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# Squid Documentation

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Contents:





Squid is an open-source molecular simulation codebase developed by the Clancy Lab at the Johns Hopkins University. The codebase includes simplified Molecular Dynamics (MD) and Density Functional Theory (DFT) simulation submission, as well as other utilities such as file I/O and post-processing.

## 1.1 Installing

For most, the easiest way to install squid is to use pip install:

```
[user@local]~% pip install clancylab-squid
```

If you wish, you may also clone the repository though:

```
[user@local]~% cd ~; git clone https://github.com/ClancyLab/squid.git
```

Note, you will need various additional software to fully take advantage of squid. We include some helper scripts to aid you in setting up these files; however, these are not robust and we do encourage you to setup your own development environment. Nevertheless, if you so choose, the following information may be of use:

### Setup on Ubuntu

1. Ensure that your system is up-to-date with relevant software. The following commands will help.

```
[user@local]~% sudo apt-get update
[user@local]~% sudo apt-get upgrade
[user@local]~% sudo apt-get install build-essential make cmake g++ git swig mpich lmod
```

2. As the above line installs lmod, we have found that there may be a bug in the default install. If you find that when you open a terminal you are getting a weird error about posix not existing, this is a bug in lua install. Simply put, take the path it wants and make a symlink to point to posix\_c.so. An example of how to do this is as follows (note, your lua version and directories may or may not be the same).

```
[user@local]~% sudo ln -s /usr/lib/x86_64-linux-gnu/lua/5.2/posix_c.so /usr/lib/x86_64-linux-gnu/lua/5.2/posix.so
```

3. Setup your directories. In this case, we want all programs installed to the *~/programs* folder, and all modules installed to *~/modules*.

```
[user@local]~% mkdir ~/programs; mkdir ~/.modules
```

4. Setup a default environment file for lmod. In this case, we are making an empty one.

```
[user@local]~% touch ~/.modules/StdEnv.lua
```

5. Ensure that lmod is setup. This can be done by ensuring that the `~/.bashrc` is updated accordingly. Note, do not blindly copy, but understand what the following lines of code do!

```
# LMOD Setup
if [ -f /usr/share/lmod/6.6/init/bash ]; then
    . /usr/share/lmod/6.6/init/bash
fi
module use /home/$USER/.modules
if [ -z "$__Init_Default_Modules" ]; then
    export __Init_Default_Modules=1;

    LMOD_SYSTEM_DEFAULT_MODULES=${LMOD_SYSTEM_DEFAULT_MODULES:-"StdEnv"}
    export LMOD_SYSTEM_DEFAULT_MODULES
    module --initial_load --no_redirect restore
else
    module refresh
fi
```

6. Install as much as possible from squid. This can be done by running the following command:

```
import os
from squid.installers import *

# Get relevant path information
home_folder = os.path.expanduser("~")
program_folder = "%s/programs" % home_folder
module_folder = "%s/.modules" % home_folder
if not os.path.exists(program_folder):
    os.makedirs(program_folder, exist_ok=True)
if not os.path.exists(module_folder):
    os.makedirs(module_folder, exist_ok=True)

# As we plan to get orca/4.2.0, we need openmpi/3.1.4
openmpi_installer(program_folder, "3.1.4", module_folder)
```

7. Note, because you may want some programs for others, it is recommended that you first setup openmpi, as above, then return to install the others. This requires that you also load the openmpi module before compiling the next programs.

```
import os
from squid.installers import *

# Get relevant path information
home_folder = os.path.expanduser("~")
program_folder = "%s/programs" % home_folder
module_folder = "%s/.modules" % home_folder
if not os.path.exists(program_folder):
    os.makedirs(program_folder, exist_ok=True)
if not os.path.exists(module_folder):
    os.makedirs(module_folder, exist_ok=True)

# LAMMPS has many install options. Here we simplify things.
# Note, we can only choose between mpi or serial.
# Note, "l6Mar18_mpi" is the name of the module in the lammps
# submodule folder. Be unique!
```

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```

lammmps_installer(
    program_folder, "16Mar18", "mpi", "16Mar18_mpi",
    compiler="mpicxx",
    extra_lammmps_packages=[
        "RIGID", "PYTHON", "REPLICA", "USER-MISC", "USER-REAXC"],
    smrff_path=None,
    MODULEDIR=module_folder
)

# Install packmol
packmol_installer(program_folder, module_folder)

# Install nlopt
nlopt_installer(program_folder, "2.6.1", module_folder)

```

8. Download Orca from <https://orcaforum.kofo.mpg.de/app.php/dlxt/> (note, you'll have to register), and make your own orca module. An example is listed below (it would be saved in the modules folder as a .lua file.)

```

help([[
For detailed instructions, go to:
    https://orcaforum.cec.mpg.de/

]])
whatis("Version: 4.2.0")
whatis("Keywords: Orca 4")
whatis("URL: https://orcaforum.cec.mpg.de/")
whatis("Description: Orca 4")

load("openmpi/3.1.4")

prepend_path("PATH", "/home/username/programs/orca/4.2.0")
prepend_path("LD_LIBRARY_PATH", "/home/username/programs/orca/4.2.0")

```

## 1.2 Contributing

If you would like to be an active developer within the Clancy Group, please contact the project maintainer to be added as a collaborator on the project. Otherwise, you are welcome to submit pull requests as you see fit, and they will be addressed.

## 1.3 Documentation

Documentation is necessary, and the following steps **MUST** be followed during contribution of new code:

### Setup

1. Download [Sphinx](#). This can be done simply if you have [pip](#) installed via `pip install -U Sphinx`
2. Wherever you have *squid* installed, you want another folder called *squid-docs* (NOT as a subfolder of *squid*).

```

[user@local]~% cd ~; mkdir squid-docs; cd squid-docs; git clone -b gh-pages_
↪git@github.com:clancylab/squid.git html

```

3. Forever more just ignore that directory (don't delete it though)

### Adding Documentation

Documentation is done using [ReStructuredText](#) format docstrings, the [Sphinx](#) python package, and indices with autodoc extensions. To add more documentation, first add the file to be included in `docs/source/conf.py` under `os.path.abspath('example/dir/to/script.py')`. Secondly, ensure that you have proper docstrings in the python file, and finally run `make full` to re-generate the documentation and commit it to your local branch, as well as the git `gh-pages` branch.

For anymore information on documentation, the tutorial follwed can be found [here](#).

## OVERVIEW

### 2.1 calcs

The calcs module contains various calculations that can be seen as an automated task. Primarily, it currently holds two NEB class objects that handle running Nudged Elastic Band.

The first object, `squid.calcs.neb.NEB`, will run a standard NEB optimization. It allows for fixes such as the procrustes superimposition method and climbing image. The second object, `squid.calcs.aneb.ANEB`, handles the automated NEB approach, which will dynamically add in frames during the optimization. The idea of ANEB is that, in the end it should require less DFT calculations to complete.

**Module Files:**

- `neb`
  - `aneb`
- 

### 2.2 files

The files module handles file input and output. Currently, the following is supported:

- `squid.files.xyz_io.read_xyz()`
- `squid.files.xyz_io.write_xyz()`
- `squid.files.cml_io.read_cml()`
- `squid.files.cml_io.write_cml()`

Note - you can import any of these function directly from the files module as:

```
from squid import files
frames = files.read_xyz("demo.xyz")
```

Alternatively, some generators have been made to speed up the reading in of larger files:

- `squid.files.xyz_io.read_xyz_gen()`

When reading in xyz files of many frames, a list of lists holding `structures.atom.Atom` objects is returned. Otherwise, a single list of `structures.atom.Atom` objects is returned.

When reading in cml files, a list of `structures.molecule.Molecule` objects is returned.

Finally, additional functionality exists within the misc module:

---

- `squid.files.misc.is_exe()` - Determine if a file is an executable.
- `squid.files.misc.last_modified()` - Determine when a file was last modified.
- `squid.files.misc.which()` - Determine where a file is on a system.

**Module Files:**

- xyz\_io
  - cml\_io
  - misc
- 

## 2.3 forcefields

To handle forcefields in Molecular Dynamics, the various components are subdivided into objects. These are then stored in an overarching `squid.forcefields.parameters.Parameters` object, which is the main interface a user should use.

Main user interface:

- `squid.forcefields.parameters.Parameters`

Subdivided objects:

- `squid.forcefields.connectors.HarmonicConnector` - A generic connector object.
- `squid.forcefields.connectors.Bond` - Derived from the `HarmonicConnector`, this handles Bonds.
- `squid.forcefields.connectors.Angle` - Derived from the `HarmonicConnector`, this handles Angles.
- `squid.forcefields.connectors.Dihedral` - Derived from the `HarmonicConnector`, this handles Dihedrals.

Supported Potentials:

- `squid.forcefields.coulomb.Coul` - An object to handle Coulombic information. This also holds other pertinent atomic information (element, mass, etc).
- `squid.forcefields.lj.LJ` - An object to handle the Lennard-Jones information.
- `squid.forcefields.morse.Morse` - An object to handle Morse information.
- `squid.forcefields.tersoff.Tersoff` - An object to handle Tersoff information.

Helper Code:

- `squid.forcefields.opls.parse_pfile()` - A function to parse the OPLS parameter file.
- `squid.forcefields.smrff.parse_pfile()` - A function to parse the SMRFF parameter file.

**Module Files:**

- coulomb
- lj
- morse
- tersoff
- opls

- `smrff`
  - `connectors`
  - `helper`
  - `parameters`
- 

## 2.4 g09

TODO

**Module Files:**

- `TODO`
- 

## 2.5 geometry

The geometry module is broken down into different sections to handle atomic/molecular/system transformations/calculations.

The transform module holds functions that handle molecular transformations.

- `squid.geometry.transform.align_centroid()` - Align list of atoms to an ellipse along the x-axis.
- `squid.geometry.transform.center_frame()` - Center a list of atomic coordinates.
- `squid.geometry.transform.center_frames()` - Center multiple frames of atomic coordinates.
- `squid.geometry.transform.interpolate()` - Linearly interpolate N frames between a given two frames.
- `squid.geometry.transform.perturbate()` - Perturbate atomic coordinates of a list of atoms.
- `squid.geometry.transform.procrustes()` - Propagate rotations along a list of atoms to minimize rigid rotation, and return the rotation matrices used.
- `squid.geometry.transform.smooth_xyz()` - Iteratively use procrustes and linear interpolation to smooth out a list of atomic coordinates.

Note, when using `squid.geometry.transform.procrustes()` the input frames are being changed! If this is not desired behaviour, and you solely wish for the rotation matrix, then pass in a copy of the frames.

The spatial module holds functions that handle understanding the spatial relationship between atoms/molecules.

- `squid.geometry.spatial.furthest_atoms()` - Return the furthest atoms in a given list of atoms.
- `squid.geometry.spatial.furthest_n_atoms_to_r()` - Return the furthest n atoms to some coordinate.
- `squid.geometry.spatial.motion_per_frame()` - Get the inter-frame RMS motion per frame.
- `squid.geometry.spatial.mvee()` - Fit a volume to a list of atomic coordinates.
- `squid.geometry.spatial.nearest_atoms()` - Return the nearest atoms in a given list of atoms.
- `squid.geometry.spatial.nearest_n_atoms_to_r()` - Return the nearest n atoms to some coordinate.

- `squid.geometry.spatial.orthogonal_procrustes()` - Find the rotation matrix that best fits one list of atomic coordinates onto another.
- `squid.geometry.spatial.random_rotation_matrix()` - Generate a random rotation matrix.
- `squid.geometry.spatial.rotation_matrix()` - Generate a rotation matrix based on angle and axis.

The `packmol` module handles the interface between Squid and `packmol` (<http://m3g.iqm.unicamp.br/packmol/home.shtml>). The main functionality here is simply calling `squid.geometry.packmol.packmol()` on a system object with a set of molecules.

The `misc` module holds functions that are not dependent on other squid modules, but can return useful information and simplify coding.

- `squid.geometry.misc.get_center_of_geometry()`
- `squid.geometry.misc.get_center_of_mass()`
- `squid.geometry.misc.rotate_atoms()`

Once again, all the above can be accessed directly from the `geometry` module, as shown in the following pseudo-code example here:

```
# NOTE THIS IS PSEUDO CODE AND WILL NOT WORK AS IS

from squid import geometry

moll = None
system_obj = None

geometry.packmol(system_obj, [moll], density=1.0)
geometry.get_center_of_geometry(system_obj.atoms)
```

**Module Files:**

- `misc`
  - `packmol`
  - `spatial`
  - `transform`
- 

## 2.6 jdftx

TODO

**Module Files:**

- `TODO`
-



## 2.7 jobs

The jobs module handles submitting simulations/calculations to either a queueing system (ex. SLURM/NBS), or locally on a machine. This is done by storing a job into a job container, which will monitor it and allow the user to assess if simulations are still running or not. The job object is mainly used within squid, and is not normally required for the user to generate on their own.

The main interface with the job module is through the queue\_manager module and the submission module; however, lower level access can be obtained through the container, nbs, slurm, and misc modules.

The queue\_manager module holds the following:

- `squid.jobs.queue_manager.get_all_jobs()` - Get a list of all jobs submitted that are currently running or pending.
- `squid.jobs.queue_manager.get_available_queues()` - Get a list of the available queue/partition names.
- `squid.jobs.queue_manager.get_pending_jobs()` - Get a list of all jobs submitted that are currently pending.
- `squid.jobs.queue_manager.get_queue_manager()` - Get the queue manager available on the system.
- `squid.jobs.queue_manager.get_running_jobs()` - Get a list of all jobs submitted that are currently running.
- `squid.jobs.queue_manager.Job()` - Get a Job object container depending on the queueing system used.

The submission module holds two function that handle submitting a job:

- `squid.jobs.submission.submit_job()` - Submit a script as a job.
- `squid.jobs.submission.pysub()` - Submit a python script as a job.

### Module Files:

- container
  - nbs
  - queue\_manager
  - slurm
  - submission
- 

## 2.8 lammps

The lammps module allows squid to interface with the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code. Due to the inherent flexibility of LAMMPS, the user is still required to write-up their own lammps input script so as to not obfuscate the science; however, tedious additional tasks can be done away with using squid.

Two main abilities exist within the lammps module: submitting simulations and parsing output. This is divided into the following:

- `squid.lammps.job.job()` - The main function that allows a user to submit a LAMMPS simulation.

- `squid.lammps.io.dump.read_dump()` - The main function that allows a user to robustly read in a LAMMPS dump file.
- `squid.lammps.io.dump.read_dump_gen()` - A generator for reading in a LAMMPS dump file, so as to improve speeds.
- `squid.lammps.io.data.write_lammps_data()` - A function to automate the writing of a LAMMPS data file.

**Module Files:**

- `io.dump`
- `io.data`
- `io.thermo`
- `job`
- `parser`

**References:**

- <https://lammps.sandia.gov/>
  - [www.cs.sandia.gov/~sjplimp/pizza.html](http://www.cs.sandia.gov/~sjplimp/pizza.html)
- 

## 2.9 maths

The maths module handles additional mathematical calculations that do not pertain to atomic coordinates.

- `squid.maths.lhs.create_lhs()` - A function to generate Latin Hypercube Sampled values.

**Module Files:**

- `lhs`

**References:**

- <https://pythonhosted.org/pyDOE/>
- 

## 2.10 optimizers

The optimizers module contains various functions aiding in optimization. Several of these approaches are founded on methods within scipy with minor alterations made here to aid in the internal use of NEB optimization. If you need to use an optimizer, we recommend going straight to Scipy and using their optimizers, as they will remain more up-to-date. These have injected features allowing for use with the internal squid NEB and ANEB calculations.

- `squid.optimizers.steepest_descent.steepest_descent()`
- `squid.optimizers.bfgs.bfgs()`
- `squid.optimizers.lbfgs.lbfgs()`
- `squid.optimizers.quick_min.quick_min()`
- `squid.optimizers.fire.fire()`

- `squid.optimizers.conjugate_gradient.conjugate_gradient()`

**Module Files:**

- `steepest_descent`
  - `bfgs`
  - `lbfgs`
  - `quick_min`
  - `fire`
  - `conjugate_gradient`
- 

## 2.11 orca

The orca module allows squid to interface with the orca DFT code.

- `squid.orca.job.job()` - Submit a simulation.
- `squid.orca.job.jobarray()` - Submit a set of simulations.
- `squid.orca.io.read()` - Read in all relevant information from an orca output simulation.
- `squid.orca.post_process.gbwh_to_cube()` - Convert the output orca gbwh file to a cube file for further processing.
- `squid.orca.post_process.mo_analysis()` - Automate the generation of molecular orbitals from an orca simulation, which will then be visualized using VMD.
- `squid.orca.post_process.pot_analysis()` - Automate the generation of an electrostatic potential mapped to the electron density surface from an orca simulation, which will then be visualized using VMD.

**Module Files:**

- `io`
- `job`
- `mep`
- `post_process`
- `utils`

**References:**

- <https://sites.google.com/site/orcainputlibrary/dft>
- 

## 2.12 post\_process

The post\_process module holds functions that will aid in common post processing procedures. They further interface with external programs to visualize or simplify the process.

- `squid.post_process.debyer.get_pdf()` - Get a Pair Distribution Function (PDF) of a list of atomic coordinates. This is done using the debyer software (requires that debyer is installed).

- `squid.post_process.vmd.plot_MO_from_cube()` - Visualize molecular orbitals in VMD from a cube file.
- `squid.post_process.vmd.plot_electrostatic_from_cube()` - Visualize the electrostatic potential in VMD from a cube file.
- `squid.post_process.ovito.ovito_xyz_to_image()` - Automate the generation of an image of atomic coordinates using ovito.
- `squid.post_process.ovito.ovito_xyz_to_gif()` - Automate the generation of a gif of a sequence of atomic coordinates using ovito.

**Module Files:**

- debyer
- ovito
- vmd

**References:**

- <https://debyer.readthedocs.io/en/latest/>
  - <https://ovito.org/>
  - <https://www.ks.uiuc.edu/Research/vmd/>
- 

## 2.13 qe

TODO

**Module Files:**

- TODO
- 

## 2.14 structures

To handle atomic manipulation in python, we break down systems into the following components:

- `squid.structures.atom.Atom` - A single atom object.
- `squid.structures.topology.Connector` - A generic object to handle bonds, angles, and dihedrals.
- `squid.structures.molecule.Molecule` - A molecule object that stores atoms and all inter-atomic connections.
- `squid.structures.system.System` - A system object that holds a simulation environment. Consider this many molecules, and system dimensions for Molecular Dynamics.

For simplicity sake, when we generate a Molecule object based on atoms and bonds, all relevant angles and dihedrals are also generated and stored.

We also store objects to hold output simulation data:

- `squid.structures.results.DFT_out` - DFT specific output
- `squid.structures.results.sim_out` - More generic output

**Module Files:**

- atom
  - molecule
  - results
  - system
  - topology
- 

## 2.15 utils

The utils module holds various utility functions that help squid internally; however, can be used externally as well.

**The cast module holds functions to handle variable type assessment:**

- `squid.utils.cast.is_array()` - Check if a variable is array like.
- `squid.utils.cast.check_vec()` - Check a vector for certain features.
- `squid.utils.cast.is_numeric()` - Check if a variable is numeric.
- `squid.utils.cast.assert_vec()` - Assert that a variable is array like with certain features.
- `squid.utils.cast.simplify_numerical_array()` - Simplify a sequence of numbers to a comma separated string with values within a range indicated using inclusive i-j.

**The print\_helper module holds functions to simplify string terminal output on Linux/Unix primarily:**

- `squid.utils.print_helper.color_set()`
- `squid.utils.print_helper.strip_color()`
- `squid.utils.print_helper.spaced_print()`
- `squid.utils.print_helper.printProgressBar()`
- `squid.utils.print_helper.bytes2human()`

**The units module holds functions to handle SI unit conversion:**

- `squid.utils.units.convert_energy()`
- `squid.utils.units.convert_pressure()`
- `squid.utils.units.convert_dist()`
- `squid.utils.units.elem_i2s()`
- `squid.utils.units.elem_s2i()`
- `squid.utils.units.elem_weight()`
- `squid.utils.units.elem_sym_from_weight()`
- `squid.utils.units.convert()`

**Module Files:**

- cast
- print\_helper
- units



## CODEBASE

### 3.1 calcs

#### 3.1.1 ANEB

The Auto ANEB module simplifies the submission of Auto Nudged Elastic Band simulations.

NOTE! This module is still in a very rough beta. It has been hacked together from the NEB module and is being tested. Do not use this expecting a miracle.

Squid Auto Nudged Elastic Band package Currently supports g09 and orca Cite ANEB:

<http://aip.scitation.org/doi/full/10.1063/1.4961868> <http://scitation.aip.org/content/aip/journal/jcp/113/22/10.1063/1.1323224>

**BFGS is the best method, cite:** [http://theory.cm.utexas.edu/henkelman/pubs/sheppard08\\_134106.pdf](http://theory.cm.utexas.edu/henkelman/pubs/sheppard08_134106.pdf)

Nudged Elastic Band. k for VASP is 5 eV/Angstrom, ie 0.1837 Hartree/Angstrom. Gtol of 1E-5 from scipy.bfgs package

The following code has been tested out to some moderate success for now:

```
new_opt_params = {'step_size': 1.0,
                  'step_size_adjustment': 0.5,
                  'max_step': 0.04,
                  'maxiter': 100,
                  'linesearch': None,
                  'accelerate': False,
                  'N_reset_hess': 10,
                  'max_steps_remembered': 5,
                  'fit_rigid': True,
                  'g_rms': units.convert("eV/Ang", "Ha/Ang", 0.001),
                  'g_max': units.convert("eV/Ang", "Ha/Ang", 0.03)}

new_auto_opt_params = {'step_size': 1.0,
                      'step_size_adjustment': 0.5,
                      'max_step': 0.04,
                      'maxiter': 20,
                      'linesearch': 'backtrack',
                      'accelerate': True,
                      'reset_step_size': 20,
                      'fit_rigid': True,
                      'g_rms': units.convert("eV/Ang", "Ha/Ang", 10.0),
                      'g_max': units.convert("eV/Ang", "Ha/Ang", 0.03)}
```

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```
nebs = aneb.ANEB("debug_auto", frames, "!HF-3c", fit_rigid=True,
                 opt='LBFGS',
                 new_opt_params=new_opt_params,
                 new_auto_opt_params=new_auto_opt_params,
                 ci_N=3,
                 ANEB_Nsim=5,
                 ANEB_Nmax=15)
```

- `g09_start_job()`
- `g09_results()`
- `orca_start_job()`
- `orca_results()`
- `ANEB`

```
class squid.calcs.aneb.ANEB(name, states, theory, extra_section="", initial_guess=None,
                             spring_atoms=None, procs=1, queue=None, mem=2000, priority=None,
                             disp=0, k=0.00367453, charge=0, fit_rigid=True, DFT='orca',
                             opt='LBFGS', start_job=None, get_results=None, new_opt_params={},
                             new_auto_opt_params={}, callback=None, ci_ANEB=False, ci_N=5,
                             ANEB_Nsim=5, ANEB_Nmax=15, add_by_energy=False)
```

A method for determining the minimum energy pathway of a reaction using DFT. Note, this method was written for atomic orbital DFT codes; however, is potentially generalizable to other programs.

#### Parameters

- name:** *str* The name of the ANEB simulation to be run.
- states:** *list, list, squid.structures.atom.Atom* A list of frames, each frame being a list of atom structures. These frames represent your reaction coordinate.
- theory:** *str* The route line for your DFT simulation.
- extra\_section:** *str, optional* Additional parameters for your DFT simulation.
- initial\_guess:** *list, str, optional* TODO - List of strings specifying a previously run ANEB simulation, allowing restart capabilities.
- spring\_atoms:** *list, int, optional* Specify which atoms will be represented by virtual springs in the ANEB calculations. Default includes all.
- procs:** *int, optional* The number of processors for your simulation.
- queue:** *str, optional* Which queue you wish your simulation to run on (queueing system dependent). When None, ANEB is run locally.
- mem:** *float, optional* Specify memory constraints (specific to your X\_start\_job method).
- priority:** *int, optional* Whether to submit a DFT simulation with some given priority or not.
- disp:** *int, optional* Specify for additional stdout information.
- charge:** *int* Charge of the system.
- k:** *float, optional* The spring constant for your ANEB simulation.



**fit\_rigid:** *bool, optional* Whether you want to use procrustes to minimize motion between adjacent frames (thus minimizing error due to excessive virtual spring forces).

**DFT:** *str, optional* Specify if you wish to use the default X\_start\_job and X\_results functions where X is either g09 or orca.

**opt:** *str, optional* Select which optimization method you wish to use from the following: LBFGS.

**start\_job:** *func, optional* A function specifying how to submit your ANEB single point calculations. Needed if DFT is neither orca nor g09.

**get\_results:** *func, optional* A function specifying how to read your ANEB single point calculations. Needed if DFT is neither orca nor g09.

**new\_opt\_params:** *dict, optional* Pass any additional parameters to the optimization algorithm. Note, these parameters are for the final calculation after frames have been added in.

**new\_auto\_opt\_params:** *dict, optional* Pass any additional parameters to the optimization algorithm. Note, these parameters are for the iterative calculations, as frames are being added to the band.

**callback:** *func, optional* A function to be run after each each to calculate().

**ci\_ANEB:** *bool, optional* Whether to use the climbing image variation of ANEB.

**ci\_N:** *int, optional* How many iterations to wait in climbing image ANEB before selecting which image to be used.

**ANEB\_Nsim:** *int, optional* The number of frames for an auto ANEB calculation. If an even number is chosen, the expansion happens around floor(ANEB\_Nsim/2).

**ANEB\_Nmax:** *int, optional* The maximum number of frames to build up to in the auto ANEB.

**add\_by\_energy:** *bool, optional* If the user wants to add frames by the largest dE instead of dR (motion per frame), then set this flag to True.

## Returns

This [ANEB](#) object.

## References

- Henkelman, G.; Jonsson, H. The Journal of Chemical Physics 2000, 113, 9978-9985.
- Jonsson, H.; Mills, G.; Jacobson, K. W. In Classical and Quantum Dynamics in Condensed Phase Simulations;
- Berne, B. J., Ciccotti, G., Coker, D. F., Eds.; World Scientific, 1998; Chapter 16, pp 385-404.
- Armijo, L. Pacific Journal of Mathematics 1966, 16.
- Sheppard, D.; Terrell, R.; Henkelman, G. The Journal of Chemical Physics 2008, 128.
- Henkelman, G.; Uberuaga, B. P.; Jonsson, H. Journal of Chemical Physics 2000, 113.
- Atomic Simulation Environment - <https://wiki.fysik.dtu.dk/ase/>
- Kolsbjerg, E. L.; Groves, M. N.; Hammer, B. The Journal of Chemical Physics 2016, 145.

**align\_coordinates** (*r, B=None, H=None, return\_matrix=False*)

Get a rotation matrix A that will remove rigid rotation from the new coordinates r. Further, if another vector needs rotating by the same matrix A, it should be passed in B and will be rotated. If a matrix also needs rotating, it can be passed as H and also be rotated.

*Parameters*

**r:** *list, float* 1D array of atomic coordinates to be rotated by procrustes matrix A.

**B:** *list, list, float, optional* A list of vectors that may also be rotated by the same matrix as *r*.

**H:** *list, list, float, optional*

A matrix that should also be rotated via:  $H = R * H * R.T$

**return\_matrix:** *bool, optional* Whether to also return the rotation matrix used or not.

#### Returns

**rotations:** *dict* A dictionary holding 'A', the rotation matrix, 'r', the rotated new coordinates, 'B', a list of all other vectors that were rotated, and 'H', a rotated matrix.

