



Software Best Practices

Code Design, Style, and Quality

Having a purposeful code design and a set style improves readability. Quality code should be efficient and effective.

- For Rosetta code, follow [Rosetta coding conventions](#)
- For PyRosetta code, follow [PyRosetta coding conventions](#)
- Follow a coding style
 - For python PEP8 is recommended
 - [PEP 8 – Style Guide for Python Code](#)
 - Enforce chosen style
- [UML diagram](#) to describe code design
- [Don't Repeat Yourself \(DRY\)](#)
 - Should avoid code duplication
 - Code is broken down into smaller functions to:
 - Increase reusability
 - Enable easier testing
- [Type Checking](#)
 - Provide and enforce types in Python
 - Possible tools for this: [pydantic](#), [mypy](#), [ty](#)
- For Python - have a standard python layout
 - Example flat layout:

```
yourlib/  
├─ yourlib/  
│ ├─ __init__.py  
│ └─ core.py  
├─ tests/  
└─ pyproject.toml
```

- Example src layout:

```
yourlib/  
├─ src/  
│   └─ yourlib/  
│       ├── __init__.py  
│       └─ core.py  
├─ tests/  
└─ pyproject.toml
```

Testing

Tests ensure that your code continues to work as expected even as more code is committed or dependencies change.

- [Unit Tests](#) - ensure small chunks of code run correctly
- [Integration Tests](#) - at minimum all examples should be included as integration tests
- Scientific Tests - Optional, but good practice
- Tests should be written in test directory
- For Rosetta, see this [guide](#)

Continuous Integration (CI)

- Implement CI to run unit tests and integration test for pull request to main
 - For Rosetta - the [testing server](#) is already setup
 - For new projects, [github actions](#) can be used to run CI

Performance

- Benchmark execution time
- Benchmark memory usage

Release and Packaging

Consistent packaging allows for more reliable and consistent installation.

- Create Docker image to publish on dockerhub
 - Should be tested for Apptainer and Singularity as well

For Python Projects:

- Pypyprojects.toml
- Requirements.txt

Documentation

- See: [☰ Good Documentation Guides](#)

Maintenance

- Discuss with devel team:
 - Who can merge PRs
 - What is the protocol when tests are failing?