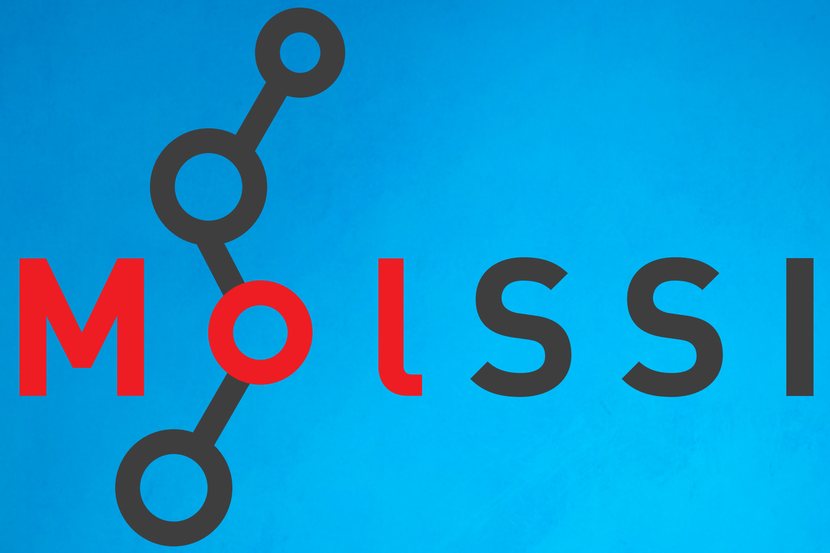
Open Source Best Practices: From Continuous Integration to Static Linters



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The Molecular Sciences Software Institute (MolSSI)

- Designed to *serve* and *enhance* the software development efforts of the broad field of computational molecular science (CMS).
- Funded at the institute level under the Software Infrastructure for Sustained Innovation (SI^2) initiative by the National Science Foundation.
- Launched August 1st, 2016

- Collaborative effort by:
  - Virginia Tech
  - Rice U.
  - Stony Brook U.
  - U.C. Berkeley
  - Stanford U.
  - Rutgers U.
  - U. Southern California
  - Iowa State U.

The Molecular Sciences Software Institute (MolSSI)

- Software Infrastructure
  - Build open-source frameworks and packages for the entire CMS community

- Education and training
  - Online materials and training guides
  - Host a number of targeted workshops, summer schools, and other training programs

- Community Engagement and Leadership
  - Interoperability standards and best practices
  - Data and API standardization targets

Talk Motivation

- Many terms thrown around:
  - **Best Practice**
  - **DevOps**
  - **Open Source**
  - **Software Sustainability**
  - **"Incorrect Software"**
  - **Manage Code**
  - **Build and Package**
  - **"Just get the physics working"**

"**Best**" is subjective and depends on your own community.

Lets discuss practical applications and how to make our lives easier!

Open Source

Open Source software is software that can be freely accessed, used, changed, and shared (in modified or unmodified form) by anyone. Open source software is made by many people, and distributed under licenses that comply with the Open Source Definition. – Open Source Initiative

- **Free Redistribution** – Program is free of charge and distributable
- **Source Code** – Source code is freely available
- **Derived Works** – Allows modification of source in derived works

