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## 7 Indices and tables

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### Python Module Index
The **freud** Python library provides a simple, flexible, powerful set of tools for analyzing trajectories obtained from molecular dynamics or Monte Carlo simulations. High performance, parallelized C++ is used to compute standard tools such as radial distribution functions, correlation functions, order parameters, and clusters, as well as original analysis methods including potentials of mean force and torque (PMFTs) and local environment matching. The **freud** library uses NumPy arrays for input and output, enabling integration with the scientific Python ecosystem for many typical materials science workflows.

When using **freud** to process data for publication, please use this citation.
The easiest ways to install \texttt{freud} are using pip:

\begin{verbatim}
pip install freud-analysis
\end{verbatim}

or conda:

\begin{verbatim}
conda install -c conda-forge freud
\end{verbatim}

\texttt{freud} is also available via containers for \texttt{Docker} or \texttt{Singularity}. If you need more detailed information or wish to install \texttt{freud} from source, please refer to the Installation Guide to compile \texttt{freud} from source.
Some other helpful links for working with freud:

- Find examples of using freud on the examples page.
- Find detailed tutorials and reference information in the freud documentation.
- View and download the code on the GitHub repository.
- Ask for help on the freud-users Google Group.
- Report issues or request features using the issue tracker.
The `freud` library is called using Python scripts. Many core features are demonstrated in the `freud` documentation. The examples come in the form of Jupyter notebooks, which can also be downloaded from the `freud` examples repository or launched interactively on Binder. Below is a sample script that computes the radial distribution function for a simulation run with HOOMD-blue and saved into a GSD file.

```python
import freud
import gsd.hoomd

# Create a freud compute object (RDF is the canonical example)
rdf = freud.density.RDF(bins=50, r_max=5)

# Load a GSD trajectory (see docs for other formats)
traj = gsd.hoomd.open('trajectory.gsd', 'rb')
for frame in traj:
    rdf.compute(frame, reset=False)

# Get bin centers, RDF data from attributes
r = rdf.bin_centers
y = rdf.rdf
```
Please visit our repository on GitHub for the library source code. Any issues or bugs may be reported at our issue tracker, while questions and discussion can be directed to our forum. All contributions to freud are welcomed via pull requests!
6.1 Introduction

The freud library is a Python package for analyzing particle simulations. The package is designed to directly use numerical arrays of data, making it easy to use for a wide range of use-cases. The most common use-case of freud is for computing quantities from molecular dynamics simulation trajectories, but it can be used for analyzing any type of particle simulation. By operating directly on numerical arrays of data, freud allows users to parse custom simulation outputs into a suitable structure for input, rather than relying specific file types or data structures.

The core of freud is analysis of periodic systems, which are represented through the freud.box.Box class. The freud.box.Box supports arbitrary triclinic systems for maximum flexibility, and is used throughout the package to ensure consistent treatment of these systems. The package’s many methods are encapsulated in various compute classes, which perform computations and populate class attributes for access. Of particular note are the various computations based on nearest neighbor finding in order to characterize particle environments. Such methods are simplified and accelerated through a centralized neighbor finding interface defined in the freud.locality.NeighborQuery family of classes in the freud.locality module of freud.

6.2 Installation

6.2.1 Installing freud

The freud library can be installed via conda or pip, or compiled from source.

Install via conda

The code below will install freud from conda-forge.

```
conda install -c conda-forge freud
```

Install via pip

The code below will install freud from PyPI.

```
pip install freud-analysis
```
Compile from source

The following are required for installing freud:

- Python (3.5+ required)
- NumPy
- Intel Threading Building Blocks (TBB)

The following are optional for installing freud:

- Cython (0.28+ required): The freud repository contains Cython-generated *.cpp files in the freud/ directory that can be used directly. However, Cython is necessary if you wish to recompile these files.

For conda users, these requirements can be met by installing the following packages from the conda-forge channel:

```
conda install -c conda-forge tbb tbb-devel numpy cython
```

The code that follows builds freud and installs it for all users (append --user if you wish to install it to your user site directory):

```
git clone --recurse-submodules https://github.com/glotzerlab/freud.git
cd freud
python setup.py install
```

You can also build freud in place so that you can run from within the folder:

```
# Run tests from the tests directory
python setup.py build_ext --inplace
```

Building freud in place has certain advantages, since it does not affect your Python behavior except within the freud directory itself (where freud can be imported after building). Additionally, due to limitations inherent to the distutils/setuptools infrastructure, building extension modules can only be parallelized using the build_ext subcommand of setup.py, not with install. As a result, it will be faster to manually run build_ext and then install (which normally calls build_ext under the hood anyway) the built packages. In general, the following options are available for setup.py in addition to the standard setuptools options (notes are included to indicate which options are only available for specific subcommands such as build_ext):

- **PRINT-WARNINGS** Specify whether or not to print compilation warnings resulting from the build even if the build succeeds with no errors.

- **ENABLE-CYTHON** Rebuild the Cython-generated C++ files. If there are any unexpected issues with compiling the C++ shipped with the build, using this flag may help. It is also necessary any time modifications are made to the Cython files.

- **-j** Compile in parallel. This affects both the generation of C++ files from Cython files and the subsequent compilation of the source files. In the latter case, this option controls the number of Python modules that will be compiled in parallel.

- **-TBB-ROOT** The root directory where TBB is installed. Useful if TBB is installed in a non-standard location or cannot be located by Python for some other reason. Note that this information can also be provided using the environment variable TBB_ROOT. The options --TBB-INCLUDE and --TBB-LINK will take precedence over --TBB-ROOT if both are specified.

- **-TBB-INCLUDE** The directory where the TBB headers (e.g. tbb.h) are located. Useful if TBB is installed in a non-standard location or cannot be located by Python for some other reason. Note that this information can also be provided using the environment variable TBB_ROOT. The options --TBB-INCLUDE and --TBB-LINK will take precedence over --TBB-ROOT if both are specified.
The directory where the TBB shared library (e.g. libtbb.so or libtbb.dylib) is located. Useful if TBB is installed in a non-standard location or cannot be located by Python for some other reason. Note that this information can also be provided using the environment variable TBB_ROOT. The options --TBB-INCLUDE and --TBB-LINK will take precedence over --TBB-ROOT if both are specified.

The following additional arguments are primarily useful for developers:

--COVERAGE Build the Cython files with coverage support to check unit test coverage.

--NTHREAD Specify the number of threads to allocate to compiling each module. This option is primarily useful for rapid development, particularly when all changes are in one module. While the -j option will not help parallelize this case, this option allows compilation of multiple source files belonging to the same module in parallel.

Note: freud makes use of git submodules. If you ever wish to manually update these, you can execute:

```
git submodule update --init
```

### 6.2.2 Unit Tests

The unit tests for freud are included in the repository and are configured to be run using the Python `unittest` library:

```
# Run tests from the tests directory
cd tests
python -m unittest discover .
```

Note that because freud is designed to require installation to run (i.e. it cannot be run directly out of the build directory), importing freud from the root of the repository will fail because it will try and import the package folder. As a result, unit tests must be run from outside the root directory if you wish to test the installed version of freud. If you want to run tests within the root directory, you can instead build freud in place:

```
# Run tests from the tests directory
python setup.py build_ext --inplace
```

This build will place the necessary files alongside the freud source files so that freud can be imported from the root of the repository.

### 6.2.3 Documentation

The documentation for freud is hosted online at ReadTheDocs, but you may also build the documentation yourself:

#### Building the documentation

The following are required for building freud documentation:

- Sphinx

You can install sphinx using conda:

```
conda install sphinx
```

or pip:

```
pip install sphinx
```
To build the documentation, run the following commands in the source directory:

```bash
cd doc
make html
# Then open build/html/index.html
```

To build a PDF of the documentation (requires LaTeX and/or PDFLaTeX):

```bash
cd doc
make latexpdf
# Then open build/latex/freud.pdf
```

### 6.3 Getting Started

Once you have installed freud, you can start using freud with any simulation data that you have on hand. As an example, we’ll assume that you have run a simulation using the HOOMD-blue and used the hoomd.dump.gsd command to output the trajectory into a file trajectory.gsd. The GSD file format provides its own convenient Python file reader that offers access to data in the form of NumPy arrays, making it immediately suitable for calculation with freud. Many other file readers and data formats are supported, see Reading Simulation Data for freud for a full list and more examples.

We start by reading the data into a NumPy array:

```python
import gsd.hoomd
traj = gsd.hoomd.open('trajectory.gsd', 'rb')
```

We can now immediately calculate important quantities. Here, we will compute the radial distribution function $g(r)$ using the freud.density.RDF compute class. Since the radial distribution function is in practice computed as a histogram, we must specify the histogram bin widths and the largest interparticle distance to include in our calculation. To do so, we simply instantiate the class with the appropriate parameters and then perform a computation on the given data:

```python
import freud
rdf = freud.density.RDF(bins=50, r_max=5)
rdf.compute(system=traj[-1])
```

We can now access the data through properties of the rdf object.

```python
r = rdf.bin_centers
y = rdf.rdf
```

Many classes in freud natively support plotting their data using Matplotlib <https://matplotlib.org/>:

```python
import matplotlib as plt
fig, ax = plt.subplots()
rdf.plot(ax=ax)
```

You will note that in the above example, we computed $g(r)$ only using the final frame of the simulation trajectory, `traj[-1]`. However, in many cases, radial distributions and other similar quantities may be noisy in simulations due to the natural fluctuations present. In general, what we are interested in are time-averaged quantities once a system has equilibrated. To perform such a calculation, we can easily modify our original calculation to take advantage of freud’s accumulation features. To accumulate, just add the argument `reset=False` with a supported compute object (such
as histogram-like computations). Assuming that you have some method for identifying the frames you wish to include in your sample, our original code snippet would be modified as follows:

```python
import freud
rdf = freud.density.RDF(bins=50, r_max=5)
for frame in traj:
    rdf.compute(frame, reset=False)
```

You can then access the data exactly as we previously did. And that’s it!

Now that you’ve seen a brief example of reading data and computing a radial distribution function, you’re ready to learn more. If you’d like a complete walkthrough please see the Tutorial. The tutorial walks through many of the core concepts in freud in greater detail, starting with the basics of the simulation systems we analyze and describing the details of the neighbor finding logic in freud. To see specific features of freud in action, look through the Examples. More detailed documentation on specific classes and functions can be found in the API documentation.

### 6.4 Tutorial

This tutorial provides a complete introduction to freud. Rather than attempting to touch on all features in freud, it focuses on common core concepts that will help understand how freud works with data and exposes computations to the user. The tutorial begins by introducing the fundamental concepts of periodic systems as implemented in freud and the concept of Compute classes, which constitute the primary API for performing calculations with freud. The tutorial then discusses the most common calculation performed in freud, finding neighboring points in periodic systems. The package’s neighbor finding tools are tuned for high performance neighbor finding, which is what enables most of other calculations in freud, which typically involve characterizing local environments of points in some way. The next part of the tutorial discusses the role of histograms in freud, focusing on the common features and properties that all histograms share. Finally, the tutorial includes a few more complete demonstrations of using freud that should provide reasonable templates for use with almost any other features in freud.

#### 6.4.1 Periodic Boundary Conditions

The central goal of freud is the analysis of simulations performed in periodic boxes. Periodic boundary conditions are ubiquitous in simulations because they permit the simulation of quasi-infinite systems with minimal computational effort. As long as simulation systems are sufficiently large, i.e. assuming that points in the system experience correlations over length scales substantially smaller than the system length scale, periodic boundary conditions ensure that the system appears effectively infinite to all points.

In order to consistently define the geometry of a simulation system with periodic boundaries, freud defines the freud.box.Box class. The class encapsulates the concept of a triclinic simulation box in a right-handed coordinate system. Triclinic boxes are defined as parallelepipeds: three-dimensional polyhedra where every face is a parallelogram. In general, any such box can be represented by three distinct, linearly independent box vectors. Enforcing the requirement of right-handedness guarantees that the box can be represented by a matrix of the form

$$
\mathbf{h} = \begin{pmatrix}
L_x & xy & xzL_z \\
0 & L_y & yzL_z \\
0 & 0 & L_z
\end{pmatrix}
$$

where each column is one of the box vectors.

As such, the box is characterized by six parameters: the box vector lengths $L_x$, $L_y$, and $L_z$, and the tilt factors $xy$, $xz$, and $yz$. The tilt factors are directly related to the angles between the box vectors. All computations in freud are built around this class, ensuring that they naturally handle data from simulations conducted in non-cubic systems. There is also native support for two-dimensional (2D) systems when setting $L_z = 0$. 

6.4. Tutorial
Boxes can be constructed in a variety of ways. For simple use-cases, one of the factory functions of the `freud.box.Box` provides the easiest possible interface:

```python
# Make a 10x10 square box (for 2-dimensional systems).
freud.box.Box.square(10)

# Make a 10x10x10 cubic box.
freud.box.Box.cube(10)
```

For more complex use-cases, the `freud.box.Box.from_box()` method provides an interface to create boxes from any object that can easily be interpreted as a box.

```python
# Create a 10x10 square box from a list of two items.
freud.box.Box.from_box([10, 10])

# Create a 10x10x10 cubic box from a list of three items.
freud.box.Box.from_box([10, 10, 10])

# Create a triclinic box from a list of six items (including tilt factors).
freud.box.Box.from_box([10, 5, 2, 0.1, 0.5, 0.7])

# Create a triclinic box from a dictionary.
freud.box.Box.from_box(dict(Lx=8, Ly=7, Lz=10, xy=0.5, xz=0.7, yz=0.2))

# Directly call the constructor.
freud.box.Box(Lx=8, Ly=7, Lz=10, xy=0.5, xz=0.7, yz=0.2, dimensions=3)
```

More examples on how boxes can be created may be found in the API documentation of the `Box` class.

**Note:** All `freud` boxes are centered at the origin, so for a given box the range of possible positions is $[-L/2, L/2)$.

### 6.4.2 Compute Classes

Calculations in `freud` are built around the concept of Compute classes, Python objects that encode a given method and expose it through a `compute` method. In general, these methods operate on a system composed of a triclinic box and a NumPy array of particle positions. The box can be provided as any object that can be interpreted as a `freud` box (as demonstrated in the examples above). We can look at the `freud.order.Hexatic` order parameter calculator as an example:

```python
import freud

positions = ...  # Read positions from trajectory file.
op = freud.order.Hexatic(k=6)
op.compute(
    system=(dict(Lx=8, Ly=7, Lz=10, xy=0.5, xz=0.7, yz=0.2)),
    neighbors=dict(r_max=3)
)

# Plot the value of the order parameter.
from matplotlib import pyplot as plt
plt.hist(np.absolute(op.particle_order))
```

Here, we are calculating the hexatic order parameter, then using Matplotlib to plot. The `freud.order.Hexatic` class constructor accepts a single argument `k`, which represents the periodicity of the calculation. If you’re unfamiliar with this order parameter, the most important piece of information here is that many compute methods in `freud` require parameters that are provided when the Compute class is constructed.
To calculate the order parameter we call `compute`, which takes two arguments, a `tuple (box, points)` and a `dict`. We first focus on the first argument. The `box` is any object that can be coerced into a `freud.box.Box` as described in the previous section; in this case, we use a dictionary to specify a square (2-dimensional) box. The `points` must be anything that can be coerced into a 2-dimensional NumPy array of shape \( (N, 3) \) In general, the points may be provided as anything that can be interpreted as an \( N \times 3 \) list of positions; for more details on valid inputs here, see `numpy.asarray()`. Note that because the hexatic order parameter is designed for two-dimensional systems, the points must be provided of the form \([x, y, 0]\) (i.e. the \( z \)-component must be 0). We’ll go into more detail about the \((box, points)\) tuple soon, but for now, it’s sufficient to just think of it as specifying the system of points we want to work with.

Now let’s return to the `neighbors` argument to `compute`, which is a dictionary is used to determine which particle neighbors to use. Many computations in `freud` (such as the hexatic order parameter) involve the bonds in the system (for example, the average length of bonds or the average number of bonds a given point has). However, the concept of a bond is sufficiently variable between different calculations; for instance, should points be considered bonded if they are within a certain distance of each other? Should every point be considered bonded to a fixed number of other points?

To accommodate this variability, `freud` offers a very general framework by which bonds can be specified, and we’ll go into more details in the next section. In the example above, we’ve simply informed the `Hexatic` class that we want it to define bonds as pairs of particles that are less than 3 distance units apart. We then access the computed order parameter as `op.particle_order` (we use `np.absolute()` because the output is a complex number and we just want to see its magnitude).

### Accessing Computed Properties

In general, `Compute` classes expose their calculations using `properties`. Any parameters to the `Compute` object (e.g. \( k \) in the above example) can typically be accessed as soon as the object is constructed:

```python
op = freud.order.Hexatic(k=6)
op.k
```

Computed quantities can also be accessed in a similar manner, but only after the `compute` method is called. For example:

```python
op = freud.order.Hexatic(k=6)

# This will raise an exception.
op.particle_order

op.compute(
    system=({'Lx': 5, 'Ly': 5, 'dimensions': 2}, positions),
    neighbors=dict(r_max=3)
)

# Now you can access this.
op.particle_order
```

**Note:** Most (but not all) of `freud`’s `Compute` classes are Python wrappers around high-performance implementations in C++. As a result, none of the data or the computations is actually stored in the Python object. Instead, the Python object just stores an instance of the C++ object that actually owns all its data, performs calculations, and returns computed quantities to the user. Python properties provide a nice way to hide this logic so that the Python code involves just a few lines.

Compute objects is that they can be used many times to calculate quantities, and the most recently calculated output
can be accessed through the property. If you need to perform a series of calculations and save all the data, you can also easily do that:

```python
# Recall that lists of length 2 automatically convert to 2D freud boxes.
box = [5, 5]

op = freud.order.Hexatic(k=6)

# Assuming that we have a list of Nx3 NumPy arrays that represents a
# simulation trajectory, we can loop over it and calculate the order
# parameter values in sequence.
trajectory = ...
# Read trajectory file into a list of positions by frame.
hexatic_values = []
for points in trajectory:
    op.compute(system=(box, points), neighbors=dict(r_max=3))
    hexatic_values.append(op.particle_order)
```

To make using freud as simple as possible, all Compute classes are designed to return self when compute is called. This feature enables a very concise method-chaining idiom in freud where computed properties are accessed immediately:

```python
particle_order = freud.order.Hexatic(k=6).compute(
    system=(box, points)).particle_order
```

### 6.4.3 Finding Neighbors

Now that you’ve been introduced to the basics of interacting with freud, let’s dive into the central feature of freud: efficiently and flexibly finding neighbors in periodic systems.

#### Problem Statement

##### Neighbor-Based Calculations

As discussed in the previous section, a central task in many of the computations in freud is finding particles’ neighbors. These calculations typically only involve a limited subset of a particle’s neighbors that are defined as characterizing its local environment. This requirement is analogous to the force calculations typically performed in molecular dynamics simulations, where a cutoff radius is specified beyond which pair forces are assumed to be small enough to neglect. Unlike in simulation, though, many analyses call for different specifications than simply selecting all points within a certain distance.

An important example is the calculation of order parameters, which can help characterize phase transitions. Such parameters can be highly sensitive to the precise way in which neighbors are selected. For instance, if a hard distance cutoff is imposed in finding neighbors for the hexatic order parameter, a particle may only be found to have five neighbors when it actually has six neighbors except the last particle is slightly outside the cutoff radius. To accommodate such differences in a flexible manner, freud allows users to specify neighbors in a variety of ways.
Finding Periodic Neighbors

Finding neighbors in periodic systems is significantly more challenging than in aperiodic systems. To illustrate the difference, consider the figure above, where the black dashed line indicates the boundaries of the system. If this system were aperiodic, the three nearest neighbors for point 1 would be points 5, 6, and 7. However, due to periodicity, point 2 is actually closer to point 1 than any of the others if you consider moving straight through the top (or equivalently, the bottom) boundary. Although many tools provide efficient implementations of algorithms for finding neighbors in aperiodic systems, they seldom generalize to periodic systems. Even more rare is the ability to work not just in cubic periodic systems, which are relatively tractable, but in arbitrary triclinic geometries as described in Periodic Boundary Conditions. This is precisely the type of calculation freud is designed for.

Neighbor Querying

To understand how Compute classes find neighbors in freud, it helps to start by learning about freud’s neighbor finding classes directly. Note that much more detail on this topic is available in the Query API topic guide; in this section we will restrict ourselves to a higher-level overview. For our demonstration, we will make use of the freud.locality.AABBQuery class, which implements one fast method for periodic neighbor finding. The primary mode of interfacing with this class (and other neighbor finding classes) is through the query interface.

```python
import numpy as np
import freud

# As an example, we randomly generate 100 points in a 10x10x10 cubic box.
L = 10
num_points = 100

# We shift all points into the expected range for freud.
points = np.random.rand(num_points)*L - L/2
box = freud.box.Box.cube(L)
aq = freud.locality.AABBQuery(box, points)

# Now we generate a smaller sample of points for which we want to find
# neighbors based on the original set.
query_points = np.random.rand(num_points/10)*L - L/2
distances = []

# Here, we ask for the 4 nearest neighbors of each point in query_points.
for bond in aq.query(query_points, dict(num_neighbors=4)):
    # The returned bonds are tuples of the form
```

(continues on next page)
Let’s dig into this script a little bit. Our first step is creating a set of 100 points in a cubic box. Note that the shifting done in the code above could also be accomplished using the `Box.wrap` method like so: `box.wrap(np.random.rand(num_points)*L)`. The result would appear different, because if plotted without considering periodicity, the points would range from $-L/2$ to $L/2$ rather than from $0$ to $L$. However, these two sets of points would be equivalent in a periodic system.

We then generate an additional set of `query_points` and ask for neighbors using the `query` method. This function accepts two arguments: a set of points, and a `dict` of `query arguments`. Query arguments are a central concept in `freud` and represent a complete specification of the set of neighbors to be found. In general, the most common forms of queries are those requesting either a fixed number of neighbors, as in the example above, or those requesting all neighbors within a specific distance. For example, if we wanted to rerun the above example but instead find all bonds of length less than or equal to 2, we would simply replace the for loop above with:

```python
for bond in aq.query(query_points, dict(r_max=2)):
    distances.append(bond[2])
```

Query arguments constitute a powerful method for specifying a query request. Many query arguments may be combined for more specific purposes. A common use-case is finding all neighbors within a single set of points (i.e. setting `query_points = points` in the above example). In this situation, however, it is typically not useful for a point to find itself as a neighbor since it is trivially the closest point to itself and falls within any cutoff radius. To avoid this, we can use the `exclude_ii` query argument:

```python
query_points = points
for bond in aq.query(query_points, dict(num_neighbors=4, exclude_ii=True)):
    pass
```

The above example will find the 4 nearest neighbors to each point, excepting the point itself. A complete description of valid query arguments can be found in `Query API`.

**Neighbor Lists**

Query arguments provide a simple but powerful language with which to express neighbor finding logic. Used in the manner shown above, `query` can be used to express many calculations in a very natural, Pythonic way. By itself, though, the API shown above is somewhat restrictive because the output of `query` is a generator. If you aren’t familiar with generators, the important thing to know is that they can be looped over, but only once. Unlike objects like lists, which you can loop over as many times as you like, once you’ve looped over a generator once, you can’t start again from the beginning.

In the examples above, this wasn’t a problem because we simply iterated over the bonds once for a single calculation. However, in many practical cases we may need to reuse the set of neighbors multiple times. A simple solution would be to simply store the bonds into a list as we loop over them. However, because this is such a common use-case, `freud` provides its own containers for bonds: the `freud.locality.NeighborList`.

Queries can easily be used to generate `NeighborList` objects using their `toNeighborList` method:
query_result = aq.query(query_points, dict(num_neighbors=4, exclude_ii))
nlist = query_result.toNeighborList()

The resulting object provides a persistent container for bond data. Using NeighborLists, our original example might instead look like this:

```python
import numpy as np
import freud

L = 10
num_points = 100

points = np.random.rand(num_points)*L - L/2
box = freud.box.Box.cube(L)
aq = freud.locality.AABBQuery(box, points)
query_points = np.random.rand(num_points/10)*L - L/2
distances = []
# Here, we ask for the 4 nearest neighbors of each point in query_points.
query_result = aq.query(query_points, dict(num_neighbors=4)):
for (i, j) in nlist:
    # Note that we have to wrap the bond vector before taking the norm;
    # this is the simplest way to compute distances in a periodic system.
    distances.append(np.linalg.norm(box.wrap(query_points[i] - points[j])))
avg_distance = np.mean(distances)
```

Note that in the above example we looped directly over the nlist and recomputed distances. However, the query_result contained information about distances: here's how we access that through the nlist:

```python
assert np.all(nlist.distances == distances)
```

The indices are also accessible through properties, or through a NumPy-like slicing interface:

```python
assert np.all(nlist.query_point_indices == nlist[:, 0])
assert np.all(nlist.point_indices == nlist[:, 1])
```

Note that the query_points are always in the first column, while the points are in the second column. freud.locality.NeighborList objects also store other properties; for instance, they may assign different weights to different bonds. This feature can be used by, for example, freud.order.Steinhardt, which is typically used for calculating Steinhardt order parameters, a standard tool for characterizing crystalline order. When provided appropriately weighted neighbors, however, the class instead computes Minkowski structure metrics, which are much more sensitive measures that can differentiate a wider array of crystal structures.

### 6.4.4 Pair Computations

Some computations in freud do not depend on bonds at all. For example, freud.density.GaussianDensity creates a “continuous equivalent” of a system of points by placing normal distributions at each point’s location to smear out its position, then summing the value of these distributions at a set of fixed grid points. This calculation can be quite useful because it allows the application of various analysis tools like fast Fourier transforms, which require regular grids. For the purposes of this tutorial, however, the importance of this class is that it is an example of a calculation where neighbors are unimportant: the calculation is performed on a per-point basis only.
The much more common pattern in freud, though, is that calculations involve the local neighborhoods of points. To support efficient, flexible computations of such quantities, various Compute classes essentially expose the same API as the query interface demonstrated in the previous section. These PairCompute classes are designed to mirror the querying functionality of freud as closely as possible.

As an example, let’s consider freud.density.LocalDensity, which calculates the density of points in the local neighborhood of each point. Adapting our code from the previous section, the simplest usage of this class would be as follows:

```python
import numpy as np
import freud

L = 10
num_points = 100
points = np.random.rand(num_points) * L - L/2
box = freud.box.Box.cube(L)

# r_max specifies how far to search around each point for neighbors
r_max = 2

# For systems where the points represent, for instance, particles with a
# specific size, the diameter is used to add fractional volumes for
# neighbors that would be overlapping the sphere of radius r_max around
# each point.
diameter = 0.001

ld = freud.density.LocalDensity(r_max, diameter)
ld.compute(system=(box, points))

# Access the density.
ld.density
```

Using the same example system we’ve been working with so far, we’ve now calculated an estimate for the number of points in the neighborhood of each point. Since we already told the computation how far to search for neighbors based on r_max, all we had to do was pass a tuple (box, points) to compute indicate where the points were located.

**Binary Systems**

Imagine that instead of a single set of points, we actually had two different types of points and we were interested in finding the density of one set of points in the vicinity of the other. In that case, we could modify the above calculation as follows:

```python
import numpy as np
import freud

L = 10
num_points = 100
points = np.random.rand(num_points) * L - L/2
query_points = np.random.rand(num_points/10) * L - L/2

r_max = 2
diameter = 0.001

ld = freud.density.LocalDensity(r_max, diameter)
ld.compute(system=(box, points), query_points=query_points)
```

(continues on next page)
The choice of names names here is suggestive of exactly what this calculation is now doing. Internally, freud.
density.LocalDensity will search for all points that are within the cutoff distance r_max of every
query_point (essentially using the query interface we introduced previously) and use that to calculate ld.
density. Note that this means that ld.density now contains densities for every query_point, i.e. it is of
length 10, not 100. Moreover, recall that one of the features of the querying API is the specification of whether or
not to count particles as their own neighbors. PairCompute classes will attempt to make an intelligent determi-
nation of this for you; if you do not pass in a second set of query_points, they will assume that you are computing
with a single set of points and automatically exclude self-neighbors, but otherwise all neighbors will be included.

So far, we have included all points within a fixed radius; however, one might instead wish to consider the density in
some shell, such as the density between 1 and 2 distance units away. To address this need, you could simply adapt the
call to compute above as follows:

```python
ld.compute(system=(box, points), query_points=query_points,
            neighbors=dict(r_max=2, r_min=1))
```

The neighbors argument to PairCompute classes allows users to specify arbitrary query arguments, making it
possible to easily modify freud calculations on-the-fly. The neighbors argument is actually more general than
query arguments you’ve seen so far; if query arguments are not precise enough to specify the exact set of neighbors
you want to compute with, you can instead provide a NeighborList directly

```python
ld.compute(system=(box, points), query_points=query_points,
            neighbors=nlist)
```

This feature allows users essentially arbitrary flexibility to specify the bonds that should be included in any bond-based
computation. A common use-case for this is constructing a NeighborList using freud.locality.Voronoi;
Voronoi constructions provide a powerful alternative method of defining neighbor relationships that can improve the
accuracy and robustness of certain calculations in freud.

You may have noticed in the last example that all the arguments are specified using keyword arguments. As the
previous examples have attempted to show, the query_points argument defines a second set of points to be used
when performing calculations on binary systems, while the neighbors argument is how users can specify which
neighbors to consider in the calculation.

The system argument is what, to this point, we have been specifying as a tuple (box, points). However, we
don’t have to use this tuple. Instead, we can pass in any freud.locality.NeighborQuery, the central class in
freud’s querying infrastructure. In fact, you’ve already seen examples of freud.locality.NeighborQuery:
the freud.locality.AABBQuery object that we originally used to find neighbors. There are also a number of
other input types that can be converted via freud.locality.NeighborQuery.from_system(), see also
Reading Simulation Data for freud. Since these objects all contain a freud.box.Box and a set of points, they can
be directly passed to computations:

```python
aq = freud.locality.AABBQuery(box, points)
ld.compute(system=aq, query_points=query_points, neighbors=nlist)
```

For more information on why you might want to use freud.locality.NeighborQuery objects instead of the
tuples, see Using freud Efficiently. For now, just consider this to be a way in which you can simplify your calls to
many freud computes in one script by storing (box, points) into another objects.

You’ve now covered the most important information needed to use freud! To recap, we’ve discussed how freud
handles periodic boundary conditions, the structure and usage of Compute classes, and methods for finding and
performing calculations with pairs of neighbors. For more detailed information on specific methods in freud, see the
Examples page or look at the API documentation for specific modules.
6.5 Examples

Examples are provided as Jupyter notebooks in a separate freud-examples repository. These notebooks may be launched interactively on Binder or downloaded and run on your own system. Visualization of data is done via Matplotlib and Bokeh, unless otherwise noted.

6.5.1 Key concepts

There are a few critical concepts, algorithms, and data structures that are central to all of freud. The freud.box.Box class defines the concept of a periodic simulation box, and the freud.locality module defines methods for finding nearest neighbors of particles. Since both of these are used throughout freud, we recommend reading the Tutorial first, before delving into the workings of specific freud analysis modules.

freud.box.Box

In this notebook, we demonstrate the basic features of the Box class, including wrapping particles back into the box under periodic boundary conditions. For more information, see the introduction to Periodic Boundary Conditions and the freud.box documentation.

Creating a Box object

Boxes may be constructed explicitly using all arguments. Such construction is useful when performing ad hoc analyses involving custom boxes. In general, boxes are assumed to be 3D and orthorhombic unless otherwise specified.

```python
[1]: import freud.box

    # All of the below examples are valid boxes.
    box = freud.box.Box(Lx=5, Ly=6, Lz=7, xy=0.5, xz=0.6, yz=0.7, is2D=False)
    box = freud.box.Box(1, 3, 2, 0.3, 0.9)
    box = freud.box.Box(5, 6, 7)
    box = freud.box.Box(5, 6, is2D=True)
    box = freud.box.Box(5, 6, xy=0.5, is2D=True)
```

From another Box object

The simplest case is simply constructing one freud box from another.

