

How to Package and Publish Your Python Code

Winter 2026 Research Computing Workshops

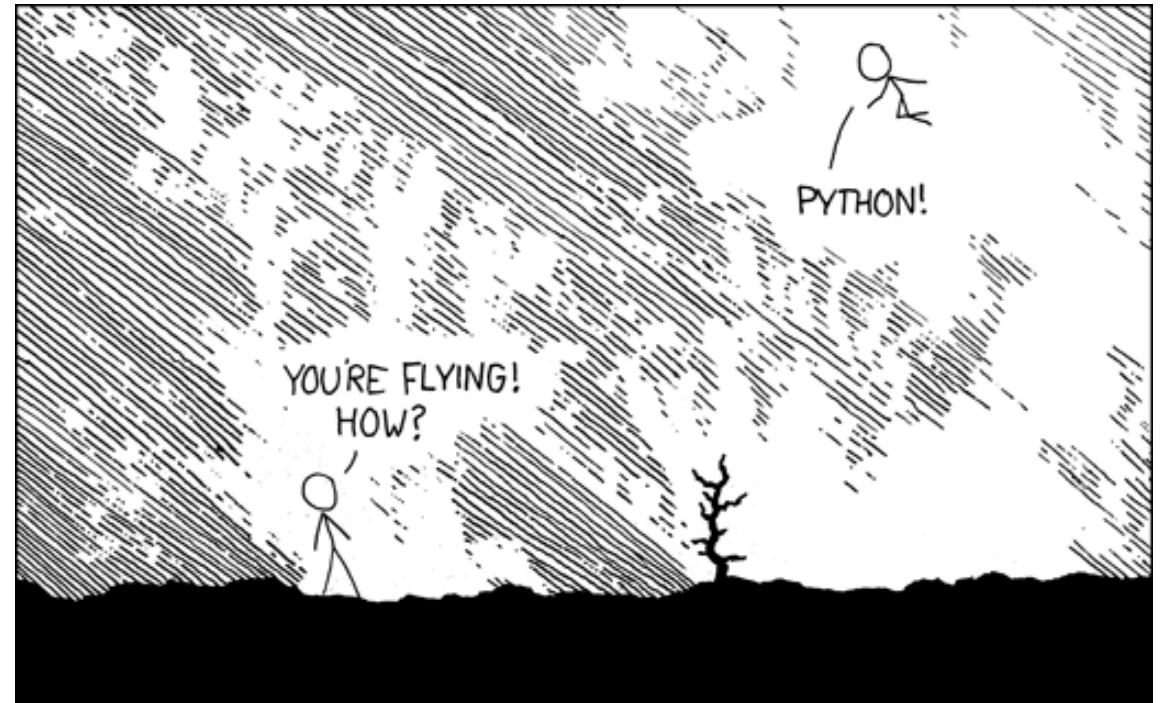
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Outline

- Python Packages
- Using a python package
- How to create a python package
 - Organization
 - Hands-on
- Summary

Python Packages: What are they & why do we care

- A reusable way to share code
- Dramatically accelerate development
- Make large projects manageable



How do we use a python package

- We install the package by using tools such as pip, conda, uv, hatch, etc.
 - Installed in the loaded environment
- Best use a virtual environment
 - Separates system and user environment
 - Provides reproducible environments
- After installation is complete, import package

Build systems

Setup tools	Poerty	Hatch/ hatchling	meson-python	scikit-build-core	uv
Industry standard	Modern	Modern build backend	Very fast builds, Esp. C/C++ ext.	Modern Cmake intergation	Extremely fast
pure Python and extension modules	Integrated env management	Both python and extensions	Good for complex projects	Good for C/C++ extensions	All-in-one tool
setup.py, setup.cfg, and pyproject.toml	Only pyproject.toml	Integrated environment management	Used by Numpy and SciPy	Requires Cmake knowledge	Grows rapidly
Multiversion	Offers lockfile	Small community	Need to learn meson	Complex for simple projects	Breaking changes possibles
Slow and complex	Can be slow	Still evolving	Maybe an overkill	Still evolving0	Features are still added