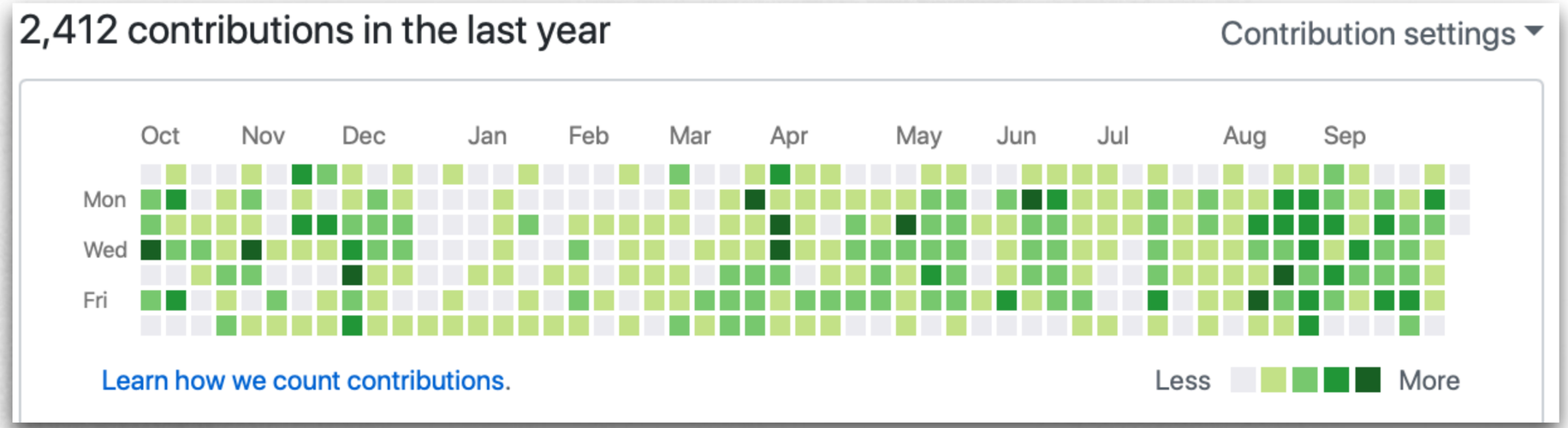
Open Source

- **Community** – Building engaged cooperative communities
- **Open Collaboration**– Anyone is free to join the community
- **Development Costs** – Allows common goal execution

Open Source

Personal Reasons

- **Improves Coding Skills** - Code reviews and feedback
- **New Technologies**- Large base of users to provide unique experience
- **Peer Recognition** - Complete portfolio of what a person has done
- **Job Prospects** - Excellent for resumes

