Scientific Software Center

IWR Interdisciplinary Center for Scientific Computing

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

Open Research Software

Best practices for reliable, maintainable software

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Scientific
Software
Center

Scientific Software Center

- Team of Research Software Engineers (currently 6)
- Offer researchers at Heidelberg University
  - Large scale software development
  - Small scale software development
  - Consultation / advice
  - Teaching / training
- Our website / github page also offers
  - Coding guidelines
  - Template repositories

ssc.iwr.uni-heidelberg.de

github.com/ssciwr

Research Software

- Is an increasingly vital part of scientific research
- Is an intrinsic part of reproducible science
- Is not only code written by “real programmers”
    - Your Python data analysis script is also research software!

For people to trust your research, they need to trust your software

- Needs to be **open**
- Needs to be **reliable**
- Needs to be **maintainable**

Best practices for reliable, maintainable software

- Open source development
- Version control
- Testing
- Documentation
- Continuous integration
- Community involvement

For each of these I will

- Describe what it is and what the benefits are
- Make some concrete recommendations
- Show an example of this from an open source library (pybind11)

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Open source development

Open source development

- Making your source code publicly available
    - e.g. GitHub, GitLab, Software Heritage, Zenodo
- Advantages
    - Makes it easier for people to reproduce your results
    - People can find mistakes and bugs
    - People can fix mistakes and bugs
    - People can offer suggestions, improvements
    - People can cite and use your work
    - Gives others confidence in the value of your code

Which platform to use?

- GitHub.com / GitLab.com / etc
  - Commercial git hosting with a (substantial) free tier of services
- Self-hosted gitlab / forgejo / etc
  - Your institute may offer self-hosted gitlab or other code hosting services
- Software Heritage
  - Public software archive, provides a SWHID for your code
- Zenodo
  - Public data archive, provides a DOI for your code
- Recommendation
  - Some form of git hosting + Software Heritage + Zenodo

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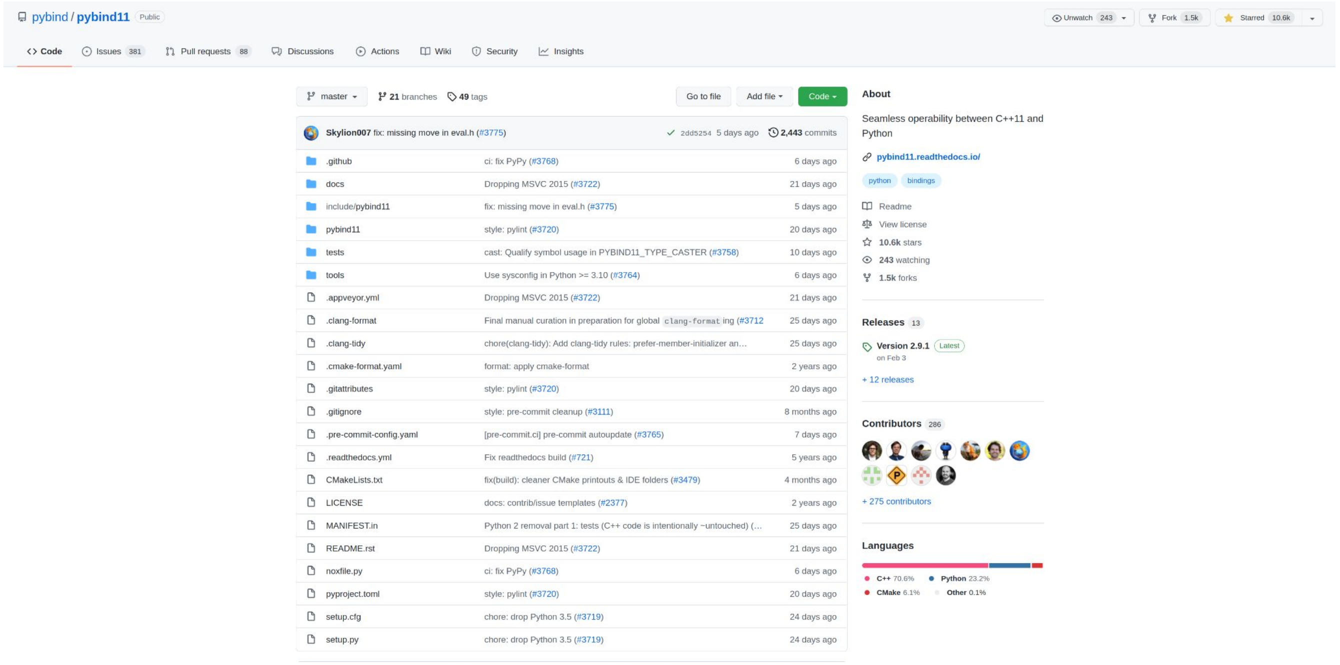
Open source development example



