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# **SEAMM Forcefield Utilities Documentation**

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## SEAMM FORCEFIELD UTILITIES

The SEAMM Forcefield Utilities read and write forcefields, assigns them to molecules, and creates energy expressions.

- Free software: BSD license
- Documentation: [https://seamm\\_ff\\_util.readthedocs.io](https://seamm_ff_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 award ACI-1547580





## INSTALLATION

### 2.1 Stable release

To install the SEAMM Forcefield Utilities, run this command in your terminal:

```
$ pip install seamm_ff_util
```

This is the preferred method to install the SEAMM Forcefield Utilities, as it will always install the most recent stable release.

If you don't have `pip` installed, this [Python installation guide](#) can guide you through the process.

### 2.2 From sources

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

You can either clone the public repository:

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

Or download the [tarball](#):

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

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

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



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## CHAPTER THREE

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### USAGE

To use the SEAMM Forcefield Utilities in a project:

```
import seamm_ff_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\\_ff\\_util/issues](https://github.com/molssi-seamm/seamm_ff_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\_FF\_Util could always use more documentation, whether as part of the official SEAMM\_FF\_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\\_ff\\_util/issues](https://github.com/molssi-seamm/seamm_ff_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\_ff\_util* for local development.

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

```
$ git clone git@github.com:your_name_here/seamm_ff_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_ff_util
$ cd seamm_ff_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_ff_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 3.5, 3.6 and 3.7, and for PyPy. Check [https://travis-ci.org/molssi-seamm/seamm\\_ff\\_util/pull\\_requests](https://travis-ci.org/molssi-seamm/seamm_ff_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_forcefield
```





## 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

### 6.1 0.1.0 (2017-12-05)

- First release on PyPI.



## INDICES AND TABLES

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