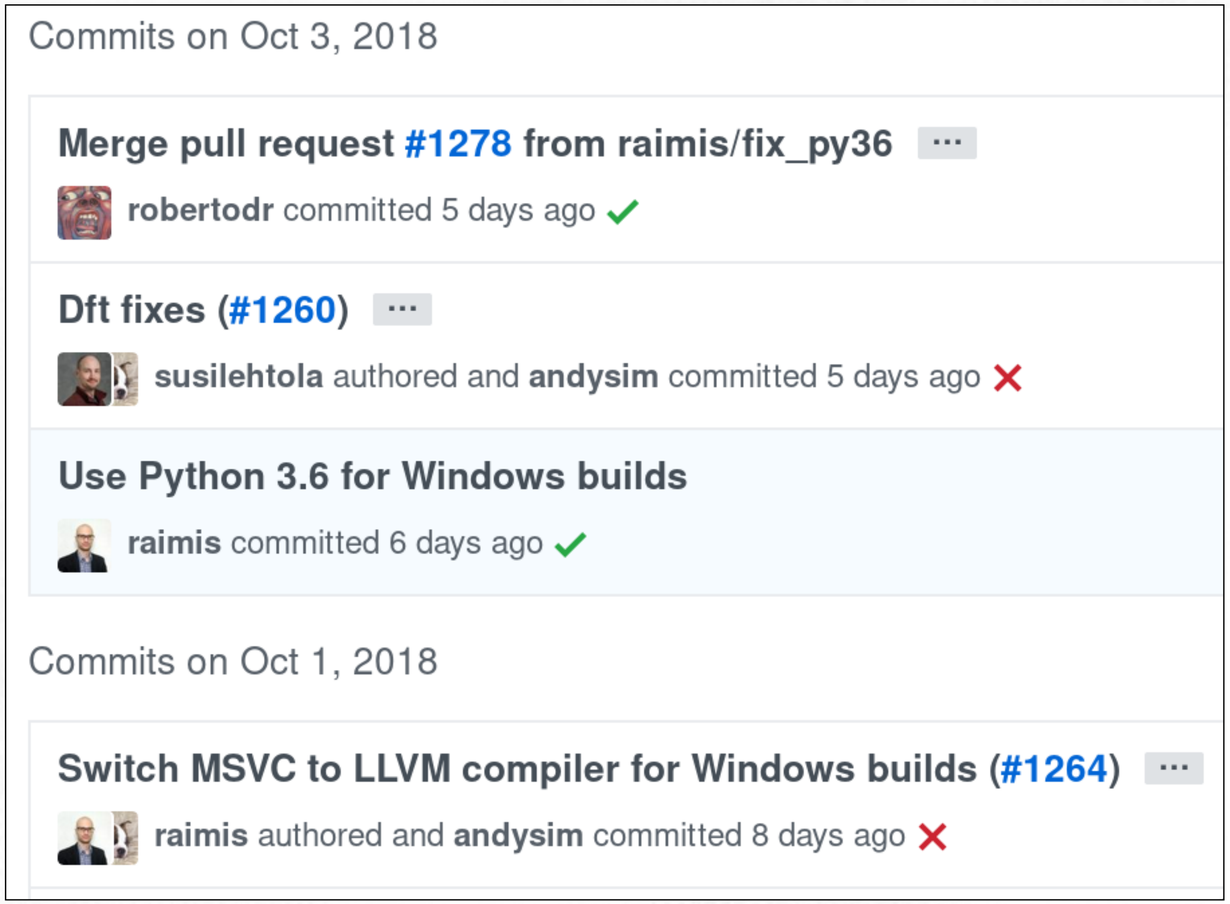


Version Control

- Tracks changes over time (and who made them)
- Allow independent development on branches, and then merging later
- Can revert inappropriate changes

- Most popular: git
- Comments at the top of source files **do not** count
- Foundation of a community

GitHub GitLab Bitbucket



Testing

"Mistakes in software erode trust in research and researchers" – Neil Chue Hong

We can improve reliability and trust in software by testing it

- **Unit Testing** – test a small unit (function)
- **Integration Testing** – test interoperation of units
- **Regression Testing** – ensure a fixed bug remains fixed
- **Smoke Testing** – sanity test of whole system
- **Acceptance Testing** – test that a feature is correctly implemented
- Testing of failure modes is also encouraged

Testing Frameworks

- Pick a common, appropriate testing framework
  - Depends on language and personal preference
  - Do **not** write your own unless you have to!

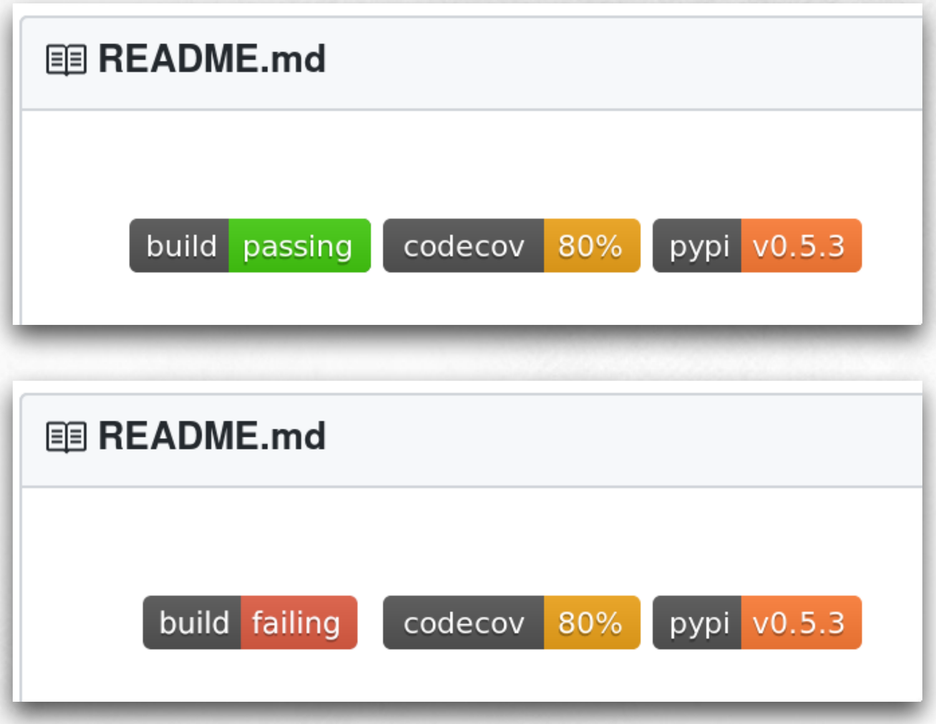
- **C/C++** – CTest, Catch2
- **Python** – PyTest
- **Fortran** – CTest

```
52/54 Test #52: gtoeri_gtoeri_4center_water_sto-3g.inp_testcreate.dat_exact ..............................   Passed  149.47 sec
      Start 53: gtoeri___create_reference
53/54 Test #53: gtoeri___create_reference ...................................................................   Passed   15.31 sec
      Start 54: reference_gtoeri_gtoeri_testref.ref
54/54 Test #54: reference_gtoeri_gtoeri_testref.ref .........................................................   Passed   15.30 sec

100% tests passed, 0 tests failed out of 54

Total Test time (real) = 1073.07 sec
```

```
basis_set_exchange/tests/test_converters.py .........          [ 47%]
basis_set_exchange/tests/test_io.py ........                   [ 89%]
basis_set_exchange/tests/test_metadata.py ..                   [100%]

=========== 19 passed, 15996 deselected in 7.86 seconds ============
```

