Things you didn't know that you thought you knew that... something

Henry Schreiner

2024-07-23

Python 3.13

Largest change to CPython ever

```
def pi(trials: int) -> float:
    Ncirc = 0
    rand = random.Random()

    for _ in range(trials):
        x = rand.uniform(-1, 1)
        y = rand.uniform(-1, 1)

        test = x * x + y * y
        if test <= 1:
            Ncirc += 1

    return 4.0 * (Ncirc / trials)
```

Threads	Time (s)
1	6.48
2	3.28
4	1.74

Running with 10M

Caveats:

"Free" thread safety gone*

(*Python has always supported concurrency)

Have to rebuild all extensions

Extensions have always been able to release the GIL

```
def pi_in_threads(threads: int, trials: int) -> float:
    with ThreadPoolExecutor(max_workers=threads) as executor:
        return statistics.mean(executor.map(pi, [trials // threads] * threads))
```

https://github.com/scikit-build/scikit-build-sample-projects/blob/main/projects/hello-free-threading

Learn some Rust

Even if you don't use it (yet)

Packaging

Modern without legacy (C++23 - C++98)

(AKA CrowdStrike) Memory Safety (compile time)

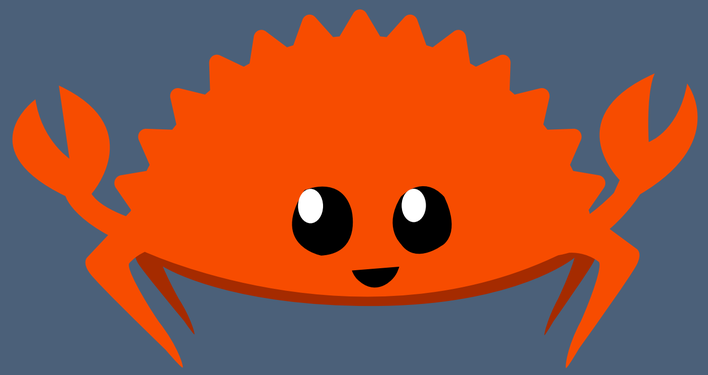
Explicit error handling

Great compiler messages

Traits

Declarative programming

Crabs are cuter than snakes



Some Rust projects

This is why it's interesting

BAT

Pretty cat replacement

PRESENTERM

Terminal presentations

PYPROJECT-FMT

Formatter for pyproject.toml

ZENITH

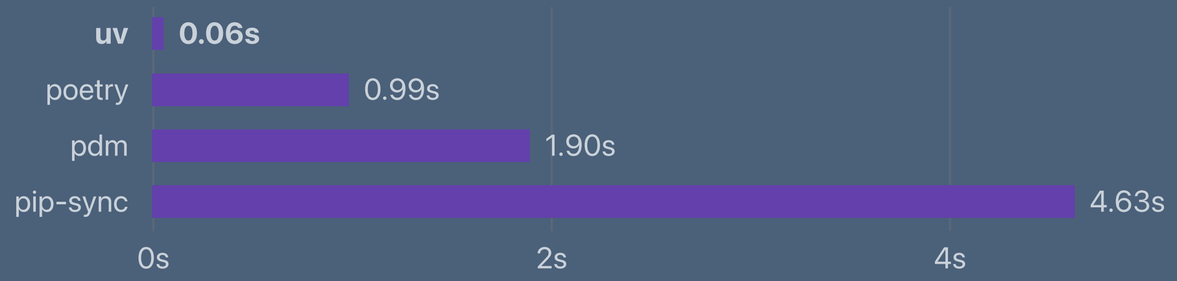
top/htop replacement

UV

Replacement for pip/venv/pip-tools

10-100x faster than pip & co.

Will be replacing more soon!