`squid.calcs.aneb.g09_results` (*ANEB, step\_to\_use, i, state*)

A method for reading in the output of Gaussian09 single point calculations for ANEB calculations. This will both (a) assign forces to the atoms stored in state and (b) return the energy and atoms.

#### Parameters

**ANEB:** *ANEB* An ANEB container holding the main ANEB simulation

**step\_to\_use:** *int* Which iteration in the ANEB sequence the output to be read in is on.

**i:** *int* The index corresponding to which image on the frame is to be simulated.

**state:** *list, squid.structures.atom.Atom* A list of atoms describing the image on the frame associated with index *i*.

#### Returns

**new\_energy:** *float* The energy of the system in Hartree (Ha).

**new\_atoms:** *list, squid.structures.atom.Atom* A list of atoms with the forces attached in units of Hartree per Angstrom (Ha/Ang).

`squid.calcs.aneb.g09_start_job` (*ANEB, i, state, charge, procs, queue, initial\_guess, extra\_section, mem, priority*)

A method for submitting a single point calculation using Gaussian09 for ANEB calculations.

#### Parameters

**ANEB:** *ANEB* An ANEB container holding the main ANEB simulation

**i:** *int* The index corresponding to which image on the frame is to be simulated.

**state:** *list, squid.structures.atom.Atom* A list of atoms describing the image on the frame associated with index *i*.

**charge:** *int* Charge of the system.

**procs:** *int* The number of processors to use during calculations.

**queue:** *str* Which queue to submit the simulation to (this is queueing system dependent).

**initial\_guess:** *str* The name of a previous simulation for which we can read in a hessian.

**extra\_section:** *str* Extra settings for this DFT method.

**mem:** *int* How many Mega Words (MW) you wish to have as dynamic memory.

**priority:** *int* Whether to submit the job with a given priority (NBS). Not setup for this function yet.

#### Returns

**g09\_job:** *squid.jobs.container.JobObject* A job container holding the g09 simulation.

`squid.calcs.aneb.orca_results` (*ANEB, step\_to\_use, i, state*)

A method for reading in the output of Orca single point calculations for ANEB calculations. This will both (a) assign forces to the atoms stored in state and (b) return the energy and atoms.

#### Parameters

**ANEB:** *ANEB* An ANEB container holding the main ANEB simulation

**step\_to\_use:** *int* Which iteration in the ANEB sequence the output to be read in is on.

**i:** *int* The index corresponding to which image on the frame is to be simulated.

**state:** *list, squid.structures.atom.Atom* A list of atoms describing the image on the frame associated with index *i*.

#### Returns

**new\_energy:** *float* The energy of the system in Hartree (Ha).

**new\_atoms:** *list, squid.structures.atom.Atom* A list of atoms with the forces attached in units of Hartree per Angstrom (Ha/Ang).

`squid.calcs.aneb.orca_start_job` (*ANEB, i, state, charge, procs, queue, initial\_guess, extra\_section, mem, priority*)

A method for submitting a single point calculation using Orca for ANEB calculations.

#### Parameters

**ANEB:** *ANEB* An ANEB container holding the main ANEB simulation

**i:** *int* The index corresponding to which image on the frame is to be simulated.

**state:** *list, squid.structures.atom.Atom* A list of atoms describing the image on the frame associated with index *i*.

**charge:** *int* Charge of the system.

**procs:** *int* The number of processors to use during calculations.

**queue:** *str* Which queue to submit the simulation to (this is queueing system dependent).

**initial\_guess:** *str* The name of a previous simulation for which we can read in a hessian.

**extra\_section:** *str* Extra settings for this DFT method.

**mem:** *int* How many MegaBytes (MB) of memory you have available per core.

**priority:** *int* Whether to submit to NBS with a given priority

#### Returns

**orca\_job:** *squid.jobs.container.JobObject* A job container holding the orca simulation.

## 3.1.2 NEB

The NEB module simplifies the submission of Nudged Elastic Band simulations.

- `g09_start_job()`
- `g09_results()`
- `orca_start_job()`
- `orca_results()`
- `NEB`

```
class squid.calcs.neb.NEB(name, states, theory, extra_section="", initial_guess=None,
                           spring_atoms=None, nprocs=1, queue=None, mem=2000, priority=None,
                           disp=0, k=0.00367453, charge=0, multiplicity=1, fit_rigid=True,
                           DFT='orca', opt='LBFGS', start_job=None, get_results=None,
                           new_opt_params={}, callback=None, ci_neb=False, ci_N=5, no_energy=False)
```

A method for determining the minimum energy pathway of a reaction using DFT. Note, this method was written for atomic orbital DFT codes; however, is potentially generalizable to other programs.

### Parameters

- name:** *str* The name of the NEB simulation to be run.
- states:** *list, list, squid.structures.atom.Atom* A list of frames, each frame being a list of atom structures. These frames represent your reaction coordinate.
- theory:** *str* The route line for your DFT simulation.
- extra\_section:** *str, optional* Additional parameters for your DFT simulation.
- initial\_guess:** *list, str, optional* TODO - List of strings specifying a previously run NEB simulation, allowing restart capabilities.
- spring\_atoms:** *list, int, optional* Specify which atoms will be represented by virtual springs in the NEB calculations. Default includes all.
- nprocs:** *int, optional* The number of processors for your simulation.
- queue:** *str, optional* Which queue you wish your simulation to run on (queueing system dependent). When None, NEB is run locally.
- mem:** *float, optional* Specify memory constraints (specific to your X\_start\_job method).
- priority:** *int, optional* Whether to submit a DFT simulation with some given priority or not.
- disp:** *int, optional* Specify for additional stdout information.
- charge:** *int* Charge of the system.
- multiplicity:** *int* Multiplicity of the system.
- k:** *float, optional* The spring constant for your NEB simulation.
- fit\_rigid:** *bool, optional* Whether you want to use procrustes to minimize motion between adjacent frames (thus minimizing error due to excessive virtual spring forces).
- DFT:** *str, optional* Specify if you wish to use the default X\_start\_job and X\_results functions where X is either g09 or orca.
- opt:** *str, optional* Select which optimization method you wish to use from the following: BFGS, LBFGS, SD, FIRE, QM, CG, scipy\_X. Note, if using scipy\_X, change X to be a valid scipy minimize method.
- start\_job:** *func, optional* A function specifying how to submit your NEB single point calculations. Needed if DFT is neither orca nor g09.
- get\_results:** *func, optional* A function specifying how to read your NEB single point calculations. Needed if DFT is neither orca nor g09. Note, this function returns two things: list of energies, list of atoms. Further, the forces are contained within each atom object. It also requires that the forces on the state object be updated within said function (for more info see example codes). Finally, if using no\_energy=True, then return None (or an empty list) for the energies.
- new\_opt\_params:** *dict, optional* Pass any additional parameters to the optimization algorithm.

**callback:** *func, optional* A function to be run after each each to calculate().

**ci\_neb:** *bool, optional* Whether to use the climbing image variation of NEB.

**ci\_N:** *int, optional* How many iterations to wait in climbing image NEB before selecting which image to be used.

**no\_energy:** *bool, optional* A flag to turn on an experimental method, in which our selection of the tangent is based on only the force, and not the energy. Note, the code still expects the `get_results` function to return two things, so just have it return (None, atoms + forces).

## Returns

This *NEB* object.

## References

- Henkelman, G.; Jonsson, H. The Journal of Chemical Physics 2000, 113, 9978-9985.
- Jonsson, H.; Mills, G.; Jacobson, K. W. In Classical and Quantum Dynamics in Condensed Phase Simulations;
- Berne, B. J., Ciccotti, G., Coker, D. F., Eds.; World Scientific, 1998; Chapter 16, pp 385-404.
- Armijo, L. Pacific Journal of Mathematics 1966, 16.
- Sheppard, D.; Terrell, R.; Henkelman, G. The Journal of Chemical Physics 2008, 128.
- Henkelman, G.; Uberuaga, B. P.; Jonsson, H. Journal of Chemical Physics 2000, 113.
- Atomic Simulation Environment - <https://wiki.fysik.dtu.dk/ase/>

**align\_coordinates** (*r, B=None, H=None, return\_matrix=False*)

Get a rotation matrix A that will remove rigid rotation from the new coordinates r. Further, if another vector needs rotating by the same matrix A, it should be passed in B and will be rotated. If a matrix also needs rotating, it can be passed as H and also be rotated.

### Parameters

**r:** *list, float* 1D array of atomic coordinates to be rotated by procrustes matrix A.

**B:** *list, list, float, optional* A list of vectors that may also be rotated by the same matrix as r.

**H:** *list, list, float, optional*

A matrix that should also be rotated via:  $H = R * H * R.T$

**return\_matrix:** *bool, optional* Whether to also return the rotation matrix used or not.

### Returns

**rotations:** *dict* A dictionary holding 'A', the rotation matrix, 'r', the rotated new coordinates, 'B', a list of all other vectors that were rotated, and 'H', a rotated matrix.

`squid.calcs.neb.g09_results` (*NEB, step\_to\_use, i, state*)

A method for reading in the output of Gaussian09 single point calculations for NEB calculations. This will both (a) assign forces to the atoms stored in state and (b) return the energy and atoms.

## Parameters

**NEB:** *NEB* An NEB container holding the main NEB simulation

**step\_to\_use:** *int* Which iteration in the NEB sequence the output to be read in is on.

**i:** *int* The index corresponding to which image on the frame is to be simulated.

**state:** *list, squid.structures.atom.Atom* A list of atoms describing the image on the frame associated with index i.

**Returns**

**new\_energy:** *float* The energy of the system in Hartree (Ha).

**new\_atoms:** *list*, *squid.structures.atom.Atom* A list of atoms with the forces attached in units of Hartree per Angstrom (Ha/Ang).

`squid.calcs.neb.g09_start_job` (*NEB*, *i*, *state*, *charge*, *multiplicity*, *nprocs*, *queue*, *initial\_guess*, *extra\_section*, *mem*, *priority*, *extra\_keywords*={})

A method for submitting a single point calculation using Gaussian09 for NEB calculations.

**Parameters**

**NEB:** *NEB* An NEB container holding the main NEB simulation

**i:** *int* The index corresponding to which image on the frame is to be simulated.

**state:** *list*, *squid.structures.atom.Atom* A list of atoms describing the image on the frame associated with index *i*.

**charge:** *int* Charge of the system.

**multiplicity:** *int* Multiplicity of the system.

**nprocs:** *int* The number of processors to use during calculations.

**queue:** *str* Which queue to submit the simulation to (this is queueing system dependent).

**initial\_guess:** *str* The name of a previous simulation for which we can read in a hessian.

**extra\_section:** *str* Extra settings for this DFT method.

**mem:** *int* How many Mega Words (MW) you wish to have as dynamic memory.

**priority:** *int* Whether to submit the job with a given priority (NBS). Not setup for this function.

**extra\_keywords:** *dict*, *optional* Specify extra keywords beyond the defaults.

**Returns**

**g09\_job:** *squid.jobs.container.JobObject* A job container holding the g09 simulation.

`squid.calcs.neb.orca_results` (*NEB*, *step\_to\_use*, *i*, *state*)

A method for reading in the output of Orca single point calculations for NEB calculations. This will both (a) assign forces to the atoms stored in state and (b) return the energy and atoms.

**Parameters**

**NEB:** *NEB* An NEB container holding the main NEB simulation

**step\_to\_use:** *int* Which iteration in the NEB sequence the output to be read in is on.

**i:** *int* The index corresponding to which image on the frame is to be simulated.

**state:** *list*, *squid.structures.atom.Atom* A list of atoms describing the image on the frame associated with index *i*.

**Returns**

**new\_energy:** *float* The energy of the system in Hartree (Ha).

**new\_atoms:** *list*, *squid.structures.atom.Atom* A list of atoms with the forces attached in units of Hartree per Angstrom (Ha/Ang).

`squid.calcs.neb.orca_start_job` (*NEB*, *i*, *state*, *charge*, *multiplicity*, *nprocs*, *queue*, *initial\_guess*, *extra\_section*, *mem*, *priority*, *extra\_keywords*={})

A method for submitting a single point calculation using Orca for NEB calculations.

**Parameters**

**NEB:** *NEB* An NEB container holding the main NEB simulation

**i:** *int* The index corresponding to which image on the frame is to be simulated.

**state:** *list*, *squid.structures.atom.Atom* A list of atoms describing the image on the frame associated with index *i*.

**charge:** *int* Charge of the system.

**multiplicity:** *int* Multiplicity of the system.

**nprocs:** *int* The number of processors to use during calculations.

**queue:** *str* Which queue to submit the simulation to (this is queueing system dependent).

**initial\_guess:** *str* The name of a previous simulation for which we can read in a hessian.

**extra\_section:** *str* Extra settings for this DFT method.

**mem:** *int* How many MegaBytes (MB) of memory you have available per core.

**priority:** *int* Whether to submit to NBS with a given priority

**extra\_keywords:** *dict*, *optional* Specify extra keywords beyond the defaults.

#### Returns

**orca\_job:** *squid.jobs.container.JobObject* A job container holding the orca simulation.

## 3.2 files

### 3.2.1 cml\_io

`squid.files.cml_io.read_cml(name)`

Read in a file written in the Chemical Markup Language (CML) format. As cml files may hold more than simple atomic coordinates, we return a list of molecules instead.

#### Parameters

**name:** *str* File name.

#### Returns

**molecules:** *list*, *squid.structures.molecule.Molecule* A list of molecules in read in from the CML file.

`squid.files.cml_io.write_cml(atoms, name=None, bonds=None)`

Write atomic coordinates and any other relevant information into a file using the Chemical Markup Language (CML) format.

#### Parameters

**atoms:** ... A list of atomic coordinates to be stored. Note, you may also input a molecule object which stores relevant bonding information. You may further pass a System object that has further information.

**name:** *str*, *optional* The name of the output file (either ending or not in .cml).

**bonds:** *list*, *squid.structures.topology.Connector*, *optional* A list of bonds within the system. This is useful when the input is a list of *squid.structures.atom.Atom*.

#### Returns

None

### 3.2.2 misc

`squid.files.misc.close_pipes(p)`

A simple function to close the pipes if they remain open.

`squid.files.misc.is_exe(fpath)`

A function to determine if a file is an executable.

#### Parameters

**fpath:** *str* Path to a file.

#### Returns

**is\_executable:** *bool* Whether the file is an executable or not.

#### References

- <http://stackoverflow.com/a/377028>

`squid.files.misc.last_modified(name)`

Determine when a file was last modified in seconds.

#### Parameters

**name:** *str* Name of the file.

#### Returns

**time:** *datetime.datetime* The last time this file was modified in the standard python datetime format.

`squid.files.misc.which(program)`

A function to return the full path of a system executable.

#### Parameters

**program:** *str* The name of the system executable to find.

#### Returns

**path:** *str or None* The path to the system executable. If none exists, then None.

#### References

- <http://stackoverflow.com/a/377028>

### 3.2.3 xyz\_io

`squid.files.xyz_io.read_xyz(name, cols=['element', 'x', 'y', 'z'], cast_elem_to_sym=True, fast=True)`

Read in a file written in the XYZ file format. This is an improved version, accounting for xyz files of varying atom numbers.

#### Parameters

**name:** *str* File name with or without .xyz file extension.

**cols:** *list, str, optional* The specific columns in this xyz file. Note - we may not support all possibilities, and order matters!

**cast\_elem\_to\_sym:** *bool, optional* Whether to cast the element into the symbol (ex. 2 becomes He).



**fast:** *bool, optional* If specified, you are promising that this xyz file has the columns [element x y z]. Further, if speed truly matters and you do not want to force cast element into symbols, we recommend setting `cast_elem_to_sym=False`.

#### Returns

**frames:** *list, list, squid.structures.atom.Atom* A list of atoms read in from the xyz file. If there is only one frame, then only a *list* of `squid.structures.atom.Atom` is returned.

```
squid.files.xyz_io.read_xyz_gen(name, cols=['element', 'x', 'y', 'z'], cast_elem_to_sym=True,
                                fast=False)
```

This will yield a frame from an xyz file.

#### Parameters

**name:** *str* File name with or without .xyz file extension.

**cols:** *list, str, optional* The specific columns in this xyz file. Note - we may not support all possibilities, and order matters!

**cast\_elem\_to\_sym:** *bool, optional* Whether to cast the element into the symbol (ex. 2 becomes He).

**fast:** *bool, optional* If specified, you are promising that this xyz file has the columns [element x y z]. Further, if speed truly matters and you do not want to force cast element into symbols, we recommend setting `cast_elem_to_sym=False`.

#### Returns

**yield:** *list, squid.structures.atom.Atom* A frame from an xyz file.

```
squid.files.xyz_io.write_xyz(frames, name='out', ID='Atoms')
Write frames of atomic conformations to a file written in the XYZ file format.
```

#### Parameters

**frames\_or\_system:** *list, squid.structures.atom.Atom* Atoms to be written to an xyz file.

**name:** *str, optional* A filename for the xyz file.

**ID:** *str, optional* What is to be written on the xyz comment line.

#### Returns

None

## 3.3 forcefields

### 3.3.1 connectors

```
class squid.forcefields.connectors.Angle(indices=None, energies=None, equilibs=None,
                                          line=None)
```

```
classmethod load_opls(angle_types, pfile_name=None, restrict=None)
```

Given a parameter file, import the Angle parameters if possible.

#### Parameters

**angle\_types:** *list, dict* Angle types from a parsed opls parameter file.

**pfile\_name:** *str* The name of a parameter file to be parsed. If specified, then pfile is ignored (you may simply pass None as pfile).

**restrict:** *list, str, optional* A list of atom labels to include when loading. If not specified, everything is loaded.

#### Returns

**angle\_objs:** *list, Angle, or None* Returns a list of Angle objects if possible, else None.

**class** squid.forcefields.connectors.**Bond** (*indices=None, energies=None, equilibs=None, line=None*)

**classmethod** **load\_opls** (*bond\_types, pfile\_name=None, restrict=None*)

Given a parameter file, import the Bond parameters if possible.

#### Parameters

**bond\_types:** *list, dict* Bond types from a parsed opls parameter file.

**pfile\_name:** *str* The name of a parameter file to be parsed. If specified, then pfile is ignored (you may simply pass None as pfile).

**restrict:** *list, str, optional* A list of atom labels to include when loading. If not specified, everything is loaded.

#### Returns

**bond\_objs:** *list, Bond, or None* Returns a list of Bond objects if possible, else None.

**class** squid.forcefields.connectors.**Dihedral** (*indices=None, energies=None, equilibs=None, line=None*)

**classmethod** **load\_opls** (*dihedral\_types, pfile\_name=None, restrict=None*)

Given a parameter file, import the Dihedral parameters if possible.

#### Parameters

**dihedral\_types:** *list, dict* Dihedral types from a parsed opls parameter file.

**pfile\_name:** *str* The name of a parameter file to be parsed. If specified, then pfile is ignored (you may simply pass None as pfile).

**restrict:** *list, str, optional* A list of atom labels to include when loading. If not specified, everything is loaded.

#### Returns

**dihedral\_objs:** *list, Dihedral, or None* Returns a list of Dihedral objects if possible, else None.

**class** squid.forcefields.connectors.**HarmonicConnector** (*indices=None, energies=None, equilibs=None, line=None*)

Initialize a general connector object. Either pass indices, energies, and equilibs, or pass a line to be parsed.

This object contains the following:

- `assign_line()`
- `fix()`
- `load_opls()`
- `load_smrff()`
- `pack()`
- `parse_line()`
- `printer()`
- `unpack()`

- `validate()`

#### Parameters

**indices:** *list or tuple, str or int* The indices of the atom types in this connection.

**energies:** *list, float* A list of energies associated with this connection.

**equilibs:** *list, float* A list of equilibrium distances/angles for this connection.

**line:** *str* A line from a parameter file to be parsed.

#### Returns

**HarmonicConnector:** `squid.forcefields.connectors.HarmonicConnector` A HarmonicConnector object.

**assign\_line** (*line*)

Parse line inputs and assign to this object.

#### Parameters

**line:** *str* A string that holds information.

#### Returns

None

**fix** (*params='all', value=None*)

This will fix these parameters by assigning bounds to the values themselves.

#### Parameters

**params:** *str, optional* Whether to fix everything (all) or just a specific parameter by name.

**value:** *float, optional* The value to fix the parameter to.

#### Returns

None

**classmethod load\_opls** (*atom\_types, pfile\_name=None, restrict=None*)

Given a parameter file, import the Coulomb parameters if possible.

#### Parameters

**atom\_types:** *list, dict, ...* Atom types from a parsed opls parameter file.

**pfile\_name:** *str* The name of a parameter file to be parsed. If specified, then pfile is ignored (you may simply pass None as pfile).

**restrict:** *list, str, optional* A list of atom labels to include when loading. If not specified, everything is loaded.

#### Returns

**coul\_objs:** *list, Coul, or None* Returns a list of Coul objects if possible, else None.

**classmethod load\_smrff** (*parsed\_file, pfile\_name=None, restrict=None*)

Given a parameter file, inport the LJ parameters if possible.

#### Parameters

**parsed\_file:** *str* A parsed smrff parameter file input string (no comments or trailing white spaces)

**pfile\_name:** *str* The name of a parameter file to be parsed. If specified, then parsed\_file is ignored (you may simply pass None as parsed\_file).

**restrict:** *list, str, optional* A list of atom labels to include when loading. If not specified, everything is loaded.

#### Returns

**obj:** *list, ..., or None* Returns a list of objects if possible, else None.

**pack** (*params, with\_indices=False*)

This function packs the LJ object from a list.

#### Parameters

**params:** *list* A list holding the indices, sigma, and epsilon (IN THAT ORDER).

**with\_indices:** *bool, optional* Whether indices are included in params or not.

#### Returns

None

**static parse\_line** (*line*)

Parse line inputs.

#### Parameters

**line:** *str* A string that holds coulomb information.

#### Returns

None

**printer** (*bounds=None, with\_indices=False, map\_indices=None*)

This prints out a representation of this LJ object, in the format that is output to the smrff parameter file.

#### Parameters

**bounds:** *int, optional* Whether to output the lower bounds (0), or upper bounds (1). If None, then the parameters themselves are output instead (default).

**with\_indices:** *bool, optional* Whether indices should be returned or not.

**map\_indices:** *func, optional* A function to map the indices. This is useful when converting from OPLS atom type to structure type.

#### Returns

**lj:** *str* A string representation of LJ. The indices, sigma, and epsilon are printed, in that precise order. Note, numbers are printed to exactly 3 decimal places.

**unpack** (*with\_indices=False*)

This function unpacks the LJ object into a list.

#### Parameters

**with\_indices:** *bool, optional* Whether to also include the indices in the list.

#### Returns

**coul:** *list, str/float* A list, holding the string of the indices and the float of the charge.

**validate** ()

This function will validate data integrity. In this case, we simply ensure data types are appropriate.

#### Returns

None

### 3.3.2 coulomb

**class** squid.forcefields.coulomb.Coul (*index=None, charge=None, mass=None, element=None, line=None*)

Initialize the coulomb object. This should be done with either individual information (index, charge, mass, element) or parsed from a string (line).

This object contains the following:

- `assign_line()`
- `ff_energy()`
- `fix()`
- `generate()`
- `load_opls()`
- `load_smrff()`
- `pack()`
- `parse_line()`
- `print_lower()`
- `print_upper()`
- `unpack()`
- `validate()`

#### Parameters

- index:** *str or int* The index of the atom type.
- charge:** *float* The charge.
- mass:** *float* The mass.
- element:** *str* The atomic element string/symbol.
- line:** *str* A line from a parameter file to be parsed.

#### Returns

- coulomb:** *squid.forcefields.coulomb.Coul* A Coul object.

**assign\_line** (*line*)

Parse line.

#### Parameters

- line:** *str* A string that holds coulomb information.

#### Returns

None

**ff\_energy** (*q1, q2, r*)

Given the current parameters, what is the energy for a given interatomic distance.

#### Parameters

- q1:** *float* The charge of one particle.
- q2:** *float* The charge of the other particle.
- r:** *float* The interatomic distance.

**Returns**

**energy:** *float* The energy predicted by coul.

**References**

- [https://lammps.sandia.gov/doc/pair\\_coul.html](https://lammps.sandia.gov/doc/pair_coul.html)

**fix** (*params='all', value=None*)

This will fix these parameters by assigning bounds to the values themselves.

**Parameters**

**params:** *str, optional* Whether to fix everything (all) or just the charge (charge)

**value:** *list, float, or float, optional* The value to fix the param to. If None, then it is fixed to the current value. If params is all, then value must be a list of values.

**Returns**

None

**classmethod generate** (*atom\_types, elems, signs*)

Randomly generate parameters for coulomb.

**Parameters**

**atom\_types:** *list, str* A list of all the atom types to have parameters generated for.

**elems:** *list, str* List of the elements (in the same order as atom\_types).

**signs:** *list, float* The list of the signs of the charges (in the same order as the atom\_types).

**Returns**

**coul\_objs:** *list, squid.forcefields.coulomb.Coul* Returns a list of Coul objects.

**classmethod load\_opls** (*atom\_types, pfile\_name=None, restrict=None*)

Given a parameter file, import the Coulomb parameters if possible.

**Parameters**

**atom\_types:** *list, dict, ...* Atom types from a parsed opls parameter file.

**pfile\_name:** *str* The name of a parameter file to be parsed. If specified, then pfile is ignored (you may simply pass None as pfile).

**restrict:** *list, str, optional* A list of atom labels to include when loading. If not specified, everything is loaded.

**Returns**

**coul\_objs:** *list, squid.forcefields.coulomb.Coul, or None* Returns a list of Coul objects if possible, else None.

**classmethod load\_smrff** (*parsed\_file, pfile\_name=None, restrict=None*)

Given a parameter file, import the coulomb parameters if possible.

**Parameters**

**parsed\_file:** *str* A parsed smrff parameter file input string (no comments or trailing white spaces)

**pfile\_name:** *str* The name of a parameter file to be parsed. If specified, then parsed\_file is ignored (you may simply pass None as parsed\_file).

**restrict:** *list, str, optional* A list of atom labels to include when loading. If not specified, everything is loaded.

**Returns**

**coul\_objs:** *list*, *squid.forcefields.coulomb.Coul*, or *None* Returns a list of Coul objects if possible, else None.

**pack** (*params*)

This function packs the coulomb object from a list.

**Parameters**

**params:** *list* A list holding the index and the charge. Note, if you wish to only assign charge, then do so manually.

**Returns**

None

**static parse\_line** (*line*)

Parse line inputs and assign to this object.

**Parameters**

**line:** *str* A string that holds coulomb information.

**Returns**

**index:** *str* The label in the line corresponding to atom type.

**charge:** *float* The atomic charge.

**element:** *str* The atomic symbol.

**mass:** *float* The atomic mass.

**print\_lower** ()

Print the lower bounds.

**Returns**

**bounds:** *str* The lower bounds.

**print\_upper** ()

Print the upper bounds.

**Returns**

**bounds:** *str* The upper bounds.

**unpack** (*with\_indices=True*, *with\_bounds=False*)

This function unpacks the coulomb object into a list.

