
User k15675

Host *-t
ProxyJump tigressgateway
```

Now you can use `ssh tiger` or `ssh tiger-t` depending on whether to tunnel or not.

SSH Escape Sequences

- !? Problem: I already have an SSH session. How can I quickly forward a port?
- Solution: SSH Escape Sequences:
 - Hit Enter ~ c (now you should see a `ssh>` prompt)
 - Add `-L 8000:localhost:8000` Enter to forward port 8000
 - More escape sequences available! More information.
- Caveat: c option not available in multiplexed sessions.

Terminal kung-fu

- Vou can quickly search through your terminal history with Ctrl R start typing
 - Hit ctrl R to navigate between different hits
- You can reference the last word of the previous command with `!\$`

```
1 mkdir /path/to/some/directory/hello-world
2 cd !$
```

- Want to fix up a complicated command that just failed? Type `fc` to edit the command in your `\$EDITOR`
- If you're using `bash`, consider switching to `zsh` (almost completely compatible) and install `oh-my-zsh` to get beautiful prompts, autocomplete on steroids and many small benefits

```
1  $ ~/D/P/x¬
2  ~/Document/Projects/xonsh/
3  $ part¬
4  this-is-part-of-a-filename
```

How to shell...

- !? Problem: `man` pages are wasting your time?
- Solution: Try `tldr` (`pipx install tldr`). Compare:



How to shell...

- !? Problem: Understanding cryptic bash commands
- Solutions: Go to explainshell.com



File navigation and completion

- !? Problem: Changing directories in the terminal is cumbersome.
- **Solution:** Autojump learns which directories you visit often. Hit `j <some part of directory name>` to directly jump there
- Installation instructions on github

Usage:

```
1  cd codas-hep # <-- autojump remembers this
2
3  cd ../../my-directory
4  cd some-subfolder
5
6  j codas # <-- get back to codas-hep folder</pre>
```

File navigation and completion

- !? Problem: I like visual file managers, but I'm working on a server...
- Solution: Use a terminal file manager, e.g., `ranger` (`pipx install ranger-fm`)



- !? Problem: I search through files a lot, but `grep` is slow/inconvenient...
- **Solution:** There are faster and more feature-rich alternatives. Example: ripgrep, `ag`, ...
- !? Problem: Even with tab completion, completing file names is cumbersome.
- Solution: Try type-ahead-searching/fuzzy matching, e.g., with <u>fzf</u> with <u>shell integration</u>, e.g.,

Python

Hot code reloading

!? Problem:

- 1. I have some code in a notebook and some code in a python file/library.
- 2. I update my python file/library.
- 3. Do I have to restart the kernel and rerun to see the changes?
- Solution: No! Python supports a number of ways to "reload" imported code.
- Easiest example: Add the following to your Jupyter notebook¹ to reload all (!) modules every time you execute code

```
1 %load_ext autoreload
2 %autoreload 2 # reload everything
```

More granular:

```
1 %load_ext autoreload
2 %autoreload 1 # <-- reload only some modules
3
4 # Mark for reloading
5 %aimport foo</pre>
```

- Warning: These tricks don't always work, but it should save you from a lot of restarts
- Try it out! Follow our instructions here.
- More information: See the autoreload documentation

Tracking Jupyter notebooks with git

- !? Problem: Tracking & collaborating on Jupyter notebooks with git is a mess because of binary outputs (images) and additional metadata:
 - `git diff` becomes unreadable
 - merge conflicts appear often
- **Solutions:** You have several options
 - 1. Always strip output from notebooks before committing (easy but half-hearted)
 - 2. Synchronize Jupyter notebooks and python files; only track python files (slightly more advanced but best option IMO)
 - 3. Do not change how you *track* Jupyter notebooks; change how you *compare* them (use if you *really* want to track outputs). Example: <code>`nbdime`</code>
 - 4. Avoid large amounts of code in notebooks so that the issue is less important; create python packages and use hot code reloading instead

Tracking Jupyter notebooks with git

Option 1: Track notebooks but strip outputs before committing. Add the following pre-commit hook:

```
1 - repo: https://github.com/kynan/nbstripout
2    rev: 0.5.0
3    hooks:
4    - id: nbstripout
```

Option 2: Synchronize Jupyter notebooks (untracked) to python files (tracked)