Note that all forms of creating boxes aside from the explicit method above use methods defined within the Box class rather than attempting to overload the constructor itself.

```python
[2]: box = freud.box.Box(1, 2, 3)
    box2 = freud.box.Box.from_box(box)
    print("The original box: \n\t".format(box))
    print("The copied box: \n\t".format(box2))

    # Boxes are always copied by value, not by reference
    box.Lx = 5
    print("The original box is modified: \n\t".format(box))
    print("The copied box is not: \n\t".format(box2))

    # Note, however, that box assignment creates a new object that
```

(continues on next page)
# still points to the original box object, so modifications to
# one are visible on the other.
box3 = box2
print("The new copy: \n\t".format(box3))
box2.Lx = 2
print("The new copy after the original is modified: \n\t".format(box3))
print("The modified original box: \n\t".format(box2))

The original box:
freud.box.Box(Lx=1.0, Ly=2.0, Lz=3.0, xy=0.0, xz=0.0, yz=0.0, is2D=False)
The copied box:
freud.box.Box(Lx=1.0, Ly=2.0, Lz=3.0, xy=0.0, xz=0.0, yz=0.0, is2D=False)
The original box is modified:
freud.box.Box(Lx=5.0, Ly=2.0, Lz=3.0, xy=0.0, xz=0.0, yz=0.0, is2D=False)
The copied box is not:
freud.box.Box(Lx=1.0, Ly=2.0, Lz=3.0, xy=0.0, xz=0.0, yz=0.0, is2D=False)
The new copy:
freud.box.Box(Lx=1.0, Ly=2.0, Lz=3.0, xy=0.0, xz=0.0, yz=0.0, is2D=False)
The new copy after the original is modified:
freud.box.Box(Lx=2.0, Ly=2.0, Lz=3.0, xy=0.0, xz=0.0, yz=0.0, is2D=False)
The modified original box:
freud.box.Box(Lx=2.0, Ly=2.0, Lz=3.0, xy=0.0, xz=0.0, yz=0.0, is2D=False)

### From a matrix

A box can be constructed directly from the box matrix representation described above using the `Box.from_matrix` method.

```python
# Matrix representation. Note that the box vectors must represent
# a right-handed coordinate system! This translates to requiring
# that the matrix be upper triangular.
box = freud.box.Box.from_matrix([[1, 1, 0], [0, 1, 0.5], [0, 0, 0.5]])
print("This is a 3D box from a matrix: \n\t".format(box))

# 2D box
box = freud.box.Box.from_matrix([[1, 0, 0], [0, 1, 0], [0, 0, 0]])
print("This is a 2D box from a matrix: \n\t".format(box))

# Automatic matrix detection using from_box
box = freud.box.Box.from_box([[1, 1, 0], [0, 1, 0.5], [0, 0, 0.5]])
print("The box matrix was automatically detected: \n\t".format(box))

# Boxes can be numpy arrays as well
import numpy as np
box = freud.box.Box.from_box(np.array([[1, 1, 0], [0, 1, 0.5], [0, 0, 0.5]]))
print("Using a 3x3 numpy array: \n\t".format(box))
```

This is a 3D box from a matrix:
freud.box.Box(Lx=1.0, Ly=1.0, Lz=0.5, xy=1.0, xz=0.0, yz=1.0, is2D=False)

This is a 2D box from a matrix:
freud.box.Box(Lx=1.0, Ly=1.0, Lz=0.0, xy=0.0, xz=0.0, yz=0.0, is2D=True)

The box matrix was automatically detected:
freud Documentation, Release 2.0.0

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Using a 3x3 numpy array:
freud.box.Box(Lx=1.0, Ly=1.0, Lz=0.5, xy=1.0, xz=0.0, yz=1.0, is2D=False)

From a namedtuple or dict

A box can be also be constructed from any object that provides an attribute for \(L_x\), \(L_y\), \(L_z\), \(x_y\), \(x_z\), and \(y_z\) (or some subset), such as a namedtuple. This method is suitable for passing in box objects constructed by some other program, for example.

```python
from collections import namedtuple

MyBox = namedtuple('mybox', ['Lx', 'Ly', 'Lz', 'xy', 'xz', 'yz'])

box = freud.box.Box.from_box(MyBox(Lx=5, Ly=3, Lz=2, xy=0, xz=0, yz=0))
print("Box from named tuple:
\t{}").format(box)

box = freud.box.Box.from_box(MyBox(Lx=5, Ly=3, Lz=0, xy=0, xz=0, yz=0))
print("2D Box from named tuple: \n\t{}").format(box)
```

Box from named tuple:
freud.box.Box(Lx=5.0, Ly=3.0, Lz=2.0, xy=0.0, xz=0.0, yz=0.0, is2D=False)
2D Box from named tuple:
freud.box.Box(Lx=5.0, Ly=3.0, Lz=0.0, xy=0.0, xz=0.0, yz=0.0, is2D=True)

Similarly, construction is also possible using any object that supports key-value indexing, such as a dict.

```python
box = freud.box.Box.from_box(dict(Lx=5, Ly=3, Lz=2))
print("Box from dict: \n\t{}").format(box)
```

Box from dict:
freud.box.Box(Lx=5.0, Ly=3.0, Lz=2.0, xy=0.0, xz=0.0, yz=0.0, is2D=False)

From a list

Finally, boxes can be constructed from any simple iterable that provides the elements in the correct order.

```python
box = freud.box.Box.from_box((5, 6, 7, 0.5, 0, 0.5))
print("Box from tuple: \n\t{}").format(box)

box = freud.box.Box.from_box([5, 6])
print("2D Box from list: \n\t{}").format(box)
```

Box from tuple:
freud.box.Box(Lx=5.0, Ly=6.0, Lz=7.0, xy=0.5, xz=0.0, yz=0.5, is2D=False)
2D Box from list:
freud.box.Box(Lx=5.0, Ly=6.0, Lz=0.0, xy=0.0, xz=0.0, yz=0.0, is2D=True)

Convenience APIs

We also provide convenience constructors for common geometries, namely square (2D) and cubic (3D) boxes.
Export

If you want to export or display the box, you can export box objects into their matrix or dictionary representations, which provide completely specified descriptions of the box.

Using boxes

Given a freud box object, you can query it for all its attributes.

Boxes also support converting between fractional and absolute coordinates.

Note that the origin in real coordinates is defined at the center of the box. This means the fractional coordinate range [0, 1] maps onto \([-L/2, L/2]\), not [0, L].
# Convert from fractional to absolute coordinates.
```python
print(box.make_absolute([[0, 0, 0], [0.5, 0.5, 0.5], [0.8, 0.3, 1]]))
print()
```

# Convert from fractional to absolute coordinates and back.
```python
print(box.make_fractional(box.make_absolute([[0, 0, 0], [0.5, 0.5, 0.5], [0.8, 0.3, -1]])))
```

```
[-5. -5. -5.]
[ 0.  0.  0.]
[ 3. -2.  5.]]

[[0.  0.  0.]]
[[0.5 0.5 0.5]]
[[0.8 0.3 1.]]
```

Finally (and most critically for enforcing periodicity), boxes support wrapping vectors from outside the box into the box. The concept of periodicity and box wrapping is most easily demonstrated visually.

```
# Construct the box and get points for plotting
Lx = Ly = 10
xy = 0.5
box = freud.box.Box.from_matrix([[Lx, xy*Ly, 0], [0, Ly, 0], [0, 0, 0]])
box.plot()
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7f2729d20518>
```

With periodic boundary conditions, what this actually represents is an infinite set of these boxes tiling space. For example, you can locally picture this box as surrounding by a set of identical boxes.

```
# Construct the box and get points for plotting
Lx = Ly = 10
xy = 0.5
box = freud.box.Box.from_matrix([[Lx, xy*Ly, 0], [0, Ly, 0], [0, 0, 0]])
box.plot()
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7f2729d20518>
```

```
for image in [[-1, 0, 0], [1, 0, 0], [0, -1, 0], [0, 1, 0]]:
    box.plot(ax=ax, image=image, linestyle='dashed', color='gray')
plt.show()
```
Any particles in the original box will also therefore be seen as existing in all the neighboring boxes.

[14]: np.random.seed(0)
fractional_coords = np.zeros((5, 3))
fractional_coords[:, :2] = np.random.rand(5, 2)
particles = box.make_absolute(fractional_coords)

[15]: fig, ax = plt.subplots(figsize=(9, 6))

# Plot the points in the original box.
box.plot(ax=ax)
ax.scatter(particles[:, 0], particles[:, 1])

# Plot particles in each of the periodic boxes.
for image in [[-1, 0, 0], [1, 0, 0], [0, -1, 0], [0, 1, 0]]:
    box.plot(ax=ax, image=image, linestyle='dashed', color='gray')
particle_images = box.unwrap(particles, image)
ax.scatter(particle_images[:, 0], particle_images[:, 1])

plt.show()
Box wrapping takes points in the periodic images of a box, and brings them back into the original box. In this context, that means that if we apply wrap to each of the sets of particles plotted above, they should all overlap.

```python
fig, axes = plt.subplots(2, 2, figsize=(12, 8))
images = [[-1, 0, 0], [1, 0, 0], [0, -1, 0], [0, 1, 0]]

# Plot particles in each of the periodic boxes.
for ax, image in zip(axes.flatten(), images):
    box.plot(ax=ax)
    box.plot(ax=ax, image=image, linestyle='dashed', color='gray')
    particle_images = box.unwrap(particles, image)
    ax.scatter(particle_images[:, 0],
               particle_images[:, 1],
               label='Images')

    wrapped_particle_images = box.wrap(particle_images)
    ax.scatter(wrapped_particle_images[:, 0],
               wrapped_particle_images[:, 1],
               label='Wrapped')

    ax.tick_params(axis="both", which="both", labelsize=14)
    ax.legend()
plt.show()
```
The `PeriodicBuffer` class is meant to replicate points beyond a single image while respecting box periodicity. This example demonstrates how we can use this to compute the radial distribution function from a sample crystal’s unit cell.

```python
%matplotlib inline
import freud
import numpy as np
import matplotlib.pyplot as plt

box = freud.box.Box(Lx=2, Ly=2, xy=np.sqrt(1/3), is2D=True)
points = np.array([[-0.5, -0.5, 0], [0.5, 0.5, 0]])
system = freud.AABBQuery(box, points)
system.plot(ax=plt.gca())
plt.show()
```

Here, we create a box to represent the unit cell and put two points inside. We plot the box and points below.

**freud.locality.PeriodicBuffer: Unit Cell RDF**

6.5. Examples
Next, we create a `PeriodicBuffer` instance and have it compute the “buffer” points that lie outside the first periodicity. These positions are stored in the `buffer_points` attribute. The corresponding `buffer_ids` array gives a mapping from the index of the buffer particle to the index of the particle it was replicated from, in the original array of `points`. Finally, the `buffer_box` attribute returns a larger box, expanded from the original box to contain the replicated points.

```python
[pbuff = freud.locality.PeriodicBuffer()
pbuff.compute(system=(box, points), buffer=6, images=True)
print(pbuff.buffer_points[:10], '...')
[[ 0.65470022  1.5          0.          ]
  [ 1.80940032  3.5          0.          ]
  [ 2.96410179  5.5          0.          ]
  [-3.96410131 -6.5          0.          ]
  [-2.80940104 -4.49999952  0.          ]
  [-1.65470016 -2.50000048  0.          ]
  [ 1.50000024 -0.5          0.          ]
  [ 2.65470076  1.5          0.          ]
  [ 3.80940032  3.5          0.          ]
  [ 4.96410179  5.5          0.          ]] ...

Below, we plot the original unit cell and the replicated buffer points and buffer box.

```python
[4]: system.plot(ax=plt.gca())
plt.scatter(pbuff.buffer_points[:, 0], pbuff.buffer_points[:, 1])
pbuff.buffer_box.plot(ax=plt.gca(), linestyle='dashed', color='gray')
plt.show()
```
Finally, we can plot the radial distribution function (RDF) of this replicated system, using a value of $r_{\text{max}}$ that is larger than the size of the original box. This allows us to see the interaction of the original points with their replicated neighbors from the buffer.

```python
[5]: rdf = freud.density.RDF(bins=250, r_max=5)
    rdf.compute(system=(pbuff.buffer_box, pbuff.buffer_points), query_points=points)
    rdf.plot(ax=plt.gca())
    plt.show()
```

The `freud.locality.Voronoi` class uses voro++ to compute the Voronoi diagram of a set of points, while respecting periodic boundary conditions (which are not handled by `scipy.spatial.Voronoi`, documentation).

These examples are two-dimensional (with $z = 0$ for all particles) for simplicity, but the `Voronoi` class works for both 2D and 3D data.
First, we generate some sample points.

```python
points = np.array([[-0.5, -0.5, 0],
                   [0.5, -0.5, 0],
                   [-0.5, 0.5, 0],
                   [0.5, 0.5, 0]])
plt.scatter(points[:, 0], points[:, 1])
plt.title('Points')
plt.xlim((-1, 1))
plt.ylim((-1, 1))
plt.gca().set_aspect('equal')
plt.show()
```

Now we create a box and a Voronoi compute object.

```python
L = 2
box = freud.box.Box.square(L)
voro = freud.locality.Voronoi()
```

Next, we use the `compute` method to determine the Voronoi polytopes (cells) and the `polytopes` property to return their coordinates. Note that we use freud’s *method chaining* here, where a compute method returns the compute object.

```python
cells = voro.compute((box, points)).polytopes
print(cells)
```

```python
[array([[-1., -1., 0.],
        [ 0., -1., 0.],
        [ 0.,  0., 0.],
        [-1.,  0., 0.])]),
 array([[ 0., -1., 0.],
        [ 1., -1., 0.],
        [ 1.,  0., 0.],
        [ 0.,  0., 0.]]),
 array([[-1.,  0., 0.],
        [ 0.,  0., 0.]])
```
The **Voronoi** class has built-in plotting methods for 2D systems.

```python
plt.figure()
ax = plt.gca()
voro.plot(ax=ax)
ax.scatter(points[:, 0], points[:, 1], s=10, c='k')
plt.show()
```

This also works for more complex cases, such as this hexagonal lattice.

```python
def hexagonal_lattice(rows=3, cols=3, noise=0, seed=None):
    if seed is not None:
        np.random.seed(seed)
    # Assemble a hexagonal lattice
    points = []
    for row in range(rows*2):
        for col in range(cols):
            x = (col + (0.5 * (row % 2)))*np.sqrt(3)
            y = row*0.5
            points.append((x, y, 0))
    points = np.asarray(points)
    points += np.random.multivariate_normal(mean=np.zeros(3), cov=np.eye(3)*noise, size=points.shape[0])
    # Set z=0 again for all points after adding Gaussian noise
    points[:, 2] = 0
    # Wrap the points into the box
    box = freud.box.Box(Lx=cols*np.sqrt(3), Ly=rows, is2D=True)
    points = box.wrap(points)
    return box, points
```

6.5. Examples
# Compute the Voronoi diagram and plot
```python
box, points = hexagonal_lattice()
voro = freud.locality.Voronoi()
voro.compute((box, points))
voro
```

For noisy data, we see that the Voronoi diagram can change substantially. We perturb the positions with 2D Gaussian noise. Coloring by the number of sides of each Voronoi cell, we can see patterns in the defects: 5-gons and 7-gons tend to pair up.

```python
# Compute the Voronoi diagram
box, points = hexagonal_lattice(rows=12, cols=8, noise=0.03, seed=2)
voro = freud.locality.Voronoi()
voro.compute((box, points))

# Plot Voronoi with points and a custom cmap
plt.figure()
ax = plt.gca()
voro.plot(ax=ax, cmap='RdBu')
ax.scatter(points[:, 0], points[:, 1], s=2, c='k')
plt.show()
```
We can also compute the volumes of the Voronoi cells. Here, we plot them as a histogram:

```
[9]: plt.hist(voro.volumes)
plt.title('Voronoi cell volumes')
plt.show()
```

The Voronoi class also computes a `freud.locality.NeighborList`, where particles are neighbors if they share an edge in the Voronoi diagram. The `NeighborList` effectively represents the bonds in the Delaunay triangulation. The neighbors are weighted by the length (in 2D) or area (in 3D) between them. The neighbor weights are stored in `voro.nlist.weights`.

```
[10]: nlist = voro.nlist
line_data = np.asarray([ points[i],
                        points[i] + box.wrap(points[j] - points[i])
                        for i, j in nlist])[:, :, :2]
line_collection = matplotlib.collections.LineCollection(line_data, alpha=0.2)
plt.figure()
ax = plt.gca()
voron.plot(ax=ax, cmap='RdBu')
```

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6.5.2 Analysis Modules

These introductory examples showcase the functionality of specific modules in freud, showing how they can be used to perform specific types of analyses of simulations.

freud.cluster.Cluster and freud.cluster.ClusterProperties

The freud.cluster module determines clusters of points and computes cluster quantities like centers of mass, gyration tensors, and radii of gyration. The example below generates random points, and shows that they form clusters. This case is two-dimensional (with $z = 0$ for all particles) for simplicity, but the cluster module works for both 2D and 3D simulations.

```python
import numpy as np
import freud
import matplotlib.pyplot as plt

First, we generate a box and random points to cluster.

```python
box = freud.Box.square(L=6)
p = np.empty(shape=(0, 2))
for center_point in [(-1.8, 0), (1.5, 1.5), (-0.8, -2.8), (1.5, 0.5)]:
    p = np.concatenate((p, np.random.multivariate_normal(mean=center_point, cov=0.08*np.eye(2),
                           size=(100,))))
p = np.hstack((p, np.zeros((p.shape[0], 1))))
points = box.wrap(points)
system = freud.AABBQuery(box, points)
system.plot(ax=plt.gca(), s=10)
plt.title('Raw points before clustering', fontsize=20)
plt.gca().tick_params(axis='both', which='both', labelsize=14, size=8)
plt.show()
```
Now we create a box and a cluster compute object.

```python
[3]: cl = freud.cluster.Cluster()

Next, we use the `computeClusters` method to determine clusters and the `clusterIdx` property to return their identities. Note that we use freud's method chaining here, where a compute method returns the compute object.

```python
cpy = cl.compute(system, neighbors={'r_max': 1.0})
print(cl.cluster_idx)
```

```
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```

```python
[4]: fig, ax = plt.subplots(1, 1, figsize=(9, 6))
for cluster_id in range(cl.num_clusters):
    cluster_system = freud.AABBQuery(system.box, system.points[cl.cluster_keys[cluster_id]])
    cluster_system.plot(ax=ax, s=10, label="Cluster {}".format(cluster_id))
    print("There are {} points in cluster {}.").format(len(cl.cluster_keys[cluster_id]), cluster_id))
ax.set_title('Clusters identified', fontsize=20)
ax.legend(loc='best', fontsize=14)
ax.tick_params(axis='both', which='both', labelsize=14, size=8)
plt.show()

There are 200 points in cluster 0.
```

(continues on next page)
There are 100 points in cluster 1.
There are 100 points in cluster 2.

We may also compute the clusters' centers of mass and gyration tensor using the `ClusterProperties` class.

```python
[6]: clp = freud.cluster.ClusterProperties()
clp.compute(system, cl.cluster_idx);
```

Plotting these clusters with their centers of mass, with size proportional to the number of clustered points:

```python
[7]: fig, ax = plt.subplots(1, 1, figsize=(9, 6))

for i in range(cl.num_clusters):
    cluster_system = freud.AABBQuery(system.box, system.points[cl.cluster_keys[i]])
    cluster_system.plot(ax=ax, s=10, label="Cluster {0}".format(i))

for i, c in enumerate(clp.centers):
    ax.scatter(c[0], c[1], s=len(cl.cluster_keys[i]), label="Cluster {0} Center".format(i))

plt.title('Center of mass for each cluster', fontsize=20)
plt.legend(loc='best', fontsize=14)
plt.gca().tick_params(axis='both', which='both', labelsize=14, size=8)
plt.gca().set_aspect('equal')
plt.show()
```
The 3x3 gyration tensors $G$ can also be computed for each cluster. For this two-dimensional case, the $z$ components of the gyration tensor are zero. The gyration tensor can be used to determine the principal axes of the cluster and radius of gyration along each principal axis. Here, we plot the gyration tensor’s eigenvectors with length corresponding to the square root of the eigenvalues (the singular values).

```python
[8]: fig, ax = plt.subplots(1, 1, figsize=(9, 6))

for i in range(cl.num_clusters):
    cluster_system = freud.AABBQuery(system.box, system.points[cl.cluster_keys[i]])
    cluster_system.plot(ax=ax, s=10, label="Cluster {0}".format(i))

for i, c in enumerate(clp.centers):
    ax.scatter(c[0], c[1], s=len(cl.cluster_keys[i]),
               label="Cluster {0} Center".format(i))

for cluster_id in range(cl.num_clusters):
    com = clp.centers[cluster_id]
    G = clp.gyrations[cluster_id]
    evals, evecs = np.linalg.eig(G[:2, :2])
    arrows = np.sqrt(evals) * evecs
    for arrow in arrows.T:
        plt.arrow(com[0], com[1], arrow[0], arrow[1], width=0.05, color='k')

plt.title('Eigenvectors of the gyration tensor for each cluster', fontsize=20)
plt.legend(loc='best', fontsize=14)
ax.tick_params(axis='both', which='both', labelsize=14, size=8)
ax.set_aspect('equal')
plt.show()
The `freud.density` module is intended to compute a variety of quantities that relate spatial distributions of particles with other particles. This example shows how correlation functions can be used to measure orientational order in 2D.

```python
[1]: import numpy as np
import freud
import matplotlib.pyplot as plt
import matplotlib.cm
from matplotlib.colors import Normalize

This helper function will make plots of the data we generate in this example.

```python
[2]: def plot_data(title, points, angles, values, box, cf, s=200):
    cmap = matplotlib.cm.viridis
    norm = Normalize(vmin=-np.pi/4, vmax=np.pi/4)
    plt.figure(figsize=(16, 6))
    plt.subplot(121)
    for point, angle, value in zip(points, angles, values):
        plt.scatter(point[0], point[1], marker=(4, 0, np.rad2deg(angle)+45),
                    edgecolor='k', c=[cmap(norm(angle))], s=s)
    plt.title(title)
    plt.gca().set_xlim([-box.Lx/2, box.Lx/2])
    plt.gca().set_ylim([-box.Ly/2, box.Ly/2])
    plt.show()

(continues on next page)
First, let’s generate a 2D structure with perfect orientational order and slight positional disorder (the particles are not perfectly on a grid, but they are perfectly aligned). The color of the particles corresponds to their angle of rotation, so all the particles will be the same color to begin with.

We create a `freud.density.CorrelationFunction` object to compute the correlation functions. Given a particle orientation \( \theta \), we compute its complex orientation value (the quantity we are correlating) as \( s = e^{4i\theta} \), to account for the fourfold symmetry of the particles. We will compute the correlation function \( C(r) = \langle s_1^*(0) \cdot s_2(r) \rangle \) by taking the average over all particle pairs and binning the results into a histogram by the distance \( r \) between the particles.

When we compute the correlations between particles, the complex conjugate of the `values` array is used internally for the query points. This way, if \( \theta_1 \) is close to \( \theta_2 \), then we get \( \langle e^{4i\theta_1} \rangle* \cdot \langle e^{4i\theta_2} \rangle \approx e^0 = 1 \).

This system has perfect spatial correlation of the particle orientations, so we see \( C(r) = 1 \) for all values of \( r \).

```python
[3]: def make_particles(L, repeats):
    uc = freud.data.UnitCell.square()
    return uc.generate_system(num_replicas=repeats, scale=L/repeats, sigma_noise=5e-3*L)

# Make a small system
box, points = make_particles(L=5, repeats=20)

# All the particles begin with their orientation at 0
angles = np.zeros(len(points))
values = np.array(np.exp(angles * 4j))

# Create the CorrelationFunction compute object and compute the correlation function
cf = freud.density.CorrelationFunction(bins=25, r_max=box.Lx/2.01)
cf.compute(system=(box, points), values=values,
            query_points=points, query_values=values)

plot_data('Particles before introducing Orientational Disorder',
          points, angles, values, box, cf)
```
Now we will generate random angles from $-\frac{\pi}{4}$ to $\frac{\pi}{4}$, which orients our squares randomly. The four-fold symmetry of the squares means that the space of unique angles is restricted to a range of $\frac{\pi}{2}$. Again, we compute a complex value for each particle, $s = e^{4i\theta}$.

Because we have purely random orientations, we expect no spatial correlations in the plot above. As we see, $C(r) \approx 0$ for all $r$.

Now we will generate random angles from $-\frac{\pi}{4}$ to $\frac{\pi}{4}$, which orients our squares randomly. The four-fold symmetry of the squares means that the space of unique angles is restricted to a range of $\frac{\pi}{2}$. Again, we compute a complex value for each particle, $s = e^{4i\theta}$.

Because we have purely random orientations, we expect no spatial correlations in the plot above. As we see, $C(r) \approx 0$ for all $r$.

```python
# Change the angles to values randomly drawn from a uniform distribution
angles = np.random.uniform(-np.pi/4, np.pi/4, size=len(points))
values = np.exp(angles * 4j)

# Recompute the correlation functions
cf.compute(system=(box, points), values=values,
            query_points=points, query_values=values)

plot_data('Particles with Orientational Disorder',
          points, angles, values, box, cf)
```

The plot below shows what happens when we intentionally introduce a correlation length by adding a spatial pattern to the particle orientations. At short distances, the correlation is very high. As $r$ increases, the oppositely-aligned part of the pattern some distance away causes the correlation to drop.
In the larger system shown below, we see the spatial autocorrelation rise and fall with damping oscillations.

```python
# Make a large system
box, points = make_particles(L=10, repeats=40)

# Use angles that vary spatially in a pattern
angles = np.pi/4 * np.cos(8*np.pi*points[:, 0]/box.Lx)
values = np.exp(angles * 4j)

cf = freud.density.CorrelationFunction(bins=25, r_max=box.Lx/2.01)
cf.compute(system=(box, points), values=values,
            query_points=points, query_values=values)

plot_data('Larger System with Spatially Correlated Orientations',
          points, angles, values, box, cf, s=80)
```
freud Documentation, Release 2.0.0

freud.density.GaussianDensity

The freud.density module is intended to compute a variety of quantities that relate spatial distributions of particles with other particles. In this notebook, we demonstrate freud’s Gaussian density calculation, which provides a way to interpolate particle configurations onto a regular grid in a meaningful way that can then be processed by other algorithms that require regularity, such as a Fast Fourier Transform.

[1]:
```python
import numpy as np
from scipy import stats
import freud
import matplotlib.pyplot as plt
```

To illustrate the basic concept, consider a toy example: a simple set of point particles with unit mass on a line. For analytical purposes, the standard way to accomplish this would be using Dirac delta functions.

[2]:
```python
n_p = 10000
np.random.seed(129)
x = np.linspace(0, 1, n_p)
y = np.zeros(n_p)
points = np.random.rand(10)
y[(points*n_p).astype('int')] = 1
plt.plot(x, y);
plt.show()
```
However, delta functions can be cumbersome to work with, so we might instead want to smooth out these particles. One option is to instead represent particles as Gaussians centered at the location of the points. In that case, the total particle density at any point in the interval \([0, 1]\) represented above would be based on the sum of the densities of those Gaussians at those points.

```python
[3]: # Note that we use a Gaussian with a small standard deviation
to emphasize the differences on this small scale
dists = [stats.norm(loc=i, scale=0.1) for i in points]
y_gaussian = 0
for dist in dists:
    y_gaussian += dist.pdf(x)
plt.plot(x, y_gaussian);
plt.show()
```

The goal of the GaussianDensity class is to perform the same interpolation for points on a 2D or 3D grid, accounting for Box periodicity.

```python
[4]: N = 1000 # Number of points
L = 10 # Box length

box, points = freud.data.make_random_system(L, N, is2D=True, seed=0)
```

(continues on next page)
aq = freud.AABBQuery(box, points)
gd = freud.density.GaussianDensity(L*L, L/3, 1)
gd.compute(aq)

fig, axes = plt.subplots(1, 2, figsize=(14, 6))
aq.plot(ax=axes[0])
gd.plot(ax=axes[1])
plt.show()
The `freud.density` module is intended to compute a variety of quantities that relate spatial distributions of particles with other particles. In this notebook, we demonstrate `freud`'s local density calculation, which can be used to characterize the particle distributions in some systems. In this example, we consider a toy example of calculating the particle density in the vicinity of a set of other points. This can be visualized as, for example, billiard balls on a table with certain regions of the table being stickier than others. In practice, this method could be used for analyzing, e.g., binary systems to determine how densely one species packs close to the surface of the other.

```python
[1]: import numpy as np
    import freud
    import matplotlib.pyplot as plt
    from matplotlib import patches

[2]: # Define some helper plotting functions.
    def add_patches(ax, points, radius=1, fill=False, color="#1f77b4", ls="solid", lw=None):
        """Add set of points as patches with radius to the provided axis""
        for pt in points:
            p = patches.Circle(pt, fill=fill, linestyle=ls, radius=radius,
                facecolor=color, edgecolor=color, lw=lw)
            ax.add_patch(p)

    def plot_lattice(box, points, radius=1, ls="solid", lw=None):
        """Helper function for plotting points on a lattice.""
        fig, ax = plt.subplots(1, 1, figsize=(9, 9))
        box.plot(ax=ax)
        add_patches(ax, points, radius, ls=ls, lw=lw)
        return fig, ax

Let us consider a set of regions on a square lattice.

```python
[3]: area = 2
    radius = np.sqrt(area/np.pi)
    spot_area = area*100

(continues on next page)
spot_radius = np.sqrt(spot_area/np.pi)
num = 6
scale = num*4
uc = freud.data.UnitCell(freud.Box.square(1), [[0.5, 0.5, 0]])
box, spot_centers = uc.generate_system(num, scale=scale)
fig, ax = plot_lattice(box, spot_centers, spot_radius, ls="dashed", lw=2.5)
plt.tick_params(axis="both", which="both", labelsize=14)
plt.show()

Now let’s add a set of points to this box. Points are added by drawing from a normal distribution centered at each of the regions above. For demonstration, we will assume that each region has some relative “attractiveness,” which is represented by the covariance in the normal distributions used to draw points. Specifically, as we go up and to the right, the covariance increases proportional to the distance from the lower right corner of the box.

[4]: points = []
fractional_distances_to_corner = np.linalg.norm(box.make_fractional(spot_centers), axis=-1)
cov_basis = 20 * fractional_distances_to_corner
for i, p in enumerate(spot_centers):
We see that the density decreases as we move up and to the right. In order to compute the actual densities, we can leverage the `LocalDensity` class. The class allows you to specify a set of query points around which the number of other points is computed. These other points can, but need not be, distinct from the query points. In our case, we want to use the blue regions as our query points with the small black dots as our data points.

When we construct the `LocalDensity` class, there are two arguments. The first is the radius from the query points within which particles should be included in the query point’s counter. The second is the circumsphere diameter of the data points, not the query points. This distinction is critical for getting appropriate density values, since these values
are used to actually check cutoffs and calculate the density.

```python
[6]: density = freud.density.LocalDensity(spot_radius, radius)
density.compute(system=(box, points), query_points=spot_centers);

[7]: fig, axes = plt.subplots(1, 2, figsize=(14, 6))
for i, data in enumerate([density.num_neighbors, density.density]):
    poly = np.poly1d(np.polyfit(cov_basis, data, 1))
    axes[i].tick_params(axis="both", which="both", labelsize=14)
    axes[i].scatter(cov_basis, data)
    x = np.linspace(*axes[i].get_xlim(), 30)
    axes[i].plot(x, poly(x), label="Best fit")
    axes[i].set_xlabel("Covariance", fontsize=16)
    axes[0].set_ylabel("Number of neighbors", fontsize=16);
    axes[1].set_ylabel("Density", fontsize=16);
plt.show()
```

As expected, we see that increasing the variance in the number of points centered at a particular query point decreases the total density at that point. The trend is noisy since we are randomly sampling possible positions, but the general behavior is clear.

**freud.density.RDF: Accumulating g(r) for a Fluid**

The `freud.density` module is intended to compute a variety of quantities that relate spatial distributions of particles with other particles. This example demonstrates the calculation of the radial distribution function \( g(r) \) for a fluid, averaged over multiple frames.

```python
[1]: import numpy as np
import freud
import matplotlib.pyplot as plt

data_path = "data/phi065"
box_data = np.load("//box_data.npy".format(data_path))
pos_data = np.load("//pos_data.npy".format(data_path))
```

(continues on next page)
def plot_rdf(box_arr, points_arr, prop, r_max=10, bins=100, label=None, ax=None):
    """Helper function for plotting RDFs."""
    if ax is None:
        fig, ax = plt.subplots(1, 1, figsize=(12, 8))
        ax.set_title(prop, fontsize=16)
    rdf = freud.density.RDF(bins, r_max)
    for box, points in zip(box_arr, points_arr):
        rdf.compute(system=(box, points), reset=False)
    if label is not None:
        ax.plot(rdf.bin_centers, getattr(rdf, prop), label=label)
    ax.legend()
    else:
        ax.plot(rdf.bin_centers, getattr(rdf, prop))
    return ax

Here, we show the difference between the RDF of one frame and an accumulated (averaged) RDF from several frames. Including more frames makes the plot smoother.

[2]: # Compute the RDF for the last frame
    box_arr = [box_data[-1].tolist()]
    pos_arr = [pos_data[-1]]
    ax = plot_rdf(box_arr, pos_arr, 'rdf', label='One frame')

    # Compute the RDF for the last 20 frames
    box_arr = [box.tolist() for box in box_data[-20:]]
    pos_arr = pos_data[-20:]
    ax = plot_rdf(box_arr, pos_arr, 'rdf', label='Last 20 frames', ax=ax)

    plt.show()
The difference between `accumulate` (which should be called on a series of frames) and `compute` (meant for a single frame) is more striking for smaller bin sizes, which are statistically noisier.

```python
[3]: # Compute the RDF for the last frame
    box_arr = [box_data[-1].tolist()]
    pos_arr = [pos_data[-1]]
    ax = plot_rdf(box_arr, pos_arr, 'rdf', bins=1000, label='One frame')

# Compute the RDF for the last 20 frames
    box_arr = [box.tolist() for box in box_data[-20:]]
    pos_arr = pos_data[-20:]
    ax = plot_rdf(box_arr, pos_arr, 'rdf', bins=1000, label='Last 20 frames', ax=ax)

plt.show()
```
The `freud.density` module is intended to compute a variety of quantities that relate spatial distributions of particles with other particles. This example demonstrates the calculation of the radial distribution function $g(r)$ using different bin sizes.

```python
import numpy as np
import freud
import matplotlib.pyplot as plt

# Define some helper plotting functions.
def plot_rdf(box, points, prop, r_max=3.5, bins_array=[20, 75, 3000]):
    """Helper function for plotting RDFs."""
    fig, axes = plt.subplots(1, len(bins_array), figsize=(16, 3))
    for i, bins in enumerate(bins_array):
        rdf = freud.density.RDF(bins, r_max)
        rdf.compute(system=(box, points))
        axes[i].plot(rdf.bin_centers, getattr(rdf, prop))
        axes[i].set_title('Bin width: {:.3f}'.format(r_max/bins), fontsize=16)
    plt.show()

To start, we construct and visualize a set of points sitting on a simple square lattice.

```python
box, points = freud.data.UnitCell.square().generate_system(5, scale=2)
aq = freud.AABBQuery(box, points)
```

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If we try to compute the RDF directly from this, we will get something rather uninteresting since we have a perfect crystal. Indeed, we will observe that as we bin more and more finely, we approach the true behavior of the RDF for perfect crystals, which is a simple delta function.

