SEAMM Documentation

Release 2020.12.4+1.g5a9300c.dirty

Paul Saxe

Dec 04, 2020

CONTENTS

Contents:

SIMULATION ENVIRONMENT FOR ATOMISTIC AND MOLECULAR SIMULATIONS (SEAMM)

The MolSSI Simulation Environment for computational molecular and materials science (CMS)

- Free software: GNU Lesser General Public License v3

- Documentation: https://seamm.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 Environment

Some of the requirements to run the SEAMM framework cannot be automatically installed using e.g. pip. A couple require a conda environment, so at the moment you will need to install either the Anaconda or conda Python environment from Continuum IO. The first dependency to install manually is RDKit. You can follow the RDKit documentation to install Anaconda, etc. but if you already have Anaconda/Conda installed you can simply do the following

```
$ conda create -c rdkit -n <env_name> python=3.6.1 rdkit
```

where you need to replace '<env_name>' with an environment name that you remember, like 'molssi'. Once you have installed RDKit, activate the environment:

```
$ source activate <env_name>
```

You also need to install Open Babel. Please consulte the Open Babel documentation for how to install on your operating system. The easiest way is to use conda:

```
$ conda install -c openbabel openbabel
```

2.2 Stable release

To install SEAMM, run this command in your terminal:

```
$ pip install seamm
```

This is the preferred method to install SEAMM, 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.

2.3 From sources

The sources for SEAMM can be downloaded from the Github repo.

You can either clone the public repository:

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

Or download the tarball:

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

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

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

USAGE

To use SEAMM in a project:

```
import seamm
```

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/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

MolSSI Workflow could always use more documentation, whether as part of the official MolSSI Workflow 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/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* for local development.

1. Fork the *seamm* repo on GitHub.

2. Clone your fork locally:

```
$ git clone git@github.com:your_name_here/seamm.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
$ cd seamm/
$ python setup.py develop
```

4. Create a branch for local development:

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

   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 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/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
```

CREDITS

5.1 Development Lead

- Paul Saxe <psaxe@molssi.org>

5.2 Contributors

None yet. Why not be the first?

HISTORY

6.1 0.1.0 (2018-01-20)

- First release on PyPI.

INDICES AND TABLES

- genindex
- modindex
- search