**Parameters**

**with\_indices:** *bool, optional* Whether to also include the indices in the list.

**with\_bounds:** *bool, optional* Whether to return bounds as well or not.

**Returns**

**coul:** *list, str/float* A list, holding the string of the index and the float of the charge.

**validate** ()

This function will validate data integrity. In this case, we simply ensure data types are appropriate.

**Returns**

None

### 3.3.3 helper

`squid.forcefields.helper.check_restriction(p, restrict)`

Checks if `p` is within the restricted set.

#### Parameters

**p:** *obj* Some parameter object, such as Coulomb, Morse, etc.

**restrict:** *list, int* A list of indices that we want to use.

#### Returns

**contained:** *bool* Whether `p` is completely in `restrict` (True) or not (False).

`squid.forcefields.helper.map_to_lmp_index(p, restrict)`

Given some set of labels, return the corresponding lammps index. For example, we hold `restrict` as a list of atom types for LAMMPS. The corresponding index in `restrict` is one less than the lammps type we output (say, in the data file). As such, this function tries to robustly convert `p` into its corresponding lammps index.

#### Parameters

**p:** *obj* Some parameter object, such as Coulomb, Morse, etc.

**restrict:** *list, int* A list of indices that we want to use.

#### Returns

**mapped\_indices:** ... Usually a list of the mapped indices.

`squid.forcefields.helper.random_in_range(bounds)`

Return a random number in the given bounds: [lower, upper).

#### Parameters

**bounds:** *list, float* A lower and upper bound.

#### Returns

**rand:** *float* A random number in the specified range.

### 3.3.4 lj

**class** `squid.forcefields.lj.LJ(index=None, sigma=None, epsilon=None, line=None)`

Initialize the LJ object. Either pass `index` + `sigma` + `epsilon`, or pass `line`. If all are passed, then an error will be thrown.

This object contains the following:

- `assign_line()`
- `ff_energy()`
- `fix()`
- `generate()`
- `load_opls()`
- `load_smrff()`
- `pack()`
- `parse_line()`
- `pair_coeff_dump()`



- `print_lower()`
- `print_upper()`
- `unpack()`
- `validate()`

#### Parameters

- index:** *str or int* The index of the atom type.
- sigma:** *float* Sigma in LJ expression.
- epsilon:** *float* Epsilon in LJ expression.
- line:** *str* A line from a parameter file to be parsed.

#### Returns

- lj:** *squid.forcefields.lj.LJ* A LJ object.

#### `assign_line(line)`

Parse line inputs and assign to this object.

#### Parameters

- line:** *str* A string that holds LJ information.

#### Returns

None

#### `ff_energy(r)`

Given the current parameters, what is the energy for a given interatomic distance.

#### Parameters

- r:** *float* The interatomic distance.

#### Returns

- energy:** *float* The energy predicted by lj.

#### References

- [https://lammps.sandia.gov/doc/pair\\_lj.html](https://lammps.sandia.gov/doc/pair_lj.html)

#### `fix(params='all', value=None)`

This will fix these parameters by assigning bounds to the values themselves.

#### Parameters

- params:** *str, optional* Whether to fix everything (all), or a specific value (sigma or epsilon).
- value:** *list, float, or float, optional* The value to fix the param to. If None, then it is fixed to the current value. If params is all, then value must be a list of values.

#### Returns

None

#### `classmethod generate(atom_types)`

Randomly generate parameters for lj sigma and epsilon.

#### Parameters

- atom\_types:** *list, str* A list of all the atom types to have parameters generated for.

#### Returns

**lj\_objs:** *list*, *squid.forcefields.lj.LJ* Returns a list of LJ objects.

**classmethod load\_opls** (*atom\_types*, *pfile\_name=None*, *restrict=None*)

Given a parameter file, import the LJ parameters if possible.

#### Parameters

**atom\_types:** *list*, *dict*, ... Atom types from a parsed opl's parameter file.

**pfile\_name:** *str* The name of a parameter file to be parsed. If specified, then pfile is ignored (you may simply pass None as pfile).

**restrict:** *list*, *str*, *optional* A list of atom labels to include when loading. If not specified, everything is loaded.

#### Returns

**lj\_objs:** *list*, *squid.forcefields.lj.LJ*, or *None* Returns a list of LJ objects if possible, else None.

**classmethod load\_smrff** (*parsed\_file*, *pfile\_name=None*, *restrict=None*)

Given a parameter file, import the coulomb parameters if possible.

#### Parameters

**parsed\_file:** *str* A parsed smrff parameter file input string (no comments or trailing white spaces)

**pfile\_name:** *str* The name of a parameter file to be parsed. If specified, then parsed\_file is ignored (you may simply pass None as parsed\_file).

**restrict:** *list*, *str*, *optional* A list of atom labels to include when loading. If not specified, everything is loaded.

#### Returns

**lj\_objs:** *list*, *squid.forcefields.lj.LJ*, or *None* Returns a list of LJ objects if possible, else None.

**pack** (*params*)

This function packs the LJ object from a list.

#### Parameters

**params:** *list* A list holding the index, sigma, and epsilon (IN THAT ORDER).

#### Returns

None

**pair\_coeff\_dump** ()

Return a string representation of the pair coefficients. In this case, it simply is the epsilon and sigma values with a space.

#### Returns

**coeff\_str:** *str* A string representation of the pair coefficients.

**static parse\_line** (*line*)

Parse line inputs.

#### Parameters

**line:** *str* A string that holds LJ information.

#### Returns

**index:** *str* The label in the line corresponding to atom type.

**sigma:** *float* The position where the potential well equals 0.

**epsilon:** *float* The depth of the well.

**print\_lower()**

This prints out a representation of this LJ object's lower bounds, in the format that is output to the smrff parameter file.

**Returns**

**lj:** *str* A string representation of LJ. The index, sigma, and epsilon are printed, in that precise order. Note, numbers are printed to exactly 2 decimal places.

**print\_upper()**

This prints out a representation of this LJ object's upper bounds, in the format that is output to the smrff parameter file.

**Returns**

**lj:** *str* A string representation of LJ. The index, sigma, and epsilon are printed, in that precise order. Note, numbers are printed to exactly 2 decimal places.

**unpack** (*with\_indices=True, with\_bounds=False*)

This function unpacks the LJ object into a list.

**Parameters**

**with\_indices:** *bool, optional* Whether to also include the indices in the list.

**with\_bounds:** *bool, optional* Whether to also return the bounds or not.

**Returns**

**coul:** *list, str/float* A list, holding the string of the index and the float of the charge.

**validate** (*warn=True*)

This function will validate data integrity. In this case, we simply ensure data types are appropriate.

**Parameters**

**warn:** *bool, optional* At times, weird parameters may exist (ex. sigma=0). If this is the case, we will push them to a more realistic lowerbound and print a warning (True) or crash (False).

**Returns**

None

### 3.3.5 morse

**class** squid.forcefields.morse.**Morse** (*indices=None, D0=None, alpha=None, r0=None, rc=None, line=None*)

Initialize the Morse object. The potential form can be found on the LAMMPS webpage ([http://lammps.sandia.gov/doc/pair\\_Morse.html](http://lammps.sandia.gov/doc/pair_Morse.html)). Either specify all the parameters, or pass a string to line, but not both. If both are specified, an error will be thrown.

This object contains the following:

- *assign\_line()*
- *ff\_energy()*
- *fix()*

- `generate()`
- `load_smrff()`
- `pack()`
- `pair_coeff_dump()`
- `parse_line()`
- `print_lower()`
- `print_upper()`
- `set_binder()`
- `set_nonbinder()`
- `unpack()`
- `validate()`

#### Parameters

**indices:** *list or tuple, str or int* The indices of the atom types in this pairwise interaction.

**D0:** *float* D0 describes the well depth (energy units) (defined relative to the dissociated atoms).

**alpha:** *float* alpha controls the ‘width’ of the potential (the smaller alpha is, the larger the well).

**r0:** *float* r0 describes the equilibrium bond distance.

**rc:** *float* rc describes the cutoff of the pairwise interaction.

**line:** *str* A line from a parameter file to be parsed.

#### Returns

**Morse:** *squid.forcefields.morse.Morse* A Morse object.

#### `assign_line(line)`

Parse line inputs and assign to this object.

#### Parameters

**line:** *str* A string that holds a three-body Morse parameter set.

#### Returns

None

#### `ff_energy(r)`

Given the current parameters, what is the energy for a given interatomic distance.

#### Parameters

**r:** *float* The interatomic distance.

#### Returns

**energy:** *float* The energy predicted by morse.

#### References

- [https://lammps.sandia.gov/doc/pair\\_morse.html](https://lammps.sandia.gov/doc/pair_morse.html)

#### `fix(params='all', value=None)`

This will fix these parameters by assigning bounds to the values themselves.

#### Parameters

**params:** *str, optional* Whether to fix everything (all), or a specific value (D0, alpha, r0, or rc).

**value:** *list, float, or float, optional* The value to fix the charge to. If None, then it is fixed to the current value. If params is all, then value must be a list of values.

#### Returns

None

**classmethod generate** (*atom\_types, gen\_rc=False*)

Randomly generate parameters for morse.

#### Parameters

**atom\_types:** *list, str* A list of all the atom types to have parameters generated for.

**gen\_rc:** *bool, optional* Whether to generate the cutoff radius, or not.

#### Returns

**morse\_objs:** *list, squid.forcefields.morse.Morse* Returns a list of Morse objects.

**classmethod load\_smrff** (*parsed\_file, pfile\_name=None, restrict=None*)

Given a parameter file, import the Morse parameters if possible.

#### Parameters

**parsed\_file:** *str* A parsed smrff parameter file input string. (no comments or trailing white spaces)

**pfile\_name:** *str* The name of a parameter file to be parsed. If specified, then parsed\_file is ignored. (you may simply pass None as parsed\_file)

**restrict:** *list, str, optional* A list of atom labels to include when loading. If not specified, everything is loaded.

#### Returns

**Morse\_objs:** *list, squid.forcefields.morse.Morse, or None* Returns a list of Morse objects if possible, else None.

**pack** (*params*)

This function packs the Morse object from a list.

#### Parameters

**params:** *list* A list holding the indices, D0, alpha, r0, rc.

#### Returns

None

**pair\_coeff\_dump** ()

Return a string representation of the pair coefficients.

#### Returns

**coeff\_str:** *str* A string representation of the pair coefficients.

**static parse\_line** (*line*)

Parse line inputs.

#### Parameters

**line:** *str* A string that holds a three-body Morse parameter set.

#### Returns

**indices:** *tuple, str* The labels in the line corresponding to atom types.

**D0:** *float* The depth of the potential well.

**alpha:** *float* The width of the potential well.

**r0:** *float* The interatomic distance associated with the minimum.

**rc:** *float* The cutoff of the potential.

**print\_lower()**

This prints out a representation of this Morse object's lower bound, in the format that is output to the smrff parameter file.

**Returns**

**Morse:** *str* A string representation of Morse parameters. It is in the following order: indices D0 alpha r0 rc

**print\_upper()**

This prints out a representation of this Morse object's upper bound, in the format that is output to the smrff parameter file.

**Returns**

**Morse:** *str* A string representation of Morse parameters. It is in the following order: indices D0 alpha r0 rc

**set\_binder()**

This will adjust bounds such that the parameters are in a range of a morse "Bond". This means that:

$$0.5 < r < 4.0$$

**Returns**

None

**set\_nonbinder()**

This will adjust bounds such that the parameters are in a range of a morse "Non-Bond". This means that:

$$4.0 < r < 10.0 \quad 0.1 < D0 < 50.0 \quad 0.1 < \alpha < 5.0$$

**Returns**

None

**unpack** (*with\_indices=True, bounds=None, with\_bounds=False*)

This function unpacks the Morse object into a list.

**Parameters**

**with\_indices:** *bool, optional* Whether to also include the indices in the list.

**bounds:** *int, optional* Whether to output the lower bounds (0), or upper bounds (1). If None, then the parameters themselves are output instead (default).

**Returns**

**Morse:** *list, str/float* A list, holding the string of the indices, D0, alpha, r0, rc.

**validate()**

This function will validate data integrity. In this case, we simply ensure data types are appropriate.

**Returns**

None

### 3.3.6 opls

`squid.forcefields.opls.parse_pfile` (*parameter\_file*='/home/hherbol/programs/squid/squid/forcefields/potentials/oplsaa',  
*pair\_style*='lj/cut')

Reads an opls parameter file written in the Tinker file format.

#### Parameters

**parameter\_file:** *str, optional* Relative or absolute path to an opls parameter file, written in the Tinker file format.

**pair\_style:** *str, optional* The pair style to be assigned.

#### Returns

**atom\_types:** *list, dict* A list of the forcefield types for atoms, stored as a dictionary.

**bond\_types:** *list, dict* A list of the forcefield types for bonds, stored as a dictionary.

**angle\_types:** *list, dict* A list of the forcefield types for angles, stored as a dictionary.

**dihedral\_types:** *list, dict* A list of the forcefield types for dihedrals, stored as a dictionary.

### 3.3.7 parameters

**class** `squid.forcefields.parameters.Parameters` (*restrict*, *opls\_file*='/home/hherbol/programs/squid/squid/forcefields/potentials/oplsaa',  
*smrff\_file*=None,  
*force\_ters\_2body\_symmetry*=False)

A Parameters object that holds force field parameters. It requires the input of which atom types to get parameters for, so as to not read in an entire force field.

This object contains the following:

- `dump_angles()`
- `dump_bonds()`
- `dump_dihedrals()`
- `dump_lj_cut_coul_cut()`
- `dump_lj_cut_coul_long()`
- `dump_morse()`
- `dump_set_charge()`
- `dump_smooths()`
- `dump_style()`
- `dump_tersoff()`
- `fix()`
- `generate()`
- `get_smrff_style()`
- `load_opls()`
- `load_smrff()`
- `mapper()`
- `num_free_parameters()`

- `pack()`
- `set_smoothed_pair_potentials()`
- `set_all_masks()`
- `set_mask()`
- `set_opls_mask()`
- `unpack()`
- `write_smrff()`

#### Parameters

**restrict:** *list, str* A list of strings specifying which types are to be used. Note, you must have unique types, lest they be overwritten. If None is passed, then everything available is read in.

**opls\_file:** *str, optional* The path to an OPLS parameter file. Default is internally stored parameters in squid.

**smrff\_file:** *str, optional* The path to a SMRFF parameter file. Default is None.

**force\_ters\_2body\_symmetry:** *bool, optional* Whether to force any read in tersoff parameters to have the 2-body symmetry we expect.

#### Returns

**params:** *squid.forcefields.parameters.Parameters* This object.

**dump\_angles** (*in\_input\_file=True*)

Get a string for lammps input in regards to assigning angle coeffs.

#### Parameters

**in\_input\_file:** *bool, optional* Whether to dump the bonds in the input file style format (True) or the data file style format (False)

#### Returns

**coeffs:** *str* A string of angle coeffs, with new line characters between different angles.

**dump\_bonds** (*in\_input\_file=True*)

Get a string for lammps input in regards to assigning bond coeffs.

#### Parameters

**in\_input\_file:** *bool, optional* Whether to dump the bonds in the input file style format (True) or the data file style format (False)

#### Returns

**coeffs:** *str* A string of bond coeffs, with new line characters between different bonds.

**dump\_dihedrals** (*in\_input\_file=True*)

Get a string for lammps input in regards to assigning dihedral coeffs.

#### Parameters

**in\_input\_file:** *bool, optional* Whether to dump the bonds in the input file style format (True) or the data file style format (False)

#### Returns

**coeffs:** *str* A string of dihedral coeffs, with new line characters between different dihedrals.



**dump\_lj\_cut\_coul\_cut ()**

This function will get the lammps command line argument for lj/cut/coul/cut of everything within the Parameters object.

**Parameters**

None

**Returns**

**cmds:** *str* A string, separated with new lines, with pair\_coeff for each lj/cut/coul/cut command possible within this parameter set.

**dump\_lj\_cut\_coul\_long ()**

This function will get the lammps command line argument for lj/cut/coul/long of everything within the Parameters object.

**Parameters**

None

**Returns**

**cmds:** *str* A string, separated with new lines, with pair\_coeff for each lj/cut/coul/long command possible within this parameter set.

**dump\_morse ()**

This function will get the lammps command line argument for morse of everything within the Parameters object.

**Parameters**

None

**Returns**

**cmds:** *str* A string, separated with new lines, with pair\_coeff for each morse command possible within this parameter set.

**dump\_set\_charge ()**

This function will get the lammps command line argument for “set type” of everything within the Parameters object.

**Parameters**

None

**Returns**

**cmds:** *str* A string, separated with new lines, with pair\_coeff for each morse command possible within this parameter set.

**dump\_smooths ()**

This function will get the lammps command line argument for smrff smooths of everything within the Parameters object.

**Parameters**

None

**Returns**

**cmds:** *str* A string, separated with new lines, with pair\_coeff for each smrff smooth command possible within this parameter set.

**dump\_style** (*style=None, tfile\_name=None, tstyle\_smrff=False, write\_file=False, in\_input\_file=True*)

This function will dump LAMMPS commands “pair\_coeff” for chosen styles.

#### Parameters

**style:** *str* Whether to ignore the universal bounds, assigned in this smrff.py file.smrff

**tfile\_name:** *str* The name of the tersoff file.

**tstyle\_smrff:** *bool, optional* Whether to output for SMRFF style (one line allocates memory, the rest overwrites the parameters) or not.

**write\_file:** *bool, optional* Whether to write any files (ex. tersoff files) or not.

**in\_input\_file:** *bool, optional* Whether to dump the bonds in the input file style format (True) or the data file style format (False)

**Returns** lammps\_command: *str*

**dump\_tersoff** (*tfile\_name, tstyle\_smrff*)

This function will get the lammps command line argument for tersoff of everything within the Parameters object.

#### Parameters

**tfile\_name:** *str* The name of the tersoff file.

**tstyle\_smrff:** *bool, optional* Whether to output for SMRFF style (one line allocates memory, the rest overwrites the parameters) or not. If True, this will NOT generate a tersoff file.

#### Returns

**cmds:** *str* A string, separated with new lines, with pair\_coeff for each tersoff command possible within this parameter set.

**fix** (*style, label, params='all', value=None*)

This function will fix a specific style (coul, lj, morse, etc), label (where label is the atom label/type you want to fix), and the component (ex, sigma in LJ).

#### Parameters

**style:** *str* Which style to fix. Options are coul, lj, morse, and ters.

**label:** ... Which atom type should be fixed. If \*, then everything. Note that for some situations this may be a list of values (as in the case of tersoff).

**params:** *str, optional* Whether to fix everything (all), or a specific value (style dependant).

**value:** *list, float, or float, optional* The value to fix the param to. If None, then it is fixed to the current value. If params is all, then value must be a list of values.

#### Returns

None

**generate** (*elems, signs=None, couple\_smooths=True, tersoff\_form='original'*)

For every mask that is true, we will generate random data.

#### Parameters

**elems:** *list, str* A list of the elements, matching 1-to-1 with the given smrff\_types.

**signs:** *list, float* A list of charge signs, matching 1-to-1 with the given smrff\_types.

**couple\_smooths:** *bool, optional* Whether to couple together like smooths. If true, when you have a situation in which, say, `sin_l` and `sin_r` match up, then this will ensure that these two overlap perfectly.

**tersoff\_form:** *str* Whether to use the original `tersoff_form` (`m=3`, `gamma=1`) or the Albe et al `tersoff_form` (`m=1`, `beta=1`) for `tersoff` parameters. Must be `original` or `albe`.

#### Returns

None

**get\_smrff\_style()**

This will return the `smrff` style.

#### Returns

**lammmps\_smrff\_style:** *str* The input script line for LAMMPS for the `smrff` pair style.

**load\_opls(fname)**

Given an OPLS file name, in the Tinker format, parse it and load it into this parameters object. Note, you should specify `restrict` before calling this function or else everything in the file will be loaded. If `restrict` is specified, then `restrict_structure` will be automatically generated during this function call.

#### Parameters

**fname:** *str* The path to the `opls` file.

#### Returns

None

**load\_smrff(fname)**

A function to read in a SMRFF parameter file.

#### Parameters

**fname:** *str* The path to a `smrff` parameter file. `???.smrff`

#### Returns

None

**mapper(x)**

A generalized function to map indices of atom types to the corresponding `lammmps` index. Note, this is generalized and should allow for a wide range of `x` objects.

#### Parameters

**x:** *list or tuple or int or str or obj* Some way of identifying the atom type. Note, if `obj`, then it will check for a `.index`, `.indices`, or `.index2s` property.

#### Returns

**mapper\_obj:** *list, str or str* The `lammmps` index, as either a list (if `bond/angle/dihedral`) or a string (if `charge/lj`).

**num\_free\_parameters()**

This function will return the number of unfixed parameters.

#### Returns

**free\_params:** *int* The number of free parameters.

**pack(params, with\_indices=False)**

Packs the parameters object from a 1D array. NOTE! This is done in primarily for parameterization; which

means the 1D array will NOT have the indices in it. This can be overridden, however, by specifying the `with_indices` flag.

Keep in mind, to maintain symmetry requirements in `tersoff` (where the two-body parameters are the same between A-B B and B-A A), this function will be tied closely to the `unpack` function.

#### Parameters

**params:** *list, float/int* A list of parameters

**with\_indices:** *bool, optional* Whether to account for the indices in the flat array.

#### Returns

None

**set\_all\_masks** (*set\_on*)

Either turn all masks to being on or off.

#### Parameters

**set\_on:** *bool* What to set all values to (True/False).

#### Returns

None

**set\_mask** (*mask*)

Given a style, turn on the respective masks.

#### Parameters

**mask:** *str* The potential for which masks should be turned on (ex. `morse`)

#### Returns

None

**set\_opls\_mask** ()

Turn off ALL masks, but leave OPLS ones on.

#### Returns

None

**set\_smoothed\_pair\_potentials** (*local\_potentials*)

This will assign masks appropriately for the input forcefield. It will also assign any necessary parameters for the desired forcefield.

NOTE! This is a rudimentary starting point and should be improved on. `pair` style `smrff` allows for N transitions, whereas the way this is currently written only allows for short-range to long-range.

#### Parameters

**local\_potentials:** *list, tuple, ...* A list of tuples, each holding three values. The first is the potential (such as `morse` or `tersoff`). The second is the global cutoff (likely in Angstroms). The final is the smooth function to apply to this potential (such as `NULL` for none, or some `sin_X smooth`).

#### Returns

None

**unpack** (*with\_indices=False, with\_bounds=False*)

Unpacks the parameters object into a 1D array for parameterization. This means that the indices are not included during unpacking! Note, this can be overridden though if needed.

**Parameters**

**with\_indices:** *bool, optional* Whether to also include the indices in the flat array.

**with\_bounds:** *bool, optional* Whether to also output the bounds for the parameters.

**Returns**

**flat\_array:** *list, float/int* A list of floats/ints of our parameters.

**bounds\_lower:** *list, float/int* If with\_bounds is specified, then the lower bounds are returned.

**bounds\_upper:** *list, float/int* If with\_bounds is specified, then the upper bounds are returned.

**write\_smrff** (*fname*)

A function to save a SMRFF parameter file.

**Parameters**

**fname:** *str* The file name to save the parameters to.

**Returns**

None

### 3.3.8 smrff

`squid.forcefields.smrff.parse_pfile` (*fname*)

This function will, given a smrff parameter file, will parse it by removing comments, trailing whitespaces, and empty lines.

**Parameters**

**fname:** *str* The name of the parameter file to be parsed.

**Returns**

**parsed:** *str* A parsed string of said parameter file.

### 3.3.9 tersoff

```
class squid.forcefields.tersoff.Tersoff (indices=None, m=None, gamma=None,  
                                         lambda3=None, c=None, d=None, cos-  
                                         theta0=None, n=None, beta=None,  
                                         lambda2=None, B=None, R=None, D=None,  
                                         lambda1=None, A=None, line=None,  
                                         form='original')
```

Initialize the Tersoff object. The potential form can be found on the LAMMPS webpage ([http://lammps.sandia.gov/doc/pair\\_tersoff.html](http://lammps.sandia.gov/doc/pair_tersoff.html)). Either specify all the parameters, or pass a string to line, but not both. If both are specified, an error will be thrown.

This object contains the following:

- `assign_line()`
- `dump_line()`
- `ff_bij()`
- `ff_energy_2body()`
- `ff_fc()`

- `fix()`
- `generate()`
- `load_smrff()`
- `pack()`
- `parse_line()`
- `print_lower()`
- `print_upper()`
- `set_default_bounds()`
- `sorted_force_2body_symmetry()`
- `tag_tersoff_for_duplicate_2bodies()`
- `turn_off()`
- `turn_off_3body()`
- `unpack()`
- `update_2body()`
- `validate()`
- `verify_tersoff_2body_symmetry()`

#### Parameters

**indices:** *list or tuple, str or int* The indices of the atom types in this three-body interaction.

**m:** *int* m is an exponential term in the zeta component of the Tersoff potential. It is either 1 or 3.

**gamma:** *float* gamma is a prefactor to g(theta) in the Tersoff potential, and is between 0 (completely off) and 1 (completely on).

**lambda3:** *float* lambda3 is the exponential coefficient of the three-body tersoff interaction.

**c:** *float* c describes the numerator part of the three-body interaction (found withing the g(theta) term).

**d:** *float* d describes the denominator part of the three-body interaction (found withing the g(theta) term).

**costheta0:** *float* costheta0 gives an equilibrium angle of sorts for the three-body interaction. As such, it is restricted between -1 and 1.

**n:** *float* n is a power that the three-body interaction is taken to (or to some function of n).

**beta:** *float* beta is some scaling to the three-body interactions, found in the b\_ij term of the Tersoff potential.

**lambda2:** *float* lambda2 is the exponential coefficient of the two-body attraction term in the tersoff interaction.

**B:** *float* B is the pre-factor to the two-body attraction term in the tersoff interaction.

**R:** *float* R is a component of the tersoff potential's cutoff distance.

**D:** *float* D is a component of the tersoff potential's cutoff distance.

**lambda1:** *float* lambda1 is the exponential coefficient of the two-body repulsion term in the tersoff interaction.

**A:** *float* A is the pre-factor to the two-body repulsion term in the tersoff interaction.

**line:** *str* A line from a parameter file to be parsed.

**form:** *str* Whether to use the original form (m=3, gamma=1) or the Albe et al form (m=1, beta=1).  
Must be original or albe.

#### Returns

**tersoff:** *squid.forcefields.tersoff.Tersoff* A Tersoff object.

**assign\_line** (*line*, *validate=True*)

Parse line inputs and assign to this object.

#### Parameters

**line:** *str* A string that holds a three-body tersoff parameter set.

**validate:** *bool, optional* Whether to validate these parameters or not.

#### Returns

None

**dump\_line** ()

This function will output the pair\_coeff line for tersoff in LAMMPS. Note - This line output only exists if SMRFF is installed.

#### Returns

**line:** *str* A pair\_coeff line output in tersoff.

**ff\_bij** (*rij*, *rik*, *theta*)

Given the current parameters, what is the bij value for a given theta, rij, and rik combination. Note - this is an approximation as in reality there exist many rij and rik.

#### Parameters

**theta:** *float* The angle, in degrees.

#### Returns

**bij\_value:** *float* The prefactor to the attractive term.

#### References

- [https://lammps.sandia.gov/doc/pair\\_tersoff.html](https://lammps.sandia.gov/doc/pair_tersoff.html)

**ff\_energy\_2body** (*r*)

Given the current parameters, what is the 2body only energy for the given interatomic distance.