In these RDFs, we see two sharply defined peaks, with the first corresponding to the nearest neighbors on the lattice (which are all at a distance 2 from each other), and the second, smaller peak caused by the particles on the diagonal (which sit at distance $\sqrt{2^2 + 2^2} \approx 2.83$).

However, in more realistic systems, we expect that the lattice will not be perfectly formed. In this case, the RDF will exhibit more features. To demonstrate this fact, we reconstruct the square lattice of points from above, but we now introduce some noise into the system.

[5]:
```python
box, clean_points = freud.data.UnitCell.square().generate_system(10, scale=2, sigma_noise=0)
box, noisy_points = freud.data.UnitCell.square().generate_system(10, scale=2, sigma_noise=0.1)
aq_clean = freud.AABBQuery(box, clean_points)
aq_clean.plot(ax=plt.gca(), c='k', s=3)
aq_noisy = freud.AABBQuery(box, noisy_points)
deviations = np.linalg.norm(box.wrap(noisy_points-clean_points), axis=-1)
_, sc = aq_noisy.plot(ax=plt.gca(), c=deviations)
cbar = plt.colorbar(sc)
```
In this RDF, we see the same rough features as we saw with the perfect lattice. However, the signal is much noisier, and in fact we see that increasing the number of bins essentially leads to overfitting of the data. As a result, we have to be careful with how we choose to bin our data when constructing the RDF object.

An alternative route for avoiding this problem can be using the cumulative RDF instead. The relationship between the cumulative RDF and the RDF is akin to that between a cumulative density and a probability density function, providing a measure of the total density of particles experienced up to some distance rather than the value at that distance. Just as a CDF can help avoid certain mistakes common to plotting a PDF, plotting the cumulative RDF may be helpful in some cases. Here, we see that decreasing the bin size slightly alters the features of the plot, but only in very minor way (i.e. decreasing the smoothness of the line due to small jitters).

6.5. Examples
freud.environment.AngularSeparation

The freud.environment module analyzes the local environments of particles. The freud.environment.AngularSeparation class enables direct measurement of the relative orientations of particles.

In order to work with orientations in freud, we need to do some math with quaternions. If you are unfamiliar with quaternions, you can read more about their definition and how they can be used to represent rotations. For the purpose of this tutorial, just consider them as 4D vectors, and know that the set of normalized (i.e. unit norm) 4D vectors can be used to represent rotations in 3D. In fact, there is a 1-1 mapping between normalized quaternions and 3x3 rotation matrices. Quaternions are more computationally convenient, however, because they only require storing 4 numbers rather than 9, and they can be much more easily chained together. The rowan library (rowan.readthedocs.io) defines many useful operations using quaternions, such as the rotations of vectors using quaternions instead of matrices.

Neighbor Angles

One usage of the AngularSeparation class is to compute angles between neighboring particles. To show how this works, we generate a simple configuration of particles with random orientations associated with each point.

```
course: use "freud"
course: import numpy as np
plt.rcParams['axes.titlepad'] = 20
from mpl_toolkits.mplot3d import Axes3D
import rowan # for quaternion math, see rowan.readthedocs.io for more information.
```

```
# Generate random, correlated particle orientations by taking identity quaternions and slightly rotating them in a random direction
np.random.seed(0)
interpolate_amount = 0.2
identity_quats = np.array([[1, 0, 0, 0]] * N)
ref_orientations = rowan.interpolate.slerp(
    identity_quats, rowan.random.rand(N), interpolate_amount)
orientations = rowan.interpolate.slerp(
    identity_quats, rowan.random.rand(N), interpolate_amount)
```

```
# To show orientations, we use arrows rotated by the quaternions.
ref_arrowheads = rowan.rotate(ref_orientations, np.array([1, 0, 0]))
arrowheads = rowan.rotate(orientations, np.array([1, 0, 0]))
```

```
fig = plt.figure(figsize=(12, 6))
ref_ax = fig.add_subplot(121, projection='3d')
ax = fig.add_subplot(122, projection='3d')
ref_ax.quiver3D(positions[:, 0], positions[:, 1], positions[:, 2],
    ref_arrowheads[:, 0], ref_arrowheads[:, 1], ref_arrowheads[:, 2])
ax.quiver3D(positions[:, 0], positions[:, 1], positions[:, 2],
    arrowheads[:, 0], arrowheads[:, 1], arrowheads[:, 2])
ref_ax.set_title("Reference orientations", fontsize=16)
ax.set_title("Orientations", fontsize=16)
plt.show()"
We can now use the AngularSeparation class to compare the orientations in these two systems.

```python
# For simplicity, we'll assume that our "particles" are completely asymmetric, i.e. there are no rotations that map the particle back onto itself. If we had a regular polyhedron, then we would want to specify all the quaternions that rotate that polyhedron onto itself.
equiv_orientations = np.array([[1, 0, 0, 0]])
ang_sep = freud.environment.AngularSeparationNeighbor()
ang_sep.compute(system=(box, positions),
                orientations=orientations,
                query_points=positions,
                query_orientations=ref_orientations,
                equiv_orientations=equiv_orientations,
                neighbors={'num_neighbors': 12})

# Convert angles from radians to degrees and plot histogram
neighbor_angles = np.rad2deg(ang_sep.angles)
plt.hist(neighbor_angles)
plt.title('Histogram of angular separations between neighbors')
plt.xlabel('Angular separation (degrees)')
plt.ylabel('Frequency')
plt.show()
```
Alternatively, the AngularSeparationGlobal class can also be used to compute the orientation of all points in the system relative to some global set of orientations. In this case, we simply provide a set of global quaternions that we want to consider. For simplicity, let’s consider $180^\circ$ rotations about each of the coordinate axes, which have very simple quaternion representations.

```python
[5]:
global_orientations = np.array([[1, 0, 0, 0], [0, 1, 0, 0], [0, 0, 1, 0], [0, 0, 0, -1]])
ang_sep = freud.environment.AngularSeparationGlobal()
ang_sep.compute(global_orientations, ref_orientations, equiv_orientations)
global_angles = np.rad2deg(ang_sep.angles)
```

```python
[6]:
plt.hist(global_angles[:, 0])
plt.title('Histogram of angular separation relative to identity quaternion')
plt.xlabel('Angular separation (degrees)')
plt.ylabel('Frequency')
plt.show()
```
As a simple check, we can ensure that for the identity quaternion \((1, 0, 0, 0)\), which performs a 0° rotation, the angles between the reference orientations and that quaternion are equal to the original angles of rotation of those quaternions (i.e. how much those orientations were already rotated relative to the identity).

```python
ref_axes, ref_angles = rowan.to_axis_angle(ref_orientations)
np.allclose(global_angles[:, 0], np.rad2deg(ref_angles), rtol=1e-4)
```

```
[7]: True
```

---

### Computing Bond Order Diagrams

The `freud.environment` module analyzes the local environments of particles. In this example, the `freud.environment.BondOrder` class is used to plot the bond order diagram (BOD) of a system of particles.

```python
import numpy as np
import freud
import matplotlib.pyplot as plt
import matplotlib
from mpl_toolkits.mplot3d import Axes3D
```

### Setup

Our sample data will be taken from an face-centered cubic (FCC) structure. The array of points is rather large, so that the plots are smooth. Smaller systems may need to gather data from multiple frames in order to smooth the resulting array’s statistics, by computing multiple times with `reset=False`.

```python
uc = freud.data.UnitCell.fcc()
box, points = uc.generate_system(40, sigma_noise=0.05)
```

Now we create a `BondOrder` compute object and create some arrays useful for plotting.
freud Documentation, Release 2.0.0

```
[3]:
n_bins_theta = 100
n_bins_phi = 100
bod = freud.environment.BondOrder((n_bins_theta, n_bins_phi))

phi = np.linspace(0, np.pi, n_bins_phi)
theta = np.linspace(0, 2*np.pi, n_bins_theta)
phi, theta = np.meshgrid(phi, theta)
x = np.sin(phi) * np.cos(theta)
y = np.sin(phi) * np.sin(theta)
z = np.cos(phi)
```

**Computing the Bond Order Diagram**

Next, we use the `compute` method and the `bond_order` property to return the array.

```
[4]:
bod_array = bod.compute(system=(box, points), neighbors={'num_neighbors': 12}).bond_order
# Clean up polar bins for plotting
bod_array = np.clip(bod_array, 0, np.percentile(bod_array, 99))
plt.imshow(bod_array.T)
plt.show()
```

**Plotting on a sphere**

This code shows the bond order diagram on a sphere as the sphere is rotated. The code takes a few seconds to run, so be patient.

```
[5]:
fig = plt.figure(figsize=(12, 8))
for plot_num in range(6):
    ax = fig.add_subplot(231 + plot_num, projection='3d')
    ax.plot_surface(x, y, z, rstride=1, cstride=1, shade=False,
                    facecolors=matplotlib.cm.viridis(bod_array / np.max(bod_array)))
    ax.set_xlim(-1, 1)
    ax.set_ylim(-1, 1)
    ax.set_zlim(-1, 1)
    ax.set_axis_off()
```

(continues on next page)
Using Custom Neighbors

We can also use a custom neighbor query to determine bonds. For example, we can filter for a range of bond lengths. Below, we only consider neighbors between $r_{\text{min}} = 2.5$ and $r_{\text{max}} = 3$ and plot the resulting bond order diagram.

```python
[6]: bod_array = bod.compute(system=(box, points), neighbors={'r_max': 3.0, 'r_min': 2.5}).
    → bond_order
# Clean up polar bins for plotting
bod_array = np.clip(bod_array, 0, np.percentile(bod_array, 99))
plt.imshow(bod_array.T)
plt.show()
```
The `freud.environment.EnvironmentCluster` class finds and clusters local environments, as determined by the vectors pointing to neighbor particles. Neighbors can be defined by a cutoff distance or a number of nearest-neighbors, and the resulting `freud.locality.NeighborList` is used to enumerate a set of vectors, defining an “environment.” These environments are compared with the environments of neighboring particles to form spatial clusters, which usually correspond to grains, droplets, or crystalline domains of a system. `EnvironmentCluster` has several parameters that alter its behavior, please see the documentation or helper functions below for descriptions of these parameters.

In this example, we cluster the local environments of hexagons. Clusters with 5 or fewer particles are colored dark gray.

```python
import numpy as np
import freud
from collections import Counter
import matplotlib.pyplot as plt

def get_cluster_arr(system, num_neighbors, threshold,
                     registration=False, global_search=False):
    """Computes clusters of particles’ local environments.
    ""

    Args:
        system: 
            Any object that is a valid argument to
            :class:`freud.locality.NeighborQuery.from_system`
        num_neighbors (int):
            Number of neighbors to consider in every particle's local environment.
        threshold (float):
            Maximum magnitude of the vector difference between two vectors,
            below which we call them matching.
        global_search (bool):
            If True, do an exhaustive search wherein the environments of
            every single pair of particles in the simulation are compared.
            If False, only compare the environments of neighboring particles.
        registration (bool):
            Controls whether we first use brute force registration to
```

orient the second set of vectors such that it minimizes the RMSD between the two sets.

Returns:

tuple(np.ndarray, dict): array of cluster indices for every particle and a dictionary mapping from cluster_index keys to vector_array pairs giving all vectors associated with each environment.

""
# Perform the env-matching calculation
neighbors = {'num_neighbors': num_neighbors}
match = freud.environment.EnvironmentCluster()
match.compute(system, threshold, neighbors=neighbors,
               registration=registration, global_search=global_search)
return match.cluster_idx, match.cluster_environments

def color_by_clust(cluster_index_arr, no_color_thresh=1,
                   no_color='#333333', cmap=plt.get_cmap('viridis')):
    """Takes a cluster_index_array for every particle and returns a dictionary of (cluster index, hexcolor) color pairs.

    Args:
        cluster_index_arr (numpy.ndarray):
            The array of cluster indices, one per particle.
        no_color_thresh (int):
            Clusters with this number of particles or fewer will be colored with no_color.
        no_color (color):
            What we color particles whose cluster size is below no_color_thresh.
        cmap (color map):
            The color map we use to color all particles whose cluster size is above no_color_thresh.
    ""
    # Count to find most common clusters
    cluster_counts = Counter(cluster_index_arr)
    # Re-label the cluster indices by size
    color_count = 0
    color_dict = {cluster[0]: counter for cluster, counter in
                  zip(cluster_counts.most_common(),
                      range(len(cluster_counts)))}

    # Don’t show colors for clusters below the threshold
    for cluster_id in cluster_counts:
        if cluster_counts[cluster_id] <= no_color_thresh:
            color_dict[cluster_id] = -1
    OP_arr = np.linspace(0.0, 1.0, max(color_dict.values())+1)

    # Get hex colors for all clusters of size greater than no_color_thresh
    for old_cluster_index, new_cluster_index in color_dict.items():
        if new_cluster_index == -1:
            color_dict[old_cluster_index] = no_color
        else:
            color_dict[old_cluster_index] = cmap(OP_arr[new_cluster_index])

    return color_dict

We load the simulation data and call the analysis functions defined above. Notice that we use 6 nearest neighbors, since our system is made of hexagons that tend to cluster with 6 neighbors.
freud Documentation, Release 2.0.0

```
[2]: ex_data = np.load('data/MatchEnv_Hexagons.npz')
    box = ex_data['box']
    positions = ex_data['positions']
    orientations = ex_data['orientations']
    aq = freud.AABBQuery(box, positions)
    
    cluster_index_arr, cluster_envs = get_cluster_arr(
        aq, num_neighbors=6, threshold=0.2,
        registration=False, global_search=False)
    color_dict = color_by_clust(cluster_index_arr, no_color_thresh=5)
    colors = [color_dict[i] for i in cluster_index_arr]

    Below, we plot the resulting clusters. The colors correspond to the cluster size.

[3]: plt.figure(figsize=(12, 12), facecolor='white')
    aq.plot(ax=plt.gca(), c=colors, s=20)
    plt.title('Clusters Colored by Particle Local Environment')
    plt.show()
```
The `freud.environment` module analyzes the local environments of particles. The `freud.environment.LocalDescriptors` class is a useful tool for analyzing identifying crystal structures in a rotationally invariant manner using local particle environments. The primary purpose of this class is to compute spherical harmonics between neighboring particles in a way that orients particles correctly relative to their local environment, ensuring that global orientational shifts do not change the output.

```python
import freud
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
```

---

**freud.environment.LocalDescriptors: Steinhardt Order Parameters from Scratch**

The `freud.environment` module analyzes the local environments of particles. The `freud.environment.LocalDescriptors` class is a useful tool for analyzing identifying crystal structures in a rotationally invariant manner using local particle environments. The primary purpose of this class is to compute spherical harmonics between neighboring particles in a way that orients particles correctly relative to their local environment, ensuring that global orientational shifts do not change the output.

---

[1]: import freud
    import numpy as np
    import matplotlib.pyplot as plt
    from mpl_toolkits.mplot3d import Axes3D
Computing Spherical Harmonics

To demonstrate the basic application of the class, let’s compute the spherical harmonics between neighboring particles. For simplicity, we consider points on a simple cubic lattice.

```python
[2]: uc = freud.data.UnitCell.sc()
    box, points = uc.generate_system(5)
    system = freud.AABBQuery(box, points)
    fig = plt.figure(figsize=(8, 6))
    ax = fig.add_subplot(111, projection='3d')
    system.plot(ax=ax)
    ax.set_title("Simple cubic crystal", fontsize=16)
    plt.show()

```

Now, let’s use the class to compute an array of spherical harmonics for the system. The harmonics are computed for each bond, where a bond is defined by a pair of particles that are determined to lie within each others’ nearest neighbor shells based on a standard neighbor list search. The number of bonds and spherical harmonics to calculate is configurable.

```python
[3]: num_neighbors = 6
    l_max = 12
    nlist = system.query(points, {'num_neighbors': num_neighbors, 'exclude_ii': True}).toNeighborList()
    ld = freud.environment.LocalDescriptors(l_max, mode='global')
    ld.compute(system, neighbors=nlist);
```

Accessing the Data

The resulting spherical harmonic array has a shape corresponding to the number of neighbors. We can now extract the spherical harmonics corresponding to a particular \((l, m)\) pair using the ordering used by the `LocalDescriptors` class: increasing values of \(l\), and for each \(l\), the nonnegative \(m\) values followed by the negative values.
Using Spherical Harmonics to Compute Steinhardt Order Parameters

The raw per bond spherical harmonics are not typically useful quantities on their own. However, they can be used to perform sophisticated crystal structure analyses with different methods; for example, the `pythia` library uses machine learning to find patterns in the spherical harmonics computed by this class. In this notebook, we’ll use the quantities for a more classical application: the computation of Steinhardt order parameters. The order parameters $q_l$ provide a rotationally invariant measure of the system that can for some structures, provide a unique identifying fingerprint. They are a particularly useful measure for various simple cubic structures such as structures with underlying simple cubic, BCC, or FCC lattices. The `freud` library actually provides additional classes to efficiently calculate these order parameters directly, but they also provide a reasonable demonstration here.

For more information on Steinhardt order parameters, see the original paper or the `freud.order.Steinhardt` documentation.

```python
[4]: sph_raw = np.mean(ld.sph, axis=0)
count = 0
sph = np.zeros((l_max+1, l_max+1), dtype=np.complex128)
for l in range(l_max+1):
    for m in range(l+1):
        sph[l, m] = sph_raw[count]
        count += 1
    for m in range(-l, 0):
        sph[l, m] = sph_raw[count]
        count += 1
```

```python
[5]: def get_ql(num_particles, descriptors, nlist, weighted=False):
    """Given a set of points and a LocalDescriptors object (and the underlying NeighborList), compute the per-particle Steinhardt ql order parameter for all $l$ values up to the maximum quantum number used in the computation of the descriptors.""
    qbar_lm = np.zeros((num_particles, descriptors.sph.shape[1]), dtype=np.complex128)
    for i in range(num_particles):
        indices = nlist.query_point_indices == i
        Ylms = descriptors.sph[indices, :]
        if weighted:
            weights = nlist.weights[indices, np.newaxis]
            weights /= np.sum(weights)
            num_neighbors = 1
        else:
            weights = np.ones_like(Ylms)
            num_neighbors = descriptors.sph.shape[0]/num_particles
        qbar_lm[i, :] = np.sum(Ylms * weights, axis=0)/num_neighbors
    ql = np.zeros((qbar_lm.shape[0], descriptors.l_max+1))
    for i in range(ql.shape[0]):
        for l in range(ql.shape[1]):
            for k in range(l**2, (l+1)**2):
                ql[i, l] += np.absolute(qbar_lm[i, k])**2
        ql[i, l] = np.sqrt(4*np.pi/(2*l + 1) * ql[i, l])
    return ql
```

Since `freud` provides the ability to calculate these parameter as well, we can directly check that our answers are
correct. Note: More information on the ‘‘Steinhardt’’ class can be found in the documentation or in the ‘‘Steinhardt’’ example.

```
[6]: L = 6
steinhardt = freud.order.Steinhardt(l=L)
steinhardt.compute(system, neighbors=nlist)
if np.allclose(steinhardt.ql, ld_ql[:, L]):
    print("Our manual calculation matches the Steinhardt class!")
```

Our manual calculation matches the Steinhardt class!

For a brief demonstration of why the Steinhardt order parameters can be useful, let’s look at the result of thermalizing our points and recomputing this measure.

```
[7]: sigmas = [0.03, 0.05, 0.1]
systems = []
nlists = []
for sigma in sigmas:
    box, points = uc.generate_system(5, sigma_noise=sigma)
    system = freud.AABBQuery(box, points)
    systems.append(system)
    nlists.append(system.query(points, {'num_neighbors': num_neighbors, 'exclude_ii': True}).toNeighborList())

[8]: fig = plt.figure(figsize=(14, 6))
axes = []
for i, v in enumerate(sigmas):
    ax = fig.add_subplot("1/1\{i+1\}", projection='3d')
    systems[i].plot(ax=ax)
    ax.set_title("$\sigma$ = \{v\}", fontsize=16);
plt.show()
```

If we recompute the Steinhardt OP for each of these data sets, we see that adding noise has the effect of smoothing the order parameter such that the peak we observed for the perfect crystal is no longer observable.
This type of identification process is what the LocalDescriptors data outputs may be used for. In the case of Steinhardt OPs, it provides a simple fingerprint for comparing thermalized systems to a known ideal structure to measure their similarity.

For reference, we can also check these values against the Steinhardt class again.

```
[11]: for i, (system, nlist) in enumerate(zip(systems, nlists)):
    steinhardt = freud.order.Steinhardt(l=L)
    steinhardt.compute(system, nlist)
    if np.allclose(steinhardt.particle_order, ld_qls[i][;,:L]):
        print("Our manual calculation matches the Steinhardt class!")
```

Our manual calculation matches the Steinhardt class!
Our manual calculation matches the Steinhardt class!
Our manual calculation matches the Steinhardt class!
Locating Particles on Interfacial Boundaries

The `freud.interface` module compares the distances between two sets of points to determine the interfacial particles.

```python
[1]:
import freud
import numpy as np
import matplotlib.pyplot as plt

To make a pretend data set, we create a large number of blue (-1) particles on a square grid. Then we place grain centers on a larger grid and draw grain radii from a normal distribution. We color the particles yellow (+1) if their distance from a grain center is less than the grain radius.

```python
[2]:
np.random.seed(0)
system_size = 100
num_grains = 4
uc = freud.data.UnitCell.square()
box, points = uc.generate_system(num_replicas=system_size, scale=1)
_, centroids = uc.generate_system(num_replicas=num_grains, scale=system_size/num_grains)
system = freud.AABBQuery(box, points)
values = np.array([-1 for p in points])
grain_radii = np.abs(np.random.normal(size=num_grains**2, loc=5, scale=2))
for center, radius in zip(centroids, grain_radii):
    for i, j, dist in system.query(center, {'r_max': radius}):
        values[j] = 1
plt.figure(figsize=(9, 9))
system.plot(ax=plt.gca(), c=values, cmap='cividis', s=12)
plt.title('System of two particle types')
plt.show()
```
This system is **phase-separated** because the yellow particles are generally near one another, and so are the blue particles.

We can use `freud.interface.InterfaceMeasure` to label the particles on either side of the yellow-blue boundary. The class can tell us how many points are on either side of the interface:

```
iface = freud.interface.Interface()
iface.compute((box, points[values > 0]), points[values < 0], neighbors={'r_max': 1.5})
print('There are {} query points (blue) on the interface.'.format(iface.query_point_count))
print('There are {} points (yellow) on the interface.'.format(iface.point_count))
```

There are 856 query points (blue) on the interface.
There are 724 points (yellow) on the interface.

Now we can plot the particles on the interface. We color the outside of the interface dark blue and the inside of the interface yellow.
freud.order.Hexatic

Hexatic Order Parameter

The hexatic order parameter measures how closely the local environment around a particle resembles perfect $k$-atic symmetry, e.g. how closely the environment resembles hexagonal/hexatic symmetry for $k = 6$. The order parameter
is given by:

\[
\psi_k (i) = \frac{1}{n} \sum_{j} e^{k i \theta_{ij}}
\]

where \( \theta_{ij} \) is the angle between the vector \( \vec{r}_{ij} \) and \((1, 0)\).

The pseudocode is given below:

```python
for each particle i:
    neighbors = nearestNeighbors(i, n):
    for each particle j in neighbors:
        r_ij = position[j] - position[i]
        theta_ij = arctan2(r_ij.y, r_ij.x)
        psi_array[i] += exp(complex(0,k*theta_ij))
```

The data sets used in this example are a system of hard hexagons, simulated in the NVT thermodynamic ensemble in HOOMD-blue, for a dense fluid of hexagons at packing fraction \( \phi = 0.65 \) and solids at packing fractions \( \phi = 0.75, 0.85 \).

[1]: import numpy as np
    import freud
    from bokeh.io import output_notebook
    from bokeh.plotting import figure, show
    # The following line imports this set of utility functions:
    # https://github.com/glotzerlab/freud-examples/blob/master/util.py
    import util
    output_notebook()

[2]: def plot_hex_order_param(data_path, title):
    # Create hexatic object
    hex_order = freud.order.Hexatic(k=6)

    # Load the data
    box_data = np.load("/box_data.npy")
    pos_data = np.load("/pos_data.npy")
    quat_data = np.load("/quat_data.npy")

    # Grab data from last frame
    box = box_data[-1].tolist()
    points = pos_data[-1]
    quats = quat_data[-1]
    angles = 2*np.arctan2(quats[:, 3], quats[:, 0])

    # Compute hexatic order for 6 nearest neighbors
    hex_order.compute(system=(box, points), neighbors={'num_neighbors': 6})
    psi_k = hex_order.particle_order
    avg_psi_k = np.mean(psi_k)

    # Create hexagon vertices
    verts = util.make_polygon(sides=6, radius=0.6204)
    # Create array of transformed positions
    patches = util.local_to_global(verts, points[:, :2], angles)
```

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# Create an array of angles relative to the average
relative_angles = np.angle(psi_k) - np.angle(avg_psi_k)
# Plot in bokeh
p = figure(title=title)
p.patches(xs=patches[:, :, 0].tolist(), ys=patches[:, :, 1].tolist(),
        fill_color=[util.cubeellipse(x) for x in relative_angles],
        line_color="black")
util.default_bokeh(p)
show(p)

[3]: plot_hex_order_param('data/phi065', 'Hexatic Order Parameter, 0.65 density')

As the density increases to $\phi = 0.75$, the shapes are forced to align more closely so that they may tile space effectively.

[4]: plot_hex_order_param('data/phi075', 'Hexatic Order Parameter, 0.75 density')

As the density increases to $\phi = 0.85$, the alignment becomes even stronger and defects are no longer visible.

[5]: plot_hex_order_param('data/phi085', 'Hexatic Order Parameter, 0.85 density')

freud.order.Nematic

Nematic Order Parameter

The freud.order module provides the tools to calculate various order parameters that can be used to identify phase transitions. This notebook demonstrates the nematic order parameter, which can be used to identify systems with strong orientational ordering but no translational ordering. For this example, we’ll start with a set of random positions in a 3D system, each with a fixed, assigned orientation. Then, we will show how deviations from these orientations are exhibited in the order parameter.

[1]: import freud
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
import rowan  # for quaternion math, see rowan.readthedocs.io for more information.

In order to work with orientations in freud, we need to do some math with quaternions. If you are unfamiliar with quaternions, you can read more about their definition and how they can be used to represent rotations. For the purpose of this tutorial, just consider them as 4D vectors, and know that the set of normalized (i.e. unit norm) 4D vectors can be used to represent rotations in 3D. In fact, there is a 1-1 mapping between normalize quaternions and 3x3 rotation matrices. Quaternions are more computationally convenient, however, because they only require storing 4 numbers...
rather than 9, and they can be much more easily chained together. For our purposes, you can largely ignore the contents of the next cell, other than to note that this is how we perform rotations of vectors using quaternions instead of matrices.

```python
# Random positions are fine for this. Order is measured
# in terms of similarity of orientations, not positions.
L = 10
N = 100
box, points = freud.data.make_random_system(L, N, seed=0)
orientations = np.array([[1, 0, 0, 0]] * N)

# To show orientations, we use arrows rotated by the quaternions.
arrowheads = rowan.rotate(orientations, [1, 0, 0])
```

The nematic order parameter provides a measure of how much of the system is aligned with respect to some provided reference vector. As a result, we can now compute the order parameter for a few simple cases. Since our original system is oriented along the x-axis, we can immediately test for that, as well as orientation along any of the other coordinate axes.

```python
nop = freud.order.Nematic([1, 0, 0])
nop.compute(orientations)
print("The value of the order parameter is {}.").format(nop.order)
The value of the order parameter is 1.0.
```

In general, the nematic order parameter is defined as the eigenvalue corresponding to the largest eigenvector of the nematic tensor, which is also computed by this class and provides an average over the orientations of all particles in the system. As a result, we can also look at the intermediate results of our calculation and see how they are related. To do so, let’s consider a more interesting system with random orientations.

```python
# We rotate identity quaternions slightly, in a random direction
np.random.seed(0)
interpolate_amount = 0.3
identity_quats = np.array([[1, 0, 0, 0]] * N)
orientations = rowan.interpolate.slerp(
```

(continues on next page)
First, we see that for this nontrivial system the order parameter now depends on the choice of director.

```python
axes = [[1, 0, 0], [0, 1, 0], [0, 0, 1], [1, 1, 0], [1, 0, 1], [0, 1, 1], [1, 1, 1]]
for ax in axes:
    nop = freud.order.Nematic(ax)
    nop.compute(orientations)
    print("For axis \{\}, the value of the order parameter is \{\:0.3f\}.".format(ax, nop.order))
```

For axis [1, 0, 0], the value of the order parameter is 0.600.
For axis [0, 1, 0], the value of the order parameter is 0.586.
For axis [0, 0, 1], the value of the order parameter is 0.587.
For axis [1, 1, 0], the value of the order parameter is 0.591.
For axis [1, 0, 1], the value of the order parameter is 0.589.
For axis [0, 1, 1], the value of the order parameter is 0.573.
For axis [1, 1, 1], the value of the order parameter is 0.578.

Furthermore, increasing the amount of variance in the orientations depresses the value of the order parameter even further.

```python
interpolate_amount = 0.4
orientations = rowan.interpolate.slerp(
    identity_quats, rowan.random.rand(N), interpolate_amount)
arrowheads = rowan.rotate(orientations, [1, 0, 0])
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
ax.quiver3D(points[:, 0], points[:, 1], points[:, 2],
            arrowheads[:, 0], arrowheads[:, 1], arrowheads[:, 2])
plt.show()
```
```python
ax.set_title("Orientations", fontsize=16);

axes = [[1, 0, 0], [0, 1, 0], [0, 0, 1], [1, 1, 0], [1, 0, 1], [0, 1, 1], [1, 1, 1]]
for ax in axes:
    nop = freud.order.Nematic(ax)
    nop.compute(orientations)
    print("For axis {}, the value of the order parameter is {:.3f}.".format(ax, nop.order))

For axis [1, 0, 0], the value of the order parameter is 0.451.
For axis [0, 1, 0], the value of the order parameter is 0.351.
For axis [0, 0, 1], the value of the order parameter is 0.342.
For axis [1, 1, 0], the value of the order parameter is 0.374.
For axis [1, 0, 1], the value of the order parameter is 0.391.
For axis [0, 1, 1], the value of the order parameter is 0.316.
For axis [1, 1, 1], the value of the order parameter is 0.344.
```

Finally, we can look at the per-particle quantities and build them up to get the actual value of the order parameter.

```python
# The per-particle values averaged give the nematic tensor
print(np.allclose(np.mean(nop.particle_tensor, axis=0), nop.nematic_tensor))
print("The nematic tensor:")
print(nop.nematic_tensor)

eig = np.linalg.eig(nop.nematic_tensor)
print("The eigenvalues of the nematic tensor:")
print(eig[0])
print("The eigenvectors of the nematic tensor:")
print(eig[1])

# The largest eigenvalue
print("The largest eigenvalue, {:.3f}, is equal to the order parameter {:.3f}.".format(np.max(eig[0]), nop.order))

True
The nematic tensor:
[[ 0.0115407  0.21569438  0.14729623]
 [ 0.21569438  0.02040018  0.14309749]
 [ 0.14729623  0.14309748 -0.03194092]]
```
The eigenvalues of the nematic tensor:
[ 0.34387365 -0.20013455 -0.14373913]
The eigenvectors of the nematic tensor:
[[ 0.6173224 0.73592573 -0.27807635]  
 [ 0.6237324 -0.6732561 -0.3970945 ]  
 [ 0.47944868 -0.07169023 0.87463677]]
The largest eigenvalue, 0.344, is equal to the order parameter 0.344.

freud.order.Steinhardt

Steinhardt Order Parameters

The freud.order module provides the tools to calculate various order parameters that can be used to identify phase transitions. In the context of crystalline systems, some of the best known order parameters are the Steinhardt order parameters $q_l$ and $w_l$. These order parameters are mathematically defined according to certain rotationally invariant combinations of spherical harmonics calculated between particles and their nearest neighbors, so they provide information about local particle environments. As a result, considering distributions of these order parameters across a system can help characterize the overall system’s ordering. The primary utility of these order parameters arises from the fact that they often exhibit certain characteristic values for specific crystal structures.

In this notebook, we will use the order parameters to identify certain basic structures: BCC, FCC, and simple cubic. FCC, BCC, and simple cubic structures each exhibit characteristic values of the order parameters for some $l$ value, meaning that in a perfect crystal all the particles in one of these structures will have the same value of $q_l$. As a result, we can use these characteristic $q_l$ values to determine whether a disordered fluid is beginning to crystallize into one structure or another. The $l$ values correspond to the $l$ quantum number used in defining the underlying spherical harmonics; for example, the $q_4$ order parameter would provide a measure of 4-fold ordering.