Continuous Integration (CI)

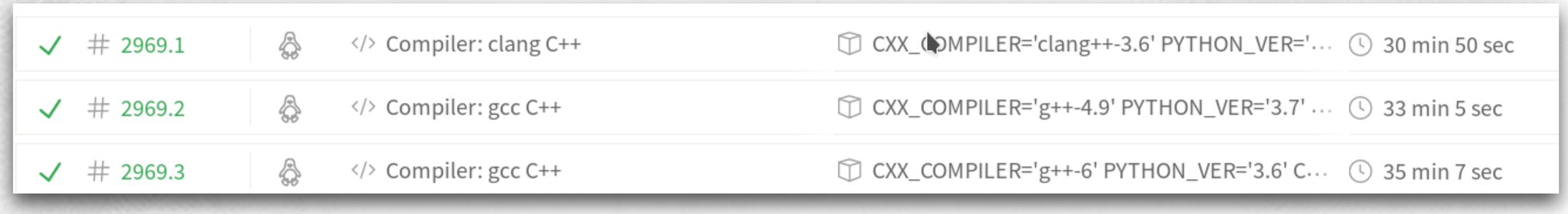
- Testing is done automatically
- Results are displayed publicly
- Develops trust in software package
- Developers feel safer contributing
- Badges!



Continuous Deployment – CI + deploy a service

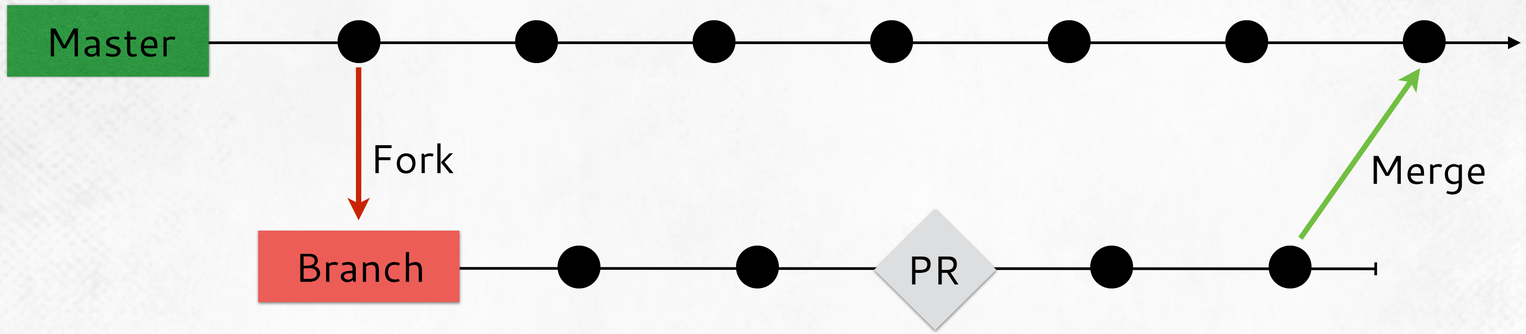
CI Features

- Matrix builds



  - Different:
    - Distributions
    - Operating systems
    - Dependency versions
  - Integrated with version control (git, GitHub, GitLab etc)
  - Integrated with social services such as Slack, etc

Development Workflow (Fork/Pull Model)



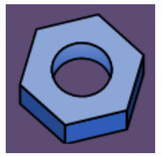
- Development happens on an independent branch/repo
- Code is reviewed/**tested** during the Pull Request (PR)
- If accepted, code is merged into the *master* branch