pybind / **pybind11** Public

Unwatch 243 · Fork 1.5k · Starred 10.6k

<> Code · Issues 381 · Pull requests 88 · Discussions · Actions · Wiki · Security · Insights

master · **21** branches · **49** tags · Go to file · Add file · Code

Skylion007 fix: missing move in eval.h (#3775) ✓ 2dd5254 5 days ago · **2,443** commits

.github	ci: fix PyPy (#3768)	6 days ago
docs	Dropping MSVC 2015 (#3722)	21 days ago
include/pybind11	fix: missing move in eval.h (#3775)	5 days ago
pybind11	style: pylint (#3720)	20 days ago
tests	cast: Qualify symbol usage in PYBIND11_TYPE_CASTER (#3758)	10 days ago
tools	Use sysconfig in Python >= 3.10 (#3764)	6 days ago
.appveyor.yml	Dropping MSVC 2015 (#3722)	21 days ago
.clang-format	Final manual curation in preparation for global `clang-format` ing (#3712	25 days ago
.clang-tidy	chore(clang-tidy): Add clang-tidy rules: prefer-member-initializer an…	25 days ago
.cmake-format.yaml	format: apply cmake-format	2 years ago
.gitattributes	style: pylint (#3720)	20 days ago
.gitignore	style: pre-commit cleanup (#3111)	8 months ago
.pre-commit-config.yaml	[pre-commit.ci] pre-commit autoupdate (#3765)	7 days ago
.readthedocs.yml	Fix readthedocs build (#721)	5 years ago
CMakeLists.txt	fix(build): cleaner CMake printouts & IDE folders (#3479)	4 months ago
LICENSE	docs: contrib/issue templates (#2377)	2 years ago
MANIFEST.in	Python 2 removal part 1: tests (C++ code is intentionally ~untouched) (…	25 days ago
README.rst	Dropping MSVC 2015 (#3722)	21 days ago
noxfile.py	ci: fix PyPy (#3768)	6 days ago
pyproject.toml	style: pylint (#3720)	20 days ago
setup.cfg	chore: drop Python 3.5 (#3719)	24 days ago
setup.py	chore: drop Python 3.5 (#3719)	24 days ago