```python
1: import freud
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
# Try to plot using KDE if available, otherwise revert to histogram
try:
    from sklearn.neighbors.kde import KernelDensity
    kde = True
except:
    kde = False
np.random.seed(1)

We first construct ideal crystals and then extract the characteristic value of $q_l$ for each of these structures. In this case, we know that simple cubic has a coordination number of 6, BCC has 8, and FCC has 12, so we are looking for the values of $q_6$, $q_8$, and $q_{12}$, respectively. Therefore, we can also enforce that we require 6, 8, and 12 nearest neighbors to be included in the calculation, respectively.

```python
[2]: L = 6
sc = freud.data.UnitCell.sc()
sc_system = sc.generate_system(5)
ql = freud.order.Steinhardt(L)
ql_sc = ql.compute(sc_system, neighbors={'num_neighbors': L}).particle_order
mean_sc = np.mean(ql_sc)
print("The Q\{\(l\)\} values computed for simple cubic are {:.3f} +/- {:.3e}".format(L, mean_sc, np.std(ql_sc)))
```

(continues on next page)
L = 8
bcc = freud.data.UnitCell.bcc()
bcc_system = bcc.generate_system(5, sigma_noise=0)
q1 = freud.order.Steinhardt(L)
q1.compute(bcc_system, neighbors={'num_neighbors': L})
q1_bcc = q1.particle_order
mean_bcc = np.mean(q1_bcc)
print("The Q{L} values computed for bcc are {mean_bcc:.3f} +/- {std:.3e}".format(
    L, mean_bcc, np.std(q1_bcc)))

L = 12
fcc = freud.data.UnitCell.fcc()
fcc_system = fcc.generate_system(5)
q1 = freud.order.Steinhardt(L)
q1_fcc = q1.compute(fcc_system, neighbors={'num_neighbors': L}).particle_order
mean_fcc = np.mean(q1_fcc)
print("The Q{L} values computed for fcc are {mean_fcc:.3f} +/- {std:.3e}".format(
    L, mean_fcc, np.std(q1_fcc)))

The Q6 values computed for simple cubic are 0.354 +/- 3.938e-08
The Q8 values computed for bcc are 0.213 +/- 1.137e-12
The Q12 values computed for fcc are 0.600 +/- 1.155e-12

Given that the per-particle order parameter values are essentially identical to within machine precision, we can be confident that we have found the characteristic value of $q_l$ for each of these systems. We can now compare these values to the values of $q_l$ in thermalized systems to determine the extent to which they are exhibiting the ordering expected of one of these perfect crystals.

```python
[3]: def make_noisy_replicas(unitcell, sigmas):
    '''Given a unit cell, return a noisy system.''
    systems = []
    for sigma in sigmas:
        systems.append(unitcell.generate_system(5, sigma_noise=sigma))
    return systems

[4]: sigmas = [0.01, 0.02, 0.03, 0.05]
sc_systems = make_noisy_replicas(sc, sigmas)
bcc_systems = make_noisy_replicas(bcc, sigmas)
fcc_systems = make_noisy_replicas(fcc, sigmas)

[5]: fig, axes = plt.subplots(1, 3, figsize=(16, 5))

# Zip up the data that will be needed for each structure type.
zip_obj = zip([sc_systems, bcc_systems, fcc_systems], [mean_sc, mean_bcc, mean_fcc],
    [6, 8, 12], ["Simple Cubic", "BCC", "FCC"])

for i, (systems, ref_val, L, title) in enumerate(zip_obj):
    ax = axes[i]
    for j, (system, sigma) in enumerate(zip(systems, sigmas)):
        q1 = freud.order.Steinhardt(L)
        q1.compute(system, neighbors={'num_neighbors': L})
        if not kde:
            ax.hist(q1.particle_order, label="$\sigma$ = {sigma}".format(sigma),
                density=True)
        else:
            padding = 0.02
```

(continues on next page)
From this figure, we can see that for each type of structure, increasing the amount of noise makes the distribution of
the order parameter values less peaked at the expected reference value. As a result, we can use this method to identify
specific structures. Choosing the appropriate parameterization for the order parameter (which quantum number \( l \)
to use, how to choose neighbors, etc.) can be very important.

In addition to the \( q_l \) parameters demonstrated here, this class can also compute the third-order invariant \( w_l \). The \( w_l \)
may be better at identifying some structures, so some experimentation and reference to the appropriate literature can
be useful (as a starting point, see Steinhardt, Nelson, and Ronchetti (1983)).

By setting `average=True` in the constructor, the `Steinhardt` class will perform an additional level of averaging
over the second neighbor shells of particles, to accumulate more information on particle environments (see Lechner
and Dellago (2008)). To get a sense for the best method for analyzing a specific system, the best course of action is
try out different parameters or to consult the literature to see how these have been used in the past.

**freud.pmft.PMFTXY**

The PMFT returns the potential energy associated with finding a particle pair in a given spatial (positional and ori-
entational) configuration. The PMFT is computed in the same manner as the RDF. The basic algorithm is described
below:

```python
for each particle i:
    for each particle j:
        v_ij = position[j] - position[i]
```

(continues on next page)
freud uses spatial data structures and parallelism to optimize this algorithm.

The data sets used in this example are a system of hard hexagons, simulated in the NVT thermodynamic ensemble in HOOMD-blue, for a dense fluid of hexagons at packing fraction $\phi = 0.65$ and solids at packing fractions $\phi = 0.75, 0.85$.

```python
import freud
freud.set_num_threads(1)
import numpy as np
import matplotlib
import matplotlib.pyplot as plt
from scipy.ndimage.filters import gaussian_filter
%mplinline
matplotlib.rcParams.update({'font.size': 20,
                           'axes.titlesize': 20,
                           'axes.labelsize': 20,
                           'xtick.labelsize': 16,
                           'ytick.labelsize': 16,
                           'savefig.pad_inches': 0.025,
                           'lines.linewidth': 2})
```

```python
def plot_pmft(data_path, phi):
    # Create the pmft object
    pmft = freud.pmft.PMFTXY(x_max=3.0, y_max=3.0, bins=300)

    # Load the data
    box_data = np.load("{}/box_data.npy".format(data_path))
    pos_data = np.load("{}/pos_data.npy".format(data_path))
    quat_data = np.load("{}/quat_data.npy".format(data_path))
    n_frames = pos_data.shape[0]
    for i in range(1, n_frames):
        # Read box, position data
        box = box_data[i].tolist()
        points = pos_data[i]
        quats = quat_data[i]
        angles = 2*np.arctan2(quats[:, 3], quats[:, 0]) % (2 * np.pi)
        pmft.compute(system=(box, points), query_orientations=angles, reset=False)

    # Get the value of the PMFT histogram bins
    pmft_arr = pmft.pmft.T

    # Do some simple post-processing for plotting purposes
    pmft_arr[np.isinf(pmft_arr)] = np.nan
    dx = (2.0 * 3.0) / pmft.nbins[0]
    dy = (2.0 * 3.0) / pmft.nbins[1]
    nan_arr = np.where(np.isnan(pmft_arr))
    for i in range(pmft.nbins[0]):
        x = -3.0 + dx * i
```

(continues on next page)
for j in range(pmft.nbins[1]):
    y = -3.0 + dy * j
    if ((x*x + y*y < 1.5) and (np.isnan(pmft_arr[j, i]))):
        pmft_arr[j, i] = 10.0
w = int(2.0 * pmft.nbins[0] / (2.0 * 3.0))
center = int(pmft.nbins[0] / 2)

# Get the center of the histogram bins
pmft_smooth = gaussian_filter(pmft_arr, 1)
pmft_image = np.copy(pmft_smooth)
pmft_image[nan_arr] = np.nan
pmft_smooth = pmft_smooth[center-w:center+w, center-w:center+w]
pmft_image = pmft_image[center-w:center+w, center-w:center+w]
x, y = pmft.bin_centers
reduced_x = x[center-w:center+w]
reduced_y = y[center-w:center+w]

# Plot figures
f = plt.figure(figsize=(12, 5), facecolor='white')
values = [-2, -1, 0, 2]
norm = matplotlib.colors.Normalize(vmin=-2.5, vmax=3.0)
n_values = [norm(i) for i in values]
colors = matplotlib.cm.viridis(n_values)
colors = colors[:, :3]
verts = util.make_polygon(sides=6, radius=0.6204)
lims = (-2, 2)
ax0 = f.add_subplot(1, 2, 1)
ax1 = f.add_subplot(1, 2, 2)
for ax in (ax0, ax1):
    ax.contour(reduced_x, reduced_y, pmft_smooth, [9, 10], colors='black')
    ax.contourf(reduced_x, reduced_y, pmft_smooth, [9, 10], hatches='X', colors='none')
    ax.plot(verts[:, 0], verts[:, 1], color='black', marker=',')
    ax.fill(verts[:, 0], verts[:, 1], color='black')
    ax.set_aspect('equal')
    ax.set_xlim(lims)
    ax.set_ylim(lims)
    ax.set_xlabel(r'$x$')
    ax.set_ylabel(r'$y$')
    ax0.set_title('PMFT Heat Map, $\phi = {}$'.format(phi))
    im = ax0.imshow(np.flipud(pmft_image),
        extent=[lims[0], lims[1], lims[0], lims[1]],
        interpolation='nearest', cmap='viridis',
        vmin=-2.5, vmax=3.0)
    ax1.set_title('PMFT Contour Plot, $\phi = {}$'.format(phi))
    ax1.contour(reduced_x, reduced_y, pmft_smooth, [-2, -1, 0, 2], colors=colors)

f.subplots_adjust(right=0.85)
cbar_ax = f.add_axes([0.88, 0.1, 0.02, 0.8])
f.colorbar(im, cax=cbar_ax)
plt.show()
65% density

The plot below shows the PMFT of hexagons at 65% density. The hexagons tend to be close to one another, in the darker regions (the lower values of the potential of mean force and torque).

The hatched region near the black hexagon in the center is a region where no data were collected: the hexagons are hard shapes and cannot overlap, so there is an excluded region of space close to the hexagon.

The ring around the hexagon where the PMFT rises and then falls corresponds to the minimum of the radial distribution function – particles tend to not occupy that region, preferring instead to be at close range (in the first neighbor shell) or further away (in the second neighbor shell).

[3]: plot_pmft('data/phi065', 0.65)

75% density

As the system density is increased to 75%, the propensity for hexagons to occupy the six sites on the faces of their neighbors increases, as seen by the deeper (darker) wells of the PMFT. Conversely, the shapes strongly dislike occupying the yellow regions, and no particle pairs occupied the white region (so there is no data).

[4]: plot_pmft('data/phi075', 0.75)
Finally, at 85% density, there is a large region where no neighbors can be found, and hexagons strictly occupy sites near those of the perfect hexagonal lattice, at the first- and second-neighbor shells. The wells are deeper and much more spatially confined than those of the systems at lower densities.

```
[5]: plot_pmft('data/phi085', 0.85)
```

**freud.pmft.PMFTXYZ: Shifting Example**

This notebook shows how to use the shifting option on PMFTXYZ to get high resolution views of PMFT features that are not centered.
First we load in our data. The particles used here are implemented with a simple Weeks-Chandler-Andersen isotropic pair potential, so particle orientation is not meaningful.

```
[2]: pos_data = np.load('data/XYZ/positions.npy')
box_data = np.load('data/XYZ/boxes.npy')
```

We calculate the PMFT the same way as shown in other examples first

```
[3]: window = 2**(1/6) # The size of the pmft calculation

bins = 100
pmft = freud.pmft.PMFTXYZ(x_max=window, y_max=window, z_max=window, bins=bins)

# This data is for isotropic particles, so we will just make some unit quaternions
# to use as the orientations
quats = np.zeros((pos_data.shape[1],4)).astype(np.float32)
quats[:,0] = 1
for i in range(10, pos_data.shape[0]):
    box = box_data[i]
    points = pos_data[i]
    pmft.compute((box, points), quats, reset=False)
unshifted = pmft.pmft
x, y, z = pmft.bin_centers
```

When we plot a centered slice of the XYZ pmft, we see that a number of wells are present at some distance from the origin

```
[4]: %matplotlib inline

plt.figure(figsize=(10,10))
plt.imshow(unshifted[int(bins/2),:,:])
plt.colorbar()
plt.show()
```
If we want a closer look at the details of those wells, then we could increase the PMFT resolution. But this will increase the computational cost by a lot, and we are wasting a big percentage of the pixels.

This use case is why the shiftvec argument was implemented. Now we will do the same calculation, but we will use a much smaller window centered on one of the wells.

To do this we need to pass a vector into the PMFTXYZ construction. The window will be centered on this vector.

```python
[5]: shiftvec = [0.82, 0.82, 0]

window = 2**(1/6)/6  # Smaller window for the shifted case

bins = 50

pmft = freud.pmft.PMFTXYZ(x_max=window, y_max=window, z_max=window, bins=50, shiftvec=shiftvec)

# This data is for isotropic particles, so we will just make some unit quaternions
# to use as the orientations
```

(continues on next page)
orientations = np.array([[1, 0, 0, 0]] * pos_data.shape[1])

for i in range(10, pos_data.shape[0]):
    box = box_data[i]
    points = pos_data[i]
    pmft.compute(system=(box, points), orientations=orientations, reset=False)

shifted = pmft.pmft
x, y, z = pmft.bin_centers

Now the PMFT is a high resolution close up of one of the bonding wells. Note that as you increase the sampling resolution, you need to increase your number of samples because there is less averaging in each bin.

[6]: %matplotlib inline
plt.figure(figsize=(10, 10))
plt.imshow(shifted[int(bins/2), :, :])
plt.colorbar()
plt.show()
6.5.3 Example Analyses

The examples below go into greater detail about specific applications of freud and use cases that its analysis methods enable, such as user-defined analyses, machine learning, and data visualization.

Implementing Common Neighbor Analysis as a custom method

Researchers commonly wish to implement their own custom analysis methods for particle simulations. Here, we show an example of how to write Common Neighbor Analysis (Honeycutt and Andersen, J. Phys. Chem. 91, 4950) as a custom method using freud and the NetworkX package.

NetworkX can be installed with pip install networkx.

First, we generate random points and determine which points share neighbors.
```python
import freud
import numpy as np
from collections import defaultdict

# Use a face-centered cubic (fcc) system
box, points = freud.data.UnitCell.fcc().generate_system(4)
aq = freud.AABBQuery(box, points)
nl = aq.query(points, {'num_neighbors': 12, 'exclude_ii': True}).toNeighborList()

# Get all sets of common neighbors.
common_neighbors = defaultdict(list)
for i, p in enumerate(points):
    for j in nl.point_indices[nl.query_point_indices == i]:
        for k in nl.point_indices[nl.query_point_indices == j]:
            if i != k:
                common_neighbors[(i, k)].append(j)

Next, we use NetworkX to build graphs of common neighbors and compute the Common Neighbor Analysis signatures.

import networkx as nx
from collections import Counter
diagrams = defaultdict(list)
particle_counts = defaultdict(Counter)

for (a, b), neighbors in common_neighbors.items():
    g = nx.Graph()
    for i in neighbors:
        for j in set(nl.point_indices[nl.query_point_indices == i]).intersection(neighbors):
            g.add_edge(i, j)

    # Define the identifiers for a CNA diagram:
    # The first integer is 1 if the particles are bonded, otherwise 2
    # The second integer is the number of shared neighbors
    # The third integer is the number of bonds among shared neighbors
    # The fourth integer is an index, just to ensure uniqueness of diagrams
    diagram_type = 2-int(b in nl.point_indices[nl.query_point_indices == a])
    key = (diagram_type, len(neighbors), g.number_of_edges())
    isomorphs = [nx.is_isomorphic(g, h) for h in diagrams[key]]
    if any(isomorphs):
        idx = isomorphs.index(True)
    else:
        diagrams[key].append(g)
        idx = diagrams[key].index(g)
    else:
        diagrams[key].append(g)
        idx = diagrams[key].index(g)
```

(continues on next page)
Looking at the counts of common neighbor signatures, we see that the first particle of the fcc structure has 12 bonds with signature \((1, 4, 2, 0)\) as we expect.

```
[5]: particle_counts[0]
[5]: Counter({(1, 4, 2, 0): 12, 
            (2, 4, 4, 0): 6, 
            (2, 1, 0, 0): 12, 
            (2, 2, 1, 0): 24})
```

**Analyzing simulation data from HOOMD-blue at runtime**

The following script shows how to use freud to compute the radial distribution function \(g(r)\) on data generated by the molecular dynamics simulation engine HOOMD-blue *during a simulation run*.

Generally, most users will want to run analyses as post-processing steps, on the saved frames of a particle trajectory file. However, it is possible to use analysis callbacks in HOOMD-blue to compute and log quantities at runtime, too. By using analysis methods at runtime, it is possible to stop a simulation early or change the simulation parameters dynamically according to the analysis results.

HOOMD-blue can be installed with `conda install -c conda-forge hoomd`.

The simulation script runs a Monte Carlo simulation of spheres, with outputs parsed with `numpy.genfromtxt`.

```
[1]: %matplotlib inline
    import hoomd
    from hoomd import hpmc
    import freud
    import numpy as np
    import matplotlib.pyplot as plt

[2]: hoomd.context.initialize('')
    system = hoomd.init.create_lattice(
        hoomd.lattice.sc(a=1), n=10)
    mc = hpmc.integrate.sphere(seed=42, d=0.1, a=0.1)
    mc.shape_param.set('A', diameter=0.5)
    rdf = freud.density.RDF(bins=50, r_max=4)
    w6 = freud.order.Steinhardt(l=6, w6='True')

    def calc_rdf(timestep):
        hoomd.util.quiet_status()
        snap = system.take_snapshot()
        hoomd.util.unquiet_status()
        rdf.compute(system=snap, reset=False)

    def calc_W6(timestep):
        hoomd.util.quiet_status()
        snap = system.take_snapshot()
        hoomd.util.unquiet_status()
        w6.compute(system=snap, neighbors={'num_neighbors': 12})
        return np.mean(w6.particle_order)
```
# Equilibrate the system a bit before accumulating the RDF.
hoomd.run(1e4)
hoomd.analyze.callback(calc_rdf, period=100)

logger = hoomd.analyze.log(filename='output.log',
    quantities=['w6'],
    period=100,
    header_prefix='#',
    overwrite=True)

logger.register_callback('w6', calc_W6)

hoomd.run(1e4)

# Store the computed RDF in a file
np.savetxt('rdf.csv', np.vstack((rdf.bin_centers, rdf.rdf)).T,
    delimiter=',', header='r, g(r)')

HOOMD-blue v2.7.0-77-g568406147 DOUBLE HPMC_MIXED MPI TBB SSE SSE2 SSE3 SSE4_1 SSE4_2, AVX AVX2
Compiled: 10/28/2019
Copyright (c) 2009-2019 The Regents of the University of Michigan.
---
You are using HOOMD-blue. Please cite the following:
---
---
You are using HPMC. Please cite the following:
---

HOOMD-blue is running on the CPU
notice(2): Group "all" created containing 1000 particles
** starting run **
Time 00:00:10 | Step 3878 / 10000 | TPS 387.761 | ETA 00:00:15
Time 00:00:20 | Step 7808 / 10000 | TPS 392.99 | ETA 00:00:05
Time 00:00:25 | Step 10000 / 10000 | TPS 398.521 | ETA 00:00:00
Average TPS: 392.122
------
notice(2): - HPMC stats:
notice(2): Average translate acceptance: 0.933106
notice(2): Trial moves per second: 1.56844e+06
notice(2): Overlap checks per second: 4.07539e+07
notice(2): Overlap checks per trial move: 25.9838
notice(2): Number of overlap errors: 0
** run complete **
** starting run **
Time 00:00:35 | Step 13501 / 20000 | TPS 349.776 | ETA 00:00:18
Time 00:00:45 | Step 17001 / 20000 | TPS 349.699 | ETA 00:00:08
Time 00:00:54 | Step 20000 / 20000 | TPS 352.224 | ETA 00:00:00
Average TPS: 350.471

(continues on next page)
Notice:

---

notice(2): - HPMC stats:
notice(2): Average translate acceptance: 0.932846
notice(2): Trial moves per second: 1.40185e+06
notice(2): Overlap checks per second: 3.63552e+07
notice(2): Overlap checks per trial move: 25.9338
notice(2): Number of overlap errors: 0

** run complete **

[3]:

rdf_data = np.genfromtxt('rdf.csv', delimiter=',')
plt.plot(rdf_data[:, 0], rdf_data[:, 1])
plt.title('Radial Distribution Function')
plt.xlabel('$r$')
plt.ylabel('$g(r)$')
plt.show()

[4]:

w6_data = np.genfromtxt('output.log')
plt.plot(w6_data[:, 0], w6_data[:, 1])
plt.title('$w_6$ Order Parameter')
plt.xlabel('$t$')
plt.ylabel('$w_6(t)$')
plt.show()
Analyzing data from LAMMPS

The following script shows how to use freud to compute the radial distribution function \( g(r) \) on data generated by the molecular dynamics simulation engine LAMMPS. The input script runs a Lennard-Jones system, which is then parsed with numpy.genfromtxt.

The input script is below. Note that we must dump images with \( ix \ iy \ iz \), so that the mean squared displacement can be calculated correctly.

![w6 Order Parameter](image)

```bash
[1]: !cat lj.in

# From http://utkstair.org/clausius/docs/mse614/text/examples.html
# define units
units lj

# specify periodic boundary conditions
boundary p p p

# define atom_style
# full covers everything
atom_style full

# define simulation volume
# If I want \( N = 512 \) atoms
# and I want a density of \( \rho = 0.5 \) atoms/lj-sigma^3
# Then I can determine the size of a cube by
# size = (N/\rho)^{1/3}
variable side equal 10
region boxid block 0.0 ${side} 0.0 ${side} 0.0 ${side}
create_box 1 boxid

# specify initial positions of atoms
# sc = simple cubic
# 0.5 = density in lj units
lattice sc 0.50
```

(continues on next page)
# place atoms of type 1 in boxid
create_atoms 1 box

# define mass of atom type 1
mass 1 1.0

# specify initial velocity of atoms
# group = all
# reduced temperature is T = 1.0 = lj-eps/kb
# seed for random number generator
# distribution is gaussian (e.g. Maxwell-Boltzmann)
velocity all create 1.0 87287 dist gaussian

# specify interaction potential
# pairwise interaction via the Lennard-Jones potential with a cut-off at 2.5 lj-sigma
pair_style lj/cut 2.5

# specify parameters between atoms of type 1 with an atom of type 1
# epsilon = 1.0, sigma = 1.0, cutoff = 2.5
pair_coeff 1 1 1.0 1.0 2.5

# add long-range tail correction
pair_modify tail yes

# specify parameters for neighbor list
# rnbr = rcut + 0.3
neighbor 0.3 bin

# specify thermodynamic properties to be output
# pe = potential energy
# ke = kinetic energy
# etotal = pe + ke
# temp = temperature
# press = pressure
# density = number density
# output every thousand steps
# norm = normalize by # of atoms (yes or no)
thermo_style custom step pe ke etotal temp press density

# report instantaneous thermo values every 100 steps
thermo 100

# normalize thermo properties by number of atoms (yes or no)
thermo_modify norm no

# specify ensemble
# fixid = 1
# atoms = all
# ensemble = nve or nvt
fix 1 all nve

# timestep 0.005

timestep 0.005

# run 1000 steps in the NVE ensemble
# (this equilibrates positions)
run 1000
# stop fix with given fixid
# fixid = 1
unfix 1

# specify ensemble
# fixid = 2
# atoms = all
# ensemble = nvt
# temp = temperature
# initial temperature = 1.0
# final temperature = 1.0
# thermostat controller gain = 0.1 (units of time, bigger is less tight control)
fix 2 all nvt temp 1.0 1.0 0.1

# run 1000 steps in the NVT ensemble
# (this equilibrates thermostat)
run 1000

# save configurations
# dumpid = 1
# all atoms
# atomic symbol is Ar
# save positions every 100 steps
# filename = output.xyz
# dump 2 all custom 100 output_custom.xyz x y z ix iy iz

# run 1000 more steps in the NVT ensemble
# (this is data production, from which configurations are saved)
run 8000

Next, we run LAMMPS to generate the output file. LAMMPS can be installed with conda install -c conda-forge lammps.

[2]: !lmp_serial -in lj.in

LAMMPS (5 Jun 2019)
Created orthogonal box = (0 0 0) to (10 10 10)
  1 by 1 by 1 MPI processor grid
Lattice spacing in x,y,z = 1.25992 1.25992 1.25992
Created 512 atoms
  create_atoms CPU = 0.00122023 secs
Neighbor list info ...
  update every 1 steps, delay 10 steps, check yes
  master list distance cutoff = 2.8
  ghost atom cutoff = 2.8
  binsize = 1.4, bins = 8 8 8
  1 neighbor lists, perpetual/occasional/extra = 1 0 0
(1) pair lj/cut, perpetual
  attributes: half, newton on
  pair build: half/bin/newton
  stencil: half/bin/3d/newton
  bin: standard
Setting up Verlet run ...
  Unit style : lj

(continues on next page)
Current step : 0
Time step : 0.005
Per MPI rank memory allocation (min/avg/max) = 6.109 | 6.109 | 6.109 Mbytes

<table>
<thead>
<tr>
<th>Step</th>
<th>PotEng</th>
<th>KinEng</th>
<th>TotEng</th>
<th>Temp</th>
<th>Press</th>
<th>Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-1804.3284</td>
<td>766.5</td>
<td>-1037.8284</td>
<td>1</td>
<td>-2.1872025</td>
<td>0.512</td>
</tr>
<tr>
<td>100</td>
<td>-1834.8127</td>
<td>774.55302</td>
<td>-1060.2596</td>
<td>1.0105062</td>
<td>-0.32671112</td>
<td>0.512</td>
</tr>
<tr>
<td>200</td>
<td>-1852.2773</td>
<td>789.53605</td>
<td>-1062.7413</td>
<td>1.0300536</td>
<td>-0.30953463</td>
<td>0.512</td>
</tr>
<tr>
<td>300</td>
<td>-1857.4621</td>
<td>795.78772</td>
<td>-1061.6744</td>
<td>1.0382097</td>
<td>-0.22960441</td>
<td>0.512</td>
</tr>
<tr>
<td>400</td>
<td>-1864.766</td>
<td>801.81089</td>
<td>-1062.9551</td>
<td>1.0460677</td>
<td>-0.24901206</td>
<td>0.512</td>
</tr>
<tr>
<td>500</td>
<td>-1860.0198</td>
<td>796.65657</td>
<td>-1063.3633</td>
<td>1.0393432</td>
<td>-0.14280039</td>
<td>0.512</td>
</tr>
<tr>
<td>600</td>
<td>-1859.1835</td>
<td>796.96259</td>
<td>-1062.221</td>
<td>1.0397425</td>
<td>-0.2828161</td>
<td>0.512</td>
</tr>
<tr>
<td>700</td>
<td>-1848.9874</td>
<td>786.01864</td>
<td>-1062.9688</td>
<td>1.0254646</td>
<td>-0.3542435</td>
<td>0.512</td>
</tr>
<tr>
<td>800</td>
<td>-1821.7263</td>
<td>759.86418</td>
<td>-1061.8622</td>
<td>0.9913427</td>
<td>-0.1766353</td>
<td>0.512</td>
</tr>
<tr>
<td>900</td>
<td>-1840.7256</td>
<td>777.68022</td>
<td>-1063.0453</td>
<td>1.0145861</td>
<td>-0.318844</td>
<td>0.512</td>
</tr>
<tr>
<td>1000</td>
<td>-1862.6606</td>
<td>799.32963</td>
<td>-1063.3309</td>
<td>1.0428306</td>
<td>-0.25224674</td>
<td>0.512</td>
</tr>
</tbody>
</table>

Loop time of 0.197457 on 1 procs for 1000 steps with 512 atoms
Performance: 2187817.275 tau/day, 5064.392 timesteps/s
99.5% CPU use with 1 MPI tasks x no OpenMP threads

MPI task timing breakdown:

<table>
<thead>
<tr>
<th>Section</th>
<th>min time</th>
<th>avg time</th>
<th>max time</th>
<th>%varavg</th>
<th>%total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pair</td>
<td>0.13402</td>
<td>0.13402</td>
<td>0.13402</td>
<td>0.0</td>
<td>67.87</td>
</tr>
<tr>
<td>Bond</td>
<td>8.2254e-05</td>
<td>8.2254e-05</td>
<td>8.2254e-05</td>
<td>0.0</td>
<td>0.04</td>
</tr>
<tr>
<td>Neigh</td>
<td>0.049226</td>
<td>0.049226</td>
<td>0.049226</td>
<td>0.0</td>
<td>24.93</td>
</tr>
<tr>
<td>Comm</td>
<td>0.0084078</td>
<td>0.0084078</td>
<td>0.0084078</td>
<td>0.0</td>
<td>4.26</td>
</tr>
<tr>
<td>Output</td>
<td>0.00015664</td>
<td>0.00015664</td>
<td>0.00015664</td>
<td>0.0</td>
<td>0.08</td>
</tr>
<tr>
<td>Modify</td>
<td>0.0042217</td>
<td>0.0042217</td>
<td>0.0042217</td>
<td>0.0</td>
<td>2.14</td>
</tr>
<tr>
<td>Other</td>
<td>0.001339</td>
<td></td>
<td></td>
<td></td>
<td>0.68</td>
</tr>
</tbody>
</table>

Nlocal: 512 ave 512 max 512 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Nghost: 1447 ave 1447 max 1447 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Neighs: 12018 ave 12018 max 12018 min
Histogram: 1 0 0 0 0 0 0 0 0 0

Total # of neighbors = 12018
Ave neighs/atom = 23.4727
Ave special neighs/atom = 0
Neighbor list builds = 100
Dangerous builds = 100
Setting up Verlet run ...
Unit style : lj
Current step : 1000
Time step : 0.005
Per MPI rank memory allocation (min/avg/max) = 6.109 | 6.109 | 6.109 Mbytes

<table>
<thead>
<tr>
<th>Step</th>
<th>PotEng</th>
<th>KinEng</th>
<th>TotEng</th>
<th>Temp</th>
<th>Press</th>
<th>Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>-1862.6606</td>
<td>799.32963</td>
<td>-1063.3309</td>
<td>1.0428306</td>
<td>-0.25224674</td>
<td>0.512</td>
</tr>
</tbody>
</table>

(continues on next page)
Loop time of 0.199068 on 1 procs for 1000 steps with 512 atoms

Performance: 2170111.968 tau/day, 5023.407 timesteps/s
99.7% CPU use with 1 MPI tasks x no OpenMP threads

MPI task timing breakdown:

<table>
<thead>
<tr>
<th>Section</th>
<th>min time</th>
<th>avg time</th>
<th>max time</th>
<th>%varavg</th>
<th>%total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pair</td>
<td>0.13415</td>
<td>0.13415</td>
<td>0.13415</td>
<td>0.0</td>
<td>67.39</td>
</tr>
<tr>
<td>Bond</td>
<td>6.5804e-05</td>
<td>6.5804e-05</td>
<td>6.5804e-05</td>
<td>0.0</td>
<td>0.03</td>
</tr>
<tr>
<td>Neigh</td>
<td>0.049349</td>
<td>0.049349</td>
<td>0.049349</td>
<td>0.0</td>
<td>24.79</td>
</tr>
<tr>
<td>Comm</td>
<td>0.0079017</td>
<td>0.0079017</td>
<td>0.0079017</td>
<td>0.0</td>
<td>4.00</td>
</tr>
<tr>
<td>Output</td>
<td>0.0013518</td>
<td>0.0013518</td>
<td>0.0013518</td>
<td>0.0</td>
<td>0.07</td>
</tr>
<tr>
<td>Modify</td>
<td>0.0060918</td>
<td>0.0060918</td>
<td>0.0060918</td>
<td>0.0</td>
<td>3.06</td>
</tr>
<tr>
<td>Other</td>
<td>0.001308</td>
<td></td>
<td></td>
<td></td>
<td>0.66</td>
</tr>
</tbody>
</table>

Nlocal:  512 ave 512 max 512 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Nghost:  1464 ave 1464 max 1464 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Neighs:  11895 ave 11895 max 11895 min
Histogram: 1 0 0 0 0 0 0 0 0 0

Total # of neighbors = 11895
Ave neighs/atom = 23.2324
Ave special neighs/atom = 0
Neighbor list builds = 100
Dangerous builds = 100
Setting up Verlet run ...