#### Parameters

**r:** *float* The interatomic distance.

#### Returns

**E\_2body:** *float* The 2body energy.

#### References

- [https://lammps.sandia.gov/doc/pair\\_tersoff.html](https://lammps.sandia.gov/doc/pair_tersoff.html)

**ff\_fc** (*r*)

Given the current parameters, what is the cutoff scalar.

#### Parameters

**r:** *float* The interatomic distance.

**Returns**

**fc\_value:** *float* The cutoff scalar.

**References**

- [https://lammps.sandia.gov/doc/pair\\_tersoff.html](https://lammps.sandia.gov/doc/pair_tersoff.html)

**fix** (*params='all', value=None*)

This will fix these parameters by assigning bounds to the values themselves.

**Parameters**

**params:** *str, optional* Whether to fix everything (all), or a specific value (m, gamma, lambda3, c, d, costheta0, n, beta, lambda2, B, R, D, lambda1, A).

**value:** *list, float, or float, optional* The value to fix the param to. If None, then it is fixed to the current value. If params is all, then value must be a list of values.

**Returns**

None

**classmethod generate** (*atom\_types, form='original'*)

Randomly generate parameters for tersoff.

**Parameters**

**atom\_types:** *list, str* A list of all the atom types to have parameters generated for.

**form:** *str* Whether to use the original form (m=3, gamma=1) or the Albe et al form (m=1, beta=1). Must be original or albe.

**Returns**

**ters\_objs:** *list, squid.forcefields.tersoff.Tersoff* Returns a list of Tersoff objects.

**classmethod load\_smrff** (*parsed\_file, pfile\_name=None, restrict=None*)

Given a parameter file, import the coulomb parameters if possible.

**Parameters**

**parsed\_file:** *str* A parsed smrff parameter file input string (no comments or trailing white spaces)

**pfile\_name:** *str* The name of a parameter file to be parsed. If specified, then parsed\_file is ignored (you may simply pass None as parsed\_file).

**restrict:** *list, str, optional* A list of atom labels to include when loading. If not specified, everything is loaded.

**Returns**

**tersoff\_objs:** *list, squid.forcefields.tersoff or None* Returns a list of Tersoff objects if possible, else None.

**pack** (*params*)

This function packs the tersoff object from a list.

**Parameters**

**params:** *list* A list holding the indices, m, gamma, lambda3, c, d, costheta0, n, beta, lambda2, B, R, D, lambda1, A.

**Returns**

None



**static parse\_line** (*line*)

Parse line inputs.

#### Parameters

**line:** *str* A string that holds a three-body tersoff parameter set.

#### Returns

**indices:** *tuple, str* Tersoff Parameter.

**m:** *float* Tersoff Parameter.

**gamma:** *float* Tersoff Parameter.

**lambda3:** *float* Tersoff Parameter.

**c:** *float* Tersoff Parameter.

**d:** *float* Tersoff Parameter.

**costheta0:** *float* Tersoff Parameter.

**n:** *float* Tersoff Parameter.

**beta:** *float* Tersoff Parameter.

**lambda2:** *float* Tersoff Parameter.

**B:** *float* Tersoff Parameter.

**R:** *float* Tersoff Parameter.

**D:** *float* Tersoff Parameter.

**lambda1:** *float* Tersoff Parameter.

**A:** *float* Tersoff Parameter.

**print\_lower** ()

This prints out a representation of this tersoff object's upper bound, in the format that is output to the smrff parameter file.

#### Returns

**tersoff:** *str* A string representation of Tersoff parameters. It is in the following order:

**indices m gamma lambda3 c d costheta0 n beta lambda2 B R D lambda1 A**

**print\_upper** ()

This prints out a representation of this tersoff object's upper bound, in the format that is output to the smrff parameter file.

#### Returns

**tersoff:** *str* A string representation of Tersoff parameters. It is in the following order:

**indices m gamma lambda3 c d costheta0 n beta lambda2 B R D lambda1 A**

**set\_default\_bounds** ()

Assign default bounds. Further, if this is the case of A-B-B vs A-B-C we can simplify the bounds as only in the case of A-B-B are two body parameters n, Beta, lambda2, lambda1, and A read in.

#### Returns

None

**turn\_off** ()

This function essentially turns off the Tersoff potential. This is accomplished by:

1. Setting a small cutoff distance.
2. Assigning an impossibly large repulsion energy (A is large)
3. Removing attractive potential (B is 0)
4. Setting beta to 0 (this removes the three-body interaction)
5. Setting all benign (unused) parameters to 1

**Returns**

None

**turn\_off\_3body ( )**

This function essentially turns off the 3-body component of the Tersoff potential. This is accomplished by:

1. Setting beta to 0 (this removes the three-body interaction)
2. Setting all benign (unused) parameters to 1

**Returns**

None

**unpack (with\_indices=True, bounds=None, with\_bounds=False, for\_output=False)**

This function unpacks the tersoff object into a list.

**Parameters**

**with\_indices:** *bool, optional* Whether to also include the indices in the list.

**bounds:** *int, optional* Whether to output the lower bounds (0), or upper bounds (1). If None, then the parameters themselves are output instead (default).

**with\_bounds:** *bool, optional* Whether to output the bounds or not.

**for\_output:** *bool, optional* Whether this is for output (in which case we disregard 2-body sym flag)

**Returns**

**tersoff:** *list, str/float* A list, holding the string of the indices, m, gamma, lambda3, c, d, cos-theta0, n, beta, lambda2, B, R, D, lambda1, A.

**update\_2body (other)**

Given a tersoff parameter object, update the current one with the 2-body parameters (n, beta, lambda1, lambda2, A, B).

**Parameters**

**other:** *squid.forcefields.tersoff.Tersoff* A Tersoff parameter object to get 2-body parameters from.

**Returns**

None

**validate ( )**

This function will validate data integrity. In this case, we simply ensure data types are appropriate.

**Returns**

None

**squid.forcefields.tersoff.sorted\_force\_2body\_symmetry (tersoff\_params)**

In the case of randomly generating parameters, we may want to randomly force the 2body symmetry condition.

**Parameters**

**tersoff\_params:** *list*, *squid.forcefields.tersoff.Tersoff* A list of Tersoff objects.

**Returns**

**corrected\_tersoff\_params:** *list*, *squid.forcefields.tersoff.Tersoff* A list of Tersoff objects with the 2body symmetry condition ensured.

`squid.forcefields.tersoff.tag_tersoff_for_duplicate_2bodies(tersoff_params)`

This function will mimic the `sorted_force_2body_symmetry` and tag the duplicates that would be set by `sorted_force_2body_symmetry`.

**Parameters**

**tersoff\_params:** *list*, *squid.forcefields.tersoff.Tersoff* A list of Tersoff objects.

**Returns**

**tagged\_tersoff\_params:** *list*, *squid.forcefields.tersoff.Tersoff* A list of the unique Tersoff objects.

**Returns**

`squid.forcefields.tersoff.verify_tersoff_2body_symmetry(tersoff_params)`

Given a list of tersoff parameters, verify that they are such that the two-body parameters are symmetric. What this means is that when we consider A-B B and B-A A, the two body parameters must be the same. This is necessary as LAMMPs will randomly isolate the two body interaction (A-B or B-A) and use the corresponding parameters.

**Parameters**

**tersoff\_params:** *list*, *squid.forcefields.tersoff.Tersoff* A list of Tersoff objects.

**Returns**

None

## 3.4 g09

TO DO

## 3.5 geometry

### 3.5.1 misc

`squid.geometry.misc.closest_atoms(atoms)`

Given a list of atomic coordinates, return the indices of the closest two atoms and the total distance. If multiple close atoms exist, it only returns the first in the list.

**Parameters**

**atoms:** *list*, *structures.atom.Atom* A list of atoms to find the closest ones.

**Returns**

**a1:** *int* The index of one of the two closest atoms.

**a2:** *int* The index of the other atom.

**dist:** *float* The interatomic distance that was deemed as close.

`squid.geometry.misc.get_center_of_geometry(atoms, skip_H=False)`

Calculate the center of geometry of the molecule.

#### Parameters

**atoms:** *list, structures.atom.Atom* A list of atoms.

**skip\_H:** *bool, optional* Whether to include Hydrogens in the calculation (False), or not (True).

#### Returns

**cog:** *np.array, float* A np.array of the x, y, and z coordinate of the center of geometry.

`squid.geometry.misc.get_center_of_mass(atoms, skip_H=False)`

Calculate the center of mass of the molecule.

#### Parameters

**atoms:** *list, structures.atom.Atom* A list of atoms.

**skip\_H:** *bool, optional* Whether to include Hydrogens in the calculation (False), or not (True).

#### Returns

**com:** *np.array, float* A np.array of the x, y, and z coordinate of the center of mass.

`squid.geometry.misc.rotate_atoms(atoms, m, around='com')`

Rotate atoms by the given matrix *m*. Note, this happens in place. That means that the atoms in the input list will themselves be rotated. This is done so that we may rotate molecules and systems using the same code! If you do not wish for this to happen, pass to `rotate_atoms` a deepcopy of the atoms.

#### Parameters

**atoms:** *list, structures.atom.Atom* A list of atoms to be rotated.

**m:** *list, list, float* A 3x3 matrix describing the rotation to be applied to this molecule.

**around:** *str, optional* Whether to rotate around the center of mass (com), center of geometry (cog), or neither ("None" or None).

#### Returns

**atoms:** *list, structures.atom.Atom* The rotated atomic coordinates.

## 3.5.2 packmol

`squid.geometry.packmol.get_packmol_obj()`

This function will find the packmol executable and handle errors accordingly.

#### Returns

**packmol\_path:** *str* The path to packmol.

`squid.geometry.packmol.packmol(system_obj, molecules, molecule_ratio=(1, ), density=1.0, seed=1, persist=True, number=None, additional="", custom=None, extra_block_at_beginning="", extra_block_at_end="", tolerance=2.0)`

Given a list of molecules, pack this system appropriately. Note, we now will pack around what is already within the system! This is done by first generating a packmol block for the system at hand, followed by a block for the solvent.

A custom script is also allowed; however, if this path is chosen, then ensure all file paths for packmol exist. We change directories within this function to a `sys_packmol` folder, where all files are expected to reside.

### Parameters

- system\_obj:** `structures.system.System` The system object to pack the molecules into.
- molecules:** *list*, `structures.molecule.Molecule` Molecules to be added to this system.
- molecule\_ratio:** *tuple, float, optional* The ration that each molecule in *molecules* will be added to the system.
- density:** *float, optional* The density of the system in g/mL
- seed:** *float, optional* Seed for random generator.
- persist:** *bool, optional* Whether to maintain the generated sys\_packmol directory or not.
- number:** *int or list, int, optional* Override density and specify the exact number of molecules to pack. When using a list of molecules, you must specify each in order within a list.
- additional:** *str, optional* Whether to add additional constraints to the standard packmol setup.
- custom:** *str, optional* A custom packmol script to run for the given input molecules. Note, you should ensure all necessary files are within the sys\_packmol folder if using this option.
- extra\_block\_at\_beginning:** *str, optional* An additional block to put prior to the standard block.
- extra\_block\_at\_end:** *str, optional* An additional block to put after the standard block.
- tolerance:** *float, optional* The tolerance around which we allow atomic overlap/proximity.

### Returns

None

### References

- Packmol - <http://www.ime.unicamp.br/~martinez/packmol/home.shtml>

## 3.5.3 spatial

`squid.geometry.spatial.furthest_atoms` (*atoms, indices=None*)

Returns the two furthest atoms in a frame. If multiple pairs end up being the same distance, then all the furthest pairs are returned.

### Parameters

- atoms:** *list*, `squid.structures.atom.Atom` A list of atom objects.
- indices:** *list, int, optional* Whether to assign specific atomic indices to each atom, or assume an enumeration. If specifying specific atom indices, these are done in order (ie. `indices[0]` holds the atom index of `atoms[0]`.)

### Returns

**furthest:** *list, tuple, ...* A list of tuples. Each tuple holds the distance the atoms are apart, and the corresponding indices.

`squid.geometry.spatial.furthest_n_atoms_to_r` (*origin, atoms, N=None, indices=None*)

Given a location and a list of atoms, we find the closest N atoms and return their corresponding indices. Note, if you specify N, then there is a chance that more atoms exist in the list that have the same distance to origin, but are not being returned.

### Parameters

- origin:** *np.array, float* A 3D location.
- atoms:** *list*, `squid.structures.atom.Atom` A list of atom objects.

**N:** *int* The closest N we should return.

**indices:** *list, int, optional* Whether to assign specific atomic indices to each atom, or assume an enumeration. If specifying specific atom indices, these are done in order (ie. `indices[0]` holds the atom index of `atoms[0]`.)

#### Returns

**dist\_index\_pairs:** *list, tuple, ...* A list of tuples holding the distance the atom is from the specified origin, and the index of said atom.

`squid.geometry.spatial.motion_per_frame(frames)`

Determine the root mean squared difference between atomic positions of adjacent frames. Note, as we have differences between frames, this means that we return `len(frames) - 1` values.

#### Parameters

**frames:** *list, list, squid.structures.atom.Atom* List of lists of atoms.

#### Returns

**motion:** *np.array, float* List of motion between consecutive frames (`frame_i` vs `frame_(i - 1)`).

`squid.geometry.spatial.mvee(points, tol=0.001)`

Generate a Minimum Volume Enclosing Ellipsoid (MVEE) around atomic species. The ellipsoid is calculated for the “center form”:  $(x-c).T * A * (x-c) = 1$

For useful values, you can get the radii as follows:

```
U, Q, V = np.linalg.svd(A)
r_i = 1/sqrt(Q[i])
vol = (4/3.) * pi * sqrt(1 / np.product(Q))
```

Further, note that V is the rotation matrix giving the orientation of the ellipsoid.

NOTE! You must have a minimum of 4 atoms for this to work.

#### Parameters

**points:** *list, squid.structures.atom.Atom* A list of Atom objects.

**tol:** *float, optional* Tolerance for ellipsoid generation.

#### Returns

**A:** *list, list, float* Positive definite symmetric matrix of the ellipsoid’s center form. This contains the ellipsoid’s orientation and eccentricity.

**c:** *list, float* Center of the ellipsoid.

#### References

- <https://www.mathworks.com/matlabcentral/fileexchange/9542-minimum-volume-enclosing-ellipsoid?requestedDomain=www.mathworks.com>
- <http://stackoverflow.com/questions/14016898/port-matlab-bounding-ellipsoid-code-to-python/14025140#14025140>

`squid.geometry.spatial.nearest_atoms(atoms, indices=None, invert=False)`

Returns the two nearest atoms in a frame. If multiple pairs end up being the same distance, then all the nearest pairs are returned.

#### Parameters

**atoms:** *list, squid.structures.atom.Atom* A list of atom objects.

**indices:** *list, int, optional* Whether to assign specific atomic indices to each atom, or assume an enumeration. If specifying specific atom indices, these are done in order (ie. `indices[0]` holds the atom index of `atoms[0]`.)

**invert:** *bool, optional* Whether to return the furthest atoms instead.

#### Returns

**nearest:** *list, tuple, ...* A list of tuples. Each tuple holds the distance the atoms are apart, and the corresponding indices.

`squid.geometry.spatial.nearest_n_atoms_to_r(origin, atoms, N=None, indices=None)`

Given a location and a list of atoms, we find the closest N atoms and return their corresponding indices. Note, if you specify N, then there is a chance that more atoms exist in the list that have the same distance to origin, but are not being returned.

#### Parameters

**origin:** *np.array, float* A 3D location.

**atoms:** *list, squid.structures.atom.Atom* A list of atom objects.

**N:** *int* The closest N we should return.

**indices:** *list, int, optional* Whether to assign specific atomic indices to each atom, or assume an enumeration. If specifying specific atom indices, these are done in order (ie. `indices[0]` holds the atom index of `atoms[0]`.)

#### Returns

**dist\_index\_pairs:** *list, tuple, ...* A list of tuples holding the distance the atom is from the specified origin, and the index of said atom.

`squid.geometry.spatial.orthogonal_procrustes(A, ref_matrix, reflection=False)`

Using the orthogonal procrustes method, we find the unitary matrix R with  $\det(R) > 0$  such that  $\|A*R - \text{ref\_matrix}\|^2$  is minimized. This varies from that within scipy by the addition of the reflection term, allowing and disallowing inversion. NOTE - This means that the rotation matrix is used for right side multiplication!

#### Parameters

**A:** *list, squid.structures.atom.Atom* A list of atoms for which R will minimize the frobenius norm  $\|A*R - \text{ref\_matrix}\|^2$ .

**ref\_matrix:** *list, squid.structures.atom.Atom* A list of atoms for which A is being rotated towards.

**reflection:** *bool, optional* Whether inversion is allowed (True) or not (False).

#### Returns

**R:** *list, list, float* Right multiplication rotation matrix to best overlay A onto the reference matrix.

**scale:** *float* Scalar between the matrices.

#### Derivation

Goal: minimize  $\|A*R - \text{ref}\|^2$ , switch to trace

$\text{trace}((A*R - \text{ref}).T*(A*R - \text{ref}))$ , now we distribute

$\text{trace}(R^T*A^T*A*R) + \text{trace}(\text{ref}.T*\text{ref}) - \text{trace}((A*R).T*\text{ref}) - \text{trace}(\text{ref}.T*(A*R))$ , trace doesn't care about order, so re-order

$\text{trace}(R^T*R.T*A.T*A) + \text{trace}(\text{ref}.T*\text{ref}) - \text{trace}(R.T*A.T*\text{ref}) - \text{trace}(\text{ref}.T*A^T*R)$ , simplify

$\text{trace}(A.T*A) + \text{trace}(\text{ref}.T*\text{ref}) - 2*\text{trace}(\text{ref}.T*A^T*R)$

Thus, to minimize we want to maximize  $\text{trace}(\text{ref.T} * A * R)$

$u * w * v.T = (\text{ref.T} * A).T$

$\text{ref.T} * A = w * u.T * v$

$\text{trace}(\text{ref.T} * A * R) = \text{trace}(w * u.T * v * R)$

differences minimized when  $\text{trace}(\text{ref.T} * A * R)$  is maximized, thus when  $\text{trace}(u.T * v * R)$  is maximized

This occurs when  $u.T * v * R = I$  (as  $u$ ,  $v$  and  $R$  are all unitary matrices so max is 1)

$R$  is a rotation matrix so  $R.T = R^{-1}$

$u.T * v * I = R^{-1} = R.T$

$R = u * v.T$

Thus,  $R = u.\text{dot}(v.t)$

### References

- [https://github.com/scipy/scipy/blob/v0.16.0/scipy/linalg/\\_procrustes.py#L14](https://github.com/scipy/scipy/blob/v0.16.0/scipy/linalg/_procrustes.py#L14)
- <http://compgroups.net/comp.soft-sys.matlab/procrustes-analysis-without-reflection/896635>

`squid.geometry.spatial.random_rotation_matrix` (*limit\_angle=None*, *lower\_bound=0.1*,  
*MAXITER=1000000*)

Generate a random rotation matrix.

### Parameters

**limit\_angle:** *float, optional* Whether to confine your random rotation (in radians).

**lower\_bound:** *float, optional* A lower bound for *limit\_angle*, at which the identity is simply returned. This is necessary as the procedure to generate the *limit\_angle* method is incredibly slow at small angles.

**MAXITER:** *int, optional* A maximum iteration for when we try to calculate a rotation matrix with some *limit\_angle* specified.

### Returns

**frames:** *np.array, list, float* A random rotation matrix.

### References

- <http://tog.acm.org/resources/GraphicsGems/>, Ed III

`squid.geometry.spatial.rotation_matrix` (*axis*, *theta*, *units='deg'*)

Obtain a left multiplication rotation matrix, given the axis and angle you wish to rotate by. By default it assumes units of degrees. If *theta* is in radians, set *units* to *rad*.

### Parameters

**axis:** *list, float* The axis in which to rotate around.

**theta:** *float* The angle of rotation.

**units:** *str, optional* The units of *theta* (deg or rad).

### Returns

**rotation\_matrix:** *list, list, float* The left multiplication rotation matrix.

### References

- <http://stackoverflow.com/questions/6802577/python-rotation-of-3d-vector/25709323#25709323>



### 3.5.4 transform

`squid.geometry.transform.align_centroid` (*atoms*, *recenter=True*, *skip\_H=True*)

Generate a Minimum Volume Enclosing Ellipsoid (MVEE) around atomic species to align the atoms along the x-axis.

#### Parameters

**atoms:** *list*, *squid.structures.atom.Atom* A list of Atom objects.

**recenter:** *bool*, *optional* Whether to recenter the new coordinates around the origin or not. Note, this is done via the center of geometry, NOT the center of mass.

**skip\_H:** *bool*, *optional* Whether to skip hydrogen during recentering (that is, do not take them into account when calculating the center of geometry).

#### Returns

**molec.atoms:** *list*, *squid.structures.atom.Atom* Rotated atomic coordinates.

**A:** *list*, *list*, *float* Rotated positive definite symmetric matrix of the ellipsoid's center form. This contains the ellipsoid's orientation and eccentricity.

`squid.geometry.transform.center_frame` (*frame*, *method\_to\_remove\_translations='com'*)

Center the atoms in a frame by either the center of geometry (cog) or center of mass (com).

#### Parameters

**frame:** *list*, *squid.structures.atom.Atom* List of atoms.

**method\_to\_remove\_translations:** *str*, *optional* How to remove the translations. Either com for center-of-mass, or cog for center-of-geometry. By default we do so using center-of-mass.

#### Returns

**frame:** *list*, *squid.structures.atom.Atom* The centered frame.

`squid.geometry.transform.center_frames` (*frames*, *method\_to\_remove\_translations='com'*)

Center the frames by either the center of geometry (cog) or center of mass (com).

#### Parameters

**frames:** *list*, *list*, *squid.structures.atom.Atom* List of lists of atoms.

**method\_to\_remove\_translations:** *str*, *optional* How to remove the translations. Either com for center-of-mass, or cog for center-of-geometry. By default we do so using center-of-mass.

#### Returns

**frames:** *list*, *list*, *squid.structures.atom.Atom* The centered frames.

`squid.geometry.transform.interpolate` (*frame\_1*, *frame\_2*, *N*)

Linearly interpolate N frames between two given frames.

#### Parameters

**frame\_1:** *list*, *squid.structures.atom.Atom* List of atoms.

**frame\_2:** *list*, *squid.structures.atom.Atom* List of atoms.

**N:** *int* Number of new frames you want to generate during interpolation.

#### Returns

**frames:** *list*, *list*, *float* List of interpolated frames, inclusive of frame\_1 and frame\_2.

`squid.geometry.transform.perturbate` (*atoms*, *dx=0.1*, *dr=5*, *around='com'*, *rotate=True*)

Given a list of atomic coordinates, randomly perturbate them and apply a slight rotation.

#### Parameters

**atoms:** *list*, *squid.structures.atom.Atom* A list of atomic coordinates to be perturbed

**dx:** *float, optional* By how much you are willing to perturbate via translation.

**dr:** *float, optional* By how much you are willing to perturbate via rotation in degrees.

**around:** *str, optional* Whether to rotate around the center of mass (com), center of geometry (cog), or neither ("None" or None).

**rotate:** *bool, optional* Whether to randomly rotate the molecule or not.

#### Returns

**perturbed\_atoms:** *list*, *squid.structures.atom.Atom* The perturbed list of atomic coordinates.

`squid.geometry.transform.procrustes` (*frames*, *count\_atoms=None*, *append\_in\_loop=True*, *reflection=False*, *method\_to\_remove\_translations='com'*)

Propagate rotation along a list of lists of atoms to smooth out transitions between consecutive frames. This is done by rigid rotation and translation (no scaling and no inversions). Rotation starts at frames[0].

#### Parameters

**frames:** *list, list*, *squid.structures.atom.Atom* List of lists of atoms.

**count\_atoms:** *list, int, optional* A list of indices for which translation and rotations will be calculated from.

**append\_in\_loop:** *bool, optional* If rotation matrices for every atom (True) is desired vs rotation matrices for every frame (False). Every rotation matrix for atoms within the same frame is the same. Thus, when this is True, multiplies will appear.

**reflection:** *bool, optional* Whether inversion is allowed (True) or not (False).

**method\_to\_remove\_translations:** *str, optional* How to remove the translations. Either com for center-of-mass, or cog for center-of-geometry. By default we do so using center-of-mass.

#### Returns

**full\_rotation:** *list, list, float* List of every rotation matrix applied. NOTE - These matrices are applied via right side multiplication.

#### See also

For more information, see `squid.geometry.spatial.orthogonal_procrustes()`.

`squid.geometry.transform.smooth_xyz` (*frames*, *R\_max=0.5*, *F\_max=25*, *N\_frames=None*, *use\_procrustes=True*, *remove\_translations=True*, *fname=None*, *verbose=False*)

Smooth out an xyz file by linearly interpolating frames to minimize the maximum motion between adjacent frames. Further, this can use procrustes to best overlap adjacent frames.

#### Parameters

**frames:** *list, list*, *squid.structures.atom.Atom* A list of lists of atoms.

**R\_max:** *float, optional* The maximum motion allowed between consecutive frames.

**F\_max:** *int, optional* The maximum number of frames allowed before failing the smooth function.

**N\_frames:** *int, optional* If this is specified, forgo the R\_max and F\_max and just interpolate out into N\_frames. Note, if more than N\_frames exists, this also cuts back into exactly N\_frames.

**use\_procrustes:** *bool, optional* Whether procrustes is to be used during smoothing (True), or not (False).

**remove\_translations:** *bool, optional* Whether to center the frames by center of mass or not. Note, if procrustes is run then this is already taken into account. This is for the edge-case of not wanting to use procrustes, but still wanting to minimize translation.

**fname:** *str, optional* An output file name for the smoothed frames (without the .xyz extension). If None, then no file is made.

**verbose:** *bool, optional* Whether additional stdout is desired (True), or not (False).

#### Returns

**frames:** *list, list, squid.structures.atom.Atom* Returns a list of smoothed frames

## 3.6 jdftx

TODO

## 3.7 jobs

### 3.7.1 container

**class** `squid.jobs.container.JobObject` (*name, process\_handle=None, job\_id=None*)

Job class to wrap simulations for queue submission.

#### Parameters

**name:** *str* Name of the simulation on the queue.

**process\_handle:** *process\_handle, optional* The process handle, returned by subprocess.Popen.

**job\_id:** *str, optional* The job id. Usually this should be unique.

#### Returns

**job\_obj:** *squid.jobs.container.JobObject* A Job object.

**get\_all\_jobs** (*detail=3*)

Get a list of all jobs that are running and/or pending.

#### Parameters

**detail:** *int, optional* How much detail to get when finding jobs on the queue.

#### Returns

**jobs\_on\_queue:** *list, ...* A list of all jobs on the queue, and any other relevant information requested.

**is\_finished** ()

Check if simulation has finished or not.

#### Returns

**is\_on\_queue:** *bool* Whether the simulation is still running (True), or not (False).

**wait** (*sleep=60, verbose=False*)

Hang until simulation has finished.

**tsleep:** *int, optional* How long to wait before checking if the job has finished in the loop. Default is 1 minute.

**verbose:** *bool, optional* Whether to print repeatedly on each check or not.

#### Returns

None

### 3.7.2 nbs

**class** `squid.jobs.nbs.Job` (*name, process\_handle=None, job\_id=None*)

Job class to wrap simulations for queue submission.