About

Seamless operability between C++11 and Python

pybind11.readthedocs.io/

python · bindings

Readme
View license
10.6k stars
243 watching
1.5k forks

Releases 13

Version 2.9.1 Latest
on Feb 3

+ 12 releases

Contributors 286

+ 275 contributors

Languages

● **C++** 70.6% ● **Python** 23.2%
● **CMake** 6.1% ● **Other** 0.1%

https://github.com/pybind/pybind11/

Version control

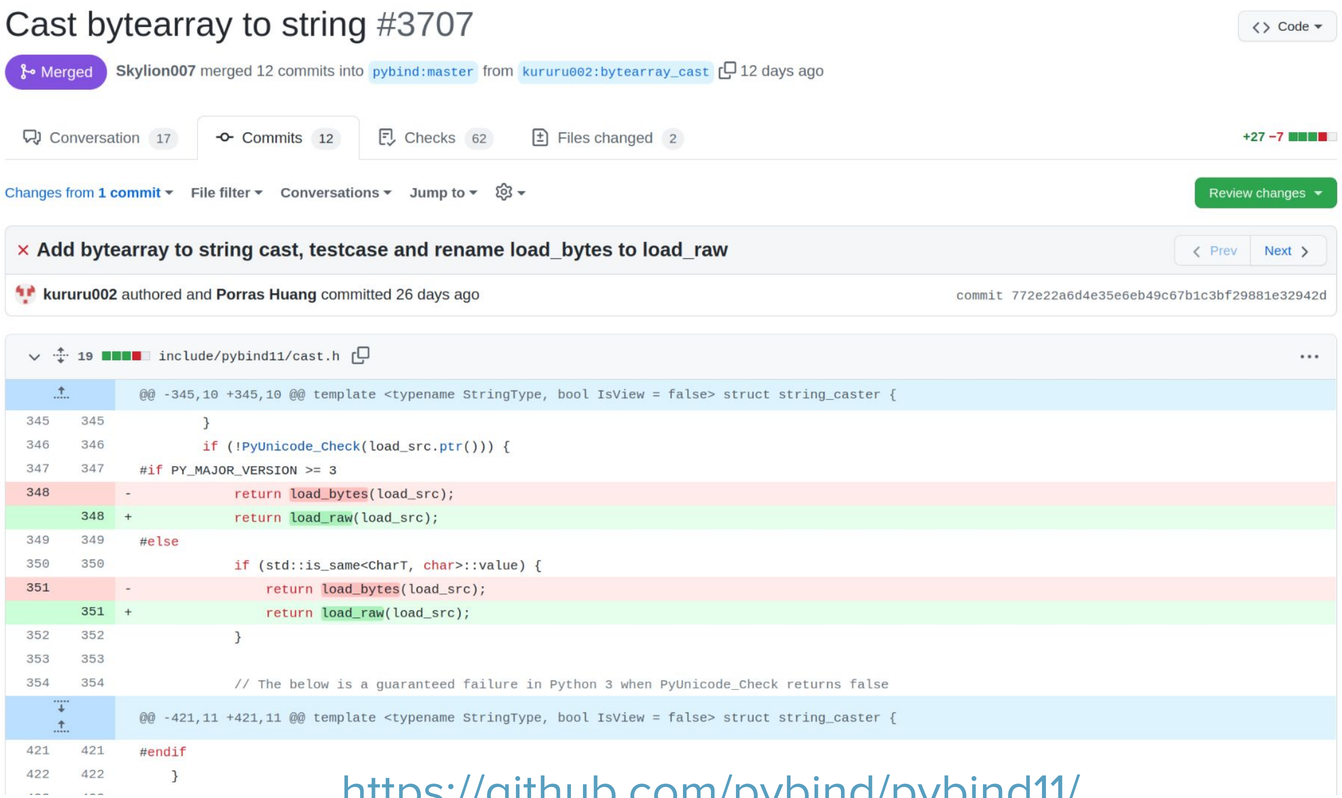
Version control

- Use a tool to track changes to your software
  - e.g. git, subversion, mercurial
- Advantages
  - Easily keep track of changes to the code
  - What changed, who changed it, when and why it changed
  - Easy to refer to specific commit, tag or version for reproducibility
  - Easy to undo or revert changes
  - Easy for multiple people to collaborate on the same code
  - Gives others confidence in the history of your code

Which version control system to use?

- Git
  - The de-facto standard, now used by the vast majority of open source projects
- Workflows
  - There are many ways to use git, known as workflows
  - Centralized workflow, Feature branching, Forking workflow
  - git-flow, gitlab-flow, github-flow, ...
- Recommendation
  - Git with a main branch
  - New code is developed on a new branch and then merged into main

Version control example



Cast bytearray to string #3707

Merged Skylion007 merged 12 commits into `pybind:master` from `kururu002:bytearray_cast` 12 days ago

Conversation 17 | Commits 12 | Checks 62 | Files changed 2 | +27 −7

Changes from 1 commit | File filter | Conversations | Jump to | Review changes

Add bytearray to string cast, testcase and rename load_bytes to load_raw

kururu002 authored and Porras Huang committed 26 days ago — commit 772e22a6d4e35e6eb49c67b1c3bf29881e32942d

19 include/pybind11/cast.h

```
@@ -345,10 +345,10 @@ template <typename StringType, bool IsView = false> struct string_caster {
         }
         if (!PyUnicode_Check(load_src.ptr())) {
#if PY_MAJOR_VERSION >= 3
-            return load_bytes(load_src);
+            return load_raw(load_src);
#else
            if (std::is_same<CharT, char>::value) {
-                return load_bytes(load_src);
+                return load_raw(load_src);
            }

            // The below is a guaranteed failure in Python 3 when PyUnicode_Check returns false
@@ -421,11 +421,11 @@ template <typename StringType, bool IsView = false> struct string_caster {
#endif
    }
```

