scverse cookiecutter template

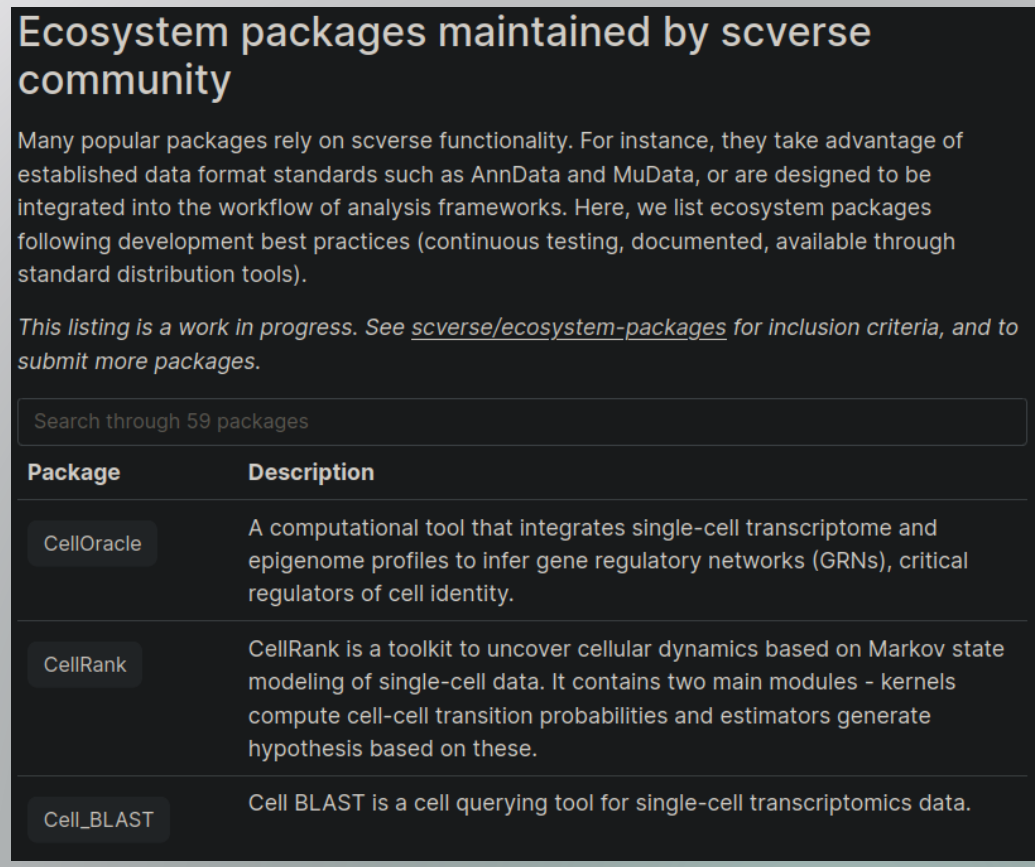
Follow along: scverse.org/cookiecutter-scverse-presentation

having impact with software

- Publish papers and get citations for academic success
- High quality software helps a lot with both
- Be part of the scverse ecosystem: ensure you meet minimum requirements for maximal impact
  - Get reviewed by PyOpenSci?
- Workshop goal: path to high quality software dev

scverse ecosystem

- Set of packages built around the scverse core packages
- Featured on the scverse ecosystem website



Ecosystem packages maintained by scverse community

Many popular packages rely on scverse functionality. For instance, they take advantage of established data format standards such as AnnData and MuData, or are designed to be integrated into the workflow of analysis frameworks. Here, we list ecosystem packages following development best practices (continuous testing, documented, available through standard distribution tools).

This listing is a work in progress. See scverse/ecosystem-packages for inclusion criteria, and to submit more packages.