Unit style : lj
Current step : 2000
Time step : 0.005
Per MPI rank memory allocation (min/avg/max) = 7.383 | 7.383 | 7.383 Mbytes

6.5. Examples 101
| 4000 | -1882.7617 | 803.22857 | -1079.5332 | 1.0479172 | -0.3189643 | 0.512 |
| 4100 | -1873.9061 | 787.05281 | -1086.8533 | 1.0268138 | -0.2660844 | 0.512 |
| 4200 | -1871.6627 | 832.59728 | -1039.0655 | 1.0862326 | -0.2904019 | 0.512 |
| 4300 | -1865.3725 | 819.61212 | -1045.7603 | 1.0692917 | -0.2259231 | 0.512 |
| 4400 | -1875.5306 | 806.71297 | -1068.8176 | 1.0524631 | -0.3160479 | 0.512 |
| 4500 | -1857.109  | 828.16158 | -1028.9474 | 1.0046546 | -0.2464398 | 0.512 |
| 4600 | -1857.8912 | 729.72570 | -1128.1655 | 0.9520231 | -0.3138504 | 0.512 |
| 4700 | -1842.205  | 734.17836 | -1108.0267 | 0.9578322 | -0.2713040 | 0.512 |
| 4800 | -1864.7696 | 776.14641 | -1088.6232 | 1.0125850 | -0.3166811 | 0.512 |
| 4900 | -1858.1103 | 793.41913 | -1064.6911 | 1.0351195 | -0.1658337 | 0.512 |
| 5000 | -1867.7818 | 815.23276 | -1052.5491 | 1.0635783 | -0.2868064 | 0.512 |
| 5100 | -1838.0477 | 725.412  | -1112.6357 | 0.9463953 | -0.2864787 | 0.512 |
| 5200 | -1810.7731 | 731.9772 | -1108.0267 | 0.9578322 | -0.2713040 | 0.512 |
| 5300 | -1837.5311 | 749.48424 | -1088.0469 | 0.9778007 | -0.3871072 | 0.512 |
| 5400 | -1873.293  | 740.70637 | -1133.2877 | 0.9663488 | -0.2603929 | 0.512 |
| 5500 | -1854.9994 | 735.97428 | -1119.0252 | 0.9601752 | -0.2822844 | 0.512 |
| 5600 | -1841.9759 | 797.06384 | -1044.9121 | 1.0398745 | -0.1914545 | 0.512 |
| 5700 | -1853.6532 | 764.84642 | -1088.8067 | 0.9978426 | -0.3224785 | 0.512 |
| 5800 | -1851.9183 | 719.20424 | -1138.4361 | 0.9382965 | -0.3224785 | 0.512 |
| 5900 | -1848.0739 | 757.0399 | -1156.9807 | 0.9753103 | -0.3846402 | 0.512 |
| 6000 | -1841.0455 | 779.78036 | -1119.4357 | 0.9756748 | -0.2607688 | 0.512 |
| 6100 | -1887.3837 | 878.92659 | -1008.4571 | 1.1466753 | -0.3466673 | 0.512 |
| 6200 | -1879.4834 | 767.25891 | -1112.2245 | 1.0009901 | -0.3331713 | 0.512 |
| 6300 | -1865.3725 | 819.61212 | -1045.7603 | 1.0692917 | -0.2259231 | 0.512 |

(continues on next page)
9700  -1878.5858  771.53563  -1107.0502  1.0065696  -0.2300855  0.512
9800  -1848.4047  752.27373  -1096.1309  0.98143997  -0.28729274  0.512
9900  -1865.561   731.41466  -1134.1464  0.95422656  -0.3874617  0.512
10000 -1887.2808  787.80237  -1099.4784  1.0277917  -0.26779032  0.512

Loop time of 1.63759 on 1 procs for 8000 steps with 512 atoms

Performance: 2110423.670 tau/day, 4885.240 timesteps/s
99.4% CPU use with 1 MPI tasks x no OpenMP threads

MPI task timing breakdown:
<table>
<thead>
<tr>
<th>Section</th>
<th>min time</th>
<th>avg time</th>
<th>max time</th>
<th>%varavg</th>
<th>%total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pair</td>
<td>1.0823</td>
<td>1.0823</td>
<td>1.0823</td>
<td>0.0</td>
<td>66.09</td>
</tr>
<tr>
<td>Bond</td>
<td>0.00054955</td>
<td>0.00054955</td>
<td>0.00054955</td>
<td>0.0</td>
<td>0.03</td>
</tr>
<tr>
<td>Neigh</td>
<td>0.39492</td>
<td>0.39492</td>
<td>0.39492</td>
<td>0.0</td>
<td>24.12</td>
</tr>
<tr>
<td>Comm</td>
<td>0.064503</td>
<td>0.064503</td>
<td>0.064503</td>
<td>0.0</td>
<td>3.94</td>
</tr>
<tr>
<td>Output</td>
<td>0.035598</td>
<td>0.035598</td>
<td>0.035598</td>
<td>0.0</td>
<td>2.17</td>
</tr>
<tr>
<td>Modify</td>
<td>0.049172</td>
<td>0.049172</td>
<td>0.049172</td>
<td>0.0</td>
<td>3.00</td>
</tr>
<tr>
<td>Other</td>
<td>0.01058</td>
<td></td>
<td></td>
<td></td>
<td>0.65</td>
</tr>
</tbody>
</table>

Nlocal: 512 ave 512 max 512 min
Histogram: 1 0 0 0 0 0 0 0 0
Nghost: 1398 ave 1398 max 1398 min
Histogram: 1 0 0 0 0 0 0 0 0
Neighs: 12036 ave 12036 max 12036 min
Histogram: 1 0 0 0 0 0 0 0 0

Total # of neighbors = 12036
Ave neighs/atom = 23.5078
Ave special neighs/atom = 0
Neighbor list builds = 800
Dangerous builds = 800
Total wall time: 0:00:02

[3]: %matplotlib inline

import freud
from matplotlib import pyplot as plt
import numpy as np
import warnings

[4]: with warnings.catch_warnings():
    warnings.simplefilter('ignore')
    # We read the number of particles, the system box, and the
    # particle positions into 3 separate arrays.
    N = int(np.genfromtxt(
        'output_custom.xyz', skip_header=3, max_rows=1))
    box_data = np.genfromtxt(
        'output_custom.xyz', skip_header=5, max_rows=3)
    data = np.genfromtxt(
        'output_custom.xyz', skip_header=9,
        invalid_raise=False)
    # Remove the unwanted text rows
    data = data[~np.isnan(data).all(axis=1)].reshape(-1, N, 6)

(continues on next page)
box = freud.box.Box.from_box(
    box_data[:, 1] - box_data[:, 0])

# We shift the system by half the box lengths to match the
# freud coordinate system, which is centered at the origin.
# Since all methods support periodicity, this shift is simply
# for consistency but does not affect any analyses.
data[..., :3] -= box.L/2
rdf = freud.density.RDF(bins=100, r_max=4, r_min=1)
for frame in data:
    rdf.compute(system=(box, frame[:, :3]), reset=False)

msd = freud.msd.MSD(box)
msd.compute(positions=data[:, :, :3], images=data[:, :, 3:])

# Plot the RDF
plt.plot(rdf.bin_centers, rdf.rdf)
plt.title('Radial Distribution Function')
plt.xlabel('$r$')
plt.ylabel('$g(r)$')
plt.show()

# Plot the MSD
plt.plot(msd.msd)
plt.title('Mean Squared Displacement')
plt.xlabel('$t$')
plt.ylabel('MSD$(t)$')
plt.show()
Using Machine Learning for Structural Identification

This notebook provides a demonstration of how a simple set of descriptors computed by freud can be coupled with machine learning for structural identification. The set of descriptors used here are not enough to identify complex crystal structures, but this notebook provides an introduction. For a more powerful set of descriptors, see the paper Machine learning for crystal identification and discovery (Spellings 2018) and the library pythia, both of which use freud for their computations.

```python
import freud
import matplotlib.pyplot as plt
import matplotlib.cm
import numpy as np
import pandas as pd
import warnings
warnings.filterwarnings("ignore")

We generate sample body-centered cubic, face-centered cubic, and simple cubic structures. Each structure has at least 4000 particles.

```python
N = 4000
noise = 0.04
structures = {}
n = round((N/2)**(1/3))
structures['bcc'] = freud.data.UnitCell.bcc().generate_system(n, sigma_noise=noise)
n = round((N/4)**(1/3))
structures['fcc'] = freud.data.UnitCell.fcc().generate_system(n, sigma_noise=noise)
n = round((N/1)**(1/3))
structures['sc'] = freud.data.UnitCell.sc().generate_system(n, sigma_noise=noise)
for name, (box, positions) in structures.items():
    print(name, 'has', len(positions), 'particles.

bcc has 4394 particles.
fcc has 4000 particles.
s c has 4096 particles.
```

Next, we compute the Steinhardt order parameters $q_l$ for $l \in \{4, 6, 8, 10, 12\}$. 

![Mean Squared Displacement](image)
We use the Voronoi neighbor list, removing neighbors whose Voronoi facets are small.

```python
[3]:
def get_features(box, positions, structure):
    voro = freud.locality.Voronoi()
    voro.compute(system=(box, positions))
    nlist = voro.nlist.copy()
    nlist.filter(nlist.weights > 0.1)
    features = {}
    for l in [4, 6, 8, 10, 12]:
        ql = freud.order.Steinhardt(l=l, weighted=True)
        ql.compute(system=(box, positions), neighbors=nlist)
        features['q{}/'.format(l)] = ql.particle_order
    return features
```

```python
[4]:
structure_features = {}
for name, (box, positions) in structures.items():
    structure_features[name] = get_features(box, positions, name)
```

Here, we plot a histogram of the $q_4$ and $q_6$ values for each structure.

```python
[5]:
for l in [4, 6]:
    plt.figure(figsize=(3, 2), dpi=300)
    for name in structures.keys():
        plt.hist(structure_features[name]['q{}/'.format(l)], range=(0, 1), bins=100, label=name, alpha=0.7)
    plt.title(r'$q_{\{l\}}$'.format(l=l))
    plt.legend()
    for lh in plt.legend().legendHandles:
        lh.set_alpha(1)
    plt.show()
```
Next, we will train a Support Vector Machine to predict particles’ structures based on these Steinhardt $Q_i$ descriptors. We build pandas data frames to hold the structure features, encoding the structure as an integer. We use `train_test_split` to train on part of the data and test the model on a separate part of the data.

```python
structure_dfs = {}
for i, structure in enumerate(structure_features):
    df = pd.DataFrame.from_dict(structure_features[structure])
    df['class'] = i
    structure_dfs[structure] = df

df = pd.concat(structure_dfs.values()).reset_index(drop=True)

from sklearn.preprocessing import normalize
from sklearn.model_selection import train_test_split
from sklearn.svm import SVC

X = df.drop('class', axis=1).values
X = normalize(X)
y = df['class'].values
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.33, random_state=42)

svm = SVC()
svm.fit(X_train, y_train)
```

(continues on next page)
Finally, we use the Uniform Manifold Approximation and Projection method (McInnes 2018, GitHub repo) to project the high-dimensional descriptors into a two-dimensional plot. Notice that some bcc particles overlap with fcc particles. This can be expected from the noise that was added to the structures. The particles that were incorrectly classified by the SVM above are probably located in this overlapping region.

```
[10]: from umap import UMAP
    umap = UMAP(random_state=42)
    X_reduced = umap.fit_transform(X)

[11]: plt.figure(figsize=(4, 3), dpi=300)
    for i in range(max(y) + 1):
        indices = np.where(y == i)[0]
        plt.scatter(X_reduced[indices, 0], X_reduced[indices, 1],
                    color=matplotlib.cm.tab10(i), s=8, alpha=0.2,
                    label=list(structure_features.keys())[i])
    plt.legend()
    for lh in plt.legend().legendHandles:
        lh.set_alpha(1)
    plt.show()
```
Calculating Strain via Voxelization

This notebook shows how to use freud’s neighbor finding to create a voxelized version of a system.

In brief, we are going to create a set of points that define the centers of our voxels, then assign all particles to one of these voxels. Then we sum up some property of the particles amongst all particles in a bin.

At the end we want to have a sampling of some particle property in our system on a regular grid (as a NumPy array).

```python
%matplotlib inline
from ipywidgets import FloatProgress
from IPython.display import display
from scipy.sparse import csr_matrix, csc_matrix
import freud
import numpy as np
import matplotlib.pyplot as plt
import re
```

This uses data from some text files that were output from the visualization software OVITO (https://ovito.org/)
The files have a header with box information, and then a list of particle info. These files have 10 fields per particle:

```
(ID#, position(x,y,z), strains(xx,yy,zz,yz,xz,xy))
```

The goal is to turn this into an \((N_x, N_y, N_z, 3, 3)\) NumPy array, where \(N_x, N_y, N_z\) are the number of bins in each dimension, and each of those bins has an averaged 3x3 strain array.

First we read in the box info from our text files and construct an average box. We need this so we can make our bin centers

```python
framefiles = ['data/strain_data/frame{f}'.format(f=f) for f in [100, 110, 120, 130]]
# read all the boxes, so we can make the grid points for voxelizing
boxes = []
for f in framefiles:
    ff = open(f, 'r')
    _ = ff.readline()
    header = ff.readline()

    match = re.match('^Lattice=".*"', header)
    boxstring = match.group(0)
    boxes.append(np.array(str.split(boxstring[9:-1]), dtype=np.float).reshape((3,3)).T)
    ff.close()

# find the average box
ave_box = np.array(boxes).mean(axis=0)
```

Now we make the bin centers using \(np.meshgrid\), but append and combine the X, Y, and Z coordinates into an array of shape \((N_x N_y N_z, 3)\) to pass to freud.

```python
res = (60, 10, 45) # The number of bins in x,y,z
xx = np.linspace(-ave_box[0,0]/2,ave_box[0,0]/2,num=res[0])
yy = np.linspace(-ave_box[1,1]/2,ave_box[1,1]/2,num=res[1])
zz = np.linspace(-ave_box[2,2]/2,ave_box[2,2]/2,num=res[2])
XX, YY, ZZ = np.meshgrid(xx,yy,zz)
XYZ = np.append(np.append(XX.flatten().reshape((-1,1)),
yz,xz,xy),
                 ...
```
Now we iterate over our files and compute the first nearest neighbor (among the bin centers) of the particles, so we
know which bin to average them in.

It is important to use scipy’s csr_matrix for this process when the number of particles is large. These files contain
>80,000 particles, and without the sparse matrix, the dot product to determine grid totals would be extremely slow.

```python
[4]: master_strains = np.zeros((XYZ.shape[0], 6)) # matrix to sum into
for i in range(len(framefiles)):
    data = np.loadtxt(framefiles[i], skiprows=2).astype(np.float32)
    box = freud.box.Box(Lx=boxes[i][0, 0],
                       Ly=boxes[i][1, 1],
                       Lz=boxes[i][2, 2],
                       yz=boxes[i][1, 2],
                       xz=boxes[i][0, 2],
                       xy=boxes[i][0, 1])
    nlist = freud.AABBQuery(box, XYZ).query(
        data[:,1:4], {'num_neighbors': 1}).toNeighborList()
    neighbors = nlist.point_indices
    sprse = csr_matrix((np.ones(len(neighbors)), (neighbors, np.
    →arange(len(neighbors)))),
                      shape=(XYZ.shape[0], len(neighbors)))
    # strain data
    sdata = data[:, 4:]
    binned = np.zeros((XYZ.shape[0], 6))
    grid_totals = sprse.dot(np.ones(len(neighbors)))
    grid_totals[grid_totals==0] = 1 # get rid of division errors
    for j in range(6):
        binned[:,j] = sprse.dot(sdata[:, j]) / grid_totals
    master_strains = master_strains + binned
master_strains = master_strains/len(framefiles) # divide by number of frames
```

Now we pack up the resulting array into the shape we want it to be: $(N_x, N_y, N_z, 3, 3)$

```python
[5]: final_matrix = np.zeros((res[1],res[0],res[2],3,3))
# this mapping turns 6 strain values into a symmetric (3,3) matrix
voigt_map = {0:(0,0), 1:(1,1), 2:(2,2), 3:(1,2), 4:(0,2), 5:(0,1)}
for i in range(6):
    v = voigt_map[i]
    final_matrix[:,:,v[0],v[1]] = master_strains[:,i].reshape(res[1],res[0],res[2])
    if v[0]!=v[1]:
        final_matrix[:,:,v[1],v[0]] = master_strains[:,i].reshape(res[1],res[0],
        →res[2])
```

Since we are only using four frames, the distribution is not very well sampled. But we can get a clue that a distinct

6.5. Examples
distribution of strain is emerging if we average along the first axis of the matrix (this particular system should not vary in that direction)

```python
[6]: plt.figure(figsize=(10,10))
plt.imshow(final_matrix[:,:,:,0,0].mean(axis=0),
    origin='lower', cmap=plt.cm.bwr,
    vmin=-0.04, vmax=0.04, interpolation='none')
plt.colorbar()
plt.show()
```

**Visualizing analyses with fresnel**

In this notebook, we simulate a system of tetrahedra, color particles according to their local density, and path-trace the resulting image with fresnel.

The cell below runs a short HOOMD-blue simulation of tetrahedra using Hard Particle Monte Carlo (HPMC).
import hoomd
import hoomd.hpmc

hoomd.context.initialize('')

# Create an 8x8x8 simple cubic lattice
system = hoomd.init.create_lattice(
    unitcell=hoomd.lattice.sc(a=1.5), n=8)

# Create our tetrahedra and configure the HPMC integrator
mc = hoomd.hpmc.integrate.convex_polyhedron(seed=42)
mc.set_params(d=0.2, a=0.1)
vertices = [(0.5, 0.5, 0.5),
            (-0.5, -0.5, 0.5),
            (-0.5, 0.5, -0.5),
            (0.5, -0.5, -0.5)]
mc.shape_param.set('A', vertices=vertices)

# Run for 5,000 steps
hoomd.run(5e3)
snap = system.take_snapshot()

Now we import the modules needed for analysis and visualization.

6.5. Examples
Next, we’ll set up the arrays needed for the scene and its geometry. This includes the analysis used for coloring particles.

```python
import fresnel
import freud
import matplotlib.cm
from matplotlib.colors import Normalize
import numpy as np
device = fresnel.Device()

poly_info = fresnel.util.convex_polyhedron_from_vertices(vertices)
positions = snap.particles.position
orientations = snap.particles.orientation
box = freud.Box.from_box(snap.box)
ld = freud.density.LocalDensity(3.0, 1.0)
ld.compute(system=snap)
colors = matplotlib.cm.viridis(Normalize()(ld.density))
box_points = np.asarray(
    box.make_absolute(
        [[0, 0, 0], [0, 0, 0], [0, 0, 0], [1, 1, 0],
         [1, 1, 0], [1, 1, 0], [0, 1, 1], [0, 1, 1],
         [0, 1, 1], [1, 0, 1], [1, 0, 1], [1, 0, 1]])
    box.make_absolute(
        [[1, 0, 0], [0, 1, 0], [0, 0, 1], [1, 0, 0],
         [0, 1, 0], [1, 1, 1], [1, 1, 1], [0, 1, 0],
         [0, 0, 1], [0, 0, 1], [1, 1, 1], [1, 0, 0]])
)

This cell creates the scene and geometry objects to be rendered by fresnel.

```python
import fresnel

geometry = fresnel.geometry.ConvexPolyhedron(
    scene, poly_info,
    position=positions,
    orientation=orientations,
    color=fresnel.color.linear(colors))

geometry.material = fresnel.material.Material(
    color=fresnel.color.linear([0.25, 0.5, 0.9]),
    roughness=0.8, primitive_color_mix=1.0)

geometry.outline_width = 0.05
box_geometry = fresnel.geometry.Cylinder(
    scene, points=box_points.swapaxes(0, 1))

box_geometry.radius[:] = 0.1
box_geometry.color[:] = np.tile([0, 0, 0], (12, 2, 1))

box_geometry.material.primitive_color_mix = 1.0

scene.camera = fresnel.camera.fit(scene, view='isometric', margin=0.1)

First, we preview the scene. (This doesn’t use path tracing, and is much faster.)

```python
fresnel.preview(scene, aa_level=3, w=600, h=600)
```
Finally, we use path tracing for a high quality image. The number of light samples can be increased to reduce path tracing noise.

```
[6]: fresnel.pathtrace(scene, light_samples=16, w=600, h=600)
```
Visualization with plato

In this notebook, we run a Lennard-Jones simulation, color particles according to their local density computed with freud, and display the results with plato. Note that plato has multiple backends – see the plato documentation for information about each backend and the features it supports.

```python
[1]: import hoomd
    import hoomd.md
    hoomd.context.initialize('')

    # Silence the HOOMD output
    hoomd.util.quiet_status()
    hoomd.option.set_notice_level(0)
```
# Create a 10x10x10 simple cubic lattice of particles with type name A
system = hoomd.init.create_lattice(unitcell=hoomd.lattice.sc(a=1.5, type_name='A'),
        n=10)

# Specify Lennard-Jones interactions between particle pairs
nl = hoomd.md.nlist.cell()
lj = hoomd.md.pair.lj(r_cut=3.0, nlist=nl)
lj.pair_coeff.set('A', 'A', epsilon=1.0, sigma=1.0)

# Integrate at constant temperature
hoomd.md.integrate.mode_standard(dt=0.005)
integrator = hoomd.md.integrate.nvt(group=hoomd.group.all(), kT=0.01, tau=0.5)
integrator.randomize_velocities(seed=42)

# Run for 10,000 time steps
hoomd.run(10e3)
snap = system.take_snapshot()

HOOMD-blue v2.6.0-151-gea140cffb DOUBLE HPMC_MIXED MPI TBB SSE SSE2 SSE3 SSE4_1
  →SSE4_2 AVX AVX2
Compiled: 09/25/2019
Copyright (c) 2009-2019 The Regents of the University of Michigan.
---
You are using HOOMD-blue. Please cite the following:
* J A Anderson, C D Lorenz, and A Travesset. "General purpose molecular dynamics
  simulations fully implemented on graphics processing units", Journal of
  Computational Physics 227 (2008) 5342-5359
* J Glaser, T D Nguyen, J A Anderson, P Liu, F Spiga, J A Millan, D C Morse, and
  S C Glotzer. "Strong scaling of general-purpose molecular dynamics simulations
  on GPUs", Computer Physics Communications 192 (2015) 97-107
---
HOOMD-blue is running on the CPU

Now we import the modules needed for visualization.

```python
# For interactive scenes, use:
import plato.draw.pythreejs as draw

# For static scenes, use:
import plato.draw.fresnel as draw
```

This code sets up the plato Scene object with the particles and colors computed above.

```python
positions = snap.particles.position
box = freud.Box.from_box(snap.box)
ld = freud.density.LocalDensity(3.0, 1.0)
ld.compute(system=snap)
colors = matplotlib.cm.viridis(Normalize()(ld.density))
radii = np.ones(len(positions)) * 0.5
box_prim = draw.Box.from_box(box, width=0.2)
sphere_prim = draw.Spheres(positions=snap.particles.position,
                           radii=radii,
                           ...
                           )
```
colors=colors,
    vertex_count=32)
scene = draw.Scene((sphere_prim, box_prim), zoom=1.5)

Click and drag the 3D scene below - it’s interactive!

```python
[4]: scene.show()
```

Renderer(camera=OrthographicCamera(bottom=-15.0,
<children=(DirectionalLight(intensity=0.692820323027551, posit...

Visualizing 3D Voronoi and Voxelization

The plato-draw package allows for visualizing particle data in 2D and 3D using a variety of backend libraries. Here, we show a 3D Voronoi diagram drawn using freenel and pythreejs. We use rowan to generate the view rotation.

To install dependencies:

- `conda install -c conda-forge freenel`
- `pip install plato-draw rowan`

```python
[1]:
    import freud
    import matplotlib.cm
    import numpy as np
    import rowan
    import plato.draw.fresnel
    backend = plato.draw.fresnel
    # For interactive scenes:
    # import plato.draw.pythreejs
    # backend = plato.draw.pythreejs

[2]:
    def plot_crystal(box, positions, colors=None, radii=None, backend=None,
                     polytopes=[], polytope_colors=None):
        if backend is None:
            backend = plato.draw.fresnel
        if colors is None:
            colors = np.array([[0.5, 0.5, 0.5, 1]] * len(positions))
        if radii is None:
            radii = np.array([0.5] * len(positions))
        sphere_prim = backend.Spheres(positions=positions, colors=colors, radii=radii)
        box_prim = backend.Box.from_box(box, width=0.1)
        if polytope_colors is None:
            polytope_colors = colors * np.array([1, 1, 1, 0.4])
        polytope_prims = []
        for p, c in zip(polytopes, polytope_colors):
            p_prim = backend.ConvexPolyhedra(
                positions=[[0, 0, 0]], colors=c, vertices=p, outline=0)
            polytope_prims.append(p_prim)
            rotation = rowan.multiply(
                rowan.from_axis_angle([1, 0, 0], np.pi/10),
                rowan.from_axis_angle([0, 1, 0], -np.pi/10))
            scene = backend.Scene((sphere_prim, box_prim, *polytope_prims),
                                   zoom=3, rotation=rotation)
        if backend is not plato.draw.fresnel:
            scene.enable('directional_light')
```
else:
    scene.enable('antialiasing')
scene.show()

We generate an fcc structure and add Gaussian noise to the positions. Colors are assigned randomly.

```python
[3]: np.random.seed(12)
    box, positions = freud.data.UnitCell.fcc().generate_system(3, scale=2, sigma_noise=0.05)
    cmap = matplotlib.cm.get_cmap('tab20')
    colors = cmap(np.random.rand(len(positions)))
```

```python
[4]: plot_crystal(box, positions, colors, backend=backend)
```

We make a Voronoi tessellation of the system and plot it in 3D. The Voronoi cells are approximately rhombic dodecahedra, which tesselate 3D space in a face-centered cubic lattice.

```python
[5]: voro = freud.locality.Voronoi()
    voro.compute(system=(box, positions))
    plot_crystal(box, positions, colors=colors,
                backend=backend, polytopes=voro.polytopes)
```
We generate a voxelization of this space by creating a dense lattice of points on a simple cubic lattice.

```
[6]: def make_cubic_grid(box, voxels_per_side):
    v_space = np.linspace(0, 1, voxels_per_side+1)
    v_space = (v_space[:-1] + v_space[1:])/2  # gets centers of the voxels
    return np.array([box.make_absolute([x, y, z])
                     for x in v_space for y in v_space for z in v_space])

[7]: voxels_per_side = 30
    cubic_grid = make_cubic_grid(box, voxels_per_side)
    # Make the spheres overlap just a bit
    radii = np.ones(len(cubic_grid)) * 0.8 * np.max(box.L) / voxels_per_side
    plot_crystal(box, cubic_grid, radii=radii, backend=backend)
```
We color the voxels by their first nearest neighbor. This is mathematically equivalent to being inside the corresponding Voronoi cell. Here, we get the neighbor indices (this can be used to separate the Voronoi cells into voxels).

```python
[8]: aq = freud.AABBQuery(box, positions)
voxel_neighbors = -np.ones(len(cubic_grid), dtype=np.int)
for i, j, distance in aq.query(cubic_grid, {'num_neighbors': 1}):
    voxel_neighbors[i] = j
```

Next, we use these indices to color and draw the voxelization.

```python
[9]: voxel_colors = np.array([colors[i] for i in voxel_neighbors])
plot_crystal(box, cubic_grid, colors=voxel_colors,
            radii=radii, backend=backend)
```
6.5.4 Benchmarks

Performance is a central consideration for freud. Below are some benchmarks comparing freud to other tools offering similar analysis methods.

Benchmarking Neighbor Finding against scipy

The neighbor finding algorithms in freud are highly efficient and rely on parallelized C++ code. Below, we show a benchmark of freud’s AABBQuery algorithm against the scipy.spatial.cKDTree. This benchmark was run on an Intel(R) Core(TM) i3-8100B CPU @ 3.60GHz.

```python
import freud
import scipy.spatial
import numpy as np
import matplotlib.pyplot as plt
import timeit
from tqdm import tqdm
```

```python
def make_scaled_system(N, Nneigh=12):
    L = (4 / 3 * np.pi * N / Nneigh)**(1/3)
    return freud.data.make_random_system(L, N)
```

[1]:
[2]:
(continues on next page)
box, points = make_scaled_system(1000)

## Timing Functions

```python
[3]: def time_statement(stmt, repeat=5, number=100, **kwargs):
    timer = timeit.Timer(stmt=stmt, globals=kwargs)
    times = timer.repeat(repeat, number)
    return np.mean(times), np.std(times)

[4]: def time_scipy_cKDTree(box, points):
    shifted_points = points + np.asarray(box.L)/2
    # SciPy only supports cubic boxes
    assert box.Lx == box.Ly == box.Lz
    assert box.xy == box.xz == box.yz == 0
    return time_statement("kdtree = scipy.spatial.cKDTree(points, boxsize=L);"
                          "kdtree.query_ball_tree(kdtree, r=rcut)",
                          scipy=scipy, points=shifted_points, L=box.Lx, rcut=1.0)

[5]: def time_freud_AABBQuery(box, points):
    return time_statement("aq = freud.locality.AABBQuery(box, points);
                           aq.query(points, {'r_max': r_max, 'exclude_ii': False})).
                          toNeighborList()",
                           freud=freud, box=box, points=points, r_max=1.0)

[6]: # Test timing functions
    kd_t = time_scipy_cKDTree(box, points)
    print(kd_t)
    abq_t = time_freud_AABBQuery(box, points)
    print(abq_t)

(0.4641454226, 0.003790939209936744)
(0.2630035949999998, 0.006359869892978881)