https://github.com/pybind/pybind11/

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Testing

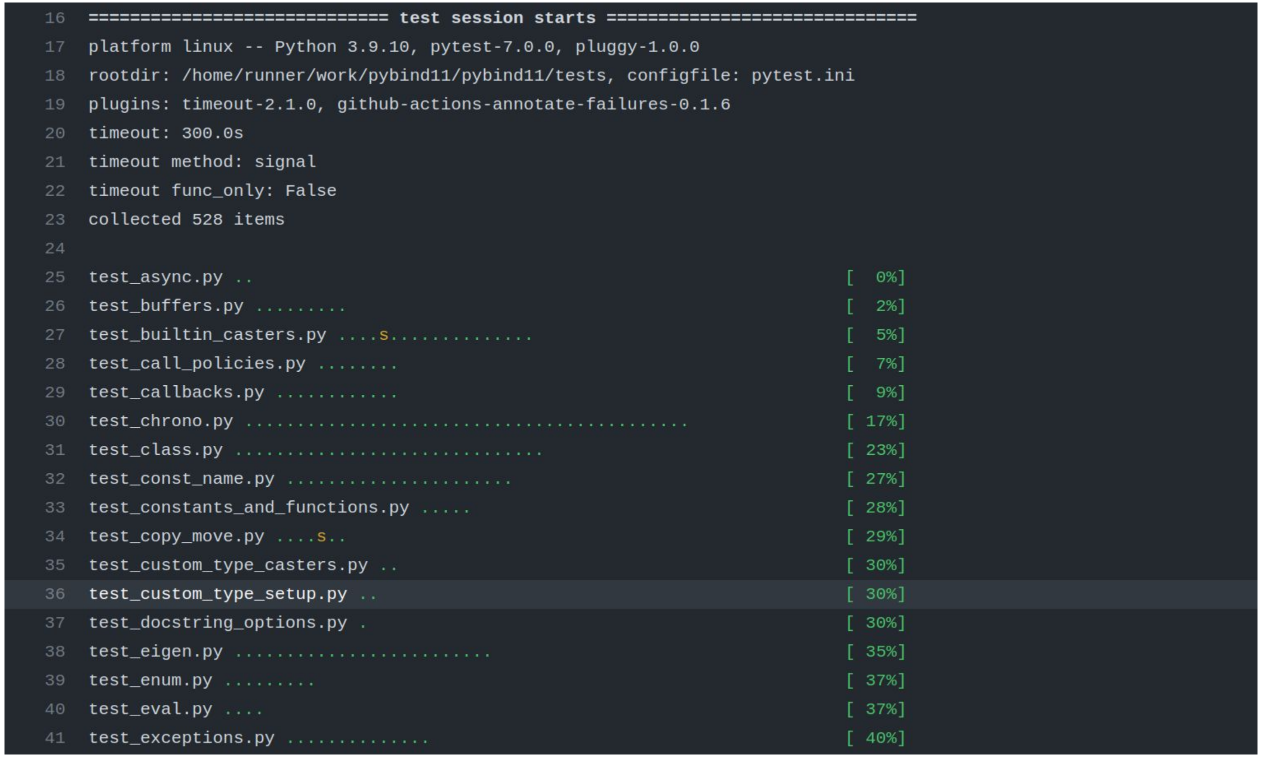
Testing

- Write automated tests that check the software is working correctly
- Advantages
  - Ensure correctness of your code
  - Maintain correctness of your code
  - Find bugs earlier and more easily
  - Make changes or refactor code without fear
  - Easier for new contributors to make positive changes
  - Complement the documentation as examples of use
  - Gives others confidence in the correctness of your code

Types of tests

- Unit tests
  - Test a small, isolated part of code
- Integration / system tests
  - Test larger, connected parts of code
- Regression tests
  - Test for a bug that was fixed to ensure it doesn't come back
- Approval tests
  - Retro-fitting tests before making changes to legacy code
- Recommendation
  - Write unit tests for new projects or new code in legacy projects
  - Write approval tests for legacy code which doesn't have any tests

Testing example



```
============================= test session starts ==============================
platform linux -- Python 3.9.10, pytest-7.0.0, pluggy-1.0.0
rootdir: /home/runner/work/pybind11/pybind11/tests, configfile: pytest.ini
plugins: timeout-2.1.0, github-actions-annotate-failures-0.1.6
timeout: 300.0s
timeout method: signal
timeout func_only: False
collected 528 items

test_async.py ..                                                         [  0%]
test_buffers.py .........                                                [  2%]
test_builtin_casters.py ....s.............                               [  5%]
test_call_policies.py ........                                           [  7%]
test_callbacks.py ............                                           [  9%]
test_chrono.py ............................................              [ 17%]
test_class.py ..............................                             [ 23%]
test_const_name.py ......................                                [ 27%]
test_constants_and_functions.py .....                                    [ 28%]
test_copy_move.py ....s..                                                [ 29%]
test_custom_type_casters.py ..                                           [ 30%]
test_custom_type_setup.py ..                                             [ 30%]
test_docstring_options.py .                                              [ 30%]
test_eigen.py .........................                                  [ 35%]
test_enum.py .........                                                   [ 37%]
test_eval.py ....                                                        [ 37%]
test_exceptions.py ..............                                        [ 40%]
```