```
pipx install jupytext
echo "*.ipynb" >> ~/.gitignore # <-- tell git to ignore noteboks
jupytext --to py mynotebook.ipynb

# Now you have mynotebook.py
git commit mynotebook.py -m "..."

git push
# People modify the file online
git pull # <-- mynotebook.py got updated
jupytext --sync # <-- update mynotebook.ipynb

# Now make changes to your mynotebook.ipynb
jupytext --sync # <-- now mynotebook.py got updated
git commit ... && git push ...</pre>
```

Satic code checkers and Jupyter notebooks

- !? Problem: I still have lots of code in my notebooks. I still want to apply tools like black, pyupgrade, ... on the notebooks.
- **Solution:** `nbqa` allows to apply a lot of tools to Jupyter notebooks

Avoiding dependency hell

- !? Problem: Python packages depend on other packages depending on other packages causing a conflict.
- Solution: Use conda or virtual environments (`venv`, `virtualenv`, `virtualenvwrapper`);

The first environment should be named `.venv`

- The Python Launcher for Unix, `py` picks up `.venv` automatically!
- Visual Studio Code does too, as do a growing number of other tools.

- !? Problem: What about `pip`-installable executables?
- Solution: Install them with `pipx` instead of `pip`! Examples:
 - pre-commit` · `black` · `cookiecutter` · `uproot-browser`

You can also use `pipx run` to install & execute in one step, cached for a week!

Lockfiles

- !? Problem: Upgrades can break things.
- **Not a solution:** Don't add upper caps to *everything*! Only things with 50%+ chance of breaking.
- **Solution:** Use lockfiles.

Your CI and/or application (including an analysis) should have a *completely pinned environment* that works. This is not your install requirements for a library!

```
pip install pip-tools
pip-compile requirements.in # -> requirements.txt
```

Now you get a locked requirements file that can be installed:

```
pip install -r requirements.txt
```

Locking package managers

Locking package managers ('pdm', 'poetry', 'pipenv') give you this with a nice all-in-one CLI:

```
pdm init # Setup environment using existing lockfile or general requirements

# Modify pyproject.toml as needed

pdm add numpy # Shortcut for adding to toml + install in venv
```

You'll also have a `pdm.lock` file tracking the environment it created. You can update the locks:

```
1 pdm update
```

Read up on how to use the environment that this makes to run your app.

Task runners

- !? Problem: There are lots of way to setup environments, lots of ways to run things.
- **Solution:** A task runner (nox, tox, hatch) can create a reproducible environment with no setup.
- Nox is nice because it uses Python for configuration, and prints what it is doing.

```
import nox

monox.session
def tests(session):
    session.install(".[test]")
    session.run("pytest")
```

Task runners

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```
import nox

nox.session

def tests(session: nox.Session) -> None:

"""

Run the unit and regular tests.

"""

session.install(".[test]")
session.run("pytest", *session.posargs)
```

Task runners

Example 1: adapted from `PyPA/manylinux`

Example 2: `python.packaging.org`

```
1  @nox.session(py="3")
2  def preview(session):
3    session.install("sphinx-autobuild")
4  build(session, autobuild=True)
```

```
@nox.session(py="3")
     def build(session, autobuild=False):
         session.install("-r", "requirements.txt")
         shutil.rmtree(target_build_dir,
                        ignore_errors=True)
         if autobuild:
             command = "sphinx-autobuild"
             extra_args = "-H", "0.0.0.0"
         else:
10
11
             command = "sphinx-build"
             extra_args = (
12
13
                 "--color".
                 "--keep-going".
14
15
16
17
         session.run(
18
             command, *extra_args,
19
             "-i". "auto".
20
             "-b", "html",
21
             "-n", "-W",
22
             *session.posargs,
23
             "source", "build",
24
```

pytest: Make testing fun

Basics

`pytest` discovers test functions named `test_...` in files `test_...`. For example:

```
1  def test_funct():
2  assert 4 == 2**2
```

To run: `pip install pytest` and then `pytest` to discover & run them all.