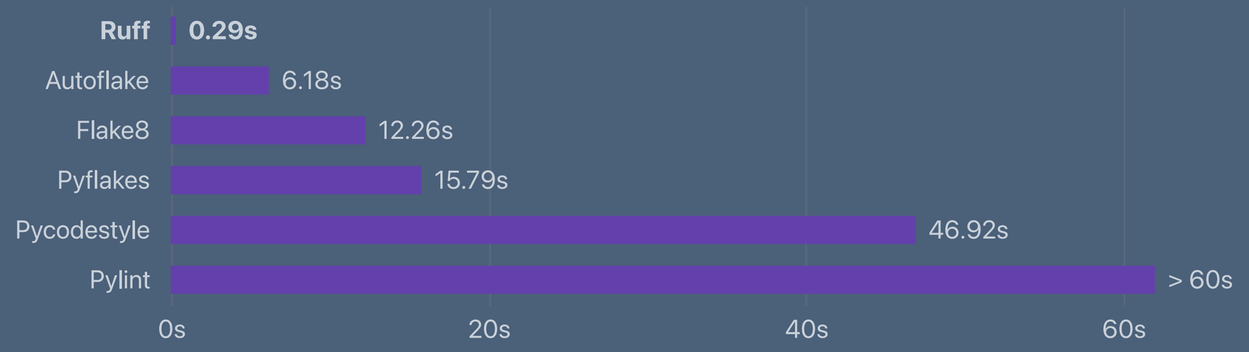


RUFF

Replacement for liners and formatters

10-100x faster

Single binary instead of 40+ packages



UV

Faster pip

```
python3 -m venv .venv
```

1.06 s

```
uv venv
```

18 ms

```
.venv/bin/pip install torch
```

Cold cache: 39.8 s
Warm cache: 21.3 s

```
uv pip install torch
```

Cold cache: 10.5 s
Warm cache: 358 ms

Practical examples:

scientific-python/cookie's CI went from 12 minutes -> 6 minutes.
nox's docs build went from 22 seconds -> 4 seconds.

Use a build system

Describe what you want, not how to get it

- **Modern** CMake isn't bad! (3.15+ at least, maybe newer)
- Or you can try Meson, build2, Bazel, etc.
- Integrates with IDEs, profilers, etc.
- Integrates with the Python builds system via scikit-build-core (or meson-python for meson)
- Integrates with OpenMP via brew on macOS* ;)
- Try using Ninja generator (more parallel than Make)

```toml
# pyproject.toml
[build-system]
requires = ["scikit-build-core"]
build-backend = "scikit_build_core.build"

[project]
name = "example"
version = "0.0.1"
```

```cmake
# CMakeLists.txt
cmake_minimum_required(VERSION 3.15...3.30)
project(example LANGUAGES C)

find_package(
  Python REQUIRED COMPONENTS
  Interpreter Development.Module)

python_add_library(example MODULE WITH_SOABI
                           example.c)

install(TARGETS example DESTINATION .)
```

* Requires a path on Apple Silicon because Homebrew moved

Pre-commit

Check and formatter framework

Make a list of checks and formatters to run

Supports over a dozen languages

Thousands of hooks

Ultra fast

Also supports git hooks (like pre-commit)

```
pre-commit run -a
check for added large files..............................................Passed
check for case conflicts.................................................Passed
check for merge conflicts................................................Passed
check for broken symlinks.....................(no files to check)Skipped
check yaml...............................................................Passed
debug statements (python)................................................Passed
fix end of files.........................................................Passed
mixed line ending........................................................Passed
python tests naming......................................................Passed
fix requirements.txt..........................(no files to check)Skipped
trim trailing whitespace.................................................Passed
ruff.....................................................................Passed
ruff-format..............................................................Passed
rst ``code`` is two backticks............................................Passed
rst directives end with two colons.......................................Passed
rst ``inline code`` next to normal text..................................Passed
blacken-docs.............................................................Passed
cmake-format.............................................................Passed
mypy.....................................................................Passed
check sdist..............................................................Passed
codespell................................................................Passed
shellcheck...............................................................Passed
Disallow improper capitalization.........................................Passed
Disallow expressions.....................................................Passed
Cog the documentation....................................................Passed
Validate pyproject.toml..................................................Passed
Validate Dependabot Config (v2)..........................................Passed
Validate GitHub Workflows................................................Passed
Validate ReadTheDocs Config..............................................Passed
Validate JSON Schema files...............................................Passed
```

Pre-commit setup

.pre-commit-config.yaml

```yaml
repos:

  - repo: https://github.com/pre-commit/pre-commit-hooks
    rev: '4.4.0'
    hooks:
      - id: check-added-large-files
      - id: check-case-conflict
      - id: check-merge-conflict
      - id: detect-private-key
      - id: end-of-file-fixer
      - id: trailing-whitespace

  - repo: https://github.com/astral-sh/ruff-pre-commit
    rev: v0.5.2
    hooks:
      - id: ruff
        args: ["--fix", "--show-fixes"]
      - id: ruff-format
```

Repo with .pre-commit-hook.yaml

Pinned for reproducibility

Repo can have any number of hooks

Can override any field (like args)