https://github.com/pybind/pybind11/

Documentation

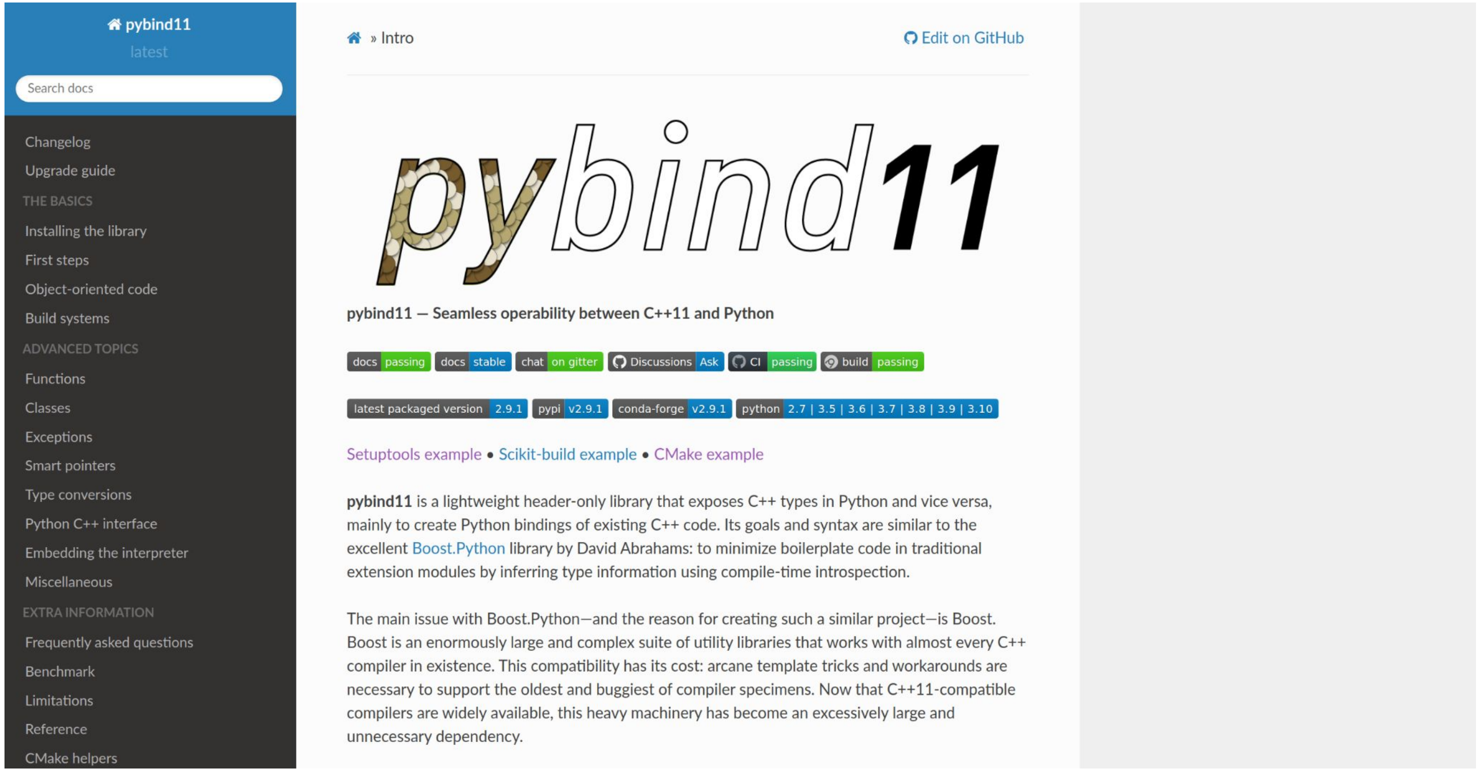
Documentation

- Document how your code works and how to use it
- Advantages
    - Helps users understand how to use the code
    - Helps developers understand how to modify the code
    - Encourages people to learn about your code
    - Gives others confidence in the usability of your code
    - By writing it you can identify hard-to-use code that could be improved