#### Parameters

**name:** *str* Name of the simulation on the queue.

**process\_handle:** *process\_handle, optional* The process handle, returned by `subprocess.Popen`.

**job\_id:** *str, optional* The job id. Usually this should be unique.

#### Returns

**job\_obj:** `squid.jobs.nbs.Job` A Job object.

**get\_all\_jobs** (*detail=3*)

Get a list of all jobs that are running and/or pending.

#### Parameters

**detail:** *int, optional* How much detail to get when finding jobs on the queue.

#### Returns

**all\_jobs:** *list* Depending on *detail*, you get the following:

- **details =0:** *list, str* List of all jobs on the queue.

- **details =1:** *list, tuple, str*

**List of all jobs on the queue as:** (job name, time run, job status)

- **details =2:** *list, tuple, str*

**List of all jobs on the queue as:**

        (**job name**, time run, job status, queue, number of processors)

`squid.jobs.nbs.get_job` (*s\_flag, detail=0*)

Get a list of all jobs currently on your queue. From this, only return the values that have *s\_flag* in them. The *detail* variable can be used to specify how much information you want returned.

#### Parameters

**s\_flag:** *str* A string to parse out job information with.

**detail:** *int, optional* The amount of information you want returned.

#### Returns

**all\_jobs:** *list* Depending on *detail*, you get the following:

- **details =0:** *list, str* List of all jobs on the queue.

- **details =1:** *list, tuple, str*

**List of all jobs on the queue as:** (job name, time run, job status)

- *details =2: list, tuple, str*

List of all jobs on the queue as:

(job name, time run, job status, queue, number of processors)

```
squid.jobs.nbs.get_nbs_queues()
```

Get a list of all available queues to submit a job to.

#### Returns

**avail\_queues:** *list, str* A list of available queues by name.

```
squid.jobs.nbs.submit_job(name, job_to_submit, **kwargs)
```

Code to submit a simulation to the specified queue and queueing system.

#### Parameters

**name:** *str* Name of the job to be submitted to the queue.

**job\_to\_submit:** *str* String holding code you wish to submit.

**queue:** *str, optional* What queue to run the simulation on (queueing system dependent).

**walltime:** *str, optional* How long to post the job on the queue for in d-h:m:s where d are days, h are hours, m are minutes, and s are seconds. Default is for 30 minutes (00:30:00).

**nprocs:** *int, optional* How many processors to run the simulation on. Note, the actual number of cores mpirun will use is procs \* ntasks.

**sub\_flag:** *str, optional* Additional strings/flags/arguments to add at the end when we submit a job using jsub. That is: jsub demo.nbs sub\_flag.

**unique\_name:** *bool, optional* Whether to force the requirement of a unique name or not. NOTE! If you submit simulations from the same folder, ensure that this is True lest you have a redundancy problem! To overcome said issue, you can set redundancy to True as well (but only if the simulation is truly redundant).

**outfile\_name:** *str, optional* Whether to give a unique output file name, or one based on the sim name.procs

**xhosts:** *str or list, str, optional* Which cpu to submit the job to.

**email:** *str, optional* An email address for sending job information to.

**priority:** *int, optional* What priority to give the submitted job.

**sandbox:** *bool, optional* Whether to sandbox the job or not.

**redundancy:** *bool, optional* With redundancy on, if the job is submitted and unique\_name is on, then if another job of the same name is running, a pointer to that job will instead be returned.

#### Returns

**job\_obj:** *squid.jobs.nbs.Job* A Job object.

### 3.7.3 queue\_manager

```
squid.jobs.queue_manager.Job(name, **kwargs)
```

This function will return a job object depending on the queue system.

#### Parameters

**name:** *str* Name of the simulation on the queue.

**process\_handle:** *process\_handle, optional* The process handle, returned by subprocess.Popen.

**job\_id:** *str, optional* The job id. Usually this should be unique.

#### Returns

**jobContainer:** *squid.jobs.container.JobObject* A job object, or a class built off of it, to handle job submission to a given queue manager.

`squid.jobs.queue_manager.get_all_jobs(detail=0)`

Get a list of all jobs currently on your queue. The *detail* variable can be used to specify how much information you want returned.

#### Parameters

**detail:** *int, optional* The amount of information you want returned.

#### Returns

**all\_jobs:** *list* Depending on *detail*, you get the following:

- *details =0: list, str* List of all jobs on the queue.
- *details =1: list, tuple, str*

**List of all jobs on the queue as:** (job name, time run, job status)

- *details =2: list, tuple, str*

**List of all jobs on the queue as:**

(job name, time run, job status, queue, number of processors)

`squid.jobs.queue_manager.get_available_queues()`

Get a list of all available queues to submit a job to.

#### Returns

**avail\_queues:** *list, str* A list of available queues by name.

`squid.jobs.queue_manager.get_pending_jobs(detail=0)`

Get a list of all jobs currently pending on your queue. The *detail* variable can be used to specify how much information you want returned.

#### Parameters

**detail:** *int, optional* The amount of information you want returned.

#### Returns

**all\_jobs:** *list* Depending on *detail*, you get the following:

- *details =0: list, str* List of all pending jobs on the queue.
- *details =1: list, tuple, str*

**List of all pending jobs on the queue as:** (job name, time run, job status)

- *details =2: list, tuple, str*

**List of all pending jobs on the queue as:**

(job name, time run, job status, queue, number of processors)

`squid.jobs.queue_manager.get_queue_manager()`

This function will determine what the current queueing system is, and return relevant functionality.

#### Returns

**queue\_manager:** *str* The name of the queue manager as either slurm, nbs, or None.

`squid.jobs.queue_manager.get_running_jobs (detail=0)`

Get a list of all jobs currently running on your queue. The *detail* variable can be used to specify how much information you want returned.

#### Parameters

**detail:** *int, optional* The amount of information you want returned.

#### Returns

**all\_jobs:** *list* Depending on *detail*, you get the following:

- **details =0:** *list, str* List of all running jobs on the queue.
- **details =1:** *list, tuple, str*

**List of all running jobs on the queue as:** (job name, time run, job status)

- **details =2:** *list, tuple, str*

**List of all running jobs on the queue as:**

(job name, time run, job status, queue, number of processors)

### 3.7.4 slurm

**class** `squid.jobs.slurm.Job (name, process_handle=None, job_id=None)`

Job class to wrap simulations for queue submission.

#### Parameters

**name:** *str* Name of the simulation on the queue.

**process\_handle:** *process\_handle, optional* The process handle, returned by subprocess.Popen.

**job\_id:** *str, optional* The job id. Usually this should be unique.

#### Returns

**job\_obj:** `squid.jobs.slurm.Job` A Job object.

**get\_all\_jobs (detail=3)**

Get a list of all jobs that are running and/or pending.

#### Parameters

**detail:** *int, optional* How much detail to get when finding jobs on the queue.

#### Returns

**all\_jobs:** *list* Depending on *detail*, you get the following:

- **details =0:** *list, str* List of all jobs on the queue.
- **details =1:** *list, tuple, str*

**List of all jobs on the queue as:** (job name, time run, job status)

- **details =2:** *list, tuple, str*

**List of all jobs on the queue as:**

(job name, time run, job status, queue, number of processors)

```
squid.jobs.slurm.get_job(s_flag, detail=0)
```

Get a list of all jobs currently on your queue. From this, only return the values that have `s_flag` in them. The `detail` variable can be used to specify how much information you want returned.

#### Parameters

**s\_flag:** *str* A string to parse out job information with.

**detail:** *int, optional* The amount of information you want returned.

#### Returns

**all\_jobs:** *list* Depending on `detail`, you get the following:

- **details =0:** *list, str* List of all jobs on the queue.

- **details =1:** *list, tuple, str*

List of all jobs on the queue as: (job name, time run, job status)

- **details =2:** *list, tuple, str*

List of all jobs on the queue as:

(job name, time run, job status, queue, number of processors)

```
squid.jobs.slurm.get_slurm_queues()
```

Get a list of all available queues to submit a job to.

#### Returns

**avail\_queues:** *list, str* A list of available queues by name.

```
squid.jobs.slurm.submit_job(name, job_to_submit, **kwargs)
```

Code to submit a simulation to the specified queue and queueing system.

#### Parameters

**name:** *str* Name of the job to be submitted to the queue.

**job\_to\_submit:** *str* String holding code you wish to submit.

**queue:** *str, optional* What queue to run the simulation on (queueing system dependent).

**walltime:** *str, optional* How long to post the job on the queue for in d-h:m:s where d are days, h are hours, m are minutes, and s are seconds. Default is for 30 minutes (00:30:00).

**cpus\_per\_task:** *int, optional* How many processors to run the simulation on. Note, the actual number of cores mpirun will use is `nprocs * ntasks`.

**ntasks:** *int, optional* How many processors to run the simulation on. Note, the actual number of cores mpirun will use is `nprocs * ntasks`.

**nodes:** *int, optional* How many nodes to run the simulation on.

**sub\_flag:** *str, optional* Additional strings/flags/arguments to add at the end when we submit a job using sbatch. That is: `sbatch demo.slurm sub_flag`.

**unique\_name:** *bool, optional* Whether to force the requirement of a unique name or not. NOTE! If you submit simulations from the same folder, ensure that this is True lest you have a redundancy problem! To overcome said issue, you can set redundancy to True as well (but only if the simulation is truly redundant).

**outfile\_name:** *str, optional* Whether to give a unique output file name, or one based on the sim name.procs

**allocation:** *str, optional* The SLURM allocation to submit the job to.



**jobarray:** *str, optional* If specified, instead of indicating a range for job arrays, we will use these specific values. For example, jobarray=1,2,4,5 would submit jobs, but skip the 3rd index by name.

**gpu:** *int, optional* How many GPUs to use, if submitting to a GPU node.

**redundancy:** *bool, optional* With redundancy on, if the job is submitted and unique\_name is on, then if another job of the same name is running, a pointer to that job will instead be returned.

#### Returns

**job\_obj:** *squid.jobs.slurm.Job* A Job object.

### 3.7.5 submission

`squid.jobs.submission.pysub(name, **kwargs)`

Submission of python scripts to run on your queue.

#### Parameters

**name:** *str* Name of the python script (with or without the .py extension).

**ompi\_threads:** *int, optional* The number OMP\_NUM\_THREADS should be manually assigned to.

**preface\_mpi:** *bool, optional* Whether to run python via mpiexec or not.

**path:** *str, optional* What directory your python script resides in. Note, this does NOT have a trailing /.

**args:** *list, str, optional* A list of arguments to pass to the python script on the queue.

**jobarray:** *tuple, int, optional* Specifies a job array of this python script should be run. In this case, the python script is submitted with a final argument corresponding to the index of the job array. NOTE - This will only work on SLURM.

**modules:** *list, str, optional* A list of modules to load prior to running this python script. Requires an installed version of lmod.

**kwargs:** ... Any other keywords necessary for a given job submission script (NBS/SLURM). See the other submission sections for more details.

#### Returns

None

`squid.jobs.submission.submit_job(name, job_to_submit, **kwargs)`

Code to submit a simulation to the specified queue and queueing system.

#### Parameters

**name:** *str* Name of the job to be submitted to the queue.

**job\_to\_submit:** *str* String holding code you wish to submit.

**kwargs:** ... Additional keyword arguments to NBS/SLURM for job submission. For more details, see the relevant section.

#### Returns

**job\_obj:** *squid.jobs.container.JobObject* A Job object.

## 3.8 lammps

### 3.8.1 io.data

`squid.lammps.io.data.write_lammps_data(system, **kwargs)`

Writes a lammps data file from the given system.

#### Parameters

**system:** *squid.structures.system.System* Atomic system to be written to a lammps data file.

**pair\_coeffs\_included:** *bool, optional* Whether to write pair coefficients into the data file (True), or not (False).

#### Returns

None

### 3.8.2 io.dump

`squid.lammps.io.dump.read_dump(fptr, ext='.dump', coordinates=['x', 'y', 'z'], extras=[])`

Function to read in a generic dump file. Currently it (1) requires element, x, y, z in the dump. You can also use xu, yu, and zu if the unwrapped flag is set to True.

Due to individual preference, the extension was separated. Thus, if you dump to .xyz, have ext=".xyz", etc.

#### Parameters

**fptr:** *str* Name of the dump file with NO extension (ex. 'run' instead of 'run.dump'). This can also be a relative path. If no relative path is given, and the file cannot be found, it will default check in lammps/fptr/fptr+ext.

**ext:** *str, optional* The extension for the dump file. Note, this is default ".dump" but can be anything (ensure you have the ".").

**coordinates:** *list, str, optional* A list of strings describing how the coordinates are specified (x vs xs vs xu vs xsu)

**extras:** *list, str, optional* An additional list of things you want to read in from the dump file.

#### Returns

**frames:** *list, list squid.structures.atom.Atom* A list of lists, each holding atom structures.

`squid.lammps.io.dump.read_dump_gen(fptr, ext='.dump', coordinates=['x', 'y', 'z'], extras=[])`

Function to read in a generic dump file. Currently it (1) requires element, x, y, z in the dump. You can also use xu, yu, and zu if the unwrapped flag is set to True.

Due to individual preference, the extension was separated. Thus, if you dump to .xyz, have ext=".xyz", etc.

#### Parameters

**fptr:** *str* Name of the dump file with NO extension (ex. 'run' instead of 'run.dump'). This can also be a relative path. If no relative path is given, and the file cannot be found, it will default check in lammps/fptr/fptr+ext.

**ext:** *str, optional* The extension for the dump file. Note, this is default ".dump" but can be anything (ensure you have the ".").

**coordinates:** *list, str, optional* A list of strings describing how the coordinates are specified (x vs xs vs xu vs xsu)

**extras:** *list, str, optional* An additional list of things you want to read in from the dump file.

#### Returns

**frames:** *list, list squid.structures.atom.Atom* A list of lists, each holding atom structures.

### 3.8.3 io.thermo

#### 3.8.4 job

`squid.lammps.job.get_lmp_obj (parallel=True)`

This function will find the lmp executable and a corresponding mpi executable. It will handle errors accordingly.

#### Parameters

**parallel:** *bool, optional* Whether to get corresponding mpiexec info or not.

#### Returns

**lmp\_path:** *str* Path to a lammps executable.

**mpi\_path:** *str* Path to an mpi executable.

`squid.lammps.job.job (run_name, input_script, system=None, queue=None, walltime='00:30:00', nprocs=1, ntasks=1, nodes=1, email=None, pair_coeffs_in_data_file=True, no_echo=False, redundancy=False, unique_name=True, allocation=None, prebash=None, postbash=None)`

Wrapper to submitting a LAMMPS simulation.

#### Parameters

**run\_name:** *str* Name of the simulation to be run.

**input\_script:** *str* Input script for LAMMPS simulation.

**system:** *squid.structures.system.System* System object for our simulation.

**queue:** *str, optional* What queue to run the simulation on (queueing system dependent).

**walltime:** *str, optional* How long to post the job on the queue for in d-h:m:s where d are days, h are hours, m are minutes, and s are seconds. Default is for 30 minutes (00:30:00).

**nprocs:** *int, optional* How many processors to run the simulation on. Note, the actual number of cores mpirun will use is nprocs \* ntasks.

**ntasks:** *int, optional* (For SLURM) The number of tasks this job will run, each task uses nprocs number of cores. Note, the actual number of cores mpirun will use is nprocs \* ntasks.

**nodes:** *int, optional* (For SLURM) The number of nodes this job requires. If requesting ntasks \* nprocs < 24 \* nodes, a warning is printed, as on MARCC each node has only 24 cores.

**email:** *str, optional* An email address for sending job information to.

**pair\_coeffs\_in\_data\_file:** *bool, optional* Whether we have included the pair coefficients to be written to our lammps data file (True) or not (False).

**no\_echo:** *bool, optional* Whether to pipe the terminal output to a file instead of printing.

**redundancy:** *bool, optional* With redundancy on, if the job is submitted and unique\_name is on, then if another job of the same name is running, a pointer to that job will instead be returned.

**unique\_name:** *bool, optional* Whether to force the requirement of a unique name or not. NOTE! If you submit simulations from the same folder, ensure that this is True lest you have a redundancy

problem! To overcome said issue, you can set redundancy to True as well (but only if the simulation is truly redundant).

**allocation:** *str, optional* Whether to use a slurm allocation for this job or not. If so, specify the name.

**prebash:** *str, optional* Code to put prior to the job\_to\_submit in the submission script. This should be bash code! Note, if nothing is passed we check if a default is specified in SQUID\_LMP\_PREBASH.

**postbash:** *str, optional* Code to put after the job\_to\_submit in the submission script. This should be bash code! Note, if nothing is passed we check if a default is specified in SQUID\_LMP\_POSTBASH.

#### Returns

**job:** *squid.jobs.container.JobObject* If running locally, return the process handle, else return the job container.

### 3.8.5 parser

The LMP\_Parser code is code from the pizza.py toolkit ([www.cs.sandia.gov/~sjplimp/pizza.html](http://www.cs.sandia.gov/~sjplimp/pizza.html)) developed by Steve Plimpton ([sjplimp@sandia.gov](mailto:sjplimp@sandia.gov)) with some additional warning interspersed through the thermo output.

- *LMP\_Parser*

---

```
class squid.lammps.parser.LMP_Parser(*list)
```

Class object to assist in parsing lammps outputs.

#### Parameters

**list:** *str* Path to the lammps log file that is to be parsed. Note, several files can be included in this string as long as they are separated by spaces.

**read\_all:** *int, optional* If this is set to 0, don't read in the whole file upon initialization. This lets you use the *next()* functionality.

#### Contains

**nvec:** *int* Number of vectors.

**nlen:** *int* Length of each vector.

**names:** *list, str* List of vector names.

**ptr:** *dict* Dictionary corresponding the thermo keys to which column of the output they reside in.  
ptr[thermo\_key] = which column this data is in

**data:** *list, list, float* Raw data from file, organized into 2d array.

**style:** *int* What style the LAMMPs log file is in. 1 = multi, 2 = one, 3 = gran

**firststr:** *str* String that begins a thermo section in log file.

**increment:** *int* 1 if log file being read incrementally

**eof:** *int* ptr into incremental file for where to start next read

#### Returns

This *LMP\_Parser* object.

**get** (\*keys)

Read specific values from thermo output.

**Parameters**

**keys:** *str* Which thermo outputs you want by ID. Not, this is as many requests as you want. ex.  
l.get("Time", "KE", ...)

**Returns**

**vecs:** *list* Desired outputs.

**next** ()

Read the next line of thermo information from the file. Note, this is used when two arguments are passed during initialization.

**Returns**

**timestep:** *int* The timestep of the parsed thermo output.

**write** (filename, \*keys)

Write parsed vectors to a file.

**Parameters**

**filename:** *str* The name of the file you want to dump all your outputs to.

**keys:** *str, optional* Which specific vectors you want output to the file. ex. >>>  
l.write("file.txt", "Time", "KE", ...)

**Returns**

None

## 3.9 maths

### 3.9.1 lhs

squid.maths.lhs.**create\_lhs** (*N\_points*, *N\_samples*, *sample\_bounds*, *params=None*)

Generate a latin hypercube sample for an n dimensional space specified by the sample\_bounds keyword. An example is to call create\_lhs to sample the lennard jones parameter space:

```
# Assuming we want to sample 5 times parameters = create_lhs(2, 5, [(0, 10), (0, 10)])
```

**Parameters**

**N\_points:** *int* The dimensionality of our system.

**N\_samples:** *int* How many samples we want to do.

**sample\_bounds:** *list, tuple, float or list, list, int/float* The min and max values for each dimension.

Note, in special cases we may want to specify that a value is discrete from a list, or specifically an integer. Finally, if neither a list nor tuple is passed, we assume the value is static. Thus, all the following cases are allowed:

- [(0, 10), (3, 20), (-3, 2)]
- [3, [2, 3], (-5., 2.3, float)]

In the second case, the first parameter is set to 3, the second parameter is chosen as either 2 or 3, and the third parameter is force cast to a float.

**params:** *list, str, optional* Current return is a list of lists, each holding the randomly chosen `N_points`. However, by specifying `params`, the return can be made into a dictionary, with each point associated with the string in `params`. Note, this is one to one with the `sample_bounds`. That is, `params[i]` has the bounds specified by `sample_bounds[i]`.

#### Returns

**params:** *list, dict/list, float* A list of lists, each holding a 1D array of points chosen from the LHC method. Note, if `params` was specified then instead a list of dictionaries is returned.

## 3.10 optimizers

### 3.10.1 bfgs

`squid.optimizers.bfgs.bfgs` (*params, gradient, NEB\_obj=None, new\_opt\_params={}*)

A Broyden-Fletcher-Goldfarb-Shanno optimizer, overloaded for NEB use.

#### Parameters

**params:** *list, float* A list of parameters to be optimized.

**gradient:** *func* A function that, given `params`, returns the gradient.

**NEB\_obj:** *neb.NEB* An NEB object to use.

**new\_opt\_params:** *dict* A dictionary holding any changes to the optimization algorithm's parameters. This includes the following -

**step\_size:** *float* Step size to take.

**step\_size\_adjustment:** *float* A factor to adjust `step_size` when a bad step is made.

**max\_step:** *float* A maximum allowable step length. If 0, any step is ok.

**target\_function:** *func* A function that will help decide if backtracking is needed or not. This function will be used to verify BFGS is minimizing. If nothing is passed, but `NEB_obj` is not `None`, the `NEB_obj.get_error` function will be called.

**armijo\_line\_search\_factor:** *float* A factor for the armijo line search.

**linesearch:** *str* Whether to use the *armijo* or *backtrack* linesearch method. If `None` is passed, a static `step_size` is used.

**reset\_when\_in\_trouble:** *bool* Whether to reset the Hessian to Identity when bad steps have been taken.

**reset\_step\_size:** *int* How many iterations of 'good' steps to take before resetting `step_size` to its initial value.

**N\_reset\_hess:** *int* A hard reset to the hessian to be applied every `N` iterations.

**start\_hess:** *int, float, or matrix* A starting matrix to use instead of the identity. If an integer or float is passed, then the starting hessian is a scaled identity matrix.

**use\_numopt\_start:** *bool* Whether to use the starting hessian guess laid out by Nocedal and Wright in the Numerical Operations textbook, page 178.  $H_0 = \langle \gamma_{ls} \rangle / \langle \gamma_{ly} \rangle * I$ . If chosen, `start_hess` is set to the identity matrix.

**accelerate:** *bool* Whether to accelerate via increasing `step_size` by  $1/\text{step\_size\_adjustment}$  when no bad steps are taken after `reset_step_size` iterations.

**maxiter:** *int* Maximum number of iterations for the optimizer to run. If None, then the code runs indefinitely.

**g\_rms:** *float* The RMS value for which to optimize the gradient to.

**g\_max:** *float* The maximum gradient value to be allowed.

**fit\_rigid:** *bool* Remove erroneous rotation and translations during NEB.

**dimensions:** *int* The number of dimensions for the optimizer to run in. By default this is 3 (for NEB atomic coordinates.)

**callback:** *func, optional* A function to be run after each optimization loop.

#### Returns

**params:** *list, float* A list of the optimized parameters.

**code:** *int* An integer describing how the algorithm converged. This can be identified in the constants file.

**iters:** *int* The number of iterations the optimizer ran for.

### 3.10.2 conjugate\_gradient

```
squid.optimizers.conjugate_gradient.conjugate_gradient(params, gradient,
                                                         NEB_obj=None,
                                                         new_opt_params={},
                                                         extra_args_gradient=None,
                                                         extra_args_target=None)
```

A conjugate gradient optimizer, overloaded for NEB use.

#### Parameters

**params:** *list, float* A list of parameters to be optimized.

**gradient:** *func* A function that, given params and an abstract list of extra arguments, returns the gradient.

**NEB\_obj:** *neb.NEB* An NEB object to use.

**new\_opt\_params:** *dict* A dictionary holding any changes to the optimization algorithm's parameters. This includes the following -

**step\_size:** *float* Step size to take.

**step\_size\_adjustment:** *float* A factor to adjust step\_size when a bad step is made.

**method:** *str* Whether to use the Fletcher-Reeves (FR) method of calculating beta, or the Polak-Ribiere (PR) method.

**max\_step:** *float* A maximum allowable step length. If 0, any step is ok.

**target\_function:** *func* A function that will help decide if backtracking is needed or not. This function will be used to verify BFGS is minimizing. If nothing is passed, but NEB\_obj is not None, the NEB\_obj.get\_error function will be called.

**armijo\_line\_search\_factor:** *float* A factor for the armijo line search.

**linesearch:** *str* Whether to use the *armijo* or *backtrack* linesearch method. If None is passed, a static step\_size is used.

**reset\_step\_size:** *int* How many iterations of 'good' steps to take before resetting step\_size to its initial value.

**accelerate:** *bool* Whether to accelerate via increasing `step_size` by `1/step_size_adjustment` when no bad steps are taken after `reset_step_size` iterations.

**maxiter:** *int* Maximum number of iterations for the optimizer to run. If `None`, then the code runs indefinitely.

**g\_rms:** *float* The RMS value for which to optimize the gradient to.

**g\_max:** *float* The maximum gradient value to be allowed.

**fit\_rigid:** *bool* Remove erroneous rotation and translations during NEB.

**dimensions:** *int* The number of dimensions for the optimizer to run in. By default this is 3 (for NEB atomic coordinates.)

**callback:** *func, optional* A function to be run after each optimization loop.

#### Returns

**params:** *list, float* A list of the optimized parameters.

**code:** *int* An integer describing how the algorithm converged. This can be identified in the constants file.

**iters:** *int* The number of iterations the optimizer ran for.

### 3.10.3 fire

`squid.optimizers.fire.fire(params, gradient, NEB_obj=None, new_opt_params={})`  
A FIRE optimizer, overloaded for NEB use.

#### Parameters

**params:** *list, float* A list of parameters to be optimized.

**gradient:** *func* A function that, given params, returns the gradient.

**NEB\_obj:** *neb.NEB* An NEB object to use.

**new\_opt\_params:** *dict* A dictionary holding any changes to the optimization algorithm's parameters. This includes the following -

**dt:** *float* Time step size to take.

**dtmax:** *float, optional* The maximum dt allowed.

**max\_step:** *float* The maximum step size to take.

**Nmin:** *int, optional* The minimum number of steps before acceleration occurs.

**finc:** *float, optional* The factor by which dt increases.

**fdec:** *float, optional* The factor by which dt decreases.

**astart:** *float, optional* The starting acceleration.

**fa:** *float, optional* The factor by which the acceleration is scaled.

**viscosity:** *float* The viscosity within a verlet step (used if euler is False).

**euler:** *bool* Whether to make an euler step or not.

**maxiter:** *int* Maximum number of iterations for the optimizer to run. If `None`, then the code runs indefinitely.

**g\_rms:** *float* The RMS value for which to optimize the gradient to.



**g\_max:** *float* The maximum gradient value to be allowed.

**fit\_rigid:** *bool* Remove erroneous rotation and translations during NEB.

**callback:** *func, optional* A function to be run after each optimization loop.

#### Returns

**params:** *list, float* A list of the optimized parameters.

**code:** *int* An integer describing how the algorithm converged. This can be identified in the constants file.

**iters:** *int* The number of iterations the optimizer ran for.

### 3.10.4 lbfgs

`squid.optimizers.lbfgs.lbfgs(params, gradient, NEB_obj=None, new_opt_params={}, extra_args_gradient=None, extra_args_target=None)`

A Limited Memory Broyden-Fletcher-Goldfarb-Shanno optimizer, overloaded for NEB use.