CI Services and Software

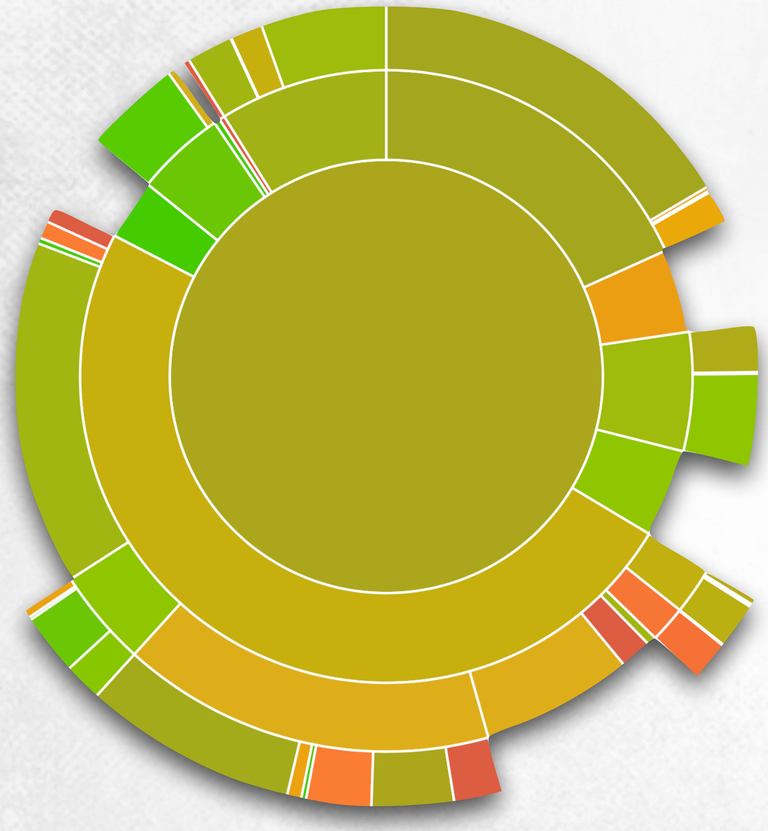
- Services can be cloud-based or you can use your own resources
- Some are free for open-source projects

- Cloud hosted:
  - TravisCI (Linux/OSX)
  - CircleCI (Linux/OSX)
  - Appveyor (Windows)
  - Azure Pipelines (Linux/OSX/Windows)

- Locally Hosted
  - Jenkins
  - Buildbot
  - TeamCity



Code Coverage



codecov.io

- Tendency to write many tests that cover a single area while completely neglecting others.
- 100% code coverage does not imply perfect code!
- General metric that informs testing competency that is difficult to fake.

Code Coverage

```
238  7      if "queue_socket" in self.objects:
239             # Add canonical queue callback
240             nanny = tornado.ioloop.PeriodicCallback(self.objects["queue_nanny"].update, 2000)
241             nanny.start()
242             self.periodic["queue_nanny_update"] = nanny
```

- Common case of missing "if" statements
- Exceptions are often not tested!

- Services: Codecov, Coveralls
- Tools: gcov (C++), coverage (Python), etc
- All languages (C, C++, Fortran, Python, Java, Julia, etc)

Code Formatters

- Automatic application of a standard format
  - Most language have a single standard (Python)
  - Several language have multiple standard (C++)
- Provides consistent code
  - Within your own software stack
  - And amongst other software stacks
- Tools: clang-format (C/C++), yapf (Python)
- Most languages (C, C++, Python, Java, Julia, etc)

example.py

```
1  x = {  'a':37,'b':42,
2
3  'c':927}
4
5  y = 'hello ''world'
6  z = 'hello '+'world'
7  a = 'hello {}'.format('world')
8  class foo  (     object  ):
9    def f    (self   ):
10     return        37*-+2
11   def g(self, x,y=42):
12       return y
13 def f  (   a ) :
14   return      37+-+a[42-x :  y**3]
15
```

YAPF

Code Quality

lgtm.co

- Statically examine the code for a variety of errors and potential errors
- Catch bugs that do not have unit tests for them.
- Automation of code review:
  - Always catches “known” errors
  - Bad news is easier from a bot

Code Quality

Actual errors

```
2150        for (iop = 0; iop < nop; ++iop) {
2151            int axis, op_ndim, op_axis;
```

Local variable 'axis' hides a `parameter of the same name`.

Possible errors

```
1440        printf("| IterIndex: %d\n", (int)NIT_ITERINDEX(iter));
1441        printf("| Iterator SizeOf: %d\n",
1442                                (int)NIT_SIZEOF_ITERATOR(itflags, ndim, nop));
```

Multiplication result may overflow 'int' before it is converted to 'unsigned long'.