First tip: your `project.toml` file

```
[tool.pytest.ini_options]
minversion = "6.0" # minimal version of pytest

# report all; check that markers are configured; check that config is OK

addopts = ["-ra", "--strict-markers", "--strict-config"]

xfail_strict = true # tests marked as failing must fail

filterwarnings = ["error"]

log_cli_level = "info"

testpaths = ["tests"] # search for tests in "test" directory
```

pytest: Make testing fun

- `--showlocals`: Show all the local variables on failure
- `--pdb`: Drop directly into a debugger on failure
- `--trace --lf`: Run the last failure & start in a debugger
- You can also add `breakpoint()` in your code to get into a debugger

Reminder: https://scikit-hep.org/developer/pytest is a great place to look for tips!

pytest: Make testing fun Fixtures allow reuse, setup, etc

Approx

This works natively on arrays, as well!

Test for errors

```
def test_raises():
    with pytest.raises(ZeroDivisionError):
    1 / 0
```

Marks

There are quite a few built-in fixtures. And you can write more:

```
1  @pytest.fixture
2  def my_complex_object():
3     mco = MyComplexObject(...)
4     mco.xyz = "asf"
5     ...
6     return mco
7
8  def test_get_value(my_complex_object):
9     assert my_complex_object.get_value() == ...
10
11  def test_other_property(my_complex_object):
12  assert my_complex_object.property == ...
```

Monkeypatching

"unit".

System IO, GUIs, hardware, slow processes; there are a lot of things that are hard to test! Use monkeypatching to keep your tests fast and

¹or any IPython system

Type checking

- !? Problem: Compilers catch lots of errors in compiled languages that are runtime errors in Python! Python can't be used for lots of code!
- **Solution:** Add types and run a type checker.

- Functions always have types in and out
- Variable definitions rarely have types

How do we use it? (requires `pipx install mypy`)

```
mypy --strict tmp.py
Success: no issues found in 1 source file
```

Some type checkers: MyPy (Python), Pyright (Microsoft), Pytype (Google), or Pyre (Meta).

Example files available here.

Type checking (details)

- Adds text but adds checked content for the reader!
- External vs. internal typing
- Libraries need to provide typing or stubs can be written
- Many stubs are available, and many libraries have types (numpy, for example)
- An active place of development for Python & libraries!

```
from __future__ import annotations
 2
 3
     def f(x: int) -> list[int]:
         return list(range(x))
 5
 6
     def g(x: str | int) -> None:
         if isinstance(x, str):
 9
             print("string", x.lower())
10
         else:
11
             print("int", x)
12
```

Type checking (Protocol)

But Python is duck-typed! Noooooo!

Duck typing can be formalized by a Protocol:

```
from typing import Protocol # or typing_extensions for < 3.8
 2
     class Duck(Protocol):
         def quack(self) -> str:
     def pester_duck(a_duck: Duck) -> None:
         print(a_duck.quack())
 9
     class MyDuck:
11
         def quack(self) -> str:
             return "quack"
12
13
     # Check explicitly that MyDuck is implementing the Duck protocol
14
     if typing.TYPE_CHECKING:
15
16
         _: Duck = typing.cast(MyDuck, None)
```

Type checking (pre-commit)

```
1  - repo: https://github.com/pre-commit/mirrors-mypy
2  rev: "v0.971"
3  hooks:
4  - id: mypy
5  files: src
6  args: []
7  additional_dependencies: [numpy==1.22.1]
```

- Args should be empty, or have things you add (pre-commit's default is poor)
- Additional dependencies can exactly control your environment for getting types

Benefits

- Covers all your code without writing tests
 - Including branches that you might forget to run, cases you might for forget to add, etc.
- Adds vital information for your reader following your code
- All mistakes displayed at once, good error messages
- Unlike compiled languages, you can lie if you need to
- You can use `mypyc` to compile (2-5x speedup for mypy, 2x speedup for black)

GitHub Actions: pages deploy

Bonus: About a week ago GitHub Actions added direct deploy to pages!

```
1  on:
2   workflow_dispatch:
3   pull_request:
4   push:
5
6  permissions:
7   contents: read
8   pages: write
9   id-token: write
10
11  concurrency:
12   group: ${{ github.workflow }}-${{ github.ref }}
13   cancel-in-progress: true
```

```
jobs:
       build:
         runs-on: ubuntu-latest
         steps:
           uses: actions/checkout@v3
           - name: Setup Pages
             id: pages
             uses: actions/configure-pages@v1
           # Static site generation, latex, etc. here
10
11
12
           - name: Upload artifact
13
             uses: actions/upload-pages-artifact@v1
             with:
14
15
               path: dist/
16
17
       deploy:
18
         if: github.ref == 'refs/heads/main'
         needs: build
19
20
         environment:
21
           name: github-pages
22
           url: ${{ steps.deployment.outputs.page_url }}
23
         runs-on: ubuntu-latest
24
         steps:
25
           - name: Deploy to GitHub Pages
26
             id: deployment
27
             uses: actions/deploy-pages@v1
```