Types of Documentation

- Source code
    - Target audience is other humans, not the computer!
- Comments
    - For you and other developers
- API Documentation
    - Technical documentation for developers / power users
- User documentation
    - Documentation written for users
- Examples
    - Very helpful
- Recommendation
    - Include your documentation in your git repository and update it alongside code changes

Documentation example



pybind11 — Seamless operability between C++11 and Python

Setuptools example • Scikit-build example • CMake example

pybind11 is a lightweight header-only library that exposes C++ types in Python and vice versa, mainly to create Python bindings of existing C++ code. Its goals and syntax are similar to the excellent Boost.Python library by David Abrahams: to minimize boilerplate code in traditional extension modules by inferring type information using compile-time introspection.

The main issue with Boost.Python—and the reason for creating such a similar project—is Boost. Boost is an enormously large and complex suite of utility libraries that works with almost every C++ compiler in existence. This compatibility has its cost: arcane template tricks and workarounds are necessary to support the oldest and buggiest of compiler specimens. Now that C++11-compatible compilers are widely available, this heavy machinery has become an excessively large and unnecessary dependency.

https://github.com/pybind/pybind11/

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Continuous integration

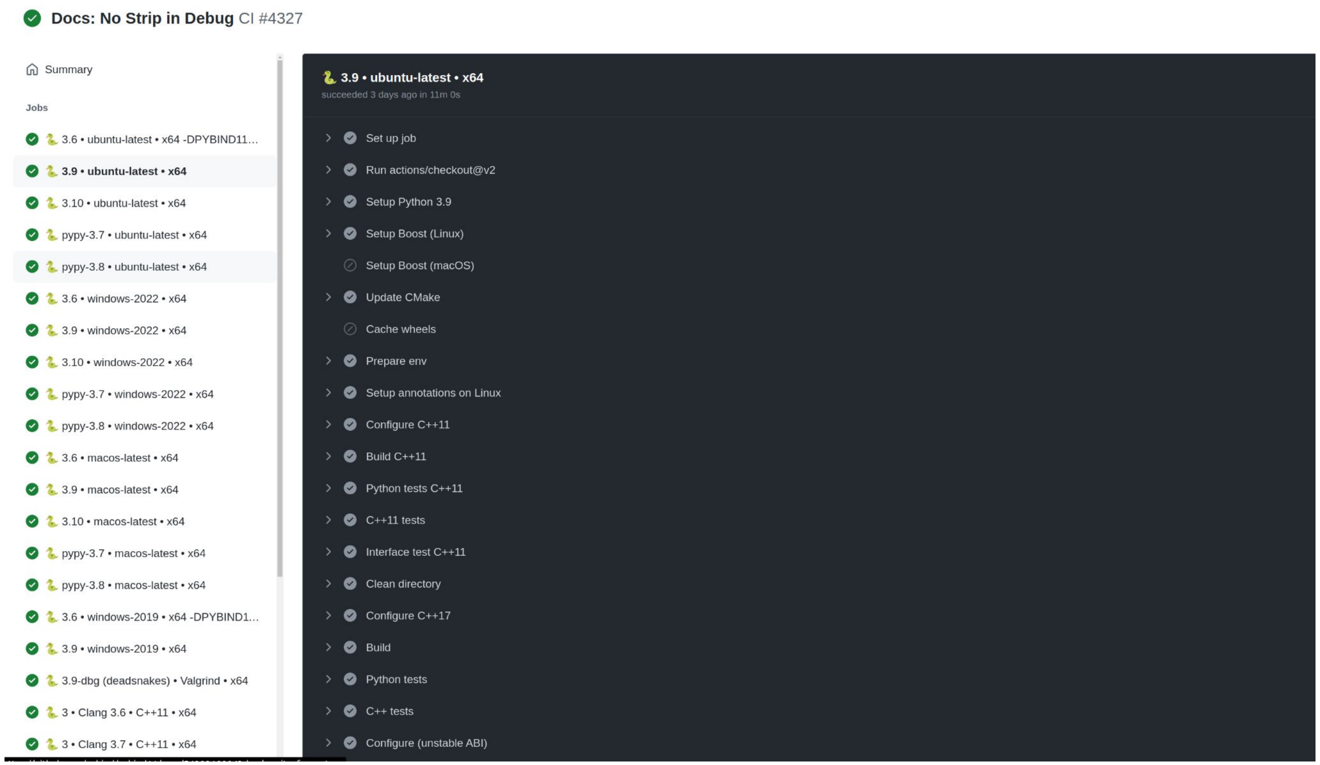
Continuous integration

- Automatic checks before code changes are accepted
- Advantages
  - Ensure all tests pass before code is changed
  - Can automatically apply uniform formatting of the code
  - Can automatically do static analysis to identify code smells or bugs