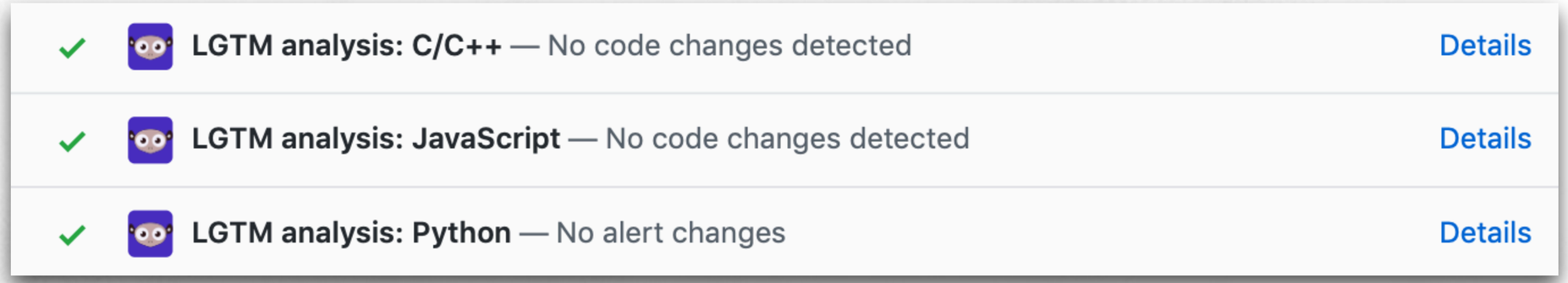
Potential code duplication

```
186     def list_final_energies(self, fragments=None, refresh_cache=False):
```

All statements in list_final_energies are similar in `list_final_molecules`.

Code Quality

- Still experimenting with code quality analysis
- Many are overzealous in their warnings
- LGTM seems to hit the "right" balance