#### Parameters

**params:** *list, float* A list of parameters to be optimized.

**gradient:** *func* A function that, given params, returns the gradient.

**NEB\_obj:** *neb.NEB* An NEB object to use.

**new\_opt\_params:** *dict* A dictionary holding any changes to the optimization algorithm's parameters. This includes the following -

- step\_size:** *float* Step size to take.
- step\_size\_adjustment:** *float* A factor to adjust step\_size when a bad step is made.
- max\_step:** *float* A maximum allowable step length. If 0, any step is ok.
- max\_steps\_remembered:** *int* The maximum number of previous iterations to save.
- target\_function:** *func* A function that will help decide if backtracking is needed or not. This function will be used to verify LBFGS is minimizing. If nothing is passed, but NEB\_obj is not None, the NEB\_obj.get\_error function will be called.
- armijo\_line\_search\_factor:** *float* A factor for the armijo line search.
- linesearch:** *str* Whether to use the *armijo* or *backtrack* linesearch method. If None is passed, a static step\_size is used.
- reset\_when\_in\_trouble:** *bool* Whether to reset the stored parameters and gradients when a bad step has been taken.
- reset\_step\_size:** *int* How many iterations of 'good' steps to take before resetting step\_size to its initial value.
- N\_reset\_hess:** *int* A hard reset to the hessian to be applied every N iterations.
- start\_hess:** *int, float, or matrix* A starting integer or float to scale the starting hessian.
- use\_numopt\_start:** *bool* Whether to use the starting hessian guess laid out by Nocedal and Wright in the Numerical Operations textbook, page 178.  $H_0 = \langle y|y \rangle / \langle y|y \rangle$   
 \* I. If chosen, start\_hess is set to the identity matrix.

**accelerate:** *bool* Whether to accelerate via increasing `step_size` by `1/step_size_adjustment` when no bad steps are taken after `reset_step_size` iterations.

**maxiter:** *int* Maximum number of iterations for the optimizer to run. If None, then the code runs indefinitely.

**g\_rms:** *float* The RMS value for which to optimize the gradient to.

**g\_max:** *float* The maximum gradient value to be allowed.

**fit\_rigid:** *bool* Remove erroneous rotation and translations during NEB.

**dimensions:** *int* The number of dimensions for the optimizer to run in. By default this is 3 (for NEB atomic coordinates.)

**callback:** *func, optional* A function to be run after each optimization loop.

#### Returns

**params:** *list, float* A list of the optimized parameters.

**code:** *int* An integer describing how the algorithm converged. This can be identified in the constants file.

**iters:** *int* The number of iterations the optimizer ran for.

### 3.10.5 quick\_min

```
squid.optimizers.quick_min.quick_min(params, gradient, NEB_obj=None,  
                                     new_opt_params={})
```

A quick min optimizer, overloaded for NEB use. Note, this will ONLY work for use within the NEB code.

#### Parameters

**params:** *list, float* A list of parameters to be optimized.

**gradient:** *func* A function that, given params, returns the gradient.

**NEB\_obj:** *neb.NEB* An NEB object to use.

**new\_opt\_params:** *dict* A dictionary holding any changes to the optimization algorithm's parameters. This includes the following -

**dt:** *float* Time step size to take.

**max\_step:** *float* The maximum step size to take.

**viscosity:** *float* The viscosity within a verlet step (used if euler is False).

**euler:** *bool* Whether to make an euler step or not.

**maxiter:** *int* Maximum number of iterations for the optimizer to run. If None, then the code runs indefinitely.

**g\_rms:** *float* The RMS value for which to optimize the gradient to.

**g\_max:** *float* The maximum gradient value to be allowed.

**fit\_rigid:** *bool* Remove erroneous rotation and translations during NEB.

**verbose:** *bool* Whether to have additional output.

**callback:** *func, optional* A function to be run after each optimization loop.

#### Returns

**params:** *list, float* A list of the optimized parameters.

**code:** *int* An integer describing how the algorithm converged. This can be identified in the constants file.

**iters:** *int* The number of iterations the optimizer ran for.

### 3.10.6 steepest\_descent

```
squid.optimizers.steepest_descent.steepest_descent (params,          gradi-
                                                    ent,          NEB_obj=None,
                                                    new_opt_params={},      ex-
                                                    tra_args_gradient=None,  ex-
                                                    tra_args_target=None)
```

A steepest descent optimizer, overloaded for NEB use.

*Parameters*

**params:** *list, float* A list of parameters to be optimized.

**gradient:** *func* A function that, given params, returns the gradient.

**NEB\_obj:** *neb.NEB* An NEB object to use.

**new\_opt\_params:** *dict* A dictionary holding any changes to the optimization algorithm's parameters. This includes the following -

**step\_size:** *float* Step size to take.

**step\_size\_adjustment:** *float* A factor to adjust step\_size when a bad step is made.

**max\_step:** *float* A maximum allowable step length. If 0, any step is ok.

**target\_function:** *func* A function that will help decide if backtracking is needed or not. This function will be used to verify BFGS is minimizing. If nothing is passed, but NEB\_obj is not None, the NEB\_obj.get\_error function will be called.

**armijo\_line\_search\_factor:** *float* A factor for the armijo line search.

**linesearch:** *str* Whether to use the *armijo* or *backtrack* linesearch method. If None is passed, a static step\_size is used.

**reset\_when\_in\_trouble:** *bool* Whether to reset the Hessian to Identity when bad steps have been taken.

**reset\_step\_size:** *int* How many iterations of 'good' steps to take before resetting step\_size to its initial value.

**accelerate:** *bool* Whether to accelerate via increasing step\_size by 1/step\_size\_adjustment when no bad steps are taken after *reset\_step\_size* iterations.

**maxiter:** *int* Maximum number of iterations for the optimizer to run. If None, then the code runs indefinitely.

**g\_rms:** *float* The RMS value for which to optimize the gradient to.

**g\_max:** *float* The maximum gradient value to be allowed.

**fit\_rigid:** *bool* Remove erroneous rotation and translations during NEB.

**dimensions:** *int* The number of dimensions for the optimizer to run in. By default this is 3 (for NEB atomic coordinates.)

**callback:** *func, optional* A function to be run after each optimization loop.

*Returns*

**params:** *list, float* A list of the optimized parameters.

**code:** *int* An integer describing how the algorithm converged. This can be identified in the constants file.

**iters:** *int* The number of iterations the optimizer ran for.

## 3.11 orca

### 3.11.1 io

`squid.orca.io.engrad_read(input_file, force='Ha/Bohr', pos='Bohr')`

General read in of all possible data from an Orca engrad file (.orca.engrad).

**Parameters**

**input\_file:** *str* Orca .orca.engrad file to be parsed.

**force:** *str, optional* Units you want force to be returned in. Default is Ha/Bohr.

**pos:** *str, optional* Units you want position to be returned in. Default is Bohr.

**Returns**

**atoms:** *list, squid.structures.atom.Atom* A list of the final atomic state, with forces appended to each atom.

**energy:** *float* The total energy of this simulation.

`squid.orca.io.read(input_file)`

General read in of all possible data from an Orca output file (.out). It should be mentioned that atomic positions are 0 indexed.

**Parameters**

**input\_file:** *str* Orca .out file to be parsed.

**Returns**

**data:** `squid.structures.results.DFT_out` Generic DFT output object containing all parsed results.

### 3.11.2 job

`squid.orca.job.job(run_name, route=None, atoms=[], extra_section="", grad=False, queue=None, walltime='00:30:00', sandbox=False, nprocs=1, ntasks=1, nodes=1, charge=0, multiplicity=1, redundancy=False, use_NBS_sandbox=False, unique_name=True, previous=None, mem=2000, priority=None, xhost=None, allocation=None, skip_ompi=False, prebash=None, postbash=None)`

Wrapper to submitting an Orca simulation.

**Parameters**

**run\_name:** *str* Name of the simulation to be run.

**route:** *str, optional* The DFT route line, containing the function, basis set, etc. Note, if route=None and previous != None, the route from the previous simulation will be used instead.

- atoms:** *list, squid.structures.atom.Atom, optional* A list of atoms for the simulation. If this is an empty list, but previous is used, then the last set of atomic coordinates from the previous simulation will be used.
- extra\_section:** *str, optional* Additional DFT simulation parameters. If None and previous is not None, then previous extra section is used.
- grad:** *bool, optional* Whether to force RunTyp Gradient.
- queue:** *str, optional* What queue to run the simulation on (queueing system dependent).
- walltime:** *str, optional* The walltime the job is given when submitted to a queue. Format is in day-hr:min:sec.
- sandbox:** *bool, optional* Whether to run the job in a sandbox or not.
- nprocs:** *int, optional* How many processors to run the simulation on. Note, the actual number requested by orca will be  $nprocs * ntasks$ .
- ntasks:** *int, optional* (For SLURM) The number of tasks this job will run, each task uses nprocs number of cores. Note, the actual number requested by orca will be  $nprocs * ntasks$ .
- nodes:** *int, optional* (For SLURM) The number of nodes this job requires. If requesting  $ntasks * nprocs < 24 * nodes$ , a warning is printed, as on MARCC each node has only 24 cores.
- charge:** *int, optional* Charge of the system. The default charge of 0 is used.
- multiplicity:** *int, optional* Multiplicity of the system. The default multiplicity of 1 is used. Recall, multiplicity  $M = 2 * S + 1$  where S is the total system spin.
- redundancy:** *bool, optional* With redundancy on, if the job is submitted and unique\_name is on, then if another job of the same name is running, a pointer to that job will instead be returned.
- use\_NBS\_sandbox:** *bool, optional* Whether to use the NBS sandboxing headers (True), or manually copy files (False).
- unique\_name:** *bool, optional* Whether to force the requirement of a unique name or not. NOTE! If you submit simulations from the same folder, ensure that this is True lest you have a redundancy problem! To overcome said issue, you can set redundancy to True as well (but only if the simulation is truly redundant).
- previous:** *str, optional* Name of a previous simulation for which to try reading in information using the MORRead method.
- mem:** *float, optional* Amount of memory per processor that is available (in MB).
- priority:** *int, optional* Priority of the simulation (queueing system dependent). Priority ranges (in NBS) from a low of 1 (start running whenever) to a high of 255 (start running ASAP).
- xhost:** *list, str or str, optional* Which processor to run the simulation on(queueing system dependent).
- allocation:** *str, optional* Whether to use a slurm allocation for this job or not. If so, specify the name.
- skip\_ompi:** *bool, optional* At times you may wish to run orca without checking if ompi is available. This can arise when you are submitting the job to a queueing system that will load ompi later, but right now you only have orca in the path. If so, set skip\_ompi=True.
- prebash:** *str, optional* Code to put prior to the job\_to\_submit in the submission script. This should be bash code! Note, if nothing is passed we check if a default is specified in SQUID\_ORCA\_PREBASH.

**postbash:** *str, optional* Code to put after the `job_to_submit` in the submission script. This should be bash code! Note, if nothing is passed we check if a default is specified in `SQUID_ORCA_POSTBASH`.

## Returns

**job:** *squid.jobs.container.JobObject* Return the job container.

```
squid.orca.job.jobarray(run_name, route, frames, n_frames=None, extra_section="",
                        grad=False, queue=None, walltime='00:30:00', sandbox=False,
                        nprocs=1, ntasks=1, nodes=1, charge=0, multiplicity=1, redundancy=False,
                        unique_name=True, previous=None, mem=2000, priority=None,
                        xhost=None, jobarray_values=None, allocation=None,
                        batch_serial_jobs=None, skip_ompi=False, prebash=None, postbash=None)
```

Wrapper to submitting various Orca simulations as a job array on a SLURM system. This is used when there are many atomic systems, stored in a list, that need to have the same DFT calculation performed on each.

Note - When requesting `nprocs`/`ntasks`/`nodes`, these will be per-job. As such, do **NOT** multiply out. For instance, if you request `ntasks=4`, and `len(frames) = 10`, you will be running 10 jobs, each with 4 tasks.

## Parameters

**run\_name:** *str* Name of the simulation to be run.

**route:** *str* The DFT route line, containing the function, basis set, etc. Note, if `route=None` and `previous != None`, the route from the previous simulation will be used instead.

**frames:** *list, squid.structures.atom.Atom* Each atomic system that needs to be simulated.

**n\_frames:** *int, optional* The number of frames.

**extra\_section:** *str, optional* Additional DFT simulation parameters. If `None` and `previous` is not `None`, then `previous` extra section is used.

**grad:** *bool, optional* Whether to force RunTyp Gradient.

**queue:** *str, optional* What queue to run the simulation on (queueing system dependent).

**walltime:** *str, optional* The walltime the job is given when submitted to a queue. Format is in day-hr:min:sec.

**sandbox:** *bool, optional* Whether to run the job in a sandbox or not.

**nprocs:** *int, optional* How many processors to run the simulation on. Note, the actual number requested by orca will be `nprocs * ntasks`.

**ntasks:** *int, optional* (For SLURM) The number of tasks this job will run, each task uses `nprocs` number of cores. Note, the actual number requested by orca will be `nprocs * ntasks`.

**nodes:** *int, optional* (For SLURM) The number of nodes this job requires. If requesting `ntasks * nprocs < 24 * nodes`, a warning is printed, as on MARCC each node has only 24 cores.

**charge:** *float, optional* Charge of the system. If this is used, then `charge_and_multiplicity` is ignored. If `multiplicity` is used, but `charge` is not, then default charge of 0 is chosen.

**multiplicity:** *int, optional* Multiplicity of the system. If this is used, then `charge_and_multiplicity` is ignored. If `charge` is used, but `multiplicity` is not, then default multiplicity of 1 is chosen.

**redundancy:** *bool, optional* With redundancy on, if the job is submitted and `unique_name` is on, then if another job of the same name is running, a pointer to that job will instead be returned.

**unique\_name:** *bool, optional* Whether to force the requirement of a unique name or not. NOTE! If you submit simulations from the same folder, ensure that this is `True` lest you have a redundancy

problem! To overcome said issue, you can set redundancy to True as well (but only if the simulation is truly redundant).

**previous:** *str, optional* Name of a previous simulation for which to try reading in information using the MORRead method.

**mem:** *float, optional* Amount of memory per processor that is available (in MB).

**priority:** *int, optional* Priority of the simulation (queueing system dependent). Priority ranges (in NBS) from a low of 1 (start running whenever) to a high of 255 (start running ASAP).

**xhost:** *list, str or str, optional* Which processor to run the simulation on(queueing system dependent).

**jobarray\_values:** *str, optional* If specified, instead of indicating a range for job arrays, we will use these specific values. For example, jobarray\_values=1,2,4,5 would submit jobs, but skip the 3rd index by name.

**allocation:** *str, optional* Whether to use a slurm allocation for this job or not. If so, specify the name.

**batch\_serial\_jobs:** *int, optional* Whether to batch jobs at N at a time (locally on serial job submission).

**skip\_ompi:** *bool, optional* At times you may wish to run orca without checking if ompi is available. This can arise when you are submitting the job to a queueing system that will load ompi later, but right now you only have orca in the path. If so, set skip\_ompi=True.

**prebash:** *str, optional* Code to put prior to the job\_to\_submit in the submission script. This should be bash code! Note, if nothing is passed we check if a default is specified in SQUID\_ORCA\_PREBASH.

**postbash:** *str, optional* Code to put after the job\_to\_submit in the submission script. This should be bash code! Note, if nothing is passed we check if a default is specified in SQUID\_ORCA\_POSTBASH.

## Returns

**job:** *squid.jobs.container.JobObject* Return the job container.

### 3.11.3 mep

(c) 2013 Marius Retegan License: BSD-2-Clause Description: Create a .cube file of the electrostatic potential using ORCA. Run: python mep.py fname npoints (e.g. python mep.py water 40) Arguments: fname - file name without the extension;

this should be the same for the .gbw and .scfp.

**npoints - number of grid points per side** (80 should be fine)

Dependencies: numpy

Source: <https://gist.github.com/mretegan/5501553>

Notes: Slight modifications made to incorporate into Squid.

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`squid.orca.mep.electrostatic_potential_cubegen` (*fname*, *npoints*=80)

Given the name of a simulation, generate the cube file.

#### Parameters

**fname:** *str* The orca simulation name.

**npoints:** *int, optional* How fine the grid should be. Larger, more fine, more expensive to calculate.

#### Returns

None

### 3.11.4 post\_process

`squid.orca.post_process.gbwn_to_cube` (*name*, *mo*, *spin*=0, *grid*=40)

Pipe in flags to `orca_plot` to generate a cube file for the given molecular orbital. Note, this is assumed to be running from the parent directory (ie, gbwn is in the orca/BASENAME/BASENAME.orca.gbwn).

#### Parameters

**name:** *str* The base name of the gbwn file. Thus, 'water' instead of 'water.orca.gbwn'.

**mo:** *int* Which molecular orbital to generate the cube file for. Note, this is 0 indexed.

**spin:** *int, optional* Whether to plot the alpha or beta (0 or 1) operator.

**grid:** *int, optional* The grid resolution, default being 40.

#### Returns

**mo\_name:** *str* The name of the output MO file.

`squid.orca.post_process.mo_analysis` (*name*, *orbital*=None, *HOMO*=True, *LUMO*=True, *wireframe*=True, *hide*=True, *iso*=0.04)

Post process an orca job using `orca_plot` and `vmd` to display molecular orbitals and the potential surface. NOTE! By default Orca does not take into account degenerate energy states when populating. To do so, ensure the following is in your `extra_section`:

'%scf FracOcc true end'.

#### Parameters

**name:** *str* Orca file name. Only use the name, such as 'water' instead of 'water.gbwn'. Note, do not pass a path as it is assumed you are in the parent directory of the job to analyze. If not, use the path variable.

**orbital:** *list, int, optional* or *int, optional* The orbital(s) to analyze (0, 1, 2, 3, ...). By default HOMO and LUMO will be analyzed, thus this only is useful if you wish to see other orbitals.

**HOMO:** *bool, optional* If you want to see the HOMO level.

**LUMO:** *bool, optional* If you want to see the LUMO level.

**wireframe:** *bool, optional* If you want to view wireframe instead of default surface.

**hide:** *bool, optional* Whether to have the representations all off by or not when opening.

**iso:** *float, optional* Isosurface magnitude. Set to 0.04 by default, but 0.01 may be better.



**Returns**

None

`squid.orca.post_process.pot_analysis` (*name*, *wireframe=True*, *npoints=80*)

Post process an orca job using orca\_plot and vmd to display the electrostatic potential mapped onto the electron density surface.

**Parameters**

**name:** *str* Orca file name. Only use the name, such as 'water' instead of 'water.gbw'. Note, do not pass a path as it is assumed you are in the parent directory of the job to analyze.

**wireframe:** *bool, optional* If you want to view wireframe instead of default surface.

**npoints:** *int, optional* The grid size for the potential surface.

**Returns**

None

### 3.11.5 utils

`squid.orca.utils.get_orca_obj` (*parallel=True*)

This function will find the orca executable and the corresponding openmpi executable. It will handle errors accordingly.

**Parameters**

**parallel:** *bool, optional* Whether we guarantee the relevant parallel openmpi is setup (True) or not (False).

**Returns**

**orca\_path:** *str* The path to the orca executable.

## 3.12 post\_process

### 3.12.1 debyer

Python hooks for the debyer code. Link: <https://debyer.readthedocs.io/en/latest/>

- `get_pdf()`

`squid.post_process.debyer.get_pdf` (*frames*, *start=0.0*, *stop=5.0*, *step=0.1*, *cutoff=10.0*, *rho=1.0*, *quanta=0.001*, *output=None*, *persist=False*)

Obtain the pair distribution function of a list of atoms using the Debyer code.

**Parameters**

**frames:** *str or list*, `squid.structures.atom.Atom` An xyz file name (with or without the .xyz extension) or an input frame to calculate the pdf for.

**start:** *float, optional* The starting radial distance in Angstroms for the calculated pattern.

**stop:** *float, optional* The ending radial distance in Angstroms for the calculated pattern.

**step:** *float, optional* Step in Angstroms for the calculated pattern.

**cutoff:** *float, optional* Cutoff distance in Angstroms for Interatomic Distance (ID) calculations.

**rho:** *float, optional* Numeric density of the system.

**quanta:** *float, optional* Interatomic Distance (ID) discretization quanta.

**output:** *str, optional* Output file name with NO extension given

**persist:** *bool, optional* Whether to persist made .g and .xyz files (True), or remove them (False)

#### Returns

**pdf:** *list, tuple, float* A list of tuples holding the pdf data (distance in Angstroms and Intensity).

#### References

- <https://debyer.readthedocs.io/en/latest/>

## 3.12.2 ovito

The visualization module automates some visualization procedures for post processing data.

An example of using this is as follows:

```
import files
import visualization as vis

vis.ovito_xyz_to_gif(files.read_xyz("CNH_HCN.xyz"), "/fs/home/hch54/tmp", renderer=
    ↪ 'Tachyon')
```

- `ovito_xyz_to_image()`
- `ovito_xyz_to_gif()`

---

```
squid.post_process.ovito.get_ovito_obj(version='2.9.0')
```

This function returns the ovito object. Note, currently the code below only works on version 2.9.0.

```
squid.post_process.ovito.ovito_xyz_to_gif(frames, scratch, fname='image', camera_pos=(10, 0, 0), camera_dir=(-1, 0, 0), size=(800, 600), delay=10, display_cell=False, renderer='OpenGLRenderer', renderer_settings={}, overwrite=False)
```

This function will, using the ovito python api, generate either a single image or a gif of the input frames. Note, a gif is only generated when more than one frame exists.

#### Parameters

**frames:** *str or list, squid.structures.atom.Atom* A list of frames you wish to generate an image for, or a path to an xyz file.

**scratch:** *str* A directory you want to have each image saved to.

**fname:** *str, optional* The prefix for the image names.

**camera\_pos:** *tuple, float, optional* A tuple of x, y, and z coordinates for the camera to be positioned.

**camera\_dir:** *tuple, float, optional* The direction the camera is facing.

**size:** *tuple, int, optional* Image size (width, height).

**delay:** *int, optional* In the event of a gif, how long it should play for.

**display\_cell:** *bool, optional* Whether to display the box around the system or not.

**renderer:** *str, optional* What kind of renderer you wish to use: OpenGL or Tachyon.

**renderer\_settings:** *dict, optional* Here you can change specific renderer settings.

**overwrite:** *bool, optional* Whether to delete any files already existing in the scratch dir.

#### Returns

None

```
squid.post_process.ovito.ovito_xyz_to_image(xyz, scratch, fname='image', camera_pos=(10, 0, 0), camera_dir=(-1, 0, 0), size=(800, 600), renderer='OpenGLRenderer', display_cell=False, renderer_settings={})
```

This function will, using the ovito python api, generate a png image of an xyz file.

#### Parameters

**xyz:** *str* A path to an xyz file.

**scratch:** *str* A directory you want to have each image saved to.

**fname:** *str, optional* The prefix for the image names.

**camera\_pos:** *tuple, float, optional* A tuple of x, y, and z coordinates for the camera to be positioned.

**camera\_dir:** *tuple, float, optional* The direction the camera is facing.

**size:** *tuple, int, optional* Image size (width, height).

**delay:** *int, optional* In the event of a gif, how long it should play for.

**renderer:** *str, optional* What kind of renderer you wish to use: OpenGL or Tachyon.

**display\_cell:** *bool, optional* Whether to display the box around the system or not.

**renderer\_settings:** *dict, optional* Here you can change specific renderer settings.

#### Returns

None

### 3.12.3 vmd

The vmd package automates various vmd post-processing tasks.

- `plot_MO_from_cube()`

```
squid.post_process.vmd.plot_MO_from_cube(fptrs, wireframe=True, hide=True, iso=0.04)
```

A function to generate a VMD visualization of a molecular orbital from a cube file.

#### Parameters

**fptrs:** *list, str, or str* Strings giving the path to the cube file.

**wireframe:** *bool, optional* If you want to view wireframe (True) or not (False) for the orbitals.

**hide:** *bool, optional* Whether to hide the representations (True) on startup, or not (False).

**iso:** *float, optional* Isosurface magnitude. Set to 0.04 by default, but 0.01 may be better.

#### Returns

None

```
squid.post_process.vmd.plot_electrostatic_from_cube(fptr_rho, fptr_pot, wire-  
                                                    frame=True)
```

A function to generate a VMD visualization of a electrostatic potential mapped onto an electron density isosurface.

#### Parameters

**fptr\_rho:** *str* Path to the electron density cube file.

**fptr\_pot:** *str* Path to the electrostatic potential cube file.

**wireframe:** *bool, optional* If you want to view wireframe (True) or not (False) for the orbitals.

#### Returns

None

## 3.13 qe

TO DO

## 3.14 structures

### 3.14.1 atom

The atom object holds atomic information in and transformations.

- [\*Atom\*](#)

---

```
class squid.structures.atom.Atom(element, x, y, z, index=None, molecule_index=1, label=None,  
                                charge=None)
```

A structure to hold atom information.

#### Parameters

**element:** *str* The atomic element.

**x:** *float* The x coordinate of the atom.

**y:** *float* The y coordinate of the atom.

**z:** *float* The z coordinate of the atom.

**index:** *int, optional* The atomic index within a molecule.

**molecule\_index:** *int, optional* Which molecule the atom is contained in.

**label:** *str, optional* The label of the atomic type within the given forcefield.

**charge:** *float, optional* The atomic charge.

#### Returns

**atom:** [\*squid.structures.atom.Atom\*](#) The Atom class container.

#### **flatten()**

Obtain simplified position output.

#### Returns

**pos:** *np.array, float* A numpy array holding the x, y, and z position of this atom.

**get\_id\_tag()**

Return the id tag of this atom. This is defined as:

molecule\_index:index

Note, if either is None then it is returned as the string. Thus:

None:1 1:None None:None

Are all possible.

**scale(v)**

Scale the atom by a vector. This can be useful if we want to change coordinate systems.

**Parameters**

**v:** *list, float* A vector of 3 floats specifying the x, y, and z scalars to be applied.

**Returns**

None

**set\_position(pos)**

Manually set the atomic positions by passing a tuple/list.

**Parameters**

**pos:** *list, float or tuple, float* A vector of 3 floats specifying the new x, y, and z coordinate.

**Returns**

None

**translate(v)**

Translate the atom by a vector.

**Parameters**

**v:** *list, float* A vector of 3 floats specifying the x, y, and z offsets to be applied.

**Returns**

None

**unravel()**

Like flatten; however, this method will unravel all properties of the atom into a tuple.

**Returns**

**props:** *tuple, ...* Return all atom properties as they are, in the following order:

element, x, y, z, index, molecule\_index, label, charge

### 3.14.2 molecule

- *Molecule*

---

```
class squid.structures.molecule.Molecule(atoms, bonds=[], angles=[], dihedrals=[],
                                           molecule_index=None, assign_indices=True)
```

A molecule object to store atoms and any/all associated interatomic connections.