## Perform Measurements

```python
[7]: def measure_runtime_scaling_N(Ns, r_max=1.0):
    result_times = []
    for N in tqdm(Ns):
        box, points = make_scaled_system(N)
        result_times.append((
            time_scipy_cKDTree(box, points),
            time_freud_AABBQuery(box, points)))
    return np.asarray(result_times)

[8]: def plot_result_times(result_times, Ns):
    plt.figure(figsize=(6, 4), dpi=200)
    plt.errorbar(Ns, result_times[:, 0, 0], result_times[:, 0, 1], label="scipy v{}
    "cKDTree".format(scipy.__version__)
    plt.errorbar(Ns, result_times[:, 1, 0], result_times[:, 1, 1], label="freud v{}
    "AABBQuery".format(freud.__version__))

(continues on next page)
plt.title(r'Neighbor finding for 12 average neighbors')
plt.xlabel(r'Number of points $N$')
plt.ylabel(r'Runtime for 100 iterations (s)')
plt.legend()
plt.show()

[9]: # Use geometrically-spaced values of N, rounded to one significant figure
    Ns = list(sorted(set(map(lambda x: int(round(x, -int(np.floor(np.log10(np.abs(x)))))),
                           np.exp(np.linspace(np.log(50), np.log(5000), 10))))))

[10]: result_times = measure_runtime_scaling_N(Ns)
    plot_result_times(result_times, Ns)

100%|| 10/10 [00:42<00:00, 4.21s/it]

---

**Benchmarking RDF against MDAnalysis**

The algorithms in freud are highly efficient and rely on parallelized C++ code. Below, we show a benchmark of `freud.density.RDF` against `MDAnalysis.analysis.rdf`. This benchmark was run on an Intel(R) Core(TM) i3-8100B CPU @ 3.60GHz.

[1]: import freud
    import gsd
import MDAnalysis
import MDAnalysis.analysis.rdf
import multiprocessing as mp
import numpy as np
import matplotlib.pyplot as plt
import timeit
from tqdm import tqdm

trajectory_filename = 'data/rdf_benchmark.gsd'
r_max = 5
r_min = 0.1
nbins = 75

trajectory = MDAnalysis.coordinates.GSD.GSDReader(trajectory_filename)
topology = MDAnalysis.core.topology.Topology(n_atoms=trajectory[0].n_atoms)
u = MDAnalysis.as_Universe(topology, trajectory_filename)

rdf = MDAnalysis.analysis.rdf.InterRDF(g1=u.atoms, g2=u.atoms,
nbins=nbins,
range=(r_min, r_max)).run()

plt.plot(rdf.bins, rdf.rdf)
plt.show()

freud_rdf = freud.density.RDF(bins=nbins, r_max=r_max, r_min=r_min)
for frame in trajectory:
    freud_rdf.compute(system=frame, reset=False)
freud_rdf
Timing Functions

[6]: `def time_statement(stmt, repeat=3, number=1, **kwargs):
    timer = timeit.Timer(stmt=stmt, globals=kwargs)
    times = timer.repeat(repeat, number)
    return np.mean(times), np.std(times)

[7]: `def time_mdanalysis_rdf(trajectory_filename, r_max, r_min, nbins):
    trajectory = MDAnalysis.coordinates.GSD.GSDReader(trajectory_filename)
    frame = trajectory[0]
    topology = MDAnalysis.core.topology.Topology(n_atoms=frame.n_atoms)
    u = MDAnalysis.as_Uuniverse(topology, trajectory_filename)
    code = """rdf = MDAnalysis.analysis.rdf.InterRDF(g1=u.atoms, g2=u.atoms, nbins=nbins, range=(r_min, r_max)).run()""
    return time_statement(code, MDAnalysis=MDAnalysis, u=u, r_max=r_max, r_min=r_min, nbins=nbins)

[8]: `def time_freud_rdf(trajectory_filename, r_max, r_min, nbins):
    trajectory = MDAnalysis.coordinates.GSD.GSDReader(trajectory_filename)
    code = """rdf = freud.density.RDF(bins=nbins, r_max=r_max, r_min=r_min)
    for frame in trajectory:
        rdf.compute(system=frame, reset=False)""
    return time_statement(code, freud=freud, trajectory=trajectory, r_max=r_max, r_min=r_min, nbins=nbins)

[9]: `# Test timing functions
    params = dict(
        trajectory_filename=trajectory_filename,
        r_max=r_max,
        r_min=r_min,
        nbins=nbins)""
def system_size(trajectory_filename, **kwargs):
    with gsd.hoomd.open(params['trajectory_filename'], 'rb') as trajectory:
        return {'frames': len(trajectory),
                'particles': len(trajectory[0].particles.position)}

print(system_size(**params))
mdanalysis_rdf_runtime = time_mdanaalysis_rdf(**params)
print('MDAnalysis:', mdanalysis_rdf_runtime)
freud_rdf_runtime = time_freud_rdf(**params)
print('freud:', freud_rdf_runtime)

{'frames': 5, 'particles': 15625}
MDAnalysis: (18.00504128, 0.054983033593944214)
freud: (2.8556541516666747, 0.05481114115556424)

Perform Measurements

[10]: def measure_runtime_scaling_r_max(r_maxes, **params):
    result_times = []
    for r_max in tqdm(r_maxes):
        params.update(dict(r_max=r_max))
        freud.parallel.set_num_threads(1)
        freud_single = time_freud_rdf(**params)
        freud.parallel.set_num_threads(0)
        result_times.append((time_mdanaalysis_rdf(**params), freud_single, time_freud_rdf(**params)))
    return np.asarray(result_times)

[11]: def plot_result_times(result_times, r_maxes, frames, particles):
    plt.figure(figsize=(6, 4), dpi=200)
    plt.errorbar(r_maxes, result_times[:, 0, 0], result_times[:, 0, 1],
                 label="MDAnalysis v\analysis.rdf.InterRDF".format(MDAnalysis.__version__))
    plt.errorbar(r_maxes, result_times[:, 1, 0], result_times[:, 1, 1],
                 label="freud v\density.RDF, 1 thread".format(freud.__version__))
    plt.errorbar(r_maxes, result_times[:, 2, 0], result_times[:, 2, 1],
                 label="freud v\density.RDF, {} threads".format(mp.cpu_count()))
    plt.title(r'RDF for \frames, \particles'.format(frames, particles))
    plt.xlabel('RDF $r_{{max}}$')
    plt.ylabel('Average Runtime (s)')
    plt.yscale('log')
    plt.legend()
    plt.show()

[12]: r_maxes = [0.2, 0.3, 0.5, 1, 2, 3]

[13]: result_times = measure_runtime_scaling_r_max(r_maxes, **params)
plot_result_times(result_times, r_maxes, **system_size(params['trajectory_filename']))
print('Speedup, parallel freud / serial freud: {:.3f}x'.format(np.average(result_times[:, 1, 0] / result_times[:, 2, 0])))
print('Speedup, parallel freud / MDAnalysis: {:.3f}x'.format(np.average(result_times[:, 0, 0] / result_times[:, 2, 0])))
print('Speedup, serial freud / MDAnalysis: {:.3f}x'.format(np.average(result_times[:, 0, 0] / result_times[:, 1, 0])))

Speedup, parallel freud / serial freud: 2.900x
Speedup, parallel freud / MDAnalysis: 7.182x
Speedup, serial freud / MDAnalysis: 2.619x

6.6 Query API

This page provides a thorough review of how neighbor finding is structured in freud. It assumes knowledge at the level of the Finding Neighbors level of the tutorial; if you’re not familiar with using the query method with query arguments to find neighbors of points, please familiarize yourself with that section of the tutorial.

The central interface for neighbor finding is the freud.locality.NeighborQuery family of classes, which provide methods for dynamically finding neighbors given a freud.box.Box. The freud.locality.NeighborQuery class defines an abstract interface for neighbor finding that is implemented by its subclasses, namely the freud.locality.LinkCell and freud.locality.AABBQuery classes. These classes represent specific data structures used to accelerate neighbor finding. These two different methods have different performance characteristics, but in most cases freud.locality.AABBQuery performs at least as well as, if not
better than, \texttt{freud.locality.LinkCell} and is entirely parameter free, so it is the default method of choice used internally in \texttt{freud}'s PairCompute classes.

In general, these data structures operate by constructing them using one set of points, after which they can be queried to efficiently find the neighbors of arbitrary other points using \texttt{freud.locality.NeighborQuery.query()}.

## 6.6.1 Query Arguments

The table below describes the set of valid query arguments.

<table>
<thead>
<tr>
<th>Query Argument</th>
<th>Definition</th>
<th>Data type</th>
<th>Legal Values</th>
<th>Valid for</th>
</tr>
</thead>
<tbody>
<tr>
<td>mode</td>
<td>The type of query to perform (distance cutoff or number of neighbors)</td>
<td>str</td>
<td>'none', 'ball', 'nearest'</td>
<td>\texttt{freud.locality.AABBQuery, freud.locality.LinkCell}</td>
</tr>
<tr>
<td>r_max</td>
<td>Maximum distance to find neighbors</td>
<td>float</td>
<td>r_max &gt; 0</td>
<td>\texttt{freud.locality.AABBQuery, freud.locality.LinkCell}</td>
</tr>
<tr>
<td>r_min</td>
<td>Minimum distance to find neighbors</td>
<td>float</td>
<td>0 \leq r_min &lt; r_max</td>
<td>\texttt{freud.locality.AABBQuery, freud.locality.LinkCell}</td>
</tr>
<tr>
<td>num_neighbors</td>
<td>Number of neighbors</td>
<td>int</td>
<td>num_neighbors &gt; 0</td>
<td>\texttt{freud.locality.AABBQuery, freud.locality.LinkCell}</td>
</tr>
<tr>
<td>exclude_ii</td>
<td>Whether or not to include neighbors with the same index in the array</td>
<td>bool</td>
<td>True/False</td>
<td>\texttt{freud.locality.AABBQuery, freud.locality.LinkCell}</td>
</tr>
<tr>
<td>r_guess</td>
<td>Initial search distance for sequence of ball queries</td>
<td>float</td>
<td>r_guess &gt; 0</td>
<td>\texttt{freud.locality.AABBQuery}</td>
</tr>
<tr>
<td>scale</td>
<td>Scale factor for r_guess when not enough neighbors are found</td>
<td>float</td>
<td>scale &gt; 1</td>
<td>\texttt{freud.locality.AABBQuery}</td>
</tr>
</tbody>
</table>

### 6.6.2 Mode Deduction

The \texttt{mode} query argument specifies the type of query that is being performed, and it therefore governs how other arguments are interpreted. In most cases, however, the query mode can be deduced from the set of query arguments. Specifically, any query with the \texttt{num_neighbors} key set is assumed to be a query with \texttt{mode='nearest'}. For completeness, users may specify the mode explicitly if they wish. The presence of the \texttt{mode} key also ensures that \texttt{freud} will not have to change its promises around mode deduction as additional query modes are added.

### 6.6.3 Query Results

Although they don’t typically need to be operated on directly, it can be useful to know a little about the objects returned by queries. The \texttt{freud.locality.NeighborQueryResult} stores the \texttt{query_points} passed to a query and returns neighbors for them one at a time (like any Python iterator). The primary goal of the result class is to support easy iteration and conversion to more persistent formats. Since it is an iterator, you can use any typical Python approach to consuming it, including passing it to \texttt{list} to build a list of the neighbors. For a more \texttt{freud}-friendly approach, you can use the \texttt{toNeighborList} method to convert the object into a \texttt{freud.locality.NeighborList}. Under the hood, the underlying C++ classes loop through candidate points and identifying neighbors for each \texttt{query_point}; this is the same process that occurs when Compute classes employ \texttt{NeighborQuery} objects for finding neighbors on-the-fly, but in that case it all happens on the C++ side.
6.6.4 Custom NeighborLists

Thus far, we’ve mostly discussed NeighborLists `<freud.locality.NeighborList` as a way to persist neighbor information beyond a single query. In Using freud Efficiently, more guidance is provided on how you can use these objects to speed up certain uses of freud. However, these objects are also extremely useful because they provide a completely customizable way to specify neighbors to freud. Of particular note here is the freud.locality.NeighborList.from_arrays() factory function that allows you to make freud.locality.NeighborList objects by directly specifying the `(i, j)` pairs that should be in the list. This kind of explicit construction of the list enables custom analyses that would otherwise be impossible. For example, consider a molecular dynamics simulation in which particles only interact via extremely short-ranged patches on their surface, and that particles should only be considered bonded if their patches are actually interacting, irrespective of how close together the particles themselves are. This type of neighbor interaction cannot be captured by any normal querying mode, but could be constructed by the user and then fed to freud for downstream analysis.

6.6.5 Nearest Neighbor Asymmetry

There is one important but easily overlooked detail associated with using query arguments with mode 'nearest'. Consider a simple example of three points on the x-axis located at -1, 0, and 2 (and assume the box is of dimensions (100, 100, 100), i.e. sufficiently large that periodicity plays no role):

```python
box = [100, 100, 100]
points = [[-1, 0, 0], [0, 0, 0], [2, 0, 0]]
query_args = dict(mode='nearest', num_neighbors=1, exclude_ii=True)
list(freud.locality.AABBQuery(box, points).query(points, query_args))
# Output: [(0, 1, 1), (1, 0, 1), (2, 1, 2)]
```

Evidently, the calculation is not symmetric. This feature of nearest neighbor queries can have unexpected side effects if a PairCompute is performed using distinct points and query_points and the two are interchanged. In such cases, users should always keep in mind that freud promises that every query_point will end up with num_neighbors points (assuming no hard cutoff `r_max` is imposed and enough points are present in the system). However, it is possible (and indeed likely) that any given point will have more or fewer than that many neighbors. This distinction can be particularly tricky for calculations that depend on vector directionality: freud imposes the convention that bond vectors always point from query_point to point, so users of calculations like PMFTs where directionality is important should keep this in mind.

6.7 Using freud Efficiently

The freud library is designed to be both fast and easy-to-use. In many cases, the library’s performance is good enough that users don’t need to worry about their usage patterns. However, in highly performance-critical applications (such as real-time visualization or on-the-fly calculations mid-simulation), uses can benefit from knowing the best ways to make use of freud. This page provides some guidance on this topic.

6.7.1 Reusing Locality Information

Perhaps the most powerful method users have at their disposal for speeding up calculations is proper reuse of the data structures in freud.locality. As one example, consider using freud to calculate multiple neighbor-based quantities for the same set of data points. It is important to recognize that internally, each time such a calculation is performed using a `(box, points)` tuple, the compute class is internally rebuilding a neighbor-finding accelerator such a freud.locality.AABBQuery object and then using it to find neighbors:
If users anticipate performing many such calculations on the same system of points, they can amortize the cost of rebuilding the `AABBQuery` object by constructing it once and then passing it into multiple computations:

```python
# Now, let's instead reuse the object for a pair of calculations:
nq = freud.locality.AABBQuery(box=box, points=points)
rdf = freud.density.RDF(bins=50, r_max=5)
rdf.compute(system=nq)

orientations = np.array([[1, 0, 0, 0]] * num_points)
pmft = freud.pmft.PMFTXYZ(r_max, r_max, r_max, bins=100)
pmft.compute(system=nq, orientations=orientations)
```

This reuse can significantly improve performance in e.g. visualization contexts where users may wish to calculate a bond order diagram and an RDF at each frame, perhaps for integration with a visualization toolkit like OVITO.

A slightly different use-case would be the calculation of multiple quantities based on exactly the same set of neighbors. If the user in fact expects to perform computations with the exact same pairs of neighbors (for example, to compute `freud.order.Steinhardt` for multiple \( l \) values), then the user can further speed up the calculation by precomputing the entire `freud.NeighborList` and storing it for future use.

```python
r_max = 3
nq = freud.locality.AABBQuery(box=box, points=points)
nlist = nq.query(points, dict(r_max=r_max))
q6_arrays = []
for l in range(3, 6):
    ql = freud.order.Steinhardt(l=1)
    q6_arrays.append(ql.compute((box, points), neighbors=nlist).particle_order)
```

Notably, if the user calls a compute method with `compute(system=(box, points))`, unlike in the examples above `freud will not construct` a `freud.locality.NeighborQuery` internally because the full set of neighbors is completely specified by the `NeighborList`. In all these cases, `freud` does the minimal work possible to find neighbors, so judicious use of these data structures can substantially accelerate your code.

### 6.7.2 Proper Data Inputs

Minor speedups may also be gained from passing properly structured data to `freud`. The package was originally designed for analyzing particle simulation trajectories, which are typically stored in single-precision binary formats. As a result, the `freud` library also operates in single precision and therefore converts all inputs to single-precision. However, NumPy will typically work in double precision by default, so depending on how data is streamed to `freud`, the package may be performing numerous data copies in order to ensure that all its data is in single-precision. To avoid this problem, make sure to specify the appropriate data types (numpy.float32) when constructing your NumPy arrays.

### 6.8 Reading Simulation Data for freud

The `freud` package is designed for maximum flexibility by making minimal assumptions about its data. However, users accustomed to the more restrictive patterns of most other tools may find this flexibility confusing. In particular,
knowing how to provide data from specific simulation sources can be a significant source of confusion. This page is intended to describe how various types of data may be converted into a form suitable for `freud`.

To simplify the examples below, we will assume in all cases that the user wishes to compute a radial distribution function over all frames in the trajectory and that the following code has already been run:

```python
import freud
rdf = freud.density.RDF(bins=50, r_max=5)
```

### 6.8.1 Native Integrations

The `freud` library offers interoperability with several popular tools for particle simulations, analysis, and visualization. Below is a list of file formats and tools that are directly supported as “system-like” objects (see `freud.locality.NeighborQuery.from_system`). Such system-like objects are data containers that store information about a periodic box and particle positions. Other attributes, such as particle orientations, are not included automatically in the system representation and must be loaded as separate NumPy arrays.

#### GSD Trajectories

Using the GSD Python API, GSD files can be easily integrated with `freud` as shown in Getting Started. This format is natively supported by HOOMD-blue. Note: the GSD format can also be read by MDAnalysis and garnett. Here, we provide an example that reads data from a GSD file.

```python
import gsd.hoomd
traj = gsd.hoomd.open('trajectory.gsd', 'rb')
for frame in traj:
    rdf.compute(frame, reset=False)
```

#### MDAnalysis Readers

The MDAnalysis package can read many popular trajectory formats, including common output formats from CHARMM, NAMD, LAMMPS, Gromacs, Tinker, AMBER, GAMESS, HOOMD-blue, and more.

DCD files are among the most familiar simulation outputs due to their longevity. Here, we provide an example that reads data from a DCD file.

```python
import MDAnalysis
reader = MDAnalysis.coordinates.DCD.DCDReader('trajectory.dcd')
for frame in reader:
    rdf.compute(system=frame, reset=False)
```

#### garnett Trajectories

The garnett package can read several trajectory formats that have historically been supported by the HOOMD-blue simulation engine, as well as other common types such as DCD and CIF. The garnett package will auto-detect supported file formats by the file extension. Here, we provide an example that reads data from a POS file.

```python
import garnett
with garnett.read('trajectory.pos') as traj:
    # (continues on next page)
```
for frame in traj:
    rdf.compute(system=frame, reset=False)

**OVITO Modifiers**

The **OVITO Open Visualization Tool** supports user-written Python modifiers. The **freud** package can be installed alongside OVITO to enable user-written Python script modifiers that leverage analyses from **freud**. Below is an example modifier that creates a user particle property in the OVITO pipeline for Steinhardt bond order parameters.

```python
import freud

def modify(frame, data):
    ql = freud.order.Steinhardt(l=6)
    ql.compute(system=data, neighbors={'num_neighbors': 6})
    data.create_user_particle_property(
        name='ql', data_type=float, data=ql.ql)
    print('Created ql property for {} particles.'.format(data.particles.count))
```

**HOOMD-blue Snapshots**

**HOOMD-blue** supports analyzers, callback functions that can perform analysis. Below is an example demonstrating how to use an analyzer to log the Steinhardt bond order parameter $q_6$ during the simulation run.

```python
import hoomd
from hoomd import md
import freud

hoomd.context.initialize()

# Create a 10x10x10 simple cubic lattice of particles with type name A
system = hoomd.init.create_lattice(
    unitcell=hoomd.lattice.sc(a=2.0, type_name='A'), n=10)

# Specify Lennard-Jones interactions between particle pairs
nl = md.nlist.cell()
lj = md.pair.lj(r_cut=3.0, nlist=nl)
lj.pair_coeff.set('A', 'A', epsilon=1.0, sigma=1.0)

# Integrate at constant temperature
md.integrate.mode_standard(dt=0.005)
hoomd.md.integrate.langevin(group=hoomd.group.all(), kT=1.2, seed=4)

# Create a Steinhardt object to analyze snapshots
ql = freud.order.Steinhardt(l=6)

def compute_q6(timestep):
    snap = system.take_snapshot()
    ql.compute(system=snap, neighbors={'num_neighbors': 6})
    return ql.order

# Register a logger that computes q6 and saves to a file
ql_logger = hoomd.analyze.log(filename='ql.dat', quantities=['q6'], period=100)
ql_logger.register_callback('q6', compute_q6)
```
6.8.2 Reading Text Files

Typically, it is best to use one of the natively supported data readers described above; however it is sometimes necessary to parse trajectory information directly from a text file. One example of a plain text format is the XYZ file format, which can be generated and used by many tools for particle simulation and analysis, including LAMMPS and VMD. Note that various readers do exist for XYZ files, including MDAnalysis, but in this example we read the file manually to demonstrate how to read these inputs as plain text. Though they are easy to parse, XYZ files usually contain no information about the system box, so this must already be known by the user. Assuming knowledge of the box used in the simulation, a LAMMPS XYZ file could be used as follows:

```python
N = int(np.genfromtxt('trajectory.xyz', max_rows=1))
traj = np.genfromtxt('trajectory.xyz', skip_header=2, invalid_raise=False)[:, 1:4].reshape(-1, N, 3)
box = freud.box.Box.cube(L=20)
for frame_positions in traj:
    rdf.compute(system=(box, frame_positions), reset=False)
```

The first line is the number of particles, so we read this line and use it to determine how to reshape the contents of the rest of the file into a NumPy array.

6.8.3 Other External Readers

For many trajectory formats, high-quality readers already exist. However sometimes these readers’ data structures must be converted into a format understood by freud. Below, we show an example that converts the MDAnalysis box dimensions from a matrix into a `freud.box.Box`. Note that MDAnalysis inputs are natively supported by freud without this extra step. For other formats not supported by a reader listed above, a similar process can be followed.

```python
import MDAnalysis
reader = MDAnalysis.coordinates.DCD.DCDReader('trajectory.dcd')
for frame in reader:
    box = freud.box.Box.from_matrix(frame.triclinic_dimensions)
    rdf.compute(system=box, frame.positions, reset=False)
```

6.9 Box Module

Overview

`freud.box.Box` The freud Box class for simulation boxes.
Details

The `Box` class defines the geometry of a simulation box. The class natively supports periodicity by providing the fundamental features for wrapping vectors outside the box back into it.

```python
class freud.box.Box
    Bases: object

    The freud Box class for simulation boxes.

    This class defines an arbitrary triclinic geometry within which all points are confined. For more information, see the documentation on boxes and periodic boundary conditions.

    Also available as `freud.Box`.
```

**Parameters**

- **Lx** (`float`, *optional*) – The x-dimension length.
- **Ly** (`float`, *optional*) – The y-dimension length.
- **Lz** (`float`, *optional*) – The z-dimension length (Default value = 0).
- **xy** (`float`, *optional*) – The xy tilt factor (Default value = 0).
- **xz** (`float`, *optional*) – The xz tilt factor (Default value = 0).
- **yz** (`float`, *optional*) – The yz tilt factor (Default value = 0).
- **is2D** (`bool`, *optional*) – Whether the box is 2-dimensional. Uses Lz == 0 if None. (Default value = None)

**L**

Get or set the box lengths along x, y, and z.

*Type* *(3,)* `numpy.ndarray`

**L_inv**

The inverse box lengths.

*Type* *(3,)* `numpy.ndarray`

**Lx**

Get or set the x-dimension length.

*Type* `float`

**Ly**

Get or set the y-dimension length.

*Type* `float`

**Lz**

Get or set the z-dimension length.

*Type* `float`

**classmethod cube(cls, L=None)**

Construct a cubic box with equal lengths.

*Parameters* `L` (*float*) – The edge length

```
```
classmethod from_box(type cls, box, dimensions=None)
Initialize a Box instance from a box-like object.

Parameters
- box – A box-like object
- dimensions (int) – Dimensionality of the box (Default value = None)

Note: Objects that can be converted to freud boxes include lists like [Lx, Ly, Lz, xy, xz, yz], dictionaries with keys 'Lx', 'Ly', 'Lz', 'xy', 'xz', 'yz', 'dimensions', objects with attributes Lx, Ly, Lz, xy, xz, yz, dimensions, 3x3 matrices (see from_matrix()), or existing freud.box.Box objects.

If any of Lz, xy, xz, yz are not provided, they will be set to 0.
If all values are provided, a triclinic box will be constructed. If only Lx, Ly, Lz are provided, an orthorhombic box will be constructed. If only Lx, Ly are provided, a rectangular (2D) box will be constructed.
If the optional dimensions argument is given, this will be used as the box dimensionality. Otherwise, the box dimensionality will be detected from the dimensions of the provided box. If no dimensions can be detected, the box will be 2D if Lz == 0, and 3D otherwise.

Returns The resulting box object.
Return type freud.box.Box

classmethod from_matrix(type cls, box_matrix, dimensions=None)
Initialize a Box instance from a box matrix.

For more information and the source for this code, see: https://hoomd-blue.readthedocs.io/en/stable/box.html

Parameters
- box_matrix (array-like) – A 3x3 matrix or list of lists
- dimensions (int) – Number of dimensions (Default value = None)

get_box_vector
Get the box vector with index i.

Parameters i (unsigned int) – Index (0 ≤ i < d) of the box vector, where d is the box dimension (2 or 3).

Returns Box vector with index i.
Return type (3,) numpy.ndarray

get_images
Returns the images corresponding to unwrapped vectors.

Parameters vecs ((3,) or (N,3) numpy.ndarray) – Coordinates of unwrapped vector(s).

Returns Image index vector(s).
Return type (3,) or (N,3) numpy.ndarray

is2D
Whether the box is 2D.

Type bool
make_absolute
Convert fractional coordinates into absolute coordinates.

Parameters fractional_coordinates ((3,) or (N, 3) numpy.ndarray) – Fractional coordinate vector(s), between 0 and 1 within parallelepipedal box.

Returns Absolute coordinate vector(s).
Return type (3,) or (N, 3) numpy.ndarray

make_fractional
Convert absolute coordinates into fractional coordinates.

Parameters absolute_coordinates ((3,) or (N, 3) numpy.ndarray) – Absolute coordinate vector(s).

Returns Fractional coordinate vector(s).
Return type (3,) or (N, 3) numpy.ndarray

periodic
Get or set the periodicity of the box in each dimension.

Type (3,) numpy.ndarray

periodic_x
Get or set the periodicity of the box in x.

Type bool

periodic_y
Get or set the periodicity of the box in y.

Type bool

periodic_z
Get or set the periodicity of the box in z.

Type bool

plot
Plot a Box object.

Parameters

- title (str) – Title of the graph. (Default value = None).
- ax (matplotlib.axes.Axes) – Axes object to plot. If None, make a new axes and figure object. If plotting a 3D box, the axes must be 3D. (Default value = None).
- image (list) – The periodic image location at which to draw the box (Default value = [0, 0, 0]).
- *args – Passed on to mpl_toolkits.mplot3d.Axes3D.plot() or matplotlib.axes.Axes.plot().
- **kwargs – Passed on to mpl_toolkits.mplot3d.Axes3D.plot() or matplotlib.axes.Axes.plot().

classmethod square(type cls, L=None)
Construct a 2-dimensional (square) box with equal lengths.

Parameters L (float) – The edge length

to_dict
Return box as dictionary.
Example::

```python
gg> box = freud.box.Box.cube(L=10)
gg> box.to_dict()
{'Lx': 10.0, 'Ly': 10.0, 'Lz': 10.0,
 'xy': 0.0, 'xz': 0.0, 'yz': 0.0, 'dimensions': 3}
```

Returns  Box parameters

Return type  dict
to_matrix
Returns the box matrix (3x3).

Example::