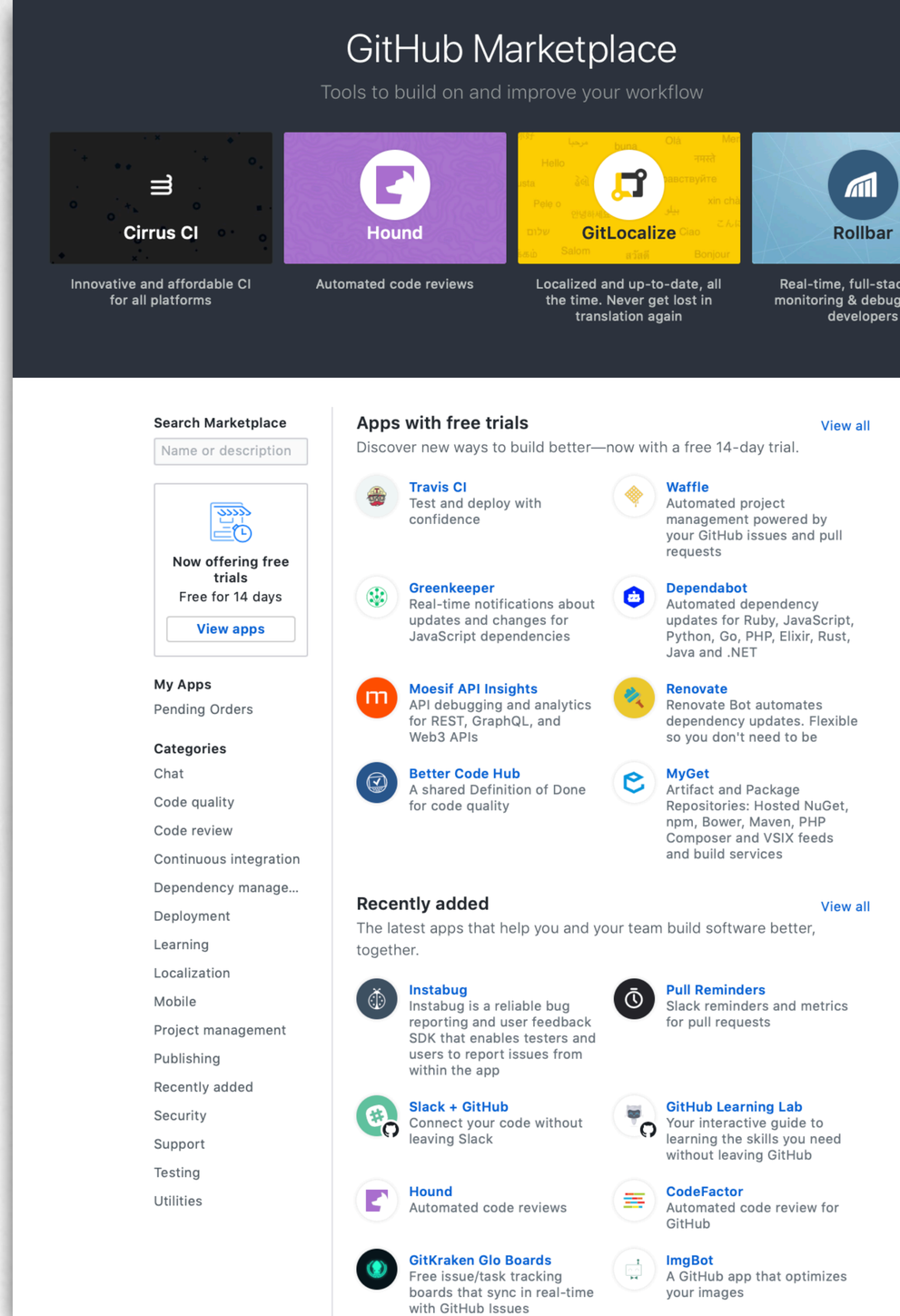


- LGTM, Code Climate, PyFlakes, …
- Most languages (C, C++, Python, Java, Julia, etc)

…and more

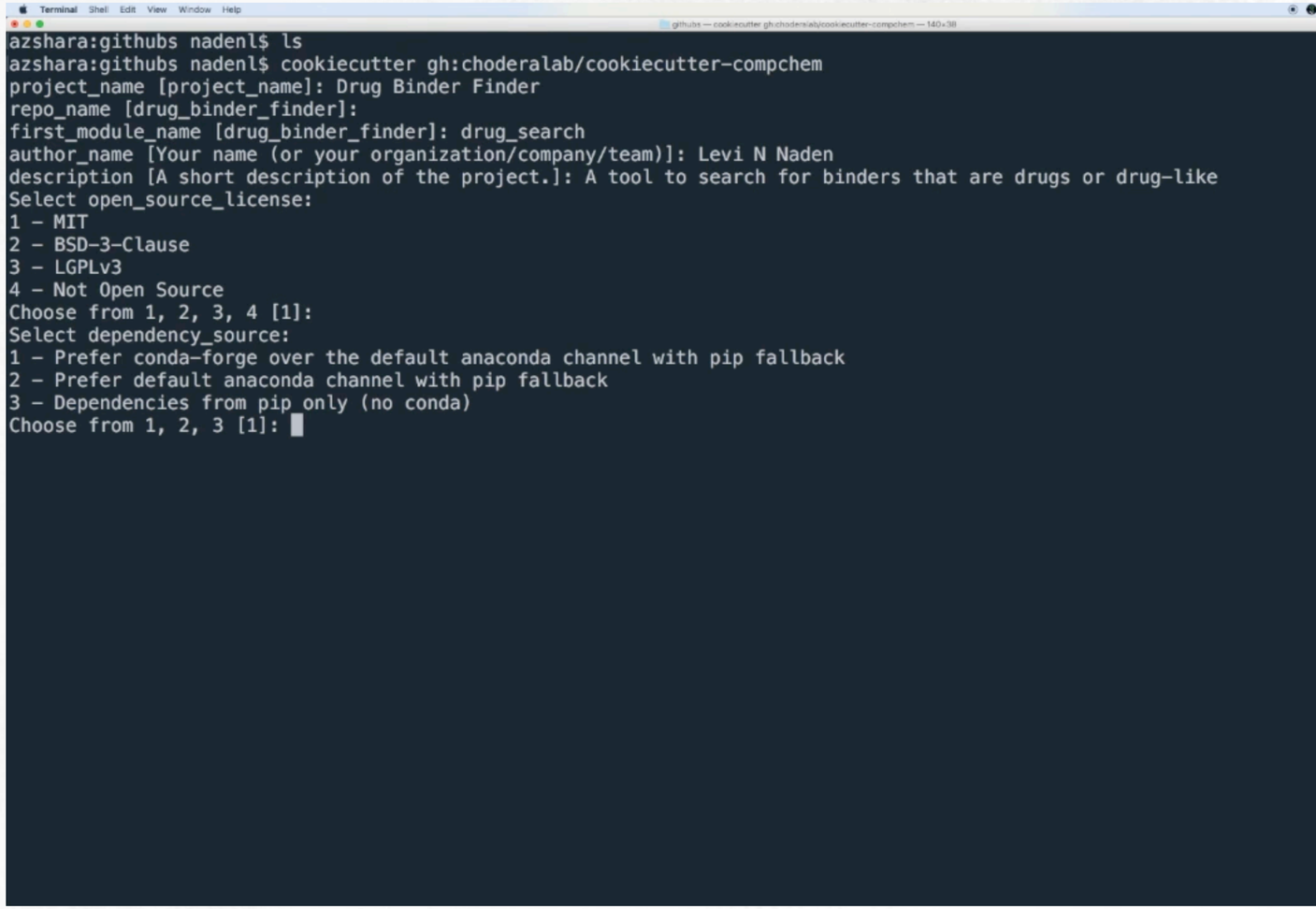
- Many other services out there
  - Dashboards
  - Agile Task Boards
  - Vulnerability Checkers
  - Dependency Management
  - ….