**Parameters**

**atoms:** *list*, *squid.structures.atom.Atom* A list of atoms.

**bonds:** *list*, *squid.structures.topology.Connector*, *optional* A list of all bonds within the system.

**angles:** *list*, *squid.structures.topology.Connector*, *optional* A list of all angles within the system.

**dihedrals:** *list*, *squid.structures.topology.Connector*, *optional* A list of all dihedrals within the system.

**molecule\_index:** *int*, *optional* The index to be assigned for this molecule.

**assign\_indices:** *bool*, *optional* Whether to assign the molecule a default index of 1 (if no other is specified), and to assign the atomic indices, indexed at 1. If molecule\_index is specified, that will take precedence over the default of 1; however, the atom re-indexing will still take place.

### Returns

**molecule:** *squid.structures.molecule.Molecule* The Molecule class container.

**assign\_angles\_and\_dihedrals()**

Given a list of atom structures with bonded information, calculate angles and dihedrals.

### Returns

None

**flatten()**

Flatten out all atoms into a 1D array.

### Returns

**atoms:** *list*, *float* A 1D array of atomic positions.

**get\_center\_of\_geometry(skip\_H=False)**

Calculate the center of geometry of the molecule.

### Parameters

**skip\_H:** *bool*, *optional* Whether to include Hydrogens in the calculation (False), or not (True).

### Returns

**cog:** *np.array*, *float* A np.array of the x, y, and z coordinate of the center of geometry.

**get\_center\_of\_mass(skip\_H=False)**

Calculate the center of mass of the molecule.

### Parameters

**skip\_H:** *bool*, *optional* Whether to include Hydrogens in the calculation (False), or not (True).

### Returns

**com:** *np.array*, *float* A np.array of the x, y, and z coordinate of the center of mass.

**merge(other, deepcopy=False)**

This function merges another molecule into this one, offsetting indices as needed. When merging, the atom indices of this molecule is reassigned. Further, if deepcopy is False, then the atom indices of the other molecule are also reassigned.

### Parameters

**deepcopy:** *bool*, *optional* Whether to merge via a deep copy, in which atoms are replicated (that is, the atom pointers are different between the molecules), or to merge via pointers, in which the other molecule has similar pointers.

**Returns**

None

**net\_charge ( )**

Return the net charge of the molecule. This requires that atoms have charges associated with them.

**Returns**

**charge:** *float* The atomic charge of the system.

**reassign\_indices (offset=0)**

Simply reassign atomic indices based on their current positions in the atoms array. This is zero indexed, unless otherwise specified. Further, assign the molecule\_index of the atoms to be the same as this molecule object.

**Parameters**

**offset:** *int, optional* What offset to use when indexing.

**Returns**

None

**rotate (m, around='com')**

Rotate the molecule by the given matrix *m*.

**Parameters**

**m:** *list, list, float* A 3x3 matrix describing the rotation to be applied to this molecule.

**around:** *str, optional* Whether to rotate around the center of mass (com), center of geometry (cog), or neither ("None" or None).

**Returns**

None

**scale (v)**

Apply a scalar to this molecule.

**Parameters**

**v:** *list, float* A vector of 3 floats specifying the x, y, and z scalars to be applied.

**Returns**

None

**set\_positions (positions, new\_atom\_list=False)**

Manually specify atomic positions of your molecule.

**Parameters**

**positions:** *list, float* A list, either 2D or 1D, of the atomic positions. Note, this should be in the same order that the atoms are stored in.

**new\_atom\_list:** *bool, optional* Whether to generate an entirely new atom list (True) or re-write atom positions of those atoms already stored (False). Note, if a new list is written, connections are wiped out.

**Returns**

None

**translate** (*v*)

Apply a translation to this molecule.

**Parameters**

**v:** *list, float* A vector of 3 floats specifying the x, y, and z offsets to be applied.

**Returns**

None

### 3.14.3 results

The results module contains data structures to hold simulation output.

- DFT\_out
- sim\_out

---

**class** `squid.structures.results.DFT_out` (*name*, *dft*='orca')

A generic class to hold dft data.

**Parameters**

**name:** *str* Given name for this simulation object.

**dft:** *str, optional* Identifier for which dft code this data is from.

**Contains**

**route:** *str* The 'route' line describing the functional, basis set, and other dft configurations.

**extra\_section:** *str* The 'extra section' in the simulation.

**charge\_and\_multiplicity:** *str* The charge and multiplicity, in that order, of the system.

**dipole:** *list, ...* The dipole of the system as a list of the magnitude and moment.

**frames:** *list, list, squid.structures.atom.Atom* A list lists of atoms describing each iteration in the dft simulation.

**atoms:** *list, squid.structures.atom.Atom* Atomic information of the last iteration in the dft simulation.

**gradients:** *list, list, float* Gradient of the potential, stored for each atom in *atoms* and *frames[-1]*.

**energy:** *float* The total energy of the last iteration.

**charges\_MULLIKEN:** *list, float* Mulliken charges for each atom in *atoms* and *frames[-1]*.

**charges\_LOEWDIN:** *list, float* Loewdin charges for each atom in *atoms* and *frames[-1]*.

**charges\_CHELPG:** *list, float* Chelpg charges for each atom in *atoms* and *frames[-1]*.

**charges:** *list, float* Charges for each atom in *atoms* and *frames[-1]*. Typically a copy of Mulliken charges.

**MBO:** *list, list, squid.structures.atom.Atom, float* A list of lists, each list holding (1) a list of atoms in the bond and (2) the Mayer Bond Order (MBO) of said bond.

**vibfreq:** *list, float* A list of the vibrational frequencies if available, otherwise None.

**convergence:** *list, str VERIFY* A list of convergence criteria and matching values.

**converged:** *bool* Whether the simulation converged (True), or not (False).



**time:** *float* Total time in seconds that the simulation ran for.

**bandgap:** *float* Bandgap of the final configuration.

**bandgaps:** *float* Bandgap of each configuration.

**orbitals:** *list, tuple, float, float* A list of tuples, each holding the information of the occupation and energy (Ha) of a molecular orbital. NOTE! This does not take into account degenerate energy states, so ensure that whatever DFT software you're using has already done so.

**finished:** *bool* Whether the simulation completed normally (True), or not (False).

**warnings:** *list, str* Warnings output by the simulation.

**class** `squid.structures.results.sim_out` (*name, program='lammps'*)  
A generic class to hold simulation data, particularly lammps trajectory files.

#### Parameters

**name:** *str* Given name for this simulation object.

**program:** *str, optional* Identifier for which program this data is from.

#### Contains

**frames:** *list, list, squid.structures.atom.Atom* A list lists of atoms describing each iteration in the simulation.

**atoms:** *list, squid.structures.atom.Atom* Atomic information of the last iteration in the simulation.

**timesteps:** *list, int* Recorded timesteps within the output.

**final\_timestep:** *int* Final timestep of the output.

**atom\_counts:** *list, int* List of how many atoms for each timestep.

**atom\_count:** *int* List of how many atoms in the final timestep.

**box\_bounds\_list:** *list, dict* List of box bounds for each timestep.

**box\_bounds:** *dict* List of box bounds for the final timestep.

### 3.14.4 system

**class** `squid.structures.system.System` (*name, box\_size=(10.0, 10.0, 10.0), box\_angles=(90.0, 90.0, 90.0), periodic=False*)

A system object to store molecules for one's simulations.

#### Parameters

**name:** *str* System Name. This is used when any files/folders are generated.

**box\_size:** *tuple, float, optional* System x, y, and z lengths.

**box\_angles:** *tuple, float, optional* System xy, yz, and xz angles in degrees.

**periodic:** *bool, optional* Whether to have periodic boundaries on or off.

#### Returns

**system:** *squid.structures.system.System* The System class container.

**add** (*molecule*, *mol\_offset=1*, *deepcopy=True*)

A function to add a molecule to this system. Note, this addition can be either a deepcopy or not. If it is not a deepcopy, then the molecule is added as a pointer and can be adjusted externally. By default it is added via a deepcopy to prevent untracked errors.

**Parameters**

**molecule:** *squid.structures.molecule.Molecule* A Molecule structure.

**mol\_offset:** *int, optional* The offset to apply to molecule\_index.

**deepcopy:** *bool, optional* Whether to add the molecule into the system via a deepcopy or not.

**Returns**

None

**contains\_molecule** (*molecule*)

Check if this system contains a molecule, based on the atoms, bonds, angles and dihedrals.

**Parameters**

**molecule:** *squid.structures.molecule.Molecule* A molecule to be checked if it resides within this system.

**Returns**

**is\_contained:** *bool* A boolean specifying if the molecule passed to this function is contained within this System object. This implies that all atoms, bonds, angles, and dihedrals within the molecule are present in a molecule within the system.

**dump\_angles\_data** ()

This function will dump all the bond information to a LAMMPS data file.

bond\_index bond\_type\_index atoms...atoms

**Returns**

**connection\_info:** *str* A string of all the connector information with proper data.

**dump\_atoms\_data** ()

This function will dump all the atom information to a LAMMPS data file.

atom\_index mol\_index type charge x y z

**Returns**

**atomic\_info:** *str* A string of all the atomic information with proper data.

**dump\_bonds\_data** ()

This function will dump all the bond information to a LAMMPS data file.

bond\_index bond\_type\_index atoms...atoms

**Returns**

**connection\_info:** *str* A string of all the connector information with proper data.

**dump\_dihedrals\_data** ()

This function will dump all the bond information to a LAMMPS data file.

bond\_index bond\_type\_index atoms...atoms

**Returns**

**connection\_info:** *str* A string of all the connector information with proper data.

**dump\_pair\_coeffs ( )**

Will try to dump all available pair coefficients. Currently, this means that Coulomb, Lennard-Jones, and Morse will be attempted. If you prefer that one or another not be output, you must set the appropriate masks to your parameter object. For example, assume this System object is called “solv\_box”, you can do the following prior to dumping the pair coeffs:

```
solv_box.parameters.coul_mask = True    solv_box.parameters.lj_mask = False
solv_box.parameters.morse_mask = False
```

Note - this function dumps pair coeffs for the input script, NOT the data file. If you wish for the alternative, see `dump_pair_coeffs_data()`

**dump\_pair\_coeffs\_data ( )**

Will try to dump all available pair coefficients. Currently, this means that Coulomb, Lennard-Jones, and Morse will be attempted. If you prefer that one or another not be output, you must set the appropriate masks to your parameter object. For example, assume this System object is called “solv\_box”, you can do the following prior to dumping the pair coeffs:

```
solv_box.parameters.coul_mask = True    solv_box.parameters.lj_mask = False
solv_box.parameters.morse_mask = False
```

Note - this function dumps pair coeffs for the data file, NOT the input script. If you wish for the alternative, see `dump_pair_coeffs()`

**get\_atom\_masses ( )**

This simplifies using data file writing by getting the masses of all the atoms in the correct order.

**Returns**

**masses:** *list, float* A list of the masses for each atom type.

**get\_center\_of\_geometry (skip\_H=False)**

Calculate the center of geometry of the system.

**Parameters**

**skip\_H:** *bool, optional* Whether to include Hydrogens in the calculation (False), or not (True).

**Returns**

**cog:** *np.array, float* A np.array of the x, y, and z coordinate of the center of geometry.

**get\_center\_of\_mass (skip\_H=False)**

Calculate the center of mass of the system.

**Parameters**

**skip\_H:** *bool, optional* Whether to include Hydrogens in the calculation (False), or not (True).

**Returns**

**com:** *np.array, float* A np.array of the x, y, and z coordinate of the center of mass.

**get\_elements ( )**

This simplifies using `dump_modify` by getting a list of the elements in this system, sorted by their weight. Note, duplicates will exist if different atom types exist within this system!

**Returns**

**elements:** *list, str* A list of the elements, sorted appropriately for something like `dump_modify`.

**reassign\_indices (mol\_offset=1, atom\_offset=1)**

Given a system of many molecules and atoms, reassign all the indices to be consistent.

**Parameters**

**mol\_offset:** *int, optional* The molecule atom offset. Do we start at 0 or 1 or 2? By default it is 0.

**atom\_offset:** *int, optional* The atom offset. Do we start at 0 or 1 or 2? By default it is 0.

#### Returns

None

**rotate** (*m*, *around*='com')

Rotate the system by the given matrix *m*.

#### Parameters

**m:** *list, list, float* A 3x3 matrix describing the rotation to be applied to this molecule.

**around:** *str, optional* Whether to rotate around the center of mass (com), center of geometry (cog), or neither ("None" or None).

#### Returns

None

**set\_types** (*opls\_file*='/home/hherbol/programs/squid/squid/structures/./forcefields/potentials/oplsaa.prm',  
*smrff\_file*=None, *params*=None)

Given the atoms, bonds, angles, and dihedrals in a system object, generate a list of the unique atom, bond, angle, dihedral types and assign that to the system object.

#### Parameters

**params:** *squid.forcefields.parameters.Parameters, optional* A parameter object that already exists.

**opls\_file:** *str, optional* A path to an opls file. By default, this points to the stored values in squid. If None, then no OPLS file is read. Otherwise, a custom file is read.

**smrff\_file:** *str, optional* A path to a smrff file. By default, none is read.

**zhi** = None

Otherwise, we have a monoclinic box. We will set the center to the euclidean origin.

### 3.14.5 topology

**class** squid.structures.topology.**Connector** (*atoms*, *length*=None, *angle*=None)

The Connector class works to hold connection information between atoms. This is used primarily for bonds, angles, and dihedrals. A corresponding length and angle can also be held in the object (defaults to None).

#### Parameters

**atoms:** *list, squid.structures.atom.Atom* A list of atoms to connect. If you connect atoms for an angle, the second atom is the center atom.

**length:** *float, optional* The bond length in Angstroms.

**angle:** *float, optional* The angle of the connection in degrees.

#### Returns

**connection:** *squid.structures.topology.Connector* This connector object.

squid.structures.topology.**get\_angle** (*a*, *center*=None, *b*=None, *deg*=True)

Determine the angle between three atoms. In this case, determine the angle a-center-b.

#### Parameters

**a:** `squid.structures.atom.Atom` First atom in the angle.  
**center:** `squid.structures.atom.Atom` Center atom of the angle.  
**b:** `squid.structures.atom.Atom` Last atom in the angle.  
**deg:** *bool, optional* Whether to return the angle in degrees (True) or radians (False).

**Returns**

**theta:** *float* Return the angle, default is degrees.

`squid.structures.topology.get_dihedral_angle(a, b=None, c=None, d=None, deg=True)`  
 Use the Praxeolitic formula to determine the dihedral angle between 4 atoms.

**Parameters**

**a:** `squid.structures.atom.Atom` First atom in the dihedral, or a tuple of all 4.  
**b:** `squid.structures.atom.Atom`, *optional* Second atom in the dihedral.  
**c:** `squid.structures.atom.Atom`, *optional* Third atom in the dihedral.  
**d:** `squid.structures.atom.Atom`, *optional* Fourth atom in the dihedral.  
**deg:** *bool, optional* Whether to return the angle in degrees (True) or radians (False).

**Returns**

**theta:** *float* Return the dihedral angle, default is degrees.

**References**

- <http://stackoverflow.com/a/34245697>

## 3.15 utils

### 3.15.1 cast

`squid.utils.cast.assert_vec(v, length=3, numeric=True)`  
 Given what should be a vector of N values, we assert that they are indeed valid.

**Parameters**

**v:** *array-like* Some array like object.  
**length:** *int, optional* The required length of the array.  
**numeric:** *bool, optional* Whether to require the array be of numerical values or not.

**Returns**

None

`squid.utils.cast.check_vec(v, length=3, numeric=True)`  
 Given what should be a vector of N values, we check that they are indeed valid.

**Parameters**

**v:** *array-like* Some array like object.  
**length:** *int, optional* The required length of the array.  
**numeric:** *bool, optional* Whether to require the array be of numerical values or not.

**Returns**

**valid:** *bool* Whether the array follows the specifications defined or not.

`squid.utils.cast.is_array(v)`  
Simply check if v is array like

#### Parameters

**v:** *array-like* Some array like object.

#### Returns

**valid:** *bool* Whether the object is array like or not.

`squid.utils.cast.is_numeric(x)`  
A simple function to test if x can be cast to a float.

#### Parameters

**v:** *numeric-object* Some variable that should be numeric.

#### Returns

**valid:** *bool* Whether the object is numeric or not.

`squid.utils.cast.simplify_numerical_array(values)`  
Given integer values, simplify to a numerical array. Note, values may also be given as a comma separated string. This is used in jobarray.

#### Parameters

**values:** *list, int or str* A list of integers, or a comma separated string of integers.

#### Returns

**simple\_string:** *str* A single string simplifying the order.

### 3.15.2 print\_helper

`squid.utils.print_helper.bytes2human(n)`  
Convert n bytes (as integer) to a human readable string. Code was found online at activestate (see references).

#### Parameters

**n:** *int* The number of bytes.

#### Returns

**n\_in\_str:** *str* The bytes in string format.

#### References

- <http://code.activestate.com/recipes/578019>

`squid.utils.print_helper.color_set(s, c)`  
Colourize a string for linux terminal output.

#### Parameters

**s:** *str* String to be formatted.

**c:** *str* Colour or format for the string, found in constants.COLOUR.

#### Returns

**s:** *str* Coloured or formatted string.

`squid.utils.print_helper.colour_set(s, c)`  
 Colourize a string for linux terminal output.

#### Parameters

**s:** *str* String to be formatted.  
**c:** *str* Colour or format for the string, found in constants.COLOUR.

#### Returns

**s:** *str* Coloured or formatted string.

`squid.utils.print_helper.printProgressBar(iteration, total, prefix="", suffix="", decimals=1, length=20, fill=' ', buf=None, pad=False)`

NOTE! THIS IS COPIED FROM STACK OVERFLOW (with minor changes), USER Greenstick Link: <https://stackoverflow.com/a/34325723>

Call in a loop to create terminal progress bar.

#### Parameters

**iteration:** *int* Current iteration.  
**total:** *int* Total number of iterations.  
**prefix:** *str, optional* Prefix for the loading bar.  
**suffix:** *str, optional* Suffix for the loading bar.  
**decimals:** *int, optional* Positive number of decimals in percent complete  
**length:** *int, optional* Character length of the loading bar.  
**fill:** *str, optional* Bar fill character.  
**pad:** *bool, optional* Whether to pad the right side with spaces until terminal width.

`squid.utils.print_helper.spaced_print(sOut, delim=['\t', ' '], buf=4)`

Given a list of strings, or a string with new lines, this will reformat the string with spaces to split columns. Note, this only works if there are no headers to the input string/list of strings.

#### Parameters

**sOut:** *str or list, str* String/list of strings to be formatted.  
**delim:** *list, str* List of delimiters in the input strings.  
**buf:** *int* The number of spaces to have between columns.

#### Returns

**spaced\_s:** *str* Appropriately spaced output string.

`squid.utils.print_helper.strip_color(s)`  
 Remove colour and/or string formatting due to linux escape sequences.

#### Parameters

**s:** *str* String to strip formatting from.

#### Returns

**s:** *str* Unformatted string.

`squid.utils.print_helper.strip_colour(s)`  
 Remove colour and/or string formatting due to linux escape sequences.

#### Parameters

**s:** *str* String to strip formatting from.

#### Returns

**s:** *str* Unformatted string.

### 3.15.3 units

`squid.utils.units.convert` (*old, new, val*)

A generic converter of fractional units. This works only for one unit in the numerator and denominator (such as Ha/Ang to eV/Bohr).

#### Parameters

**old:** *str* Units for which val is in.

**new:** *str* Units to convert to.

**val:** *float* Value to convert.

#### Returns

**new\_val:** *float* Converted value in units of new.

`squid.utils.units.convert_dist` (*d0, d1, d\_val*)

Convert distance units.

#### Parameters

**d0:** *str* Unit of distance that d\_val is in.

**d1:** *str* Unit of distance that you wish to convert to.

**d\_val:** *float* Value to be converted.

#### Returns

**distance:** *float* Converted d\_val to units of d1.

`squid.utils.units.convert_energy` (*e0, e1, e\_val*)

Convert energy units.

#### Parameters

**e0:** *str* Unit of energy that e\_val is in.

**e1:** *str* Unit of energy that you wish to convert to.

**e\_val:** *float* Value to be converted.

#### Returns

**energy:** *float* Converted e\_val to units of e1.

`squid.utils.units.convert_pressure` (*p0, p1, p\_val*)

Convert pressure units.

#### Parameters

**p0:** *str* Unit of pressure that p\_val is in.

**p1:** *str* Unit of pressure that you wish to convert to.

**p\_val:** *float* Value to be converted.

#### Returns

**pressure:** *float* Converted p\_val to units of p1.



`squid.utils.units.elem_i2s(elem_int)`

Get the elemental symbol, given its atomic number.

**Parameters**

**elem\_int:** *int* Atomic number of an element.

**Returns**

**elem\_sym:** *str* Elemental symbol.

`squid.utils.units.elem_s2i(elem_sym)`

Get the atomic number, given its elemental symbol.

**Parameters**

**elem\_sym:** *str* Elemental symbol of an element.

**Returns**

**elem\_int:** *int* Atomic number.

`squid.utils.units.elem_sym_from_weight(weight, delta=0.1)`

Get the element that best matches the given weight (in AMU).

**Parameters**

**weight:** *float* Weight of an element in AMU.

**delta:** *float, optional* How close you permit the matching to be in AMU.

**Returns**

**elem\_sym:** *str* The elemental symbol.

`squid.utils.units.elem_weight(elem)`

Get the weight of an element, given its symbol or atomic number.

**Parameters**

**elem:** *str or int* Elemental symbol or atomic number.

**Returns**

**elem\_weight:** *float* Weight of the element in AMU.



## CONSOLE SCRIPTS

Various console scripts exist to aid users in simple tasks.

### 4.1 chkDFT

This command allows one to post-process a dft (orca or g09) output file and summarize the findings to the terminal.

```
chkDFT
-----
A command to quickly get a glimpse of a DFT simulation.
chkDFT [Sim_Name] [Options]

      Flag      Default      Description
-help, -h      :           : Print this help menu
-dft           : orca      : Specify what type of dft simulation you want to
                        parse. By default it is 'g09', but can be
                        'orca' or 'jdftx'.
-units, -u      : Ha       : Specify the units you want the output to be in.
                        By default this is Hartree.
-scale         : 1.0       : Scale all energies by this value
-out, -o        : out      : Make an output file with this name holding all
                        xyz coordinates. If no xyz data is available
                        this will not run. Default output name is
                        'out.xyz' but user can choose their own using
                        this command.
-vmd, -v        :           : Opens output xyz file in vmd. Flag turns on.
-ovito, -ov     :           : Opens output xyz file in ovito. Flag turns on.
-me            :           : Forces the .xyz file to be saved to ~/out.xyz

ex. chkDFT water -dft orca -u kT_300
```

### 4.2 scanDFT

This command allows one to compile together a Nudged Elastic Band reaction pathway from various output DFT calculations. It will both graph the energy pathway, and generate a final xyz file of the last frames.

```
scanDFT
-----
A command to view the energy landscape over several configurations.
There are two ways to implement this:
```

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1.  
Note, the START STOP range is inclusive on either end.

```
scanDFT [Sim_Name%d] START STOP [Options]
```

2.  
scanDFT Sim\_Name

The first method is useful when utilizing flags. The second method will prompt the user for information. Note, in the second instance it will assume an appendage of -%d-%d, describing the iteration and frame. It also assumes and NEB scan is desired.

Flag	Default	Description
-help, -h	:	: Print this help menu
-dft	: orca	: Specify what type of dft simulation you want to get the energy landscape of. Other options include 'orca'.
-units, -u	: kT_300	: Specify the units you want the output to be in.
-scale	: 1.0	: Scale all energies by this value. Applied AFTER unit conversion from simulation units ('Ha') to -units.
-out, -o	: out	: Make an output file with this name holding all xyz coordinates of what you're scanning over.
-step	: 1.0	: Steps to take between your start and stop range
-c	:	: Compile multiple energy landscapes on the same graph. Takes three arguments, separated by commas with no spaces: char,start,stop The character is a unique identifier in the Sim_Name that will be replaced with values from start to stop (inclusive)
-neb	:	: In NEB calculations, each iteration after the first does not include the first and last energies. Giving this flag and a run name for the first in the NEB list will tack on these energies to the rest of the simulations.
-title, -t	:	: Title for the output graph
-lx	:	: Label for the x-axis
-ly	:	: Label for the y-axis
-xrange	:	: Set the x-axis range
-yrange	:	: Set the y-axis range
-xvals	:	: Set a custom label for x-axis (comma separated).
-print, -p	:	: Print out the values that are plotted.
-save, -s	:	: Whether to save the graph to out.png (True) or not (False). Note, when saving it will not display the graph.

```
ex: scanDFT water
ex: scanDFT water_ 1 10
ex: scanDFT water_%d 1 10
ex: scanDFT water%d_opt 1 10
ex: scanDFT water_^%d 1 10 -c ^,0,4 -dft orca
ex: scanDFT water_^%d 1 10 -c ^,2,4 -dft orca -neb water_0_0,water_0_10
ex: scanDFT water_opt_%d 1 10 -t "Water Optimization" -xrange 0,5
```

## 4.3 procrustes

This command allows one to quickly, from the command line, clean-up an xyz file of several frames. It will remove the rigid rotations between consecutive frames, and also allows for linear interpolation.

```
procrustes
-----
A command line tool to run procrustes along an xyz file.

procrustes [file.xyz] [Options]

      Flag           Default      Description
-help, -h         :             : Print this help menu
-overwrite, -o    :             : Overwrite the initial file
-append, -a       : _proc      : Change the appended name alteration
-interpolate, -i :             : This will turn on linear interpolation
-rmax              : 0.5       : The default max rms for interpolation
-fmax              : 25        : The default max number of frames for
                           interpolation
-nframes, -n      :             : If specified, interpolate to exactly n
                           frames.
-between, -b      :             : If specified, then interpolation is only
                           run between the two frames. Note, this
                           is [x, y) inclusive.

Default behaviour is to use procrustes on an xyz to best align
the coordinates, and then to save a new xyz file with the name
OLD_proc.xyz (where OLD is the original xyz file name).

NOTE! If you specify -o and -a, then appending will occur instead
of overwritting.

Ex.

procrustes demo.xyz
procrustes demo.xyz -i -n 20
procrustes demo.xyz -i -rmax 0.1 -fmax 30
procrustes demo.xyz -i -b 5 8 -n 6
```

## 4.4 pysub

This command allows one to quickly submit a python script to run either in the background locally, or on a queue/partition within a cluster.

```
pysub
-----
A command line tool to submit jobs to the queue.

pysub [script.py] [Options]

      Flag           Default      Description
-help, -h         :             : Print this help menu
-n                 : 1         : Number of processors to use
-nt, -tasks       : 1         : Number of tasks this job will run
```

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```
-o, -omp      :      : Manually specify what OMP_NUM_THREADS should be.
-mpi          :      : Whether to run python with mpirun or not.
-q            :      : Which queue to submit to
-walltime, -t : 00:30:00 : The walltime to use
-priority, -p :      : Manually specify job priority
-unique, -u   : False   : Whether to require a unique simulation name.

-jobarray, -ja : None    : Whether to run a job array.  If this flag is
                        specified, it MUST be followed by two values to
                        indicate the lower and upper bounds of the
                        indexing.