ACT (for GitHub Actions)

- !? Problem: You use GitHub Actions for everything. But what if you want to test the run out locally?
- **Solution:** Use ACT (requires Docker)!

```
# Install with something like brew install act
act
act # Runs on: push
act pull_request -j test # runs the test job as if it was a pull request
```

If you use a task runner, like nox, you should be able to avoid this most of the time. But it's handy in a pinch! https://github.com/nektos/act

Python libraries: Rich, Textual, Rich-cli

Textualize is one of the fastest growing library families. Recently Rich was even vendored into Pip!

progress bar demo (Using Python 3.11 TaskGroups, because why not)

```
from rich.progress import Progress
import asyncio

async def lots_of_work(n: int, progress: Progress) -> None:
    for i in progress.track(range(n), description=f"[red]Computing {n}..."):
        await asyncio.sleep(.1)

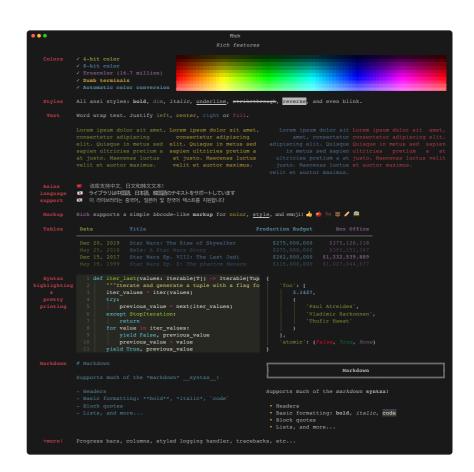
async def main():
    with Progress() as progress:
        async with asyncio.TaskGroup() as g:
        g.create_task(lots_of_work(40, progress))
        g.create_task(lots_of_work(30, progress))

asyncio.run(main())
```

Rich: Beautiful terminal output

Rich is not just a "color terminal" library.

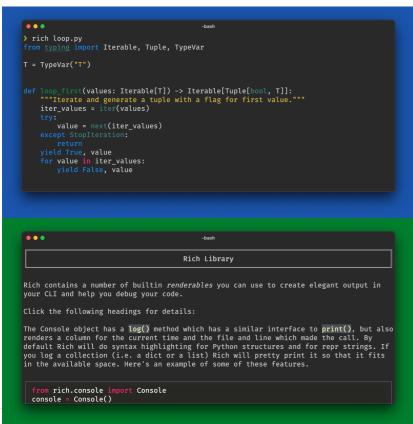
- Color and styles
- Console markup
- Syntax highlighting
- Tables, panels, trees
- Progress bars and live displays
- Logging handlers
- Inspection
- Traceback formatter
- Render to SVG



Textual: GUI? No, TUI!

New "CSS" version coming soon!

Rich-cli: Rich as a command line tool



```
• • •
                                                      Rich CLI v1.2.2 🤮
                                          Rich text and formatting in the terminal
Usage: rich [OPTIONS] <PATH, TEXT, URL, or '-'>
                                               Print console markup. See
                                                                    edocs.io/en/latest/markup.html
                                               Display a horizontal rule.
    -m --markdown
                                                Display as <u>JSON</u>.
    -h --head LINES
                                                Display as markdown
                                                Display first LINES of the file.
    -t --tail LINES
                                                Display last LINES of the file.
                                                Enable emoji code. e.g. :sparkle:
                                                Align to left.
                                                Align to center.
                                                Justify text to left.
                                                Justify text to right.
                                                Justify text to both left and right edges.
                                                Enable soft wrapping of text (requires --print).
        --expand
                                                Expand to full width (requires --panel).
                                                Fit output to SIZE characters.
        --width SIZE
                                                Set maximum width to SIZE characters.
                                                Set text style to STYLE.
        --style STYLE
         --rule-style STYLE
                                                Set rule style to STYLE.
                                                Use CHARACTER to generate a line with --rule.
         --rule-char CHARACTER
    -d --padding TOP,RIGHT,BOTTOM,LEFT Padding around output. 1, 2 or 4 comma separated integers, e.g. 2,4 a --panel BOX set panel type to BOX. ascii, ascii2, double, heavy, none, raunded,
                                                Set the panel style to STYLE (requires --panel).
                                                Set syntax theme to THEME. See https://pygments.org/styles/
         --theme THEME
                                               Enable line number in syntax.
                                               Enable indentation guides in syntax highlighting
                                               Use LEXER for syntax highlighting. See
        --lexer LEXER
                                               Render hyperlinks in markdown.
                                               Don't word wrap syntax highlighted files.
                                               Set panel title to TEXT.
                                               Force terminal output when not writing to a terminal.
         --title TEXT
         --caption TEXT
                                               Write HTML to PATH.
         --force-terminal
                                               Show this message and exit.
        --export-html PATH
```