What will we use

- Github
 - Please create a github project named picalc_[netid]
- Uv
- Adroit
- <https://test.pypi.org>
 - Please create an account
 - Please create an API key
 - Copy the key and save it in a text document for now

How to create a python package

- uv can be installed easily on nearly any system and doesn't rely on python
 - <https://docs.astral.sh/uv/getting-started/installation/>
- Clone your empty repo first
- The following command will create a new directory called picalc_ip8725 for our package
 - uv init --package picalc_ip8725 -build_backend setuptools

How to create a python package

- pyproject.toml file
- Specific folder structure
- Tools like uv does it automatically

```
[ip8725@adroit5 picalc_ip8725]$ tree .
.
├── pyproject.toml
└── README.md
    └── src
        └── picalc_ip8725
            └── __init__.py

2 directories, 3 files
[ip8725@adroit5 picalc_ip8725]$
```

```
[build-system]
requires = ["setuptools>=61.0.0"]
build-backend =
"setuptools.build_meta"

[project]
name = " picalc_ip8725"
version = "0.1.0"
description = "A short description
of my project"
readme = "README.md"
requires-python = ">=3.8"
```

Adding dependencies

- Through uv
- By changing pyproject.toml
- Optional dependencies
 - We will use later

```
[project]
name = "picalc-ip8725"
version = "0.1.0"
description = "Add your description here"
readme = "README.md"
requires-python = ">=3.9"
dependencies = [
    "numpy>=2.0.2",
]
[project.scripts]
example-package = "example_package:main"
[build-system]
requires = ["setuptools>=61"]
build-backend = "setuptools.build_meta"
[dependency-groups]
dev = [
    "pytest>=8.4.2",
]
```

How do we add more code? Build?

- Let's add a pi calculation
- We need to add an `__init__.py`
- Add a script in `pyproject`:

```
[project.scripts]
picalc-ip8725 = "picalc_ip8725:main"
example-pi = "picalc_ip8725.pi.pi:main"
```
- Install it
 - Through uv
 - With pip
- uv build

```
[ip8725@adroit5 example_package]$ tree .
.
├── pyproject.toml
└── README.md
src
└── example_package
    ├── __init__.py
    └── pi
        ├── __init__.py
        └── pi.py
3 directories, 5 files
[ip8725@adroit5 example_package]$ █
```

Let's use the optional dependencies

- We will create a test
- Install everything
 - Through uv
- Run pytests

Let's publish it

- Setup `pypirc` first
- `uv tool install twine`
- `uv tool run twine upload --repository testpypi dist/*`

The screenshot shows the PyPI account dashboard. On the left, there is a sidebar with options: Your account, Your projects (which is selected and highlighted in blue), Your organizations, Account settings, and Publishing. The main area is titled "Your projects" and shows three items:

- picalc-ip8725** | SOLE OWNER
Last released 3 minutes ago
Add your description here
Manage View
- iceberg-rivers.search** | SOLE OWNER
Last released Mar 30, 2021
The ICEBERG Rivers usecase package
Manage View
- iceberg-penguins.search**
Last released Feb 20, 2020
The ICEBERG Penguin colony usecase package
Manage View

From Github workflows

- Create a release.yaml github workflow
- Add a publisher on pypi
- Create a github release

GitHub GitLab Google ActiveState

Read more about GitHub Actions' OpenID Connect support [here](#).

Owner (required)
owner
The GitHub organization name or GitHub username that owns the repository

Repository name (required)
repository
The name of the GitHub repository that contains the publishing workflow

Workflow name (required)
workflow.yml
The filename of the publishing workflow. This file should exist in the `.github/workflows/` directory in the repository configured above.

Environment name (optional)
release
The name of the [GitHub Actions environment](#) that the above workflow uses for publishing. This should be configured under the repository's settings. While not required, a dedicated publishing environment is strongly encouraged, especially if your repository has maintainers with commit access who shouldn't have PyPI publishing access.

Add