Search through 59 packages

Package	Description
CellOracle	A computational tool that integrates single-cell transcriptome and epigenome profiles to infer gene regulatory networks (GRNs), critical regulators of cell identity.
CellRank	CellRank is a toolkit to uncover cellular dynamics based on Markov state modeling of single-cell data. It contains two main modules - kernels compute cell-cell transition probabilities and estimators generate hypothesis based on these.
Cell_BLAST	Cell BLAST is a cell querying tool for single-cell transcriptomics data.

scverse ecosystem requirements

- Metadata: name, description, OSI-approved license, ...
- Versioned releases installable from PyPI &/or Conda
- Tests automated via continuous integration (CI)
- Docs for API and use-cases
- Scverse datastructures used where appropriate

how to get into the scverse ecosystem

Instructions to add your package are on the scverse ecosystem repository

- Submit existing package, or
- Easiest way: scverse cookiecutter template

scverse cookiecutter template

- Project template for scverse packages[1]
- Best practice structure
- Many features such as continuous integration, documentation setup, …
- Automatically ticks all scverse ecosystem requirements

[1]Much is applicable elsewhere

steps

1. Set up global environment to create project
2. Create project using scverse cookiecutter template
3. Set up project specific development environment
4. Develop your package
5. Submit to scverse ecosystem

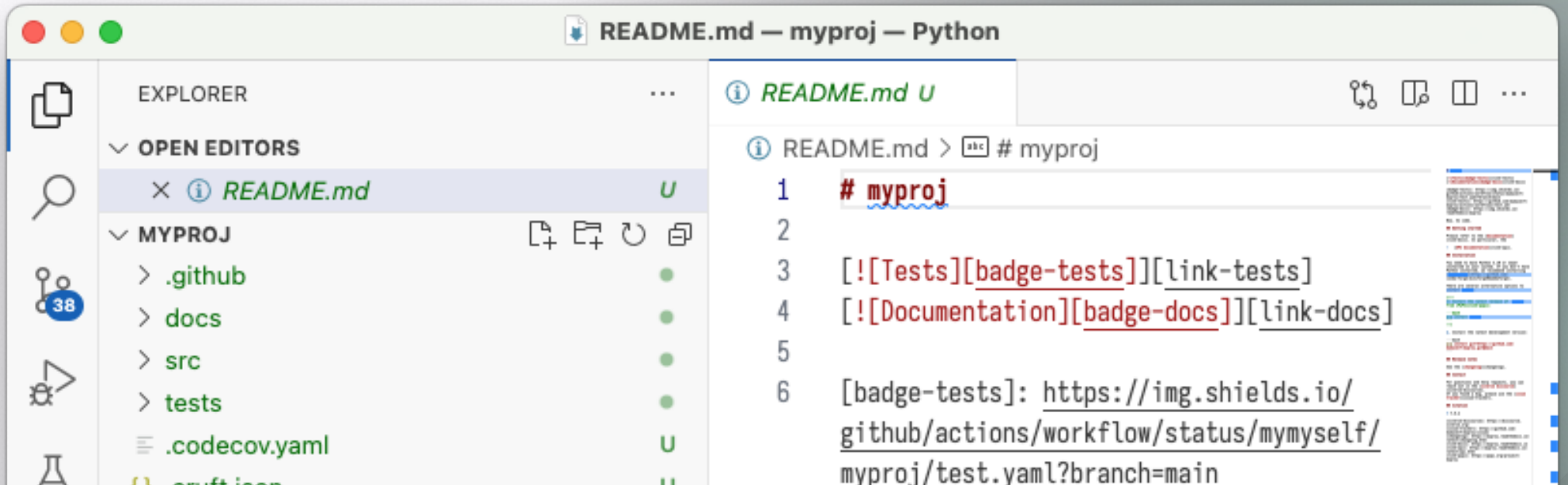
step 1: global environment

- Install using a package manager or installer:
  - `code`, `hatch`, & `git`
  - `uv` or `pipx`
- Install using a package manager, `pipx`, or `uv`:
  - `cruft` & `pre-commit`

```
$ pipx install cruft pre-commit  # or
$ uv tool install cruft pre-commit
```

step 2: creating the project

```
$ cruft create https://github.com/scverse/cookiecutter-scverse
  project_name (project-name): myproj
  […]
$ code myproj
```



step 3: environment management

Hatch envs basic usage:

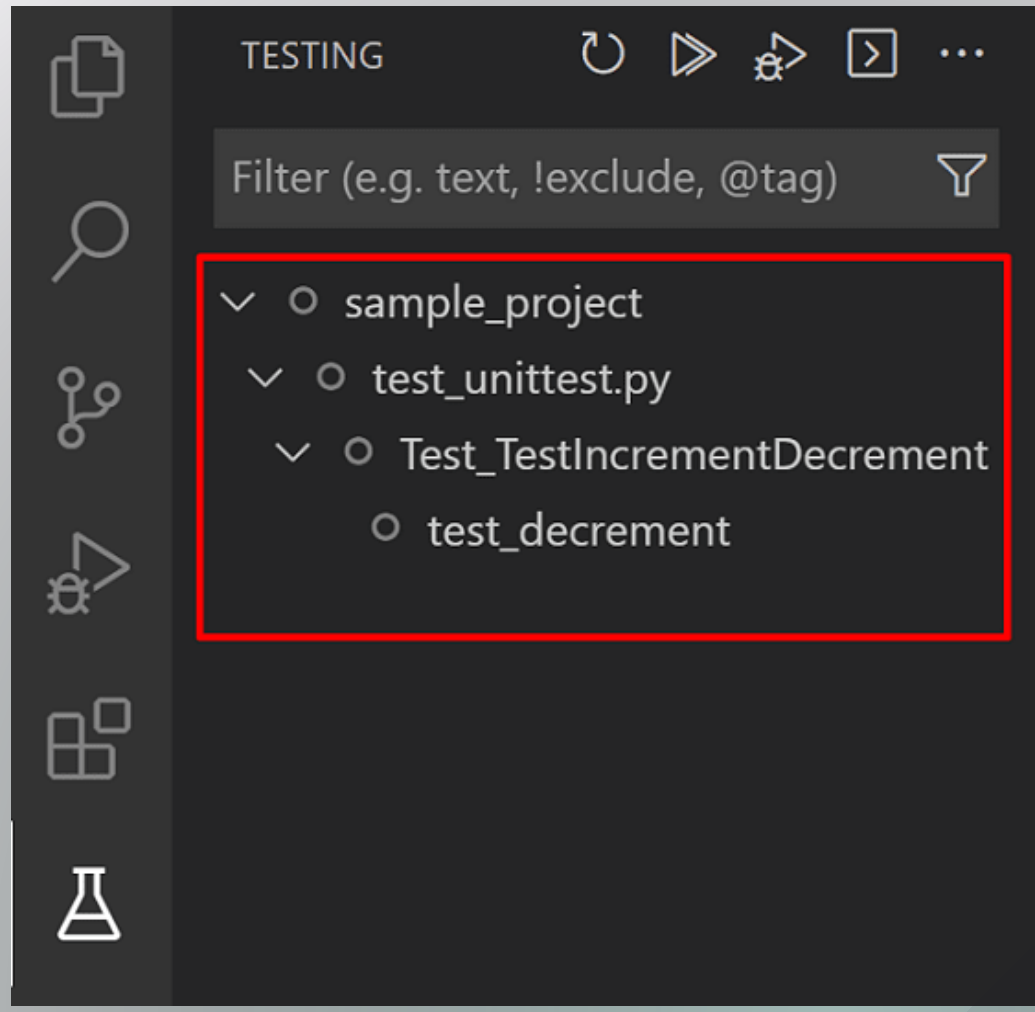
```
$ hatch run [env:]command [...args] # e.g. `… docs:build -T`
$ hatch test [...args]
$ hatch env remove <name> # or `hatch env prune` for all
$ hatch env find hatch-test
~/.local/share/hatch/env/virtual/myproj/FsejNibV/hatch-test.py3.12
[…]
```

Make sure it exists, then tell VS Code:

⌘|^+␣+P → Python: Select Interpreter

running tests

```
$ hatch test --help
[…]
Options:
  -r, --randomize
  -p, --parallel
  -c, --cover
  -a, --all
  -py, --python=X.Y
  -i, --include=VAR=VAL
  -x, --exclude=VAR=VAL
  -s, --show
…otherwise same as `pytest`
```