  - Can require that new code is covered by tests
  - Test the code on multiple platforms (e.g. Windows, Mac, Linux)
  - Can automatically deploy new releases of software
  - Helps others improve the quality of their proposed code changes

Types of continuous integration

- Integrated into git hosting service
  - GitHub Actions, GitLab CI/CD, ...
- External services
  - Travis CI, Circle CI, ...
- Self hosted
  - Jenkins, ...
- Recommendation
  - Typically easiest to use the CI provided by your git hosting service
  - E.g. for code on GitHub use GitHub Actions

Continuous integration example



✓ **Docs: No Strip in Debug** CI #4327

Summary

Jobs

- ✓ 3.6 • ubuntu-latest • x64 -DPYBIND11...
- ✓ **3.9 • ubuntu-latest • x64**
- ✓ 3.10 • ubuntu-latest • x64
- ✓ pypy-3.7 • ubuntu-latest • x64
- ✓ pypy-3.8 • ubuntu-latest • x64
- ✓ 3.6 • windows-2022 • x64
- ✓ 3.9 • windows-2022 • x64
- ✓ 3.10 • windows-2022 • x64
- ✓ pypy-3.7 • windows-2022 • x64
- ✓ pypy-3.8 • windows-2022 • x64
- ✓ 3.6 • macos-latest • x64
- ✓ 3.9 • macos-latest • x64
- ✓ 3.10 • macos-latest • x64
- ✓ pypy-3.7 • macos-latest • x64
- ✓ pypy-3.8 • macos-latest • x64
- ✓ 3.6 • windows-2019 • x64 -DPYBIND1...
- ✓ 3.9 • windows-2019 • x64
- ✓ 3.9-dbg (deadsnakes) • Valgrind • x64
- ✓ 3 • Clang 3.6 • C++11 • x64
- ✓ 3 • Clang 3.7 • C++11 • x64

3.9 • ubuntu-latest • x64
succeeded 3 days ago in 11m 0s

- ✓ Set up job
- ✓ Run actions/checkout@v2
- ✓ Setup Python 3.9
- ✓ Setup Boost (Linux)
- Setup Boost (macOS)
- ✓ Update CMake
- Cache wheels
- ✓ Prepare env
- ✓ Setup annotations on Linux
- ✓ Configure C++11
- ✓ Build C++11
- ✓ Python tests C++11
- ✓ C++11 tests
- ✓ Interface test C++11
- ✓ Clean directory
- ✓ Configure C++17
- ✓ Build
- ✓ Python tests
- ✓ C++ tests
- ✓ Configure (unstable ABI)