WebAssembly

- !? Problem: Distributing code is hard. Binder takes time to start & requires running the code one someone else's machine.
- **Solution:** Use the browser to *run* the code with a WebAssembly distribution, like Pyodide. Python 3.11 officially supports it now too! Binaries may be provided around 3.12!

Pyodide

A distribution of CPython 3.10 including ~100 binary packages like SciPy, Pandas, boost-histogram (Hist), etc.

Examples:

- https://henryiii.github.io/level-up-your-python/live/lab/index.html
- https://scikit-hep.org/developer/reporeview

PyScript

An Python interface for Pyodide in HTML.

WebAssembly - PyScript

```
<!DOCTYPF html>
     <html lang="en">
     <head>
       <meta charset="utf-8">
       <meta name="viewport" content="width=device-width, initial-scale=1">
       <title>Hello, World!</title>
       <link rel="stylesheet" href="https://pyscript.net/alpha/pyscript.css" />
       <script defer src="https://pyscript.net/alpha/pyscript.js"></script>
 9
     </head>
10
     <body>
11
       <py-script>print("Hello, World!")</py-script>
12
     </body>
13
     </html>
```

https://realpython.com/pyscript-python-in-browser

Modern packaging

- !? Problem: Making a package is hard.
- Solution: It's not hard anymore. You just need to use modern packaging and avoid old examples.

```
1  [build-system]
2  requires = ["hatchling"]
3  build-backend = "hatchling.build"
4  
5  [project]
6  name = "package"
7  version = "0.0.1"
```

Other metadata should go there too, but that's the minimum. See links:

- https://scikit-hep.org/developer/pep621
- https://packaging.python.org/en/latest/tutorials/packaging-projects

[`]scikit-hep/cookie` supports 11 backends; hatching is recommended for pure Python. For compiled extensions: See next slides(s). $\ensuremath{\mathbb{\omega}}$

Binary packaging

- !? Problem: Making a package with binaries is hard.
- **Solution:** Some parts are easy, and I'm working on making the other parts easy too!

Making the code

Use a tool like pybind11, Cython, or MyPyC. It's hard to get the C API right!

```
#include <pybind11/pybind11.hpp>

int add(int i, int j) {
    return i + j;
}

PYBIND11_MODULE(example, m) {
    m.def("add", &add);
}
```

Header only, pure C++! No dependencies, no pre-compile step, no new language.

Configuring the build

I'm working on scikit-build for the next three years! CMake for Python packaging.

Currently based on distutils & setuptools - but will be rewritten!

Org of several packages:

- Scikit-build
- CMake for Python
- Ninja for Python
- moderncmakedomain
- Examples

Building the binaries

Redistributable wheel builder.

- Targeting macOS 10.9+
- Apple Silicon cross-compiling 3.8+
- All variants of manylinux (including emulation)
- musllinux
- PyPy 3.7-3.9
- Repairing and testing wheels
- Reproducible pinned defaults (can unpin)

Local runs supported too!

```
1 pipx run cibuildwheel --platform linux
```

GitHub actions example

```
on: [push, pull_request]
     jobs:
       build wheels:
          runs-on: ${{ matrix.os }}
         strategy:
           matrix:
              08:
             - ubuntu-22.04
             - windows-2022
10
11
             - macos-11
12
13
         steps:
         - uses: actions/checkout@v4
14
15
          - name: Build wheels
16
17
           uses: pypa/cibuildwheel@v2.8.1
18
19
         - uses: actions/upload-artifact@v3
           with:
20
21
             path: ./wheelhouse/*.whl
```