```python
gg> box = freud.box.Box.cube(L=10)
gg> box.to_matrix()
array([[10., 0., 0.],
       [ 0., 10., 0.],
       [ 0., 0., 10.]])
```

Returns  Box matrix

Return type  \((3,3)\) numpy.ndarray
unwrap
Unwrap an array of vectors inside the box back into real space, using an array of image indices that
determine how many times to unwrap in each dimension.

Parameters

• **vecs** \(((3,)\) or \((N,3)\) numpy.ndarray) – Vector(s) to be unwrapped.

• **imgs** \(((3,)\) or \((N,3)\) numpy.ndarray) – Image indices for vector(s).

Returns  Unwrapped vector(s).

Return type  \((3,3)\) or \((N,3)\) numpy.ndarray

v1
The first box vector \((L_x, 0, 0)\).

Type  \((3,)\) np.ndarray

v2
The second box vector \((xy * L_y, L_y, 0)\).

Type  \((3,)\) np.ndarray

v3
The third box vector \((xz * L_z, yz * L_z, L_z)\).

Type  \((3,)\) np.ndarray

volume
The box volume (area in 2D).

Type  float
wrap

Wrap an array of vectors into the box, using periodic boundaries.

**Note:** Since the origin of the box is in the center, wrapping is equivalent to applying the minimum image convention to the input vectors.

**Parameters**

vecs (($3,)$ or ($N,3$) numpy.ndarray) – Unwrapped vector(s).

Returns

Vector(s) wrapped into the box.

Return type

($3,)$ or ($N,3$) numpy.ndarray

**xy**

Get or set the $xy$ tilt factor.

Type float

**xz**

Get or set the $xz$ tilt factor.

Type float

**yz**

Get or set the $yz$ tilt factor.

Type float

### 6.10 Cluster Module

**Overview**

<table>
<thead>
<tr>
<th>Class Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>freud.cluster.Cluster</td>
<td>Finds clusters using a network of neighbors.</td>
</tr>
<tr>
<td>freud.cluster.ClusterProperties</td>
<td>Routines for computing properties of point clusters.</td>
</tr>
</tbody>
</table>

**Details**

The freud.cluster module aids in finding and computing the properties of clusters of points in a system.

**class** freud.cluster.Cluster

**Bases:** freud.locality._PairCompute

Finds clusters using a network of neighbors.

Given a set of points and their neighbors, freud.cluster.Cluster will determine all of the connected components of the network formed by those neighbor bonds. That is, two points are in the same cluster if and only if a path exists between them on the network of bonds. The class attribute cluster_idx holds an array of cluster indices for each point. By the definition of a cluster, points that are not bonded to any other point end up in their own 1-point cluster.

Identifying micelles is one use-case for finding clusters. This operation is somewhat different, though. In a cluster of points, each and every point belongs to one and only one cluster. However, because a string of points belongs to a polymer, that single polymer may be present in more than one cluster. To handle this situation, an optional layer is presented on top of the cluster_idx array. Given a key value per point (e.g. the polymer id), the compute function will process clusters with the key values in mind and provide a list of keys that are
present in each cluster in the attribute `cluster_keys`, as a list of lists. If keys are not provided, every point is assigned a key corresponding to its index, and `cluster_keys` contains the point ids present in each cluster.

**property cluster_idx**

The cluster index for each point.

Type *(N_points)* `numpy.ndarray`

**property cluster_keys**

A list of lists of the keys contained in each cluster.

Type `list(list)`

**compute**

Compute the clusters for the given set of points.

Parameters

- **system** – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.
- **keys** *(N_points)* `numpy.ndarray` – Membership keys, one for each point.
- **neighbors** *(freud.locality.NeighborList or dict, optional)* – Either a `NeighborList` of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).

**default_query_args**

No default query arguments.

**property num_clusters**

The number of clusters.

Type `int`

**plot**

Plot cluster distribution.

Parameters

- **ax** *(matplotlib.axes.Axes, optional)* – Axis to plot on. If None, make a new figure and axis. (Default value = None)

Returns Axis with the plot.

Return type *(matplotlib.axes.Axes)*

**class freud.cluster.ClusterProperties**

Bases: `freud.util._Compute`

Routines for computing properties of point clusters.

Given a set of points and cluster ids (from `Cluster` or another source), this class determines the following properties for each cluster:

- Center of mass
- Gyration tensor
- Size (number of points)

The center of mass for each cluster (properly handling periodic boundary conditions) can be accessed with `centers` attribute. The $3 \times 3$ symmetric gyration tensors $G$ can be accessed with `gyrations` attribute.

**property centers**

The centers of mass of the clusters.

Type *(N_clusters, 3)* `numpy.ndarray`
compute
Compute properties of the point clusters. Loops over all points in the given array and determines the center of mass of the cluster as well as the gyration tensor. These can be accessed after the call to compute() with the centers and gyrations attributes.

Parameters

- **system** – Any object that is a valid argument to freud.locality.NeighborQuery.from_system.
- **cluster_idx** (\((N_{points},)\) np.ndarray) – Cluster indexes for each point.

**property gyrations**
The gyration tensors of the clusters.

Type \((N_{clusters}, 3, 3)\) numpy.ndarray

**property radii_of_gyration**
The radius of gyration of each cluster.

Type \((N_{clusters})\) numpy.ndarray

**property sizes**
The cluster sizes.

Type \((N_{clusters})\) numpy.ndarray

### 6.11 Data Module

#### Overview

**freud.data.UnitCell**
Class to represent the unit cell of a crystal structure.

### Details

The `freud.data` module provides certain sample data sets and utility functions that are useful for testing and examples.

#### Stability

`freud.data` is unstable. When upgrading from version 2.x to 2.y (y > x), existing freud scripts may need to be updated. The API will be finalized in a future release.

**class** `freud.data.UnitCell`

Bases: object

Class to represent the unit cell of a crystal structure.

This class represents the unit cell of a crystal structure, which is defined by a lattice and a basis. It provides the basic attributes of the unit cell as well as enabling the generation of systems of points (optionally with some noise) from the unit cell.

**Parameters**

- **box** – A box-like object (see `from_box()`) containing the lattice vectors of the unit cell.
- **basis_positions** (\((N_{points}, 3)\) numpy.ndarray) – The basis of the unit cell in fractional coordinates (Default value = \([[0, 0, 0]]\)).
**property a1**
The first lattice vector.

    Type (3,) np.ndarray

**property a2**
The second lattice vector.

    Type (3,) np.ndarray

**property a3**
The third lattice vector.

    Type (3,) np.ndarray

**property basis_positions**
The basis positions.

    Type (Npoints,3) np.ndarray

**classmethod bcc()**
Create a body-centered cubic crystal.

    Returns A bcc unit cell.

    Return type UnitCell

**property box**
The box instance containing the lattice vectors.

    Type freud.box.Box

**property dimensions**
The dimensionality of the unit cell.

    Type int

**classmethod fcc()**
Create a face-centered cubic crystal.

    Returns An fcc unit cell.

    Return type UnitCell

**generate_system(num_replicas=1, scale=1, sigma_noise=0, seed=None)**
Generate a system from the unit cell.

    The box and the positions are expanded by scale, and then Gaussian noise with standard deviation sigma_noise is added to the positions. All points are wrapped back into the box before being returned.

    Parameters

        • **num_replicas** (tuple or int) – If provided as a single number, the number of replicas in all dimensions. If a tuple, the number of times replicated in each dimension. Must be of the form (nx, ny, 1) for 2D boxes (Default value = 1).

        • **scale** (float) – Factor by which to scale the unit cell (Default value = 1).

        • **sigma_noise** (float) – The standard deviation of the normal distribution used to add noise to the positions in the system (Default value = 0).

        • **seed** (int) – If provided, used to seed the random noise generation. Not used unless sigma_noise > 0 (Default value = None).

    Returns A system-like object (see from_system).

    Return type tuple (freud.box.Box, np.ndarray)
property lattice_vectors
  The matrix of lattice vectors.
  Type (3, 3) np.ndarray

classmethod sc()
  Create a simple cubic crystal.
  Returns An sc unit cell.
  Return type UnitCell

classmethod square()
  Create a square crystal.
  Returns A square unit cell.
  Return type UnitCell

def make_random_system(box_size, num_points, is2D=False, seed=None)
  Helper function to make random points with a cubic or square box.
  This function has a side effect, by setting the random seed of numpy if a seed is specified.

  Parameters
  • box_size (float) – Size of box.
  • num_points (int) – Number of points.
  • is2D (bool) – If true, creates a 2D system. (Default value = False).
  • seed (int) – Random seed to use. (Default value = None).

  Returns Generated box and points.
  Return type tuple (freud.box.Box, (num_points, 3) numpy.ndarray)

6.12 Density Module

Overview

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<th>Module</th>
<th>Description</th>
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<tr>
<td>freud.density.CorrelationFunction</td>
<td>Computes the complex pairwise correlation function.</td>
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<tr>
<td>freud.density.GaussianDensity</td>
<td>Computes the density of a system on a grid.</td>
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<tr>
<td>freud.density.LocalDensity</td>
<td>Computes the local density around a particle.</td>
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<tr>
<td>freud.density.RDF</td>
<td>Computes the RDF ( g(r) ) for supplied data.</td>
</tr>
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</table>

Details

The freud.density module contains various classes relating to the density of the system. These functions allow evaluation of particle distributions with respect to other particles.

class freud.density.CorrelationFunction
  Bases: freud.locality._SpatialHistogram1D

  Computes the complex pairwise correlation function.

  The correlation function is given by \( C(r) = (s_1(0) \cdot s_2(r)) \) between two sets of points \( p_1 \) (points) and \( p_2 \) (query_points) with associated values \( s_1 \) (values) and \( s_2 \) (query_values). Computing the correlation function results in an array of the expected (average) product of all values at a given radial distance \( r \).
The values of $r$ where the correlation function is computed are controlled by the $r_{\text{max}}$ and $dr$ parameters to the constructor. $r_{\text{max}}$ determines the maximum distance at which to compute the correlation function and $dr$ is the step size for each bin.

**Note:** **Self-correlation:** It is often the case that we wish to compute the correlation function of a set of points with itself. If `query_points` is the same as `points`, not provided, or `None`, we omit accumulating the self-correlation value in the first bin.

### Parameters

- **bins** *(unsigned int)* – The number of bins in the RDF.
- **$r_{\text{max}}$** *(float)* – Maximum pointwise distance to include in the calculation.

**bin_centers**

The centers of each bin in the histogram.

Type *(Nbins,)* `numpy.ndarray`

**property bin_counts**

The bin counts in the histogram.

Type `numpy.ndarray`

**bin_edges**

The edges of each bin in the histogram. Is one element larger because each bin has a lower and upper bound.

Type *(Nbins + 1,)* `numpy.ndarray`

**bounds**

A tuple indicating upper and lower bounds of the histogram.

Type `tuple`

**property box**

The box object used in the last computation.

Type `freud.box.Box`

**compute**

Calculates the correlation function and adds to the current histogram.

### Parameters

- **system** – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.
- **values** *(Npoints)* `numpy.ndarray` – Values associated with the system points used to calculate the correlation function.
- **query_points** *(Nquery_points, 3)* `numpy.ndarray`, optional) – Query points used to calculate the correlation function. Uses the system’s points if `None` (Default value = `None`).
- **query_values** *(Nquery_points)* `numpy.ndarray`, optional) – Query values used to calculate the correlation function. Uses values if `None`. (Default value = `None`).
- **neighbors** *(freud.locality.NeighborList or dict, optional)* – Either a `NeighborList` of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: `None`).
• **reset** (*bool*) – Whether to erase the previously computed values before adding the new computation; if False, will accumulate data (Default value: True).

**property correlation**

Expected (average) product of all values at a given radial distance.

Type *(\(N_{bins}\)) numpy.ndarray*

**default_query_args**

The default query arguments are `{mode': 'ball', 'r_max': self.r_max}`.

**nbins**

The number of bins in the histogram

Type *int*

**plot**

Plot complex correlation function.

Parameters *

<table>
<thead>
<tr>
<th>Parameter</th>
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<tr>
<td><strong>ax</strong> (<em>matplotlib.axes.Axes</em>, optional)</td>
<td>Axis to plot on. If None, make a new figure and axis. (Default value = None)</td>
</tr>
</tbody>
</table>

Returns *Axis with the plot.*

Return type *(matplotlib.axes.Axes)*

**class freud.density.GaussianDensity**

**Bases:** *freud.util._Compute*

Computes the density of a system on a grid.

Replaces particle positions with a Gaussian blur and calculates the contribution from each to the proscribed grid based upon the distance of the grid cell from the center of the Gaussian. The resulting data is a regular grid of particle densities that can be used in standard algorithms requiring evenly spaced point, such as Fast Fourier Transforms. The dimensions of the image (grid) are set in the constructor, and can either be set equally for all dimensions or for each dimension independently.

**Parameters**

• **width** (*int or list or tuple*) – The number of bins to make the image in each direction (identical in all dimensions if a single integer value is provided).

• **r_max** (*float*) – Distance over which to blur.

• **sigma** (*float*) – Sigma parameter for Gaussian.

**property box**

Box used in the calculation.

Type *freud.box.Box*

**compute**

Calculates the Gaussian blur for the specified points.

Parameters *

<table>
<thead>
<tr>
<th>Parameter</th>
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<tbody>
<tr>
<td><strong>system</strong></td>
<td>Any object that is a valid argument to freud.locality.NeighborQuery.from_system.</td>
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</table>

**property density**

The image grid with the Gaussian density.

Type *(\(w_x, w_y, w_z\)) numpy.ndarray*

**plot**

Plot Gaussian Density.
Parameters **ax** *(matplotlib.axes.Axes, optional)* – Axis to plot on. If None, make a new figure and axis. (Default value = None)

Returns Axis with the plot.

Return type *(matplotlib.axes.Axes)*

**r_max**
Distance over which to blur.

**Type float**

**sigma**
Sigma parameter for Gaussian.

**Type float**

**width**
The number of bins to make the image in each direction (identical in all dimensions if a single integer value is provided).

**Type int or list or tuple**

**class** freud.density.LocalDensity

**Bases:** freud.locality._PairCompute

Computes the local density around a particle.

The density of the local environment is computed and averaged for a given set of query points in a sea of data points. Providing the same points calculates them against themselves. Computing the local density results in an array listing the value of the local density around each query point. Also available is the number of neighbors for each query point, giving the user the ability to count the number of particles in that region. Note that the computed density is essentially a number density (that allows for fractional values as described below). If your particles have a specific volume, you can compute a volume density by simply multiplying the output by the volume of the particles.

In order to provide sufficiently smooth data, data points can be fractionally counted towards the density. Rather than perform compute-intensive area (volume) overlap calculations to determine the exact amount of overlap area (volume), the LocalDensity class performs a simple linear interpolation relative to the centers of the data points. Specifically, a point is counted as one neighbor of a given query point if it is entirely contained within the *r_max*, half of a neighbor if the distance to its center is exactly *r_max*, and zero if its center is a distance greater than or equal to *r_max + diameter* from the query point’s center. Graphically, this looks like:
Parameters

- `r_max (float)` – Maximum distance over which to calculate the density.
- `diameter (float)` – Diameter of particle circumsphere.

**property box**

Box used in the calculation.

**Type** `freud.box.Box`

**compute**

Calculates the local density for the specified points.

**Parameters**

- `system` – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.
- `query_points ((N_query_points, 3) numpy.ndarray, optional)` – Query points used to calculate the correlation function. Uses the system’s points if `None` (Default value = `None`).
- `neighbors (freud.locality.NeighborList or dict, optional)` – Either a `NeighborList` of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: `None`).

**default_query_args**

The default query arguments are `{'mode': 'ball', 'r_max': self.r_max + 0.5*self.diameter}`.

**property density**

Density of points per query point.
Type \( (N_{points}) \) numpy.ndarray

**diameter**
Diameter of particle circumsphere.

Type float

**property num_neighbors**
Number of neighbor points for each query point.

Type \( (N_{points}) \) numpy.ndarray

**r_max**
Maximum distance over which to calculate the density.

Type float

**class freud.density.RDF**
Bases: freud.locality._SpatialHistogram1D
Computes the RDF \( g(r) \) for supplied data.

Note that the RDF is defined strictly according to the pair correlation function, i.e.

\[
g(r) = V \frac{N - 1}{N} \langle \delta(r) \rangle
\]

In the thermodynamic limit, the fraction tends to unity and the limiting behavior of \( \lim_{r \to \infty} g(r) = 1 \) is recovered. However, for very small systems the long range behavior of the radial distribution will instead tend to \( \frac{N^2}{N} \). If you are analyzing a very small system but wish to recover the more familiar behavior, you may use the `normalize` flag to enforce this requirement upon construction of this object. Note that this will have little to no effect on larger systems (for example, for systems of 100 particles the RDF will differ by 1%).

Note: 2D: freud.density.RDF properly handles 2D boxes. The points must be passed in as \([x, y, 0]\).

**Parameters**

- **bins** *(unsigned int)* – The number of bins in the RDF.
- **r_max** *(float)* – Maximum interparticle distance to include in the calculation.
- **r_min** *(float, optional)* – Minimum interparticle distance to include in the calculation (Default value = 0).
- **normalize** *(bool, optional)* – Scale the RDF values by \( \frac{N_{query\_points} + 1}{N_{query\_points}} \). This argument primarily exists to deal with standard RDF calculations where no special query_points or neighbors are provided, but where the number of query_points is small enough that the long-ranged limit of \( g(r) \) deviates significantly from 1. It should not be used if query_points is provided as a different set of points, or if unusual query arguments are provided to compute(), specifically if :code:`exclude_ii` is set to False. This normalization is not meaningful in such cases and will simply convolute the data.

**bin_centers**
The centers of each bin in the histogram.

Type \( (N_{bins}) \) numpy.ndarray
property bin_counts
    The bin counts in the histogram.
    Type numpy.ndarray

bin_edges
    The edges of each bin in the histogram. Is one element larger because each bin has a lower and upper bound.
    Type (N_bins + 1,) numpy.ndarray

bounds
    A tuple indicating upper and lower bounds of the histogram.
    Type tuple

property box
    The box object used in the last computation.
    Type freud.box.Box

calculate
    Calculates the RDF and adds to the current RDF histogram.

    Parameters
    • system – Any object that is a valid argument to freud.locality.NeighborQuery.from_system.
    • query_points ((N_query_points, 3) numpy.ndarray, optional) – Query points used to calculate the RDF. Uses the system’s points if None (Default value = None).
    • neighbors (freud.locality.NeighborList or dict, optional) – Either a NeighborList of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).
    • reset (bool) – Whether to erase the previously computed values before adding the new computation; if False, will accumulate data (Default value: True).

default_query_args
    The default query arguments are {'mode': 'ball', 'r_max': self.r_max}.

property n_r
    Histogram of cumulative bin_counts values. More precisely, n_r[i] is the average number of points contained within a ball of radius R[i]+dr/2 centered at a given query_point averaged over all query_points in the last call to calculate().
    Type (N_bins,) numpy.ndarray

nbins
    The number of bins in the histogram
    Type int

plot
    Plot radial distribution function.

    Parameters
    • ax (matplotlib.axes.Axes, optional) – Axis to plot on. If None, make a new figure and axis. (Default value = None)

    Returns
    Axis with the plot.
    Return type (matplotlib.axes.Axes)
6.13 Environment Module

Overview

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<td>freud.environment.BondOrder</td>
<td>Compute the bond orientational order diagram for the system of particles.</td>
</tr>
<tr>
<td>freud.environment.LocalDescriptors</td>
<td>Compute a set of descriptors (a numerical “fingerprint”) of a particle’s local environment.</td>
</tr>
<tr>
<td>freud.environment.EnvironmentCluster</td>
<td>Clusters particles according to whether their local environments match or not, according to various shape matching metrics.</td>
</tr>
<tr>
<td>freud.environment.EnvironmentMotifMatch</td>
<td>Find matches between local arrangements of a set of points and a provided motif.</td>
</tr>
<tr>
<td>freud.environment.AngularSeparationGlobal</td>
<td>Calculates the minimum angles of separation between orientations and global orientations.</td>
</tr>
<tr>
<td>freud.environment.AngularSeparationNeighbor</td>
<td>Calculates the minimum angles of separation between orientations and query orientations.</td>
</tr>
<tr>
<td>freud.environment.LocalBondProjection</td>
<td>Calculates the maximal projection of nearest neighbor bonds for each particle onto some set of reference vectors, defined in the particles’ local reference frame.</td>
</tr>
</tbody>
</table>

Details

The freud.environment module contains functions which characterize the local environments of particles in the system. These methods use the positions and orientations of particles in the local neighborhood of a given particle to characterize the particle environment.

class freud.environment.AngularSeparationGlobal

Bases: freud.util._Compute

Calculates the minimum angles of separation between orientations and global orientations.

property angles

\((N_{orientations}, N_{global orientations})\) numpy.ndarray: The global angles in radians.

compute

Calculates the minimum angles of separation between global_orientations and orientations, checking for underlying symmetry as encoded in equiv_orientations. The result is stored in the global_angles class attribute.

Parameters

- `global_orientations` ((\(N_{global}\), 4) numpy.ndarray) – Set of global orientations to calculate the order parameter.
- `orientations` ((\(N_{particles}\), 4) numpy.ndarray) – Orientations to calculate the order parameter.
- `equiv_orientations` ((\(N_{equiv}\), 4) numpy.ndarray, optional) – The set of all equivalent quaternions that map the particle to itself (the elements of its rotational sym-
metric group). Important: equiv_orientations must include both $q$ and $-q$, for all included quaternions. Note that this calculation assumes that all points in the system share the same set of equivalent orientations. (Default value = $[[1, 0, 0, 0]]$)

class freud.environment.AngularSeparationNeighbor
Bases: freud.locality._PairCompute

Calculates the minimum angles of separation between orientations and query orientations.

**property angles**
The neighbor angles in radians. The angles are stored in the order of the neighborlist object.

Type \((N_{\text{bonds}})\) numpy.ndarray

**compute**
Calculates the minimum angles of separation between orientations and query_orientations, checking for underlying symmetry as encoded in equiv_orientations. The result is stored in the neighbor_angles class attribute.

Parameters

- **system** — Any object that is a valid argument to freud.locality.NeighborQuery.from_system.
- **orientations** \((N_{\text{points}}, 4)\) numpy.ndarray — Orientations associated with system points that are used to calculate bonds.
- **query_points** \((N_{\text{query_points}}, 3)\) numpy.ndarray, optional) — Query points used to calculate the correlation function. Uses the system's points if None (Default value = None).
- **query_orientations** \((N_{\text{query_points}}, 4)\) numpy.ndarray, optional) — Query orientations used to calculate bonds. Uses orientations if None. (Default value = None).
- **equiv_orientations** \((N_{\text{equiv}}, 4)\) numpy.ndarray, optional) — The set of all equivalent quaternions that map the particle to itself (the elements of its rotational symmetry group). Important: equiv_orientations must include both $q$ and $-q$, for all included quaternions. Note that this calculation assumes that all points in the system share the same set of equivalent orientations. (Default value = $[[1, 0, 0, 0]]$)
- **neighbors** (freud.locality.NeighborList or dict, optional) — Either a NeighborList of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).

**default_query_args**
No default query arguments.

**property nlist**
The neighbor list from the last compute.

Type freud.locality.NeighborList

class freud.environment.BondOrder
Bases: freud.locality._SpatialHistogram

Compute the bond orientational order diagram for the system of particles.

The bond orientational order diagram (BOOD) is a way of studying the average local environments experienced by particles. In a BOOD, a particle and its nearest neighbors (determined by either a prespecified number of neighbors or simply a cutoff distance) are treated as connected by a bond joining their centers. All of the bonds in the system are then binned by their azimuthal ($\theta$) and polar ($\phi$) angles to indicate the location of a particle’s neighbors relative to itself. The distance between the particle and its neighbor is only important when
determining whether it is counted as a neighbor, but is not part of the BOOD; as such, the BOOD can be viewed as a projection of all bonds onto the unit sphere. The resulting 2D histogram provides insight into how particles are situated relative to one-another in a system.

This class provides access to the classical BOOD as well as a few useful variants. These variants can be accessed via the `mode` arguments to the `compute()` method. Available modes of calculation are:

- **'bod'** (Bond Order Diagram, default): This mode constructs the default BOOD, which is the 2D histogram containing the number of bonds formed through each azimuthal ($\theta$) and polar ($\phi$) angle.

- **'lbod'** (Local Bond Order Diagram): In this mode, a particle’s neighbors are rotated into the local frame of the particle before the BOOD is calculated, *i.e.* the directions of bonds are determined relative to the orientation of the particle rather than relative to the global reference frame. An example of when this mode would be useful is when a system is composed of multiple grains of the same crystal; the normal BOOD would show twice as many peaks as expected, but using this mode, the bonds would be superimposed.

- **'obcd'** (Orientation Bond Correlation Diagram): This mode aims to quantify the degree of orientational as well as translational ordering. As a first step, the rotation that would align a particle’s neighbor with the particle is calculated. Then, the neighbor is rotated around the central particle by that amount, which actually changes the direction of the bond. One example of how this mode could be useful is in identifying plastic crystals, which exhibit translational but not orientational ordering. Normally, the BOOD for a plastic crystal would exhibit clear structure since there is translational order, but with this mode, the neighbor positions would actually be modified, resulting in an isotropic (disordered) BOOD.

- **'oocd'** (Orientation Orientation Correlation Diagram): This mode is substantially different from the other modes. Rather than compute the histogram of neighbor bonds, this mode instead computes a histogram of the directors of neighboring particles, where the director is defined as the basis vector $\hat{z}$ rotated by the neighbor's quaternion. The directors are then rotated into the central particle's reference frame. This mode provides insight into the local orientational environment of particles, indicating, on average, how a particle’s neighbors are oriented.

**Parameters**

- **bins** *(unsigned int or sequence of length 2)* – If an unsigned int, the number of bins in $\theta$ and $\phi$. If a sequence of two integers, interpreted as $(\text{num}_\theta, \text{num}_\phi)$.

- **mode** *(str, optional)* – Mode to calculate bond order. Options are 'bod', 'lbod', 'obcd', or 'oocd' (Default value = 'bod').

**bin_centers**

The centers of each bin in the histogram (has the same shape as the histogram itself).

Type `numpy.ndarray`

**property bin_counts**

The bin counts in the histogram.

Type `numpy.ndarray`

**bin_edges**

The edges of each bin in the histogram (is one element larger in each dimension than the histogram because each bin has a lower and upper bound).

Type `numpy.ndarray`

**property bond_order**

Bond order.

Type $(N_\phi, N_\theta)$ `numpy.ndarray`
bounds
   A list of tuples indicating upper and lower bounds of each axis of the histogram.
   Type list(tuple)

property box
   Box used in the calculation.
   Type freud.box.Box

calculate
   Calculates the correlation function and adds to the current histogram.

Parameters
   • system – Any object that is a valid argument to freud.locality.NeighborQuery.from_system.
   • orientations ((N_points, 4) numpy.ndarray) – Orientations associated with system points that are used to calculate bonds. Uses identity quaternions if None (Default value = None).
   • query_points ((N_query_points, 3) numpy.ndarray, optional) – Query points used to calculate the correlation function. Uses the system’s points if None (Default value = None).
   • query_orientations ((N_query_points, 4) numpy.ndarray, optional) – Query orientations used to calculate bonds. Uses orientations if None. (Default value = None).
   • neighbors (freud.locality.NeighborList or dict, optional) – Either a NeighborList of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).
   • reset (bool) – Whether to erase the previously computed values before adding the new computation; if False, will accumulate data (Default value: True).

default_query_args
   No default query arguments.

mode
   Bond order mode.
   Type str

nbins
   The number of bins in each dimension of the histogram
   Type list

class freud.environment.EnvironmentCluster
   Bases: freud.environment._MatchEnv

   Clusters particles according to whether their local environments match or not, according to various shape matching metrics.

   property cluster_environments
      (N_clusters, N_neighbors, 3) numpy.ndarray): The environments for all clusters.

   property cluster_idx
      The per-particle index indicating cluster membership.
      Type (N_particles) numpy.ndarray
compute
Determine clusters of particles with matching environments.

In general, it is recommended to specify a number of neighbors rather than just a distance cutoff as part of your neighbor querying when performing this computation. Using a distance cutoff alone could easily lead to situations where a point doesn’t match a cluster because a required neighbor is just outside the cutoff.

Parameters

• **system** – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.

• **threshold** *(float)* – Maximum magnitude of the vector difference between two vectors, below which they are “matching”. Typically, a good choice is between 10% and 30% of the first well in the radial distribution function (this has distance units).

• **neighbors** *(freud.locality.NeighborList or dict, optional)* – Either a `NeighborList` of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).

• **env_neighbors** *(freud.locality.NeighborList or dict, optional)* – Either a `NeighborList` of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None). This argument is used to define the neighbors of the environment that motifs are registered against.

• **registration** *(bool, optional)* – If True, first use brute force registration to orient one set of environment vectors with respect to the other set such that it minimizes the RMSD between the two sets. (Default value = False)

• **global_search** *(bool, optional)* – If True, do an exhaustive search wherein the environments of every single pair of particles in the simulation are compared. If False, only compare the environments of neighboring particles. (Default value = False)

**default_query_args**
No default query arguments.

**property num_clusters**
The number of clusters.

  Type unsigned int

**plot**
Plot cluster distribution.

  Parameters **ax** *(matplotlib.axes.Axes, optional)* – Axis to plot on. If None, make a new figure and axis. (Default value = None)

  Returns Axis with the plot.

  Return type *(matplotlib.axes.Axes)*

**property point_environments**

  *(Npoints, Nneighbors, 3)* `numpy.ndarray`: All environments for all points.

**class** `freud.environment.EnvironmentMotifMatch`

Bases: `freud.environment._MatchEnv`

Find matches between local arrangements of a set of points and a provided motif.

In general, it is recommended to specify a number of neighbors rather than just a distance cutoff as part of your neighbor querying when performing this computation since it can otherwise be very sensitive. Specifically, it is highly recommended that you choose a number of neighbors query that requests at least as many neighbors as
the size of the motif you intend to test against. Otherwise, you will struggle to match the motif. However, this
is not currently enforced.

**compute**
Determine clusters of particles that match the motif provided by motif.

**Parameters**

- **system** – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.
- **motif** ([N\text{points}, 3] \text{numpy.ndarray}) – Vectors that make up the motif against which we are matching.
- **threshold** (float) – Maximum magnitude of the vector difference between two vectors, below which they are “matching”. Typically, a good choice is between 10% and 30% of the first well in the radial distribution function (this has distance units).
- **neighbors** ([freud.locality.NeighborList or dict, optional) – Either a `NeighborList` of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).
- **registration** (bool, optional) – If True, first use brute force registration to orient one set of environment vectors with respect to the other set such that it minimizes the RMSD between the two sets (Default value = False).

**default_query_args**
No default query arguments.

**property matches**
A boolean array indicating whether each point matches the motif.

Type ([N\text{points},]) \text{numpy.ndarray}

**property point_environments**
(N\text{points}, N\text{neighbors}, 3) \text{numpy.ndarray}: All environments for all points.

**class** `freud.environment.LocalBondProjection`
**Bases:** `freud.locality._PairCompute`
Calculates the maximal projection of nearest neighbor bonds for each particle onto some set of reference vectors, defined in the particles’ local reference frame.

**compute**
Calculates the maximal projections of nearest neighbor bonds (between `points` and `query_points`) onto the set of reference vectors `proj_vecs`, defined in the local reference frames of the `points` as defined by the orientations `orientations`. This computation accounts for the underlying symmetries of the reference frame as encoded in `equiv_orientations`.

**Parameters**

- **system** – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.
- **orientations** ([N\text{points}, 4] \text{numpy.ndarray}) – Orientations associated with system points that are used to calculate bonds.
- **proj_vecs** ([N\text{vectors}, 3] \text{numpy.ndarray}) – The set of projection vectors, defined in the query particles’ reference frame, to calculate maximal local bond projections onto.
- **query_points** ([N\text{query_points}, 3] \text{numpy.ndarray}, optional) – Query points used to calculate the correlation function. Uses the system’s points if None (Default value = None). (Default value = None).
• **equiv_orientations** ([N\textsubscript{equiv}, 4] numpy.ndarray, optional) – The set of all equivalent quaternions that map the particle to itself (the elements of its rotational symmetry group). Important: equiv_orientations must include both \(q\) and \(-q\), for all included quaternions. Note that this calculation assumes that all points in the system share the same set of equivalent orientations. (Default value = \([[1, 0, 0, 0]]\))

• **neighbors** (freud.locality.NeighborList or dict, optional) – Either a NeighborList of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).

**default_query_args**
No default query arguments.

**property nlist**
The neighbor list from the last compute.

Type: freud.locality.NeighborList

**property normed_projections**
\((N\textsubscript{bonds}, N\textsubscript{projection}_\textsubscript{vecs})\) numpy.ndarray: The projection of each bond between query particles and their neighbors onto each of the projection vectors, normalized by the length of the bond.

**property projections**
\((N\textsubscript{bonds}, N\textsubscript{projection}_\textsubscript{vecs})\) numpy.ndarray: The projection of each bond between query particles and their neighbors onto each of the projection vectors.

class freud.environment.LocalDescriptors
Bases: freud.locality._PairCompute

Compute a set of descriptors (a numerical “fingerprint”) of a particle’s local environment.

The resulting spherical harmonic array will be a complex-valued array of shape \((\text{num}_\text{bonds}, \text{num}_\text{sphs})\). Spherical harmonic calculation can be restricted to some number of nearest neighbors through the num_neighbors argument; if a particle has more bonds than this number, the last one or more rows of bond spherical harmonics for each particle will not be set.

**Parameters**

• **l_max** (unsigned int) – Maximum spherical harmonic \(l\) to consider.

• **negative_m** (bool, optional) – True if we should also calculate \(Y_{lm}\) for negative \(m\). (Default value = True)

• **mode** (str, optional) – Orientation mode to use for environments, either ’neighborhood’ to use the orientation of the local neighborhood, ’particle_local’ to use the given particle orientations, or ’global’ to not rotate environments (Default value = ’neighborhood’).

**compute**
Calculates the local descriptors of bonds from a set of source points to a set of destination points.

**Parameters**

• **system** – Any object that is a valid argument to freud.locality.NeighborQuery.from_system.

• **query_points** ([N\textsubscript{query_points}, 3] numpy.ndarray, optional) – Query points used to calculate the correlation function. Uses the system’s points if None (Default value = None).

• **orientations** ([N\textsubscript{points}, 4] numpy.ndarray) – Orientations associated with system points that are used to calculate bonds.
• **neighbors** *(freud.locality.NeighborList or dict, optional)* – Either a NeighborList of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).

**default_query_args**
No default query arguments.

**l_max**
The maximum spherical harmonic $l$ calculated for.

  Type  unsigned int

**mode**
Orientation mode to use for environments, either 'neighborhood' to use the orientation of the local neighborhood, 'particle_local' to use the given particle orientations, or 'global' to not rotate environments.

  Type  str

**negative_m**
True if we also calculated $Y_{lm}$ for negative $m$.

  Type  bool

**property nlist**
The neighbor list from the last compute.

  Type  freud.locality.NeighborList

**property num_sphs**
The last number of spherical harmonics computed. This is equal to the number of bonds in the last computation, which is at most the number of points multiplied by the lower of the num_neighbors arguments passed to the last compute call or the constructor (it may be less if there are not enough neighbors for every particle).

  Type  unsigned int

**property sph**
$(N_{bonds}, \text{SphWidth})$ numpy.ndarray: The last computed spherical harmonic array.

## 6.14 Interface Module

### Overview

| **freud.interface.Interface** | Measures the interface between two sets of points. |

### Details

The **freud.interface** module contains functions to measure the interface between sets of points.

**class freud.interface.Interface**

  Bases: freud.locality._PairCompute

  Measures the interface between two sets of points.

  **compute**

  Compute the particles at the interface between two sets of points.

  **Parameters**
• **system** – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.

• **query_points** (`(N_{query\_points}, 3) \text{numpy.ndarray}`, optional) – Second set of points (in addition to the system points) to calculate the interface.

• **neighbors** (`freud.locality.NeighborList` or dict, optional) – Either a `NeighborList` of neighbor pairs to use in the calculation, or a dictionary of `query arguments` (Default value: None).

```python
default_query_args
    No default query arguments.
```

```python
@property
    def point_count(self):
        """Number of particles from points on the interface."
        return int

@property
    def point_ids(self):
        """The particle IDs from points."
        return np.ndarray

@property
    def query_point_count(self):
        """Number of particles from query_points on the interface."
        return int

@property
    def query_point_ids(self):
        """The particle IDs from query_points."
        return np.ndarray
```

### 6.15 Locality Module

#### Overview

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#### Details

The `freud.locality` module contains data structures to efficiently locate points based on their proximity to other points.

```python
class freud.locality.AABBQuery
    Bases: freud.locality.NeighborQuery

    Use an AABB tree to find neighbors.
```
Also available as `freud.AABBQuery`.

**box**

The box object used by this data structure.

*Type* `freud.box.Box`

**classmethod from_system**( `type cls, system` )

Create a `NeighborQuery` from any system-like object.

The standard concept of a system in `freud` is any object that provides a way to access a box-like object (anything that can be coerced to a box by `freud.box.Box.from_box()`) and an array-like (according to NumPy’s definition) object that turns into a $N \times 3$ array.

Supported types for `system` include:

- `AABBQuery`
- `LinkCell`
- A sequence of `(box, points)` where `box` is a `Box` and `points` is a `numpy.ndarray`.
- Objects with attributes `box` and `points`.
- `MDAnalysis.coordinates.base.Timestep`
- `gsd.hoomd.Snapshot`
- `garnett.trajectory.Frame`
- `ovito.data.DataCollection`
- `hoomd.data.snapshot`

**Parameters**

- `system` *(system-like object)* – Any object that can be converted to a `NeighborQuery`.

**Returns**

The same `NeighborQuery` object if one is given, or an instance of `NeighborQuery` built from an inferred `box` and `points`.

**Return type** `freud.locality.NeighborQuery`

**plot**

Plot system box and points.

**Parameters**

- `ax` *(matplotlib.axes.Axes)* – Axis to plot on. If None, make a new figure and axis. The axis projection (2D or 3D) must match the dimensionality of the system (Default value = None).
- `title` *(str)* – Title of the plot (Default value = None).
- `*args` – Passed on to `mpl_toolkits.mplot3d.Axes3D.plot()` or `matplotlib.axes.Axes.plot()`.
- `**kwargs` – Passed on to `mpl_toolkits.mplot3d.Axes3D.plot()` or `matplotlib.axes.Axes.plot()`.

**Returns**

Axis with the plot.

**Return type** `matplotlib.axes.Axes`

**points**

The array of points in this data structure.
Type np.ndarray

query
Query for nearest neighbors of the provided point.

Parameters

• query_points ((N, 3) numpy.ndarray) – Points to query for.
• query_args (dict) – Query arguments determining how to find neighbors. For information on valid query argument, see the Query API.

Returns Results object containing the output of this query.

Return type NeighborQueryResult
class freud.locality.LinkCell
Bases: freud.locality.NeighborQuery

Supports efficiently finding all points in a set within a certain distance from a given point.

Also available as freud.LinkCell.

Parameters

• box (freud.box.Box) – Simulation box.
• points (np.ndarray) – The points to bin into the cell list.
• cell_width (float, optional) – Width of cells. If not provided, ~.LinkCell will estimate a cell width based on the number of points and the box size assuming constant density of points throughout the box.

box

The box object used by this data structure.

Type freud.box.Box
cell_width
Cell width.

Type float
classmethod from_system (type cls, system)
Create a NeighborQuery from any system-like object.

The standard concept of a system in freud is any object that provides a way to access a box-like object (anything that can be coerced to a box by freud.box.Box.from_box()) and an array-like (according to NumPy's definition) object that turns into a N x 3 array.

Supported types for system include:

• AABBQuery
• LinkCell
• A sequence of (box, points) where box is a Box and points is a numpy.ndarray.
• Objects with attributes box and points.
• MDAnalysis.coordinates.base.Timestep
• gsd.hoomd.Snapshot
• garnett.trajectory.Frame
• ovito.data.DataCollection
• `hoomd.data` snapshot

**Parameters**

`system (system-like object)` – Any object that can be converted to a `NeighborQuery`.

**Returns**

The same `NeighborQuery` object if one is given, or an instance of `NeighborQuery` built from an inferred box and points.

**Return type** `freud.locality.NeighborQuery`}

```python
plot

Plot system box and points.

**Parameters**

- `ax (matplotlib.axes.Axes)` – Axis to plot on. If None, make a new figure and axis. The axis projection (2D or 3D) must match the dimensionality of the system (Default value = None).
- `title (str)` – Title of the plot (Default value = None).
- `*args` – Passed on to `mpl_toolkits.mplot3d.Axes3D.plot()` or `matplotlib.axes.Axes.plot()`.
- `**kwargs` – Passed on to `mpl_toolkits.mplot3d.Axes3D.plot()` or `matplotlib.axes.Axes.plot()`.

**Returns**

Axis with the plot.

**Return type** `matplotlib.axes.Axes`
```

```python
points

The array of points in this data structure.