https://github.com/pybind/pybind11/

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Community involvement

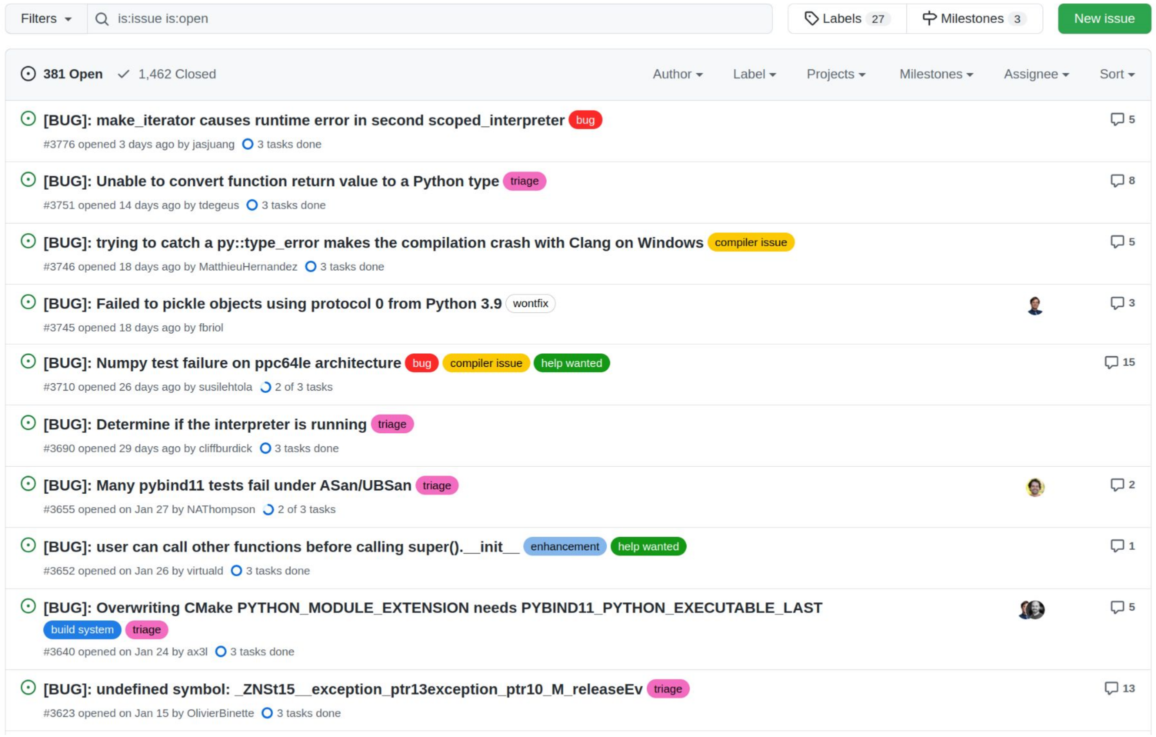
Community involvement

- Enable people to contribute bug reports, feature requests and code
- Advantages
    - People can find mistakes and bugs
    - People can fix mistakes and bugs
    - People can improve the documentation
    - People can offer suggestions, improvements
    - People can help each other to use your code
    - More contributors can make a project more sustainable
    - Helps others to use and contribute to your work

Communication channels

- Issue trackers on git hosting service
- Mailing list
- Contact email for support / questions
- Wiki pages
- Recommendation
    - Use public issue trackers for all feedback / discussions / bugs / features

Community involvement example



Filters is:issue is:open Labels 27 Milestones 3 New issue

381 Open ✓ 1,462 Closed Author Label Projects Milestones Assignee Sort

[BUG]: make_iterator causes runtime error in second scoped_interpreter bug 5
#3776 opened 3 days ago by jasjuang 3 tasks done

[BUG]: Unable to convert function return value to a Python type triage 8
#3751 opened 14 days ago by tdegeus 3 tasks done

[BUG]: trying to catch a py::type_error makes the compilation crash with Clang on Windows compiler issue 5
#3746 opened 18 days ago by MatthieuHernandez 3 tasks done

[BUG]: Failed to pickle objects using protocol 0 from Python 3.9 wontfix 3
#3745 opened 18 days ago by fbriol

[BUG]: Numpy test failure on ppc64le architecture bug compiler issue help wanted 15
#3710 opened 26 days ago by susilehtola 2 of 3 tasks

[BUG]: Determine if the interpreter is running triage
#3690 opened 29 days ago by cliffburdick 3 tasks done

[BUG]: Many pybind11 tests fail under ASan/UBSan triage 2
#3655 opened on Jan 27 by NAThompson 2 of 3 tasks

[BUG]: user can call other functions before calling super().__init__ enhancement help wanted 1
#3652 opened on Jan 26 by virtuald 3 tasks done

[BUG]: Overwriting CMake PYTHON_MODULE_EXTENSION needs PYBIND11_PYTHON_EXECUTABLE_LAST build system triage 5
#3640 opened on Jan 24 by ax3l 3 tasks done

[BUG]: undefined symbol: _ZNSt15__exception_ptr13exception_ptr10_M_releaseEv triage 13
#3623 opened on Jan 15 by OlivierBinette 3 tasks done

https://github.com/pybind/pybind11/

Summary

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Best practices for reliable, maintainable software

- Open source development
- Version control
- Testing
- Documentation
- Continuous integration
- Community involvement

Getting started

- Start from a template repository
- Basic project ready to go
    - Open source development
    - Version control
    - Testing
    - Documentation
    - Continuous integration
    - Community involvement

Basic C++ Project Template

github.com/ssciwr/cpp-project-template

Basic Python Project Template

github.com/ssciwr/python-project-template

Advanced C++ Project Template

github.com/ssciwr/cookiecutter-cpp-project