-xhost, -x     :      : If needed, specify computer
-args, -a      :      : A list of arguments for the python code
-mods, -m      :      : Specify the modules you wish to use here.
-mo           : False   : Whether to override the default modules.
-keep, -k      :      : Whether to keep the submission file

-py3          :      : Whether to use python 3, or 2 (2 is default).
-alloc, -A     : None    : Whether to specify a SLURM Allocation.
-gpu          : None    : The number of desired GPUs you want.
```

Default behaviour is to generate a job with the same name as the python script and to generate a .log file with the same name as well.

When using -mpi, it will only be effective **if** nprocs > 1.

NOTE! If using xhost or args, make sure it is the last flag as we assume all remaining inputs are the desired strings. This means that only xhost or args can be used at a **time** (both would lead to errors).

## EXAMPLES

On the squid github repo, we include an examples folder that describes simple use cases. These are replicated here:

- Using NEB to find the MEP of CNH Isomerization
- Calculating and visualizing the molecular orbitals of Water
- Calculating and visualizing the electrostatic potential surface of Water
- Using procrustes and linear interpolation to smooth predicted reaction pathways
- Equilibrating a box of benzene and acetone in Molecular Dynamics

### 5.1 Nudged Elastic Band Demo

The below code shows how one can generate a reaction pathway, and ultimately run NEB on it to find the minimum energy pathway (MEP). Further, it automates the submission of an eigenvector following Transition State optimization from the peak, and verifies a transition state was found. Note, the endpoints and NEB should use the same DFT level of theory, otherwise your endpoints may not remain local minima within the potential energy surface.

```
from squid import orca
from squid import files
from squid import geometry
from squid.calcs import NEB
from squid import structures

if __name__ == "__main__":
    # In this example we will generate the full CNH-HCN isomerization using
    # only squid. Then we optimize the endpoints in DFT, smooth the frames,
    # and subsequently run NEB

    # Step 1 - Generate the bad initial guess
    print("Step 1 - Generate the bad initial guess...")
    H_coords = [(2, 0), (2, 0.5), (1, 1), (0, 1), (-1, 0.5), (-1, 0)]
    CNH_frames = [
        structures.Atom("C", 0, 0, 0),
        structures.Atom("N", 1, 0, 0),
        structures.Atom("H", x, y, 0)]
        for x, y in H_coords
    ]
    # Save initial frames
    files.write_xyz(CNH_frames, "bad_guess.xyz")
```

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```

# Step 2 - Optimize the endpoints
print("Step 2 - Optimize endpoints...")
frame_start_job = orca.job(
    "frame_start", "! HF-3c Opt", atoms=CNH_frames[0], queue=None
)
frame_last_job = orca.job(
    "frame_last", "! HF-3c Opt", atoms=CNH_frames[-1], queue=None
)
# Wait
frame_start_job.wait()
frame_last_job.wait()

# Step 3 - Read in the final coordiantes, and update the band
print("Step 3 - Store better endpoints...")
CNH_frames[0] = orca.read("frame_start").atoms
CNH_frames[-1] = orca.read("frame_last").atoms
# Save better endpoints
files.write_xyz(CNH_frames, "better_guess.xyz")

# Step 4 - Smooth out the band to 10 frames
print("Step 4 - Smooth out the band...")
CNH_frames = geometry.smooth_xyz(
    CNH_frames, N_frames=8,
    use_procrustes=True
)
# Save smoothed band
files.write_xyz(CNH_frames, "smoothed_guess.xyz")

# Step 5 - Run NEB
print("Step 5 - Run NEB...")
neb_handle = NEB(
    "CNH", CNH_frames, "! HF-3c",
    nprocs=1, queue=None, ci_neb=True
)
CNH_frames = neb_handle.optimize()[-1]
# Save final band
files.write_xyz(CNH_frames, "final.xyz")

# Step 6 - Isolate the peak frame, and converge to the transition state
print("Step 6 - Calculating Transition State...")
ts_job = orca.job(
    "CNH_TS", "! HF-3c OptTS NumFreq",
    extra_section='''
%geom
  Calc_Hess true
  NumHess true
  Recalc_Hess 5
end
'''
    atoms=CNH_frames[neb_handle.highest_energy_frame_index], queue=None
)
ts_job.wait()

# Ensure we did find the transition state
data = orca.read("CNH_TS")
vib_freq = data.vibfreq
if sum([int(v < 0) for v in vib_freq]) == 1:
    print("    Isolated a transition state with exactly 1 negative vibfreq.")

```

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```

print("    Saving it to CNH_ts.xyz")
files.write_xyz(data.atoms, "CNH_ts.xyz")
else:
print("FAILED!")

```

Example output is as follows:

```

-----
↪-----
Run_Name = CNH
DFT Package = orca
Spring Constant for NEB: 0.00367453 Ha/Ang = 0.1 eV/Ang
Running Climbing Image, starting at iteration 5

Running neb with optimization method LBFGS
    step_size = 1
    step_size_adjustment = 0.5
    max_step = 0.04
    Using numerical optimization starting hessian approximation.
    Will reset stored parameters and gradients when stepped bad.
    Will reset step_size after 20 good steps.
    Will accelerate step_size after 20 good steps.
    Will use procrustes to remove rigid rotations and translations
Convergence Criteria:
    g_rms = 0.001 (Ha/Ang) = 0.0272144 (eV/Ang)
    g_max = 0.001 (Ha/Ang) = 0.0272144 (eV/Ang)
    maxiter = 1000
-----
Step      RMS_F (eV/Ang)  MAX_F (eV/Ang)  MAX_E (kT_300)  Energies (kT_300)
-----
0   28.7949    44.5242    223.9    -92.232 + 109.6 215.5 223.9 182.8  62.4  62.4 ↪
↪-24.8
1   15.339    21.7786    161.1    -92.232 +  44.3 143.0 161.1  88.4  13.7  20.3 ↪
↪-24.8
2   14.6517    20.8575    158.0    -92.232 +  41.7 139.4 158.0  86.2  11.9  17.2 ↪
↪-24.8
3    6.0258     9.376    122.9    -92.232 +  15.2 100.8 122.9  62.8  -5.4  -9.2 ↪
↪-24.8
4    5.6856     8.8098    121.5    -92.232 +  14.5  99.4 121.5  61.5  -5.7  -9.3 ↪
↪-24.8
5    1.8606     3.0362    107.7    -92.232 +   9.4  86.9 107.7  50.6  -8.2 -10.1 ↪
↪-24.8
6    1.1459     3.024    105.3    -92.232 +   9.3  85.5 105.3  49.1  -8.4 -11.0 ↪
↪-24.8
7    0.945     2.5354    105.2    -92.232 +   9.4  84.9 105.2  48.5  -8.5 -11.3 ↪
↪-24.8
8    0.9274     2.0697    107.9    -92.232 +   9.5  84.5 107.9  48.8  -8.5 -11.9 ↪
↪-24.8
9    0.8502     1.9055    110.2    -92.232 +   9.4  84.5 110.2  49.1  -8.6 -12.3 ↪
↪-24.8
10   0.9637     1.7608    114.3    -92.232 +   9.5  85.0 114.3  49.5  -8.4 -13.0 ↪
↪-24.8
11   0.8564     1.4446    115.4    -92.232 +   9.5  84.9 115.4  49.4  -8.4 -13.4 ↪
↪-24.8
12   0.8252     1.2095    116.8    -92.232 +   9.7  84.6 116.8  49.6  -8.2 -14.5 ↪
↪-24.8
13   0.3625     0.742    115.6    -92.232 +   9.6  84.2 115.6  49.3  -8.4 -14.3 ↪
↪-24.8

```

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```

14  0.8296      1.4249      116.8      -92.232 +    9.9  84.3 116.8  49.9  -8.1 -15.6
↪-24.8
15  0.6218      1.0318      116.8      -92.232 +    9.8  84.2 116.8  49.8  -8.2 -15.6
↪-24.8
16  0.2493      0.5738      116.4      -92.232 +    9.7  83.9 116.4  49.6  -8.2 -15.2
↪-24.8
17  0.1849      0.3175      116.4      -92.232 +    9.7  83.9 116.4  49.6  -8.2 -15.1
↪-24.8
18  0.1046      0.2349      116.3      -92.232 +    9.8  83.8 116.3  49.7  -8.2 -15.1
↪-24.8
19  0.0459      0.1069      116.3      -92.232 +    9.8  83.8 116.3  49.7  -8.1 -15.1
↪-24.8
20  0.0221      0.0458      116.3      -92.232 +    9.8  83.7 116.3  49.7  -8.1 -15.1
↪-24.8

```

NEB converged the RMS force.

-----

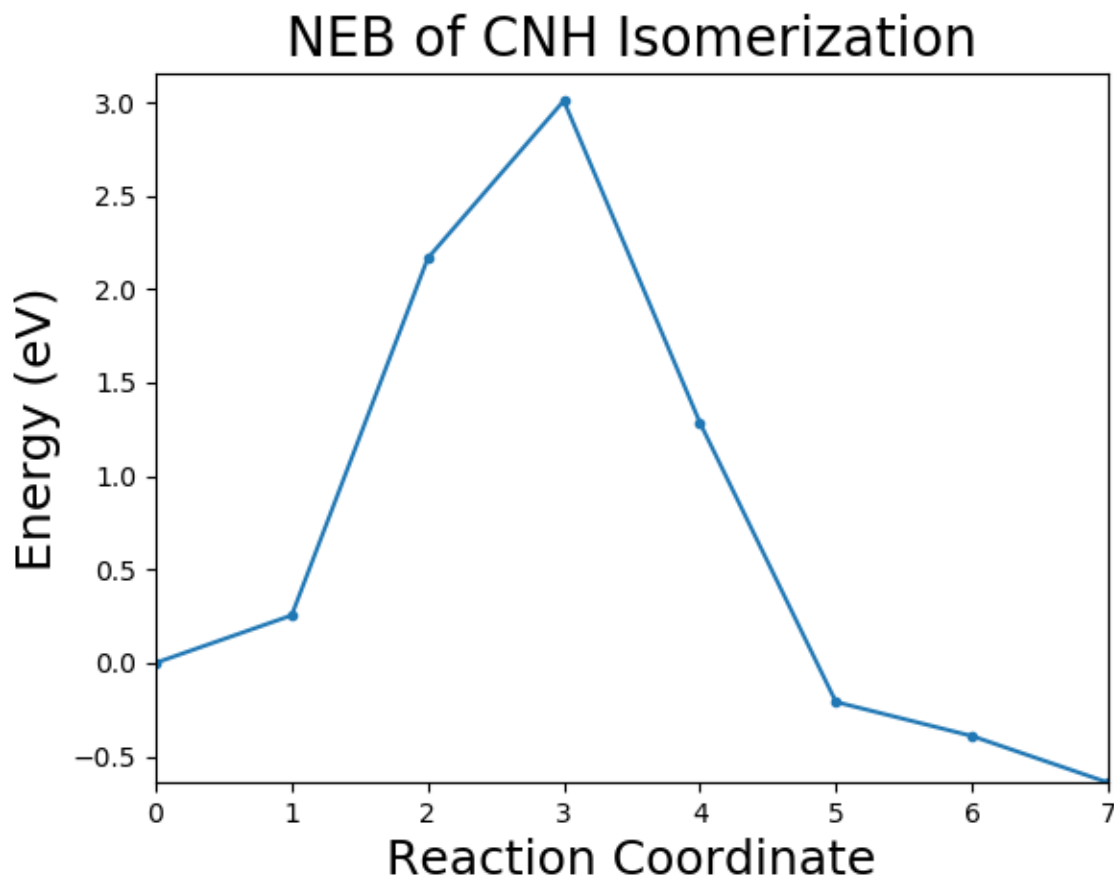
↪----

With the following graph made using the scanDFT command line tool:

```

scanDFT CNH-20-%d 1 6 -neb CNH-0-0,CNH-0-7 -t "NEB of CNH Isomerization" -lx
↪ "Reaction Coordinate" -ly "Energy" -u eV

```



## 5.2 Molecular Orbital Visualization Demo

The below code shows how one can visualize molecular orbitals of a molecule (in this case water) using VMD.

```
from squid import orca
from squid import files

if __name__ == "__main__":
    # First, calculate relevant information
    frames = files.read_xyz('water.xyz')
    job_handle = orca.job(
        'water',
        '! PW6B95 def2-TZVP D3BJ OPT NumFreq',
        atoms=frames,
        queue=None)
    job_handle.wait()

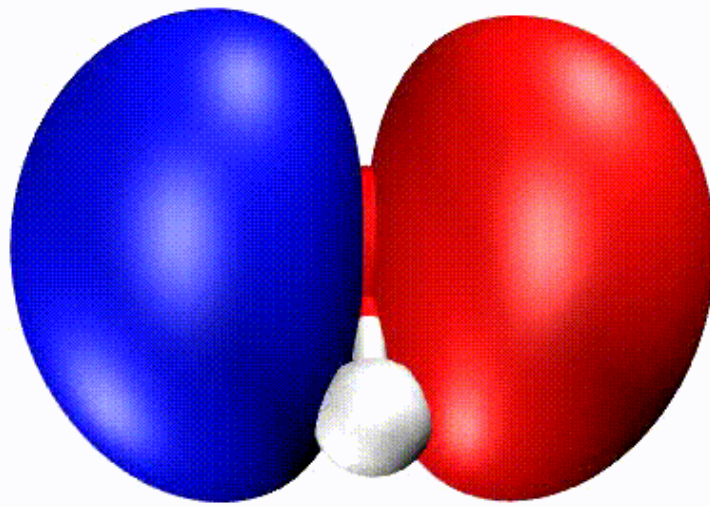
    # Next, post process it
    orca.mo_analysis(
        "water", orbital=None,
        HOMO=True, LUMO=True,
        wireframe=False, hide=True, iso=0.04
    )
```

In the console output it'll show the following in blue:

Representations are as follows:

- 1 - CPK of atoms
- 2 - LUMO Positive
- 3 - HOMO Positive
- 4 - LUMO Negative
- 5 - HOMO Negative
- 6 - Potential Surface
- 7 - MO 3

Choosing only displays 1, 3, and 5 we can see the HOMO level of water as follows (positive being blue and negative being red):



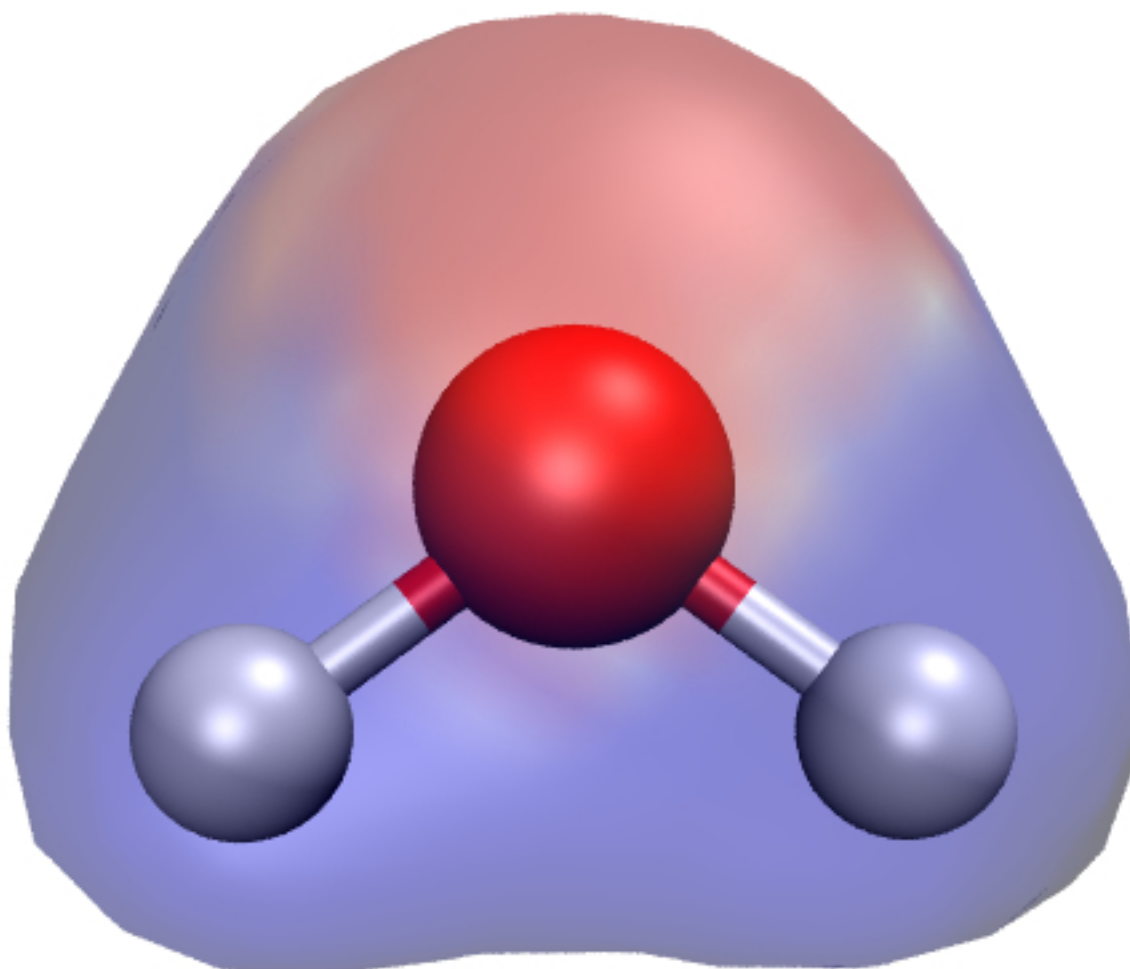
## 5.3 DFT - Electrostatic Potential Mapped on Electron Density Post Processing

We can also readily generate an electrostatic potential mapped onto an electron density isosurface using squid. One thing to note is that the final results are subjective depending on two primary values, which the user may set in VMD. These values are found under the *Graphics > Representations* tab as the *Isovalue* listed in *Draw Style* and the *Color Scale Data Range* listed under *Trajectory*.

```
from squid import orca
from squid import files

if __name__ == "__main__":
    # First, calculate relevant information
    frames = files.read_xyz('water.xyz')
    job_handle = orca.job(
        'water',
        '! PW6B95 def2-TZVP D3BJ OPT NumFreq',
        atoms=frames,
        queue=None)
    job_handle.wait()

    # Next, post process it
    orca.pot_analysis(
        "water", wireframe=False, npoints=80
    )
```



## 5.4 Geometry - Smoothing out a Reaction Coordinate

The below code shows how we can smooth out xyz coordinates in a reaction pathway using linear interpolation and procrustes superimposition.

```
import os
import shutil
from squid import files
from squid import geometry
from squid import structures
from squid.post_process.ovito import ovito_xyz_to_gif
```

```
def example_1(): # In this example, we will generate a smooth CNH-HCN isomerization # guessed pathway
    # Step 1 - Generate the bad initial guess
    print("Step 1 - Generate the bad initial guess...")
    H_coords = [(2, 0), (2, 1), (1, 1), (0, 1), (-1, 1), (-1, 0)]
    CNH_frames = [
        structures.Atom("C", 0, 0, 0),
        structures.Atom("N", 1, 0, 0),
        structures.Atom("H", x, y, 0) for x, y in H_coords
    ]
    # Further, randomly rotate the atoms
    CNH_frames = [
        geometry.perturbate(frame, dx=0.0, dr=360) for frame in CNH_frames
    ]
```

```

] files.write_xyz(CNH_frames, "rotated_pathway.xyz")

# Step 2 - Use procrustes to remove rotations print("Step 2 - Use Procrustes to remove rotations...") geometry.procrustes(CNH_frames) files.write_xyz(CNH_frames, "procrustes_pathway.xyz")

# Step 3 - Smooth out the band by minimizing the RMS atomic motion between # consecutive frames until it is below 0.1 (with a max of 50 frames). print("Step 3 - Smooth out the band...") CNH_frames = geometry.smooth_xyz(
    CNH_frames, R_max=0.1, F_max=50, use_procrustes=True
) # Save smoothed band files.write_xyz(CNH_frames, "smoothed_pathway.xyz")

if __name__ == "__main__": example_1()

```

Further, we can automate the generation of gifs using the ovitos python interface. Note, this is not always guaranteed to be a pretty image, as you would need to know exactly where to point the camera. In some situations it may be obvious where it should be placed; however, in many we simply recommend opening up Ovito and using their GUI interface directly.

```

import os
import shutil
from squid import files
from squid import geometry
from squid import structures
from squid.post_process.ovito import ovito_xyz_to_gif

```

```

def example_2(): # In this example, we illustrate how we can automate the generation of # gifs of the reactions in example_1
    print("Step 4 - Generating gifs...")

    # Generate a scratch folder for image generation scratch_folder = "/tmp" if os.path.exists(scratch_folder):
        shutil.rmtree(scratch_folder)

    print("rotated_pathway.gif") os.mkdir(scratch_folder) ovito_xyz_to_gif(
        files.read_xyz("rotated_pathway.xyz"), scratch_folder, fname="rotated_pathway", camera_pos=(0, 0, -10), camera_dir=(0, 0, 1))

    shutil.rmtree(scratch_folder)

    print("procrustes_pathway.gif") os.mkdir(scratch_folder) ovito_xyz_to_gif(
        files.read_xyz("procrustes_pathway.xyz"), scratch_folder, fname="procrustes_pathway", camera_pos=(0, 0, -10), camera_dir=(0, 0, 1))

    shutil.rmtree(scratch_folder)

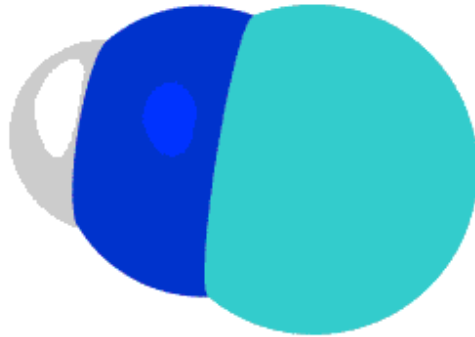
    print("smoothed_pathway.gif") os.mkdir(scratch_folder) ovito_xyz_to_gif(
        files.read_xyz("smoothed_pathway.xyz"), scratch_folder, fname="smoothed_pathway", camera_pos=(0, 0, -10), camera_dir=(0, 0, 1))

    shutil.rmtree(scratch_folder)

if __name__ == "__main__": example_2()

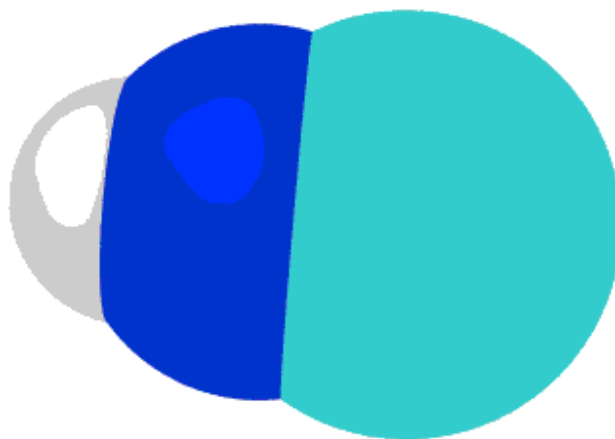
```

The rough reaction coordinate with rotations, shown below, would not lend itself to linear interpolation, as neighbouring frames would lead to atoms overlapping.

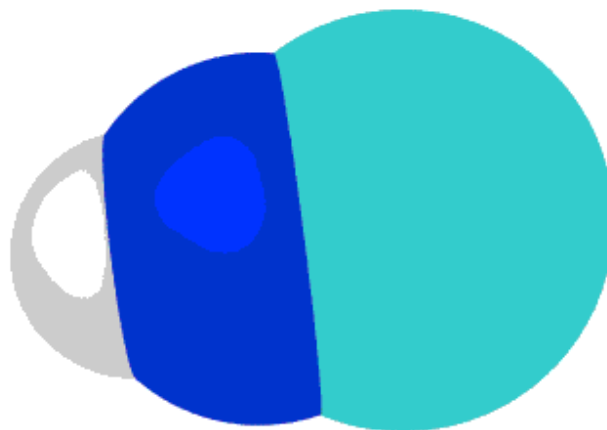


However, when using the procrustes method we remove the rigid rotation associated with this change of coordinate system, making it appear much better.





Finally, with the added linear interpolations we end up with a smooth reaction coordinate.



## 5.5 Molecular Dynamics Solvent Box Equilibration

In this example, we equilibrate an MD box of two benzene molecules (offset by 10, 10, 10) and acetone (packed to a density of 1.0 using packmol).

```
from squid import files
from squid import lammps
from squid import geometry
from squid import structures

if __name__ == "__main__":
    # In this example, we discuss how to handle running MD using LAMMPS and
    # squid. We start by generating a System object, add in some molecules,
    # and then pack this system object with solvents. We then equilibrate
    # the system.

    # Step 1 - Generate the system
    world = structures.System(
        "solv_box", box_size=(15.0, 15.0, 15.0), periodic=True)

    # Step 2 - Get any molecules you want
    mol1 = files.read_cml("benzene.cml")[0]
    mol2 = mol1 + (10, 10, 10)
```

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```

solv = files.read_cml("acetone.cml")[0]

# Step 3 - Add them however you want
world.add(mol1)
world.add(mol2)
geometry.packmol(world, [solv], persist=False, density=1.0)

# Step 4 - Run a simulation
world.set_types()

input_script = """units real
atom_style full
pair_style lj/cut/coul/cut 10.0
bond_style harmonic
angle_style harmonic
dihedral_style opls

boundary p p p
read_data solv_box.data

pair_modify mix geometric

""" + world.dump_pair_coeffs() + """

dump 1 all xyz 100 solv_box.xyz
dump_modify 1 element "" + ' '.join(world.get_elements()) + ""

compute pe all pe/atom
dump forces all custom 100 forces.dump id element x y z fx fy fz c_pe
dump_modify forces element "" + ' '.join(world.get_elements()) + ""

thermo_style custom ke pe temp press
thermo 100

minimize 1.0e-4 1.0e-6 1000 10000

velocity all create 300.0 23123 rot yes dist gaussian
timestep 1.0

fix motion_npt all npt temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
run 10000
unfix motion_npt

fix motion_nvt all nvt temp 300.0 300.0 300.0
run 10000
unfix motion_nvt
"""

job_handle = lammps.job("solv_box", input_script, system=world, nprocs=1)
job_handle.wait()

```

In this example, we want to write a lammps data file without knowing any parameters, so we strip away all relevant information and write the file.

```

from squid import files
from squid import lammps
from squid import geometry

```

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```
from squid import structures

if __name__ == "__main__":
    # Step 1 - Generate the system
    world = structures.System(
        "solv_box", box_size=(15.0, 15.0, 15.0), periodic=True)

    # Step 2 - Get any molecules you want
    mol1 = files.read_cml("benzene.cml")[0]
    mol2 = mol1 + (10, 10, 10)
    solv = files.read_cml("acetone.cml")[0]

    # Step 3 - In the case that we do not know the atom types, but we still
    # want to generate a lammps data file, we can still do so! We must first
    # in this example strip away all relevant bonding information. Further,
    # and this is important: YOU MUST SET a.label and a.charge to the element
    # and some value (in this example I set it to 0.0).
    for mol in [mol1, mol2, solv]:
        for a in mol.atoms:
            a.label = a.element
            a.charge = 0.0
        mol.bonds = []
        mol.angles = []
        mol.dihedrals = []

    # Step 4 - Add them however you want
    world.add(mol1)
    world.add(mol2)
    geometry.packmol(world, [solv], persist=False, density=1.0)

    # Step 5 - Run a simulation
    world.set_types()
    lammps.write_lammps_data(world)
```

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