…you can have too many services!



Cookiecutters [Python]

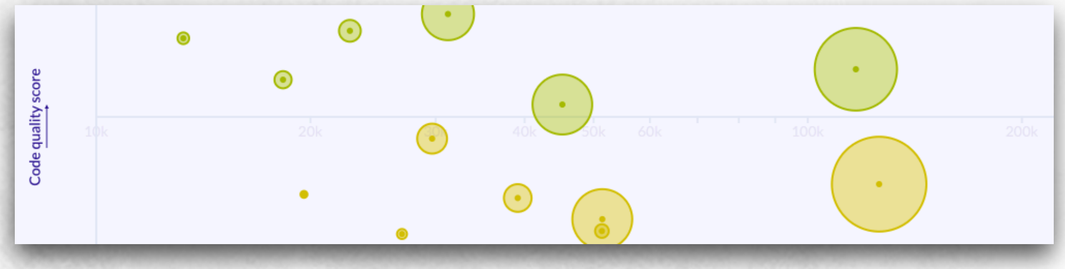
- Automatic setup:
  - Version Control (git)
  - License (MIT/BSD/LGPL/Other)
  - CI (Travis CI/Appveyor)
  - Testing (PyTest)
  - Code Coverage (Codecov)
  - Documentation (Sphinx)
- Takes ~5 minutes to integrate



https://github.com/MolSSI/cookiecutter-cms

Summary

- Version Control
- Testing
- Continuous Integration
- Code Coverage
- Formatters



- Saves developer time
- Builds trust with your community base
- Makes your code more welcoming to new developers
- Best practices are a balance of developer and user time

Communities of Practice

"**Best**" is subjective and depends on your own community.

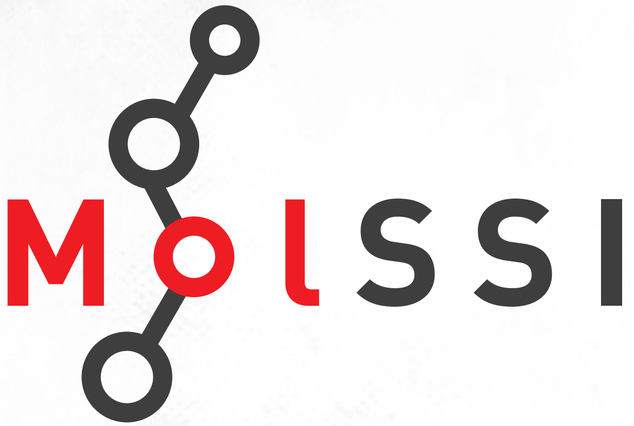
- We believe these practices are optimal for our community and are derived from many other communities
- Depends greatly on:
  - Target audience
  - Size of the project
  - Activity level of the project
- Still core "good ideas" that can be widely applied

Example Repositories

- **Molecular Dynamics:**
  - LAMMPS – GitHub, CI (Jenkins),
  - OpenMM – GitHub, CI (Travis/Appveyor)
- **Quantum Mechanics:**
  - NWChem – GitHub, CI (Travis)
  - Psi4 – GitHub, CI (Travis/Appveyor), Code Coverage
- **Python Utility Codes:**
  - opt_einsum – GitHub, CI, Code Coverage
  - QCFractal – GitHub, CI, Code Coverage, Static Analysis

Learn More about MolSSI

- Twitter: @molssi_nsf
- Best Practices: https://molssi.org/education/best-practices/
- E-Mail List: MolSSI Mailing List
- Cookiecutter: https://github.com/MolSSI/cookiecutter-cms



Watch molssi.org for the latest information!

Tools

Version Control

GitHub

GitLab

Bitbucket

Code Coverage

- Services: Codecov, Coveralls
- Tools: gcov (C++), coverage (Python)

Static Analysis

- LGTM, Code Climate, PyFlakes

Continuous Integration

- Cloud hosted:
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