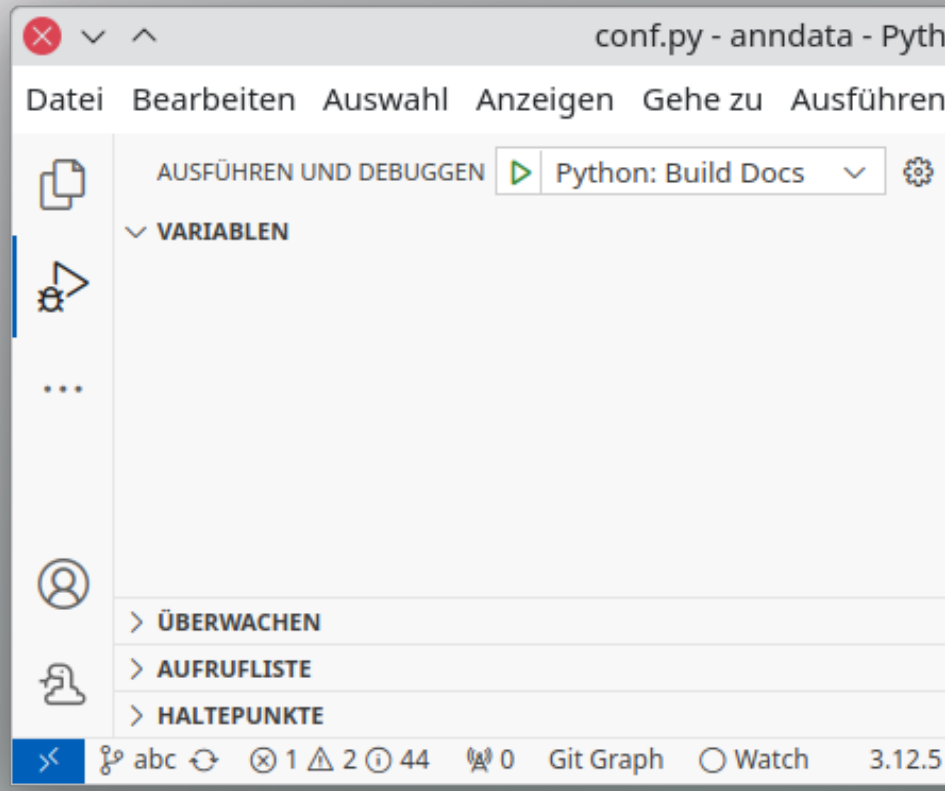


building docs

```
$ hatch run docs:build
$ hatch run docs:open
$ hatch run docs:clean
```

See `pyproject.toml`:

```
[tools.hatch.envs.docs]
scripts.build = "..."
...
```



formatting and linting

VS Code:

```
{
  "[python]": {
    "editor.formatOnSave": true,
    "editor.defaultFormatter": "charliermarsh.ruff",
    "editor.codeActionsOnSave": { ... },
  }, ...
}
```

CLI: `pre-commit` (or `hatch run pre-commit`)

```
$ pre-commit install # `git commit` hook
$ pre-commit run --all-files
```

