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# **SEAMM Util Documentation**

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This is documentation for developers! There is nothing here for users, since this is part of the underlying framework of SEAMM. Anything a users sees is documented either in the main SEAMM documentation or in the plug-in documentation.

Contents:



## SEAMM UTIL

Utility classes and functions that support other SEAMM tools

- Free software: BSD license
- Documentation: <https://seamm-util.readthedocs.io>.

### 1.1 Features

- TODO

### 1.2 Credits

This package was created with [Cookiecutter](#) and the [molssi-seamm/cookiecutter-seamm-plugin](#) project template.

Developed by the Molecular Sciences Software Institute (MolSSI), which receives funding from the [National Science Foundation](#) under awards OAC-1547580 and CHE-2136142





## INSTALLATION

### 2.1 Stable release

Some of the requirements to run the SEAMM framework cannot be automatically installed using e.g. pip but can be using Conda Forge. Please use the [SEAMM installer](#) to install this module and the other core modules that comprise SEAMM.

### 2.2 From sources

The sources for SEAMM Util can be downloaded from the [Github repo](#).

You can either clone the public repository:

```
$ git clone git://github.com/molssi-seamm/seamm_util
```

Or download the [tarball](#):

```
$ curl -OL https://github.com/molssi-seamm/seamm_util/tarball/master
```

Once you have a copy of the source, you can install it with:

```
$ python setup.py install
```

or more simply:

```
$ make install
```

*make* or *make help* will provide a list of all the targets.:

```
$ make
make
clean                remove all build, test, coverage and Python artifacts
clean-build          remove build artifacts
clean-pyc             remove Python file artifacts
clean-test           remove test and coverage artifacts
lint                 check style with black and flake8
format               reformat with with yapf and isort
typing              check typing
test                 run tests quickly with the default Python
test-all            run tests on every Python version with tox
```

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coverage	check code coverage quickly with the default Python
docs	generate Sphinx HTML documentation, including API docs
servedocs	compile the docs watching for changes
release	package and upload a release
dist	builds source and wheel package
install	install the package to the active Python's site-packages
uninstall	uninstall the package
\$	

Typically it is a good idea to check the formatting of your changes using *black* and *flake8* which is what the *lint* target does, e.g.:

```
$ make lint install
```

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## CHAPTER THREE

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### USAGE

To use SEAMM Util in a project:

```
import seamm_util
```



## CONTRIBUTING

Contributions are welcome, and they are greatly appreciated! Every little bit helps, and credit will always be given. You can contribute in many ways:

### 4.1 Types of Contributions

#### 4.1.1 Report Bugs

Report bugs at [https://github.com/molssi-seamm/seamm\\_util/issues](https://github.com/molssi-seamm/seamm_util/issues).

If you are reporting a bug, please include:

- Your operating system name and version.
- Any details about your local setup that might be helpful in troubleshooting.
- Detailed steps to reproduce the bug.

#### 4.1.2 Fix Bugs

Look through the GitHub issues for bugs. Anything tagged with “bug” and “help wanted” is open to whoever wants to implement it.

#### 4.1.3 Implement Features

Look through the GitHub issues for features. Anything tagged with “enhancement” and “help wanted” is open to whoever wants to implement it.

#### 4.1.4 Write Documentation

SEAMM Util could always use more documentation, whether as part of the official SEAMM Util docs, in docstrings, or even on the web in blog posts, articles, and such.

### 4.1.5 Submit Feedback

The best way to send feedback is to file an issue at [https://github.com/molssi-seamm/seamm\\_util/issues](https://github.com/molssi-seamm/seamm_util/issues).

If you are proposing a feature:

- Explain in detail how it would work.
- Keep the scope as narrow as possible, to make it easier to implement.
- Remember that this is a volunteer-driven project, and that contributions are welcome :)

## 4.2 Get Started!

Ready to contribute? Here's how to set up *seamm\_util* for local development.

1. Fork the *seamm\_util* repo on GitHub.
2. Clone your fork locally:

```
$ git clone git@github.com:your_name_here/seamm_util.git
```

3. Install your local copy into a virtualenv. Assuming you have virtualenvwrapper installed, this is how you set up your fork for local development:

```
$ mkvirtualenv seamm_util
$ cd seamm_util/
$ python setup.py develop
```

4. Create a branch for local development:

```
$ git checkout -b name-of-your-bugfix-or-feature
```

Now you can make your changes locally.

5. When you're done making changes, check that your changes pass flake8 and the tests, including testing other Python versions with tox:

```
$ flake8 seamm_util tests
$ python setup.py test or py.test
$ tox
```

To get flake8 and tox, just pip install them into your virtualenv.

6. Commit your changes and push your branch to GitHub:

```
$ git add .
$ git commit -m "Your detailed description of your changes."
$ git push origin name-of-your-bugfix-or-feature
```

7. Submit a pull request through the GitHub website.

## 4.3 Pull Request Guidelines

Before you submit a pull request, check that it meets these guidelines:

1. The pull request should include tests.
2. If the pull request adds functionality, the docs should be updated. Put your new functionality into a function with a docstring, and add the feature to the list in README.rst.
3. The pull request should work for Python 2.6, 2.7, 3.3, 3.4 and 3.5, and for PyPy. Check [https://travis-ci.org/molssi-seamm/seamm\\_util/pull\\_requests](https://travis-ci.org/molssi-seamm/seamm_util/pull_requests) and make sure that the tests pass for all supported Python versions.

## 4.4 Tips

To run a subset of tests:

```
$ py.test tests.test_seamm_util
```





## CREDITS

### 5.1 Development Lead

- Paul Saxe <[psaxe@molssi.org](mailto:psaxe@molssi.org)>

### 5.2 Contributors

None yet. Why not be the first?



## HISTORY

### 2023.6.4 – Added more unit conversions to support thermochemistry

- added  $E_h/K \rightarrow kJ/mol/K$

### 2023.4.6 – Added more unit conversions to support Buckingham potentials

- added e.g.  $eV \cdot \text{\AA}^6$  to  $kcal/mol \cdot \text{\AA}^6$  to support Buckingham potentials

### 2023.2.28 – Added a compact JSON encoder

- To make the schema-type JSON more human-readable.

### 2022.11.3 – More conversions involving substance (mol) to number

- Added  $energy/mol/\text{\AA}^2 \rightarrow energy/\text{\AA}^2$  for force constants
- Added  $energy/mol/\text{\AA}^3 \rightarrow energy/\text{\AA}^3$  for stress/pressure/elastic constants

### 0.1.0 (2017-12-07)

- First release on PyPI.



## INDICES AND TABLES

- `genindex`
  - `modindex`
  - `search`
-



## DOCUMENTATION VERSIONS