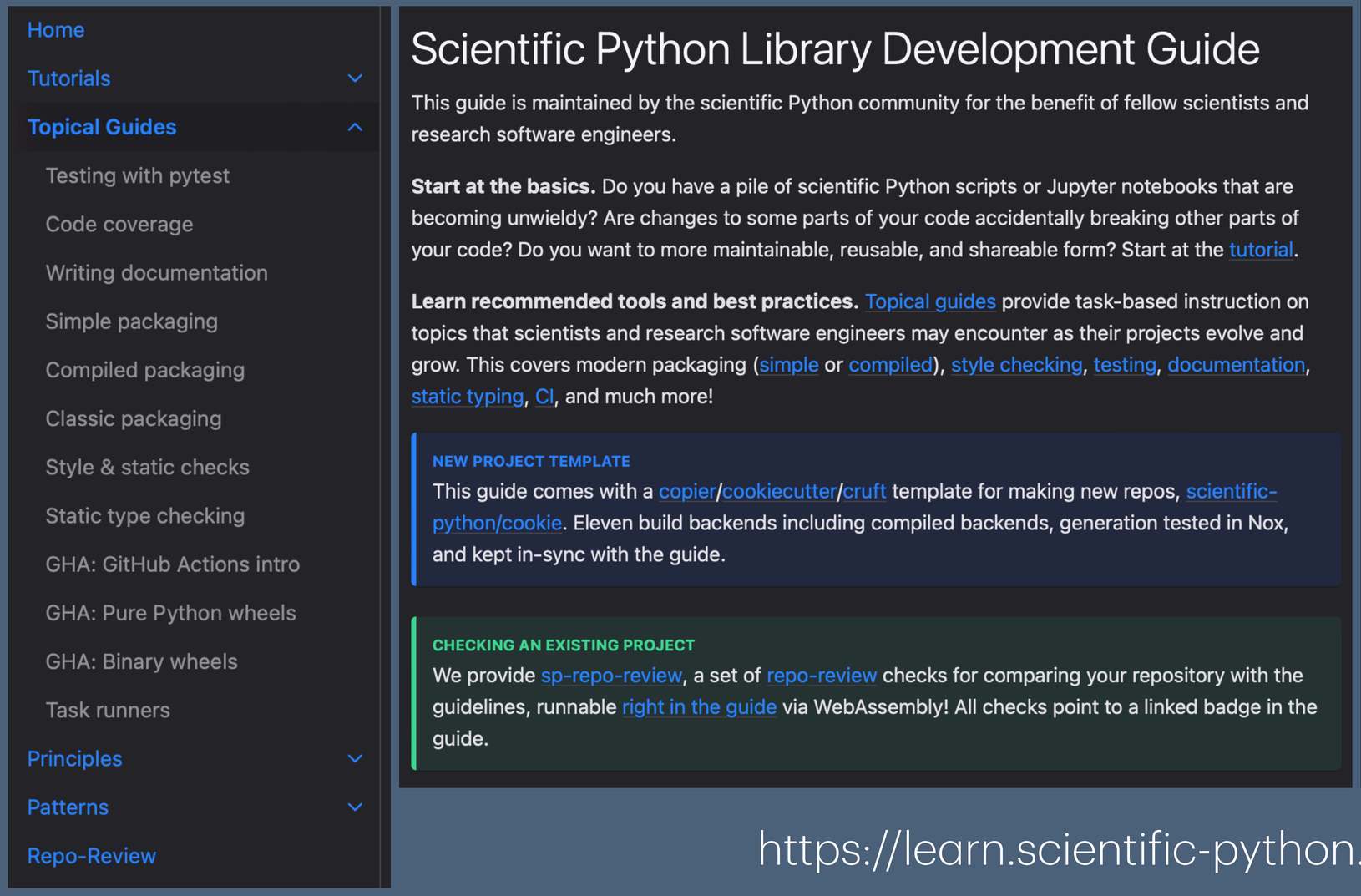
Pre-commit: other features

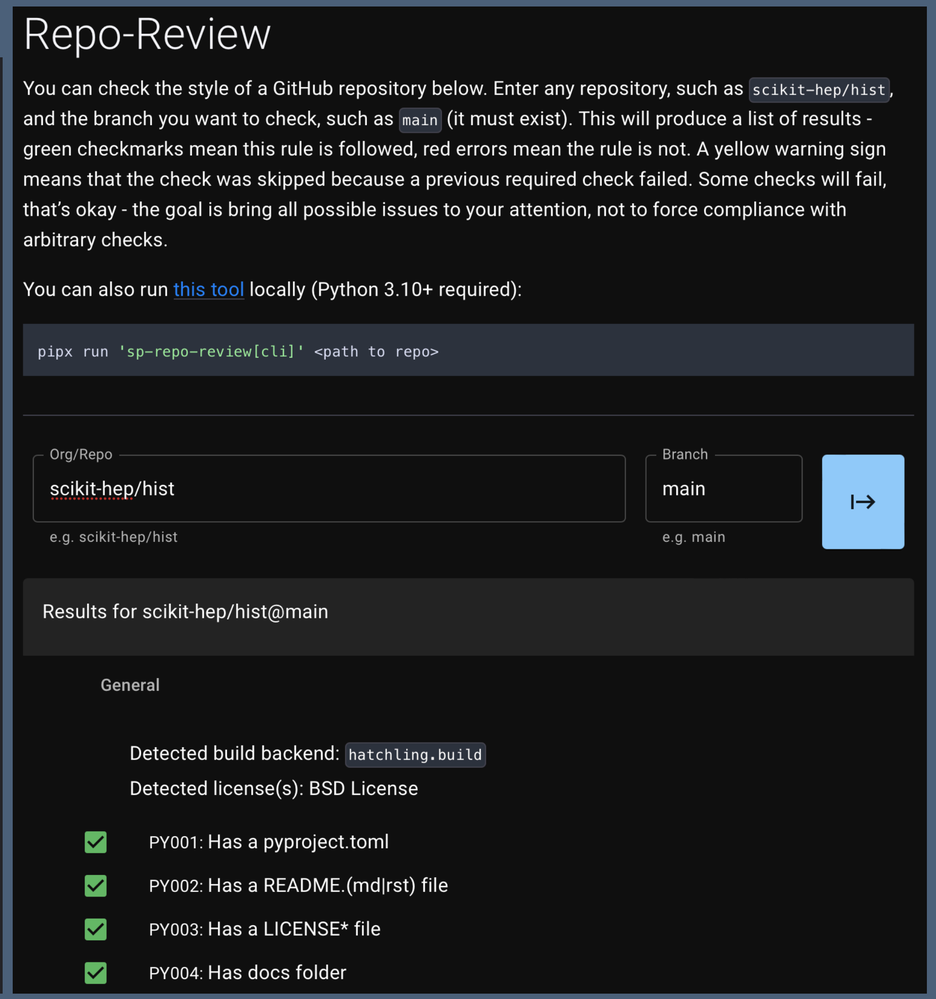
More good stuff

- Every check globally cached (fast)
- pre-commit install -> will run as git hook on all commits (-n to skip)
- pre-commit autoupdate —parallel -> will update all pins
- Local hooks - can disallow greps for content or files, etc.
- pre-commit.ci: free-for-open-source service
  - Update your pins weekly/monthly/quarterly
  - Auto-commit fixes to PRs
  - Ultra fast with global caching

Scientific Python Development Guide

One stop for all about Python packaging





https://learn.scientific-python.org/development

More info

Links to projects / tutorials

ISciNumPy.dev

A random collection of Science, Numerics, C++, CMake, and Python related topics.

Favorite posts and series

C++ 11 14 17 20 23 • macOS (AS) / Windows Setup • Azure DevOps (Python Wheels) • Conda-Forge ROOT • CLI11 • GooFit • cibuildwheel • Hist • Python Bindings • Python 2→3 3.7 3.8 3.9 3.10 3.11 3.12 3.13 • SSH

My classes and books

Modern CMake • CompClass • se-for-sci

My workshops

CMake Workshop • Python CPU, GPU, Compiled minicourses • Level Up Your Python • Packaging

My projects

pybind11 (python_example, cmake_example, scikit_build_example) • cibuildwheel • build • pipx • nox • pyproject-metadata • scikit-build (core, cmake, ninja, moderncmakedomain) • boost-histogram • Hist • UHI • Vector • GooFit • Particle • DecayLanguage • Conda-Forge ROOT • Jekyll-Indico • uproot-browser • Scientific-Python/cookie • repo-review • CLI11 • meson-python • Plumbum • validate-pyproject(-schema-store) • pytest GHA annotate-failures • flake8-errmsg • check-sdist • beautifulhugo • POVM • hypernewsviewer

My sites

Scientific-Python Development Guide • IRIS-HEP • Scikit-HEP • CLARIPHY