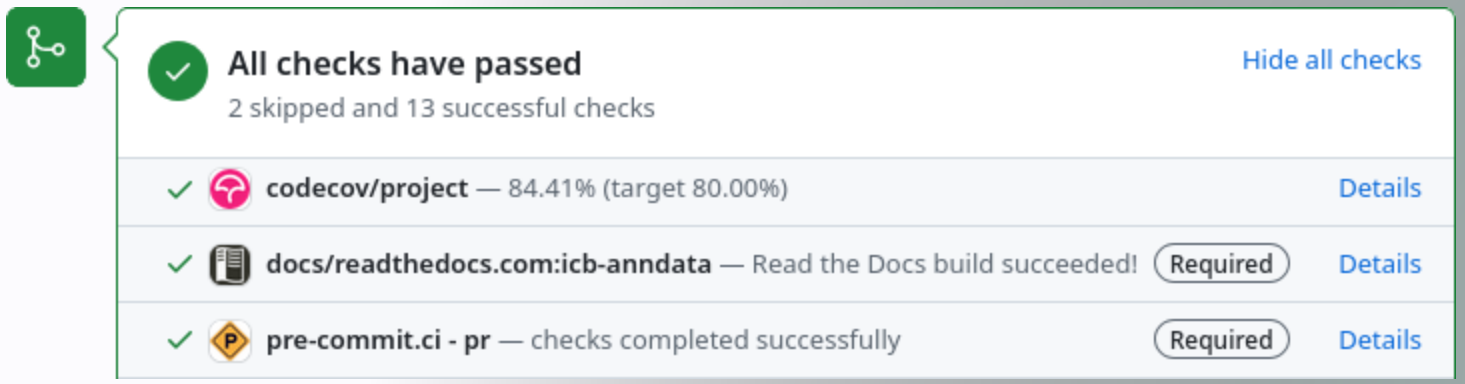
existing project

- Simple project
  1. Instantiate template
  2. Replace `src/*` directory with your package
  3. Edit `[project]` table in `pyproject.toml`
- Complex project
  1. Step by step PRs: formatter, …
  2. We can help!

follow along

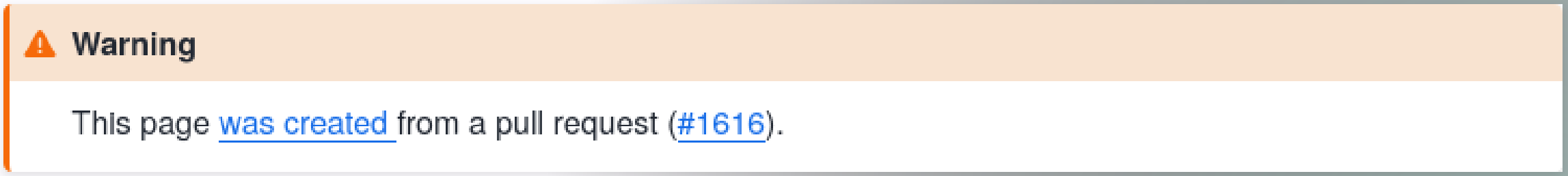
step 4: committing code

- Use PRs, don't push to `main`
- Set up pre-commit.ci, codecov.io on github.com/<you>/<yourpackage>/settings/installation



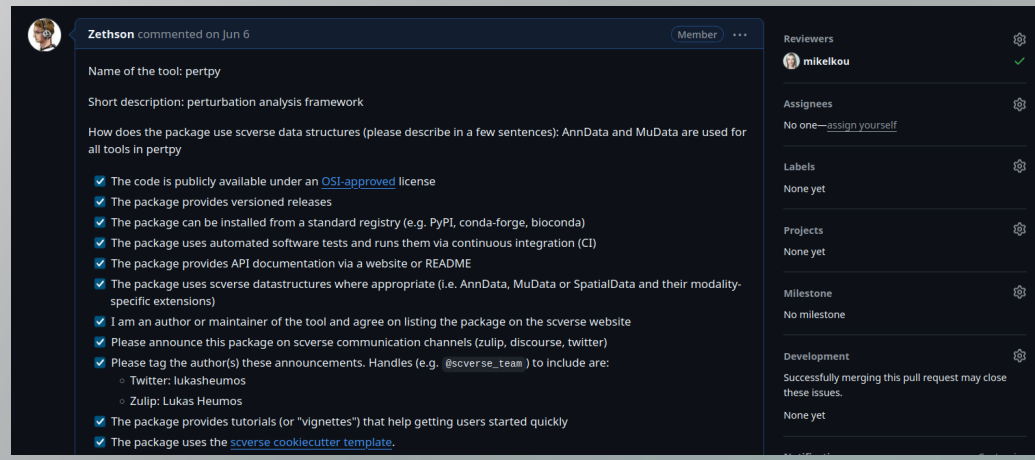
ReadTheDocs

- Set up readthedocs.org and its PR previews:



step 5: submit to scverse ecosystem

1. Follow the instructions
2. Submit a pull request
3. Maybe get reviewed by PyOpenSci



Thank You!