**Type** `np.ndarray`

```python
query

Query for nearest neighbors of the provided point.

**Parameters**

- `query_points ((N, 3) numpy.ndarray)` – Points to query for.
- `query_args (dict)` – Query arguments determining how to find neighbors. For information on valid query argument, see the Query API.

**Returns**

Results object containing the output of this query.

**Return type** `NeighborQueryResult`
```

```python
class `freud.locality.NeighborList`

**Bases:** `object`

Class representing bonds between two sets of points.

Compute classes contain a set of bonds between two sets of position arrays (“query points” and “points”) and hold a list of index pairs \((i, j)\) where \(i < N_{query\_points}, j < N_{points}\) corresponding to neighbor pairs between the two sets.

For efficiency, all bonds must be sorted by the query point index, from least to greatest. Bonds have an query point index \(i\) and a point index \(j\). The first bond index corresponding to a given query point can be found in \(\log(N_{bonds})\) time using `find_first_index()` , because bonds are ordered by the query point index.
Note: Typically, there is no need to instantiate this class directly. In most cases, users should manipulate `freud.locality.NeighborList` objects received from a neighbor search algorithm, such as `freud.locality.LinkCell`, `freud.locality.AABBQuery`, or `freud.locality.Voronoi`.

Also available as `freud.NeighborList`.

Example:

```python
# Assume we have position as Nx3 array
aq = freud.locality.AABBQuery(box, positions)
nlist = aq.query(positions, {'r_max': 3}).toNeighborList()

# Get all vectors from central particles to their neighbors
rijs = (positions[nlist.point_indices] -
        positions[nlist.query_point_indices])
rijs = box.wrap(rijs)
```

The NeighborList can be indexed to access bond particle indices. Example:

```python
for i, j in nlist[]:
    print(i, j)
```

`copy`

Create a copy. If other is given, copy its contents into this object. Otherwise, return a copy of this object.

**Parameters**

- **other** (`freud.locality.NeighborList`, optional) – A NeighborList to copy into this object (Default value = `None`).

`distances`

The distances for each bond.

**Type** `(N_{bonds})\text{np.ndarray}`

`filter`

Removes bonds that satisfy a boolean criterion.

**Parameters**

- **filt** (`np.ndarray`) – Boolean-like array of bonds to keep (True means the bond will not be removed).

Note: This method modifies this object in-place.

Example:

```python
# Keep only the bonds between particles of type A and type B
nlist.filter(types[nlist.query_point_indices] != types[nlist.point_indices])
```

`filter_r`

Removes bonds that are outside of a given radius range.

**Parameters**

- **r_max** (`float`) – Maximum bond distance in the resulting neighbor list.
- **r_min** (`float`, optional) – Minimum bond distance in the resulting neighbor list (Default value = 0).

`find_first_index`

Returns the lowest bond index corresponding to a query particle with an index \( \geq i \).
Parameters $i$ *(unsigned int)* – The particle index.

**classmethod from_arrays** *(type cls, num_query_points, num_points, query_point_indices, point_indices, distances, weights=None)*

Create a NeighborList from a set of bond information arrays.

Parameters

- **num_query_points** *(int)* – Number of query points (corresponding to *query_point_indices*).
- **num_points** *(int)* – Number of points (corresponding to *point_indices*).
- **query_point_indices** *(np.ndarray)* – Array of integers corresponding to indices in the set of query points.
- **point_indices** *(np.ndarray)* – Array of integers corresponding to indices in the set of points.
- **distances** *(np.ndarray)* – Array of distances between corresponding query points and points.
- **weights** *(np.ndarray, optional)* – Array of per-bond weights (if None is given, use a value of 1 for each weight) (Default value = None).

**neighbor_counts**

A neighbor count array indicating the number of neighbors for each query point.

*Type* *(N_{query\_points}) np.ndarray*

**point_indices**

The point indices for each bond. This array is read-only to prevent breakage of *find_first_index()*.

Equivalent to indexing with [:, 1].

*Type* *(N_{bonds}) np.ndarray*

**query_point_indices**

The query point indices for each bond. This array is read-only to prevent breakage of *find_first_index()*.

Equivalent to indexing with [:, 0].

*Type* *(N_{bonds}) np.ndarray*

**segments**

A segment array indicating the first bond index for each query point.

*Type* *(N_{query\_points}) np.ndarray*

**weights**

The weights for each bond. By default, bonds have a weight of 1.

*Type* *(N_{bonds}) np.ndarray*

**class freud.locality.NeighborQuery**

*Bases: object*

Class representing a set of points along with the ability to query for neighbors of these points.

**Warning:** This class should not be instantiated directly. The subclasses *AABBQuery* and *LinkCell* provide the intended interfaces.

The *NeighborQuery* class represents the abstract interface for neighbor finding. The class contains a set of points and a simulation box, the latter of which is used to define the system and the periodic boundary conditions required for finding neighbors of these points. The primary mode of interacting with the *NeighborQuery* is

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through the `query()` and `queryBall()` functions, which enable finding either the nearest neighbors of a point or all points within a distance cutoff, respectively. Subclasses of NeighborQuery implement these methods based on the nature of the underlying data structure.

**Parameters**

- `box (freud.box.Box)` – Simulation box.
- `points ((N, 3) numpy.ndarray)` – Point coordinates to build the structure.

**box**

The box object used by this data structure.

**Type** `freud.box.Box`

**classmethod from_system** *(type cls, system)*

Create a `NeighborQuery` from any system-like object.

The standard concept of a system in `freud` is any object that provides a way to access a box-like object (anything that can be coerced to a box by `freud.box.Box.from_box()`) and an array-like (according to NumPy’s definition) object that turns into a $N \times 3$ array.

Supported types for `system` include:

- `AABBQuery`
- `LinkCell`
- A sequence of `(box, points)` where `box` is a `Box` and `points` is a `numpy.ndarray`.
- Objects with attributes `box` and `points`.
- `MDAnalysis.coordinates.base.Timestep`
- `gsd.hoomd.Snapshot`
- `garnett.trajectory.Frame`
- `ovito.data.DataCollection`
- `hoomd.data.snapshot`

**Parameters** `system` *(system-like object)* – Any object that can be converted to a `NeighborQuery`.

**Returns** The same `NeighborQuery` object if one is given, or an instance of `NeighborQuery` built from an inferred `box` and `points`.

**Return type** `freud.locality.NeighborQuery`

**plot**

Plot system box and points.

**Parameters**

- `ax (matplotlib.axes.Axes)` – Axis to plot on. If None, make a new figure and axis. The axis projection (2D or 3D) must match the dimensionality of the system (Default value = None).
- `title (str)` – Title of the plot (Default value = None).
- `*args` – Passed on to `mpl_toolkits.mplot3d.Axes3D.plot()` or `matplotlib.axes.Axes.plot()`.
- `**kwargs` – Passed on to `mpl_toolkits.mplot3d.Axes3D.plot()` or `matplotlib.axes.Axes.plot()`.
Returns Axis with the plot.

Return type matplotlib.axes.Axes

points
The array of points in this data structure.

Type np.ndarray

query
Query for nearest neighbors of the provided point.

Parameters

• query_points ((N, 3) numpy.ndarray) – Points to query for.

• query_args (dict) – Query arguments determining how to find neighbors. For information on valid query argument, see the Query API.

Returns Results object containing the output of this query.

Return type NeighborQueryResult

class freud.locality.NeighborQueryResult
Bases: object

Class encapsulating the output of queries of NeighborQuery objects.

Warning: This class should not be instantiated directly, it is the return value of all query* functions of NeighborQuery. The class provides a convenient interface for iterating over query results, and can be transparently converted into a list or a NeighborList object.

The NeighborQueryResult makes it easy to work with the results of queries and convert them to various natural objects. Additionally, the result is a generator, making it easy for users to lazily iterate over the object.

toNeighborList
Convert query result to a freud NeighborList.

Returns A freud NeighborList containing all neighbor pairs found by the query generating this result object.

Return type NeighborList

class freud.locality.PeriodicBuffer
Bases: freud.util._Compute

Replicate periodic images of points inside a box.

property buffer_box
The buffer box, expanded to hold the replicated points.

Type freud.box.Box

property buffer_ids
The buffer point ids.

Type (N_{buffer}) numpy.ndarray

property buffer_points
The buffer point positions.

Type (N_{buffer}, 3) numpy.ndarray
compute
Compute the periodic buffer.

Parameters

- **system** – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.

- **buffer** *(float or list of 3 floats)* – Buffer distance for replication outside the box.

- **images** *(bool, optional)* – If False, buffer is a distance. If True, buffer is a number of images to replicate in each dimension. Note that one image adds half of a box length to each side, meaning that one image doubles the box side lengths, two images triples the box side lengths, and so on. (Default value = False).

class freud.locality.Voronoi
Bases: freud.util._Compute

Computes Voronoi diagrams using voro++.

Voronoi diagrams (Wikipedia) are composed of convex polytopes (polyhedra in 3D, polygons in 2D) called cells, corresponding to each input point. The cells bound a region of Euclidean space for which all contained points are closer to a corresponding input point than any other input point. A ridge is defined as a boundary between cells, which contains points equally close to two or more input points.

The voro++ library [Ryc09] is used for fast computations of the Voronoi diagram.

compute
Compute Voronoi diagram.

Parameters **system** – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.

property nlist
Returns the computed `NeighborList`.

The `NeighborList` computed by this class is weighted. In 2D systems, the bond weight is the length of the ridge (boundary line) between the neighboring points’ Voronoi cells. In 3D systems, the bond weight is the area of the ridge (boundary polygon) between the neighboring points’ Voronoi cells. The weights are not normalized, and the weights for each query point sum to the surface area (perimeter in 2D) of the polytope.

It is possible for pairs of points to appear multiple times in the neighbor list. For example, in a small unit cell, points may neighbor one another on multiple sides because of periodic boundary conditions.

Returns `NeighborList`.

Return type ` NeighborList`

plot
Plot Voronoi diagram.

Parameters **ax** *(matplotlib.axes.Axes)* – Axis to plot on. If None, make a new figure and axis. (Default value = None)

**color_by_sides** *(bool)*: If True, color cells by the number of sides. If False, random colors are used for each cell. (Default value = True)

**cmap** *(str)*: Colormap name to use (Default value = None).

Returns Axis with the plot.
Return type: `matplotlib.axes.Axes`

**property polytopes**

A list of `numpy.ndarray` defining Voronoi polytope vertices for each cell.

Type: `list[numpy.ndarray]`

**property volumes**

Returns an array of Voronoi cell volumes (areas in 2D).

Type: `(N_points) numpy.ndarray`

## 6.16 MSD Module

### Overview

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<th>Compute the mean squared displacement.</th>
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### Details

The `freud.msd` module provides functions for computing the mean-squared-displacement (MSD) of particles in periodic systems.

```python
class freud.msd.MSD
    Bases: freud.util._Compute

    Compute the mean squared displacement.
```

The mean squared displacement (MSD) measures how much particles move over time. The MSD plays an important role in characterizing Brownian motion, since it provides a measure of whether particles are moving according to diffusion alone or if there are other forces contributing. There are a number of definitions for the mean squared displacement. This function provides access to the two most common definitions through the mode argument.

- 'window' *(default)*: This mode calculates the most common form of the MSD, which is defined as

\[
MSD(m) = \frac{1}{N_{\text{particles}}} \sum_{i=1}^{N_{\text{particles}}} \frac{1}{N - m} \sum_{k=0}^{N-m-1} (\vec{r}_i(k + m) - \vec{r}_i(k))^2
\]

where \( \vec{r}_i(t) \) is the position of particle \( i \) in frame \( t \). According to this definition, the mean squared displacement is the average displacement over all windows of length \( m \) over the course of the simulation. Therefore, for any \( m \), \( MSD(m) \) is averaged over all windows of length \( m \) and over all particles. This calculation can be accessed using the ‘window’ mode of this function.

The windowed calculation can be quite computationally intensive. To perform this calculation efficiently, we use the algorithm described in [CPC+11] as described in this StackOverflow thread.

**Note:** The most intensive part of this calculation is computing an FFT. To maximize performance, freud attempts to use the fastest FFT library available. By default, the order of preference is pyFFTW, SciPy, and then NumPy. If you are experiencing significant slowdowns in calculating the MSD, you may benefit from installing a faster FFT library, which freud will automatically detect. The performance change will be especially noticeable if the length of your trajectory is a number whose prime factorization consists of extremely large prime factors. The standard Cooley-Tukey FFT algorithm performs very poorly in this case, so installing pyFFTW will significantly improve performance.
Note that while pyFFTW is released under the BSD 3-Clause license, the FFTW library is available under either GPL or a commercial license. As a result, if you wish to use this module with pyFFTW in code, your code must also be GPL licensed unless you purchase a commercial license.

• 'direct': Under some circumstances, however, we may be more interested in calculating a different quantity described by

\[
MSD(t) = \frac{1}{N_{\text{particles}}} \sum_{i=1}^{N_{\text{particles}}} (r_i(t) - r_i(0))^2
\]

In this case, at each time point (i.e. simulation frame) we simply compute how much particles have moved from their initial position, averaged over all particles. For more information on this calculation, see the Wikipedia page.

**Note:** The MSD is only well-defined when the box is constant over the course of the simulation. Additionally, the number of particles must be constant over the course of the simulation.

**Parameters**

- **box** *(freud.box.Box, optional)* – If not provided, the class will assume that all positions provided in calls to *compute()* are already unwrapped. (Default value = *None*).

- **mode** *(str, optional)* – Mode of calculation. Options are 'window' and 'direct'. (Default value = 'window').

**box**

Box used in the calculation.

**Type** *freud.box.Box*

**compute**

Calculate the MSD for the positions provided.

**Note:** Unlike most methods in freud, accumulation for the MSD is split over points rather than frames of a simulation. The reason for this choice is that efficient computation of the MSD requires using the entire trajectory for a given particle. As a result, when setting *reset=False*, you must provide the positions of each point over the full length of the trajectory, but you may call *compute* multiple times with different subsets the points to calculate the MSD over the full set of positions. The primary use-case is when the trajectory is so large that computing an MSD on all particles at once is prohibitively expensive.

**Parameters**

- **positions** *((N_{frames}, N_{particles}, 3)) numpy.ndarray* – The particle positions over a trajectory. If neither box nor images are provided, the positions are assumed to be unwrapped already.

- **images** *((N_{frames}, N_{particles}, 3)) numpy.ndarray, optional* – The particle images to unwrap with if provided. Must be provided along with a simulation box (in the constructor) if particle positions need to be unwrapped. If neither are provided, positions are assumed to be unwrapped already. (Default value = *None*).

- **reset** *(bool)* – Whether to erase the previously computed values before adding the new computation; if False, will accumulate data (Default value: True).
property msd
The mean squared displacement.

Type \((N_{frames},)\) numpy.ndarray

plot
Plot MSD.

Parameters

- \(ax\) (matplotlib.axes.Axes, optional) – Axis to plot on. If None, make a new figure and axis. (Default value = None)

Returns

Axis with the plot.

Return type (matplotlib.axes.Axes)

6.17 Order Module

Overview

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Details

The freud.order module contains functions which compute order parameters for the whole system or individual particles. Order parameters take bond order data and interpret it in some way to quantify the degree of order in a system using a scalar value. This is often done through computing spherical harmonics of the bond order diagram, which are the spherical analogue of Fourier Transforms.

class freud.order.Cubatic

Bases: freud.util._Compute

Compute the cubatic order parameter [HAG15] for a system of particles using simulated annealing instead of Newton-Raphson root finding.

Parameters

- \(t_{initial}\) (float) – Starting temperature.
- \(t_{final}\) (float) – Final temperature.
- \(scale\) (float) – Scaling factor to reduce temperature.
- \(n_{replicates}\) (unsigned int, optional) – Number of replicate simulated annealing runs. (Default value = 1).
• `seed (unsigned int, optional)` – Random seed to use in calculations. If `None`, system time is used. (Default value = `None`).

**compute**

Calculates the per-particle and global order parameter.

Parameters `orientations ((N\text{\_particles}, 4) \text{ numpy.\_ndarray})` – Orientations as angles to use in computation.

**property cubatic\_tensor**

Rank 4 homogeneous tensor representing the optimal system-wide coordinates.

Type \((3, 3, 3, 3) \text{ numpy.\_ndarray}\)

**property global\_tensor**

Rank 4 tensor corresponding to the global orientation. Computed from all orientations.

Type \((3, 3, 3, 3) \text{ numpy.\_ndarray}\)

**property order**

Cubatic order parameter of the system.

Type `float`

**property orientation**

The quaternion of global orientation.

Type \((4) \text{ numpy.\_ndarray}\)

**property particle\_order**

Order parameter.

Type \((N\text{\_particles}) \text{ numpy.\_ndarray}\)

**scale**

The scale.

Type `float`

**seed**

Random seed to use in calculations.

Type `unsigned int`

**t\_final**

The value of the final temperature.

Type `float`

**t\_initial**

The value of the initial temperature.

Type `float`

**class freud.order.Hexatic**

Bases: `freud.localization._PairCompute`

Calculates the \(k\)-atic order parameter for 2D systems.

The \(k\)-atic order parameter (called the hexatic order parameter for \(k = 6\)) is analogous to Steinhardt order parameters, and is used to measure order in the bonds of 2D systems.

The \(k\)-atic order parameter for a particle \(i\) and its \(n\) neighbors \(j\) is given by:

\[
\psi_k (i) = \frac{1}{n} \sum_{j} c^{k\phi_{ij}}
\]
The parameter $k$ governs the symmetry of the order parameter and typically matches the number of neighbors to be found for each particle. The quantity $\phi_{ij}$ is the angle between the vector $r_{ij}$ and $(1, 0)$.

**Note:** 2D: `freud.order.Hexatic` is only defined for 2D systems. The points must be passed in as $[x, y, 0]$.

**Parameters**

- **k** *(unsigned int, optional)* – Symmetry of order parameter. (Default value = 6).

**compute**
Calculates the hexatic order parameter.

**Parameters**

- **system** – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.
- **neighbors** *(freud.locality.NeighborList or dict, optional)* – Either a `NeighborList` of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).

**default_query_args**
The default query arguments are {'mode': 'nearest', 'num_neighbors': self.k}.

**k**
Symmetry of the order parameter.

**property particle_order**
Order parameter.

**class freud.order.Nematic**
Bases: `freud.util._Compute`

Compute the nematic order parameter for a system of particles.

**Parameters**

- **u** *(3)* `numpy.ndarray` – The nematic director of a single particle in the reference state (without any rotation applied).

**compute**
Calculates the per-particle and global order parameter.

**Parameters**

- **orientations** *(N_{particles}, 4)* `numpy.ndarray` – Orientations to calculate the order parameter.

**property director**
The average nematic director.

**property nematic_tensor**
3x3 matrix corresponding to the average particle orientation.

**property order**
Nematic order parameter of the system.
property particle_tensor

\((N_{\text{particles}}, 3, 3)\) \text{numpy.ndarray}: One 3x3 matrix per-particle corresponding to each individual particle orientation.

\(u\)

The normalized reference director (the normalized vector provided on construction).

\textbf{Type} \(3\) \text{numpy.ndarray}

class freud.order.RotationalAutocorrelation

\textbf{Bases:} \text{freud.util._Compute}

Calculates a measure of total rotational autocorrelation.

For any calculation of rotational correlations of extended (i.e. non-point) particles, encoding the symmetries of these particles is crucial to appropriately determining correlations. For systems of anisotropic particles in three dimensions, representing such equivalence can be quite mathematically challenging. This calculation is based on the hyperspherical harmonics as laid out in [KDvAG19]. Generalizations of spherical harmonics to four dimensions, hyperspherical harmonics provide a natural basis for periodic functions in 4 dimensions just as harmonic functions (sines and cosines) or spherical harmonics do in lower dimensions. The idea behind this calculation is to embed orientation quaternions into a 4-dimensional space and then use hyperspherical harmonics to find correlations in a symmetry-aware fashion.

The choice of the hyperspherical harmonic parameter \(l\) determines the symmetry of the functions. The output is not a correlation function, but rather a scalar value that measures total system orientational correlation with an initial state. As such, the output can be treated as an order parameter measuring degrees of rotational (de)correlation. For analysis of a trajectory, the compute call needs to be done at each trajectory frame.

\textbf{Parameters}

\(l\) \text{(int)} – Order of the hyperspherical harmonic. Must be a positive, even integer.

\textbf{compute}

Calculates the rotational autocorrelation function for a single frame.

\textbf{Parameters}

- \textbf{ref_orientations} \((N_{\text{orientations}}, 4)\) \text{numpy.ndarray} – Orientations for the initial frame.
- \textbf{orientations} \((N_{\text{orientations}}, 4)\) \text{numpy.ndarray} – Orientations for the frame of interest.

\(l\)

The azimuthal quantum number, which defines the order of the hyperspherical harmonic.

\textbf{Type} \text{int}

property order

Autocorrelation of the system.

\textbf{Type} \text{float}

property particle_order

Rotational autocorrelation values calculated for each orientation.

\textbf{Type} \((N_{\text{orientations}})\) \text{numpy.ndarray}

class freud.order.SolidLiquid

\textbf{Bases:} \text{freud.locality._PairCompute}

Identifies solid-like clusters using dot products of \(q_{lm}\).

The solid-liquid order parameter [tW95][FHND10] uses a Steinhardt-like approach to identify solid-like particles. First, a bond parameter \(q_{lm}\) is computed for each neighbor bond.
If `normalize_q` is true (default), the bond parameter is given by
\[ q_l(i, j) = \frac{\sum_{m=-l}^{l} \text{Re} q_{lm}(i)^* q_{lm}(j)}{\sqrt{\sum_{m=-l}^{l} |q_{lm}(i)|^2} \sqrt{\sum_{m=-l}^{l} |q_{lm}(j)|^2}} \]

If `normalize_q` is false, then the denominator of the above expression is left out.

Next, the bonds are filtered to keep only “solid-like” bonds with \( q_l(i, j) \) above a cutoff value \( q_{\text{threshold}} \). If a particle has more than \( S_{\text{threshold}} \) solid-like bonds, then the particle is considered solid-like. Finally, solid-like particles are clustered.

**Parameters**

- `l (unsigned int)` – Spherical harmonic quantum number \( l \).
- `q_threshold (float)` – Value of dot product threshold when evaluating \( q_l(i, j) \) to determine if a bond is solid-like. For \( l = 6 \), 0.7 is generally good for FCC or BCC structures [FHND10].
- `solid_threshold (unsigned int)` – Minimum required number of adjacent solid-like bonds for a particle to be considered solid-like for clustering. For \( l = 6 \), 6-8 is generally good for FCC or BCC structures.
- `normalize_q (bool)` – Whether to normalize the dot product (Default value = True).

**property cluster_idx**

\((N_{\text{particles}})\text{ numpy.ndarray}\): Solid-like cluster indices for each particle.

**property cluster_sizes**

The sizes of all clusters.

Type \((N_{\text{clusters}},)\text{ np.ndarray}\)

**compute**

Compute the order parameter.

**Parameters**

- `system` – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.
- `neighbors` (`freud.locality.NeighborList` or dict, optional) – Either a `NeighborList` of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).

**default_query_args**

No default query arguments.

\( l \)

Spherical harmonic quantum number \( l \).

Type unsigned int

**property largest_cluster_size**

The largest cluster size.

Type unsigned int

**property nlist**

Neighbor list of solid-like bonds.

Type `freud.locality.NeighborList`

**normalize_q**

Whether the dot product is normalized.

Type bool
property num_connections
The number of solid-like bonds for each particle.

Type \((N_{\text{particles}})\) numpy.ndarray

plot
Plot solid-like cluster distribution.

Parameters

- \(ax\) (matplotlib\'s Axes, optional) – Axis to plot on. If None, make a new figure and axis. (Default value = None)

Returns
Axis with the plot.

Return type
(matplotlib\'s Axes)

q_threshold
Value of dot product threshold.

Type float

property ql_ij
Bond dot products \(q_l(i,j)\). Indexed by the elements of self.nlist.

Type \((N_{\text{bonds}})\) numpy.ndarray

solid_threshold
Value of number-of-bonds threshold.

Type float

class freud.order.Steinhardt
Bases: freud.locality._PairCompute

Compute the local Steinhardt [Ste83] rotationally invariant \(Q_l\) \(W_l\) order parameter for a set of points.

Implements the local rotationally invariant \(q_l\) or \(w_l\) order parameter described by Steinhardt. For a particle \(i\), we calculate the average order parameter by summing the spherical harmonics between particle \(i\) and its neighbors \(j\) in a local region:

\[
\bar{q}_{lm}(i) = \frac{1}{N_b} \sum_{j=1}^{N_b} Y_{lm}(\theta(\vec{r}_{ij}), \phi(\vec{r}_{ij}))
\]

The particles included in the sum are determined by the \(r_{\text{max}}\) argument to the constructor.

For \(q_l\), this is then combined in a rotationally invariant fashion to remove local orientational order as follows:

\[
q_l(i) = \sqrt{\frac{4\pi}{2l+1} \sum_{m=-l}^{l} |\bar{q}_{lm}|^2}
\]

For \(w_l\), it is then defined as a weighted average over the \(\bar{q}_{lm}(i)\) values using Wigner 3j symbols (Clebsch-Gordan coefficients). The resulting combination is rotationally (i.e. frame) invariant.

The average argument in the constructor provides access to a variant of this parameter that performs a average over the first and second shell combined [LD08]. To compute this parameter, we perform a second averaging over the first neighbor shell of the particle to implicitly include information about the second neighbor shell. This averaging is performed by replacing the value \(\bar{q}_{lm}(i)\) in the original definition by the average value of \(\bar{q}_{lm}(k)\) over all the \(k\) neighbors of particle \(i\) as well as itself.

The norm attribute argument provides normalized versions of the order parameter, where the normalization is performed by averaging the \(q_{lm}\) values over all particles before computing the order parameter of choice.

Parameters

- \(l\) (unsigned int) – Spherical harmonic quantum number \(l\).
- average (bool, optional) – Determines whether to calculate the averaged Steinhardt order parameter. (Default value = False)
• \texttt{wl} (bool, optional) – Determines whether to use the $w_l$ version of the Steinhardt order parameter. (Default value = False)

• \texttt{weighted} (bool, optional) – Determines whether to use neighbor weights in the computation of spherical harmonics over neighbors. If enabled and used with a Voronoi neighbor list, this results in the Minkowski Structure Metrics $q'_l$. (Default value = False)

• \texttt{wl_normalize} (bool, optional) – Determines whether to normalize the $w_l$ version of the Steinhardt order parameter. (Default value = False)

\textbf{average}

Whether the averaged Steinhardt order parameter was calculated.

Type bool

\textbf{compute}

Compute the order parameter.

\textbf{Parameters}

• \texttt{system} – Any object that is a valid argument to \texttt{freud.locality.NeighborQuery.from_system}.

• \texttt{neighbors} (\texttt{freud.locality.NeighborList or dict, optional}) – Either a \texttt{NeighborList} of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).

\textbf{default_query_args}

No default query arguments.

\textbf{l}

Spherical harmonic quantum number $l$.

Type unsigned int

\textbf{property order}

The system wide normalization of the $q_l$ or $w_l$ order parameter.

Type float

\textbf{property particle_order}

Variant of the Steinhardt order parameter for each particle (filled with nan for particles with no neighbors).

Type ($N_{\text{particles}}$) numpy.ndarray

\textbf{plot}

Plot order parameter distribution.

\textbf{Parameters} \texttt{ax} (matplotlib.axes.Axes, optional) – Axis to plot on. If None, make a new figure and axis. (Default value = None)

\textbf{Returns} Axis with the plot.

\textbf{Return type} (matplotlib.axes.Axes)

\textbf{property ql}

($N_{\text{particles}}$) numpy.ndarray: $q_l$ Steinhardt order parameter for each particle (filled with nan for particles with no neighbors). This is always available, no matter which options are selected.

\textbf{weighted}

Whether neighbor weights were used in the computation of spherical harmonics over neighbors.

Type bool
Whether the $W_l$ version of the Steinhardt order parameter was used.

**Type** bool

**class freud.order.Translational**

**Bases:** freud.locality._PairCompute

Compute the translational order parameter for each particle.

**Note:** 2D: freud.order.Translational is only defined for 2D systems. The points must be passed in as $[x, y, 0]$.

**Parameters**

- $k$ *(float, optional)* – Symmetry of order parameter. (Default value = 6.0).

**compute**

Calculates the local descriptors.

**Parameters**

- $system$ – Any object that is a valid argument to freud.locality.NeighborQuery.from_system.

- $neighbors$ *(freud.locality.NeighborList or dict, optional)* – Either a NeighborList of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).

**default_query_args**

`{'mode': 'nearest', 'num_neighbors': int(self.k)}`.

**Type** The default query arguments are

**Type** code

$k$

Normalization of the order parameter.

**Type** unsigned int

**property particle_order**

Order parameter.

**Type** $(N_{\text{particles}})$ numpy.ndarray

## 6.18 Parallel Module

**Overview**

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<td>Get the number of threads for parallel computation.</td>
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<td>Set the number of threads for parallel computation.</td>
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</table>
Details

The `freud.parallel` module controls the parallelization behavior of freud, determining how many threads the TBB-enabled parts of freud will use. freud uses all available threads for parallelization unless directed otherwise.

```python
class freud.parallel.NumThreads
    Bases: object

    Context manager for managing the number of threads to use.

    Parameters
    N (int, optional) -- Number of threads to use in this context. If None, which will use all available threads. (Default value = None).

freud.parallel.get_num_threads
    Get the number of threads for parallel computation.

    Returns
    Number of threads.

    Return type
    (int)

freud.parallel.set_num_threads
    Set the number of threads for parallel computation.

    Parameters
    nthreads (int, optional) -- Number of threads to use. If None, use all threads available. (Default value = None).
```

6.19 PMFT Module

Overview

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<td>Computes the PMFT [vAKA+14][vAAS+13] in a 2D system described by $r, \theta_1, \theta_2$.</td>
</tr>
<tr>
<td><code>freud.pmft.PMFTXYT</code></td>
<td>Computes the PMFT [vAKA+14][vAAS+13] for systems described by coordinates $x, y, \theta$.</td>
</tr>
<tr>
<td><code>freud.pmft.PMFTXY</code></td>
<td>Computes the PMFT [vAKA+14][vAAS+13] in coordinates $x, y$.</td>
</tr>
<tr>
<td><code>freud.pmft.PMFTXYZ</code></td>
<td>Computes the PMFT [vAKA+14][vAAS+13] in coordinates $x, y, z$.</td>
</tr>
</tbody>
</table>

Details

The `freud.pmft` module allows for the calculation of the Potential of Mean Force and Torque (PMFT) [vAKA+14][vAAS+13] in a number of different coordinate systems. The shape of the arrays computed by this module depend on the coordinate system used, with space discretized into a set of bins created by the PMFT object’s constructor. Each query point’s neighboring points are assigned to bins, determined by the relative positions and/or orientations of the particles. Next, the pair correlation function (PCF) is computed by normalizing the binned histogram, by dividing out the number of accumulated frames, bin sizes (the Jacobian), and query point number density. The PMFT is then defined as the negative logarithm of the PCF. For further descriptions of the numerical methods used to compute the PMFT, refer to the supplementary information of [vAKA+14].

Note: The coordinate system in which the calculation is performed is not the same as the coordinate system in which particle positions and orientations should be supplied. Only certain coordinate systems are available for certain particle positions and orientations:

- 2D particle coordinates (position: $[x, y, 0]$, orientation: $\theta$):
Note: For any bins where the histogram is zero (i.e. no observations were made with that relative position/orientation of particles), the PMFT will return nan.

class freud.pmft.PMFTR12
    Bases: freud.pmft._PMFT
    Computes the PMFT [vAKA+14][vAAS+13] in a 2D system described by $r, \theta_1, \theta_2$.

    Parameters
    • $r_{max}$ (float) – Maximum distance at which to compute the PMFT.
    • bins (unsigned int or sequence of length 3) – If an unsigned int, the number of bins in $r, \theta_1, \text{and } \theta_2$. If a sequence of three integers, interpreted as (num_bins_r, num_bins_t1, num_bins_t2).

    bin_centers
        The centers of each bin in the histogram (has the same shape as the histogram itself).
        Type numpy.ndarray

    property bin_counts
        The bin counts in the histogram.
        Type numpy.ndarray

    bin_edges
        The edges of each bin in the histogram (is one element larger in each dimension than the histogram because each bin has a lower and upper bound).
        Type numpy.ndarray

    bounds
        A list of tuples indicating upper and lower bounds of each axis of the histogram.
        Type list(tuple)

    property box
        The box object used in the last computation.
        Type freud.box.Box

    compute
        Calculates the PMFT.
        Parameters
• **system** – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.

• **orientations** `((N_{points}, 4) \text{ or } (N_{points},) \text{ numpy.ndarray})` – Orientations associated with system points that are used to calculate bonds. If the array is one-dimensional, the values are treated as angles in radians corresponding to **counterclockwise** rotations about the z axis.

• **query_points** `((N_{query\_points}, 3) \text{ numpy.ndarray}, \text{ optional})` – Query points used to calculate the PMFT. Uses the system’s points if None (Default value = None).

• **query_orientations** `((N_{query\_points}, 4) \text{ numpy.ndarray}, \text{ optional})` – Query orientations associated with query points that are used to calculate bonds. If the array is one-dimensional, the values are treated as angles in radians corresponding to **counterclockwise** rotations about the z axis. Uses orientations if None. (Default value = None).

• **neighbors** (`freud.locality.NeighborList or dict, \text{ optional}`) – Either a `NeighborList` of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).

• **reset** (`bool`) – Whether to erase the previously computed values before adding the new computation; if False, will accumulate data (Default value: True).

```python
default_query_args
    The default query arguments are {'mode': 'ball', 'r_max': self.r_max}.
```

```python
nbins
    The number of bins in each dimension of the histogram
    Type list
```

```python
property pmft
    The discrete potential of mean force and torque.
    Type np.ndarray
```

**class freud.pmft.PMFTXY**
Bases: freud.pmft._PMFT

Computes the PMFT [vAKA+14][vAAS+13] in coordinates x, y.

Since there are 3 degrees of translational and rotational freedom in 2 dimensions, this class is implicitly integrating out one of them. Specifically, by comparison to `PMFTXYT` we see that the missing dimension is the relative orientation of the second particle. Note that this degree of freedom is still accounted for in the Jacobian of this calculation.

**Note:** 2D: `freud.pmft.PMFTXY` is only defined for 2D systems. The points must be passed in as `[x, y, 0]`.

**Parameters**

- **x_max** (`float`) – Maximum x distance at which to compute the PMFT.

- **y_max** (`float`) – Maximum y distance at which to compute the PMFT.

- **bins** (`unsigned int or sequence of length 2`) – If an unsigned int, the number of bins in x and y. If a sequence of two integers, interpreted as `(num_bins_x, num_bins_y)`.
bin_centers
The centers of each bin in the histogram (has the same shape as the histogram itself).
Type numpy.ndarray

property bin_counts
The bin counts in the histogram.
Type numpy.ndarray

bin_edges
The edges of each bin in the histogram (is one element larger in each dimension than the histogram because each bin has a lower and upper bound).
Type numpy.ndarray

bounds
A list of tuples indicating upper and lower bounds of each axis of the histogram.
Type list (tuple)

property box
The box object used in the last computation.
Type freud.box.Box

compute
Calculates the PMFT.

Note: The orientations of the system points are irrelevant for this calculation because that dimension is integrated out. The provided query_orientations are therefore always associated with query_points (which are equal to the system points if no query_points are explicitly provided).

Parameters

- system – Any object that is a valid argument to freud.locality.NeighborQuery.from_system.

- query_orientations ((N_query_points, 4) or (N_query_points,)) numpy.ndarray – Query orientations associated with query points that are used to calculate bonds. If the array is one-dimensional, the values are treated as angles in radians corresponding to counterclockwise rotations about the z axis.

- query_points ((N_query_points, 3)) numpy.ndarray, optional) – Query points used to calculate the PMFT. Uses the system’s points if None (Default value: None).

- neighbors (freud.locality.NeighborList or dict, optional) – Either a NeighborList of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).

- reset (bool) – Whether to erase the previously computed values before adding the new computation; if False, will accumulate data (Default value: True).

default_query_args
The default query arguments are {'mode': 'ball', 'r_max': self.r_max}.

nbins
The number of bins in each dimension of the histogram
Type list
**plot**
Plot PMFTXY.

**Parameters**
- `ax` *(matplotlib.axes.Axes, optional)* – Axis to plot on. If None, make a new figure and axis. (Default value = None)

**Returns**
Axis with the plot.

**Return type** *(matplotlib.axes.Axes)*

**property pmft**
The discrete potential of mean force and torque.

**Type** *np.ndarray*

**class freud.pmft.PMFTXYT**
Bases: freud.pmft._PMFT

Computes the PMFT [vAKA+14][vAAS+13] for systems described by coordinates $x, y, \theta$.

**Note:** 2D: `freud.pmft.PMFTXYT` is only defined for 2D systems. The points must be passed in as $[x, y, 0]$.

**Parameters**
- `x_max` (*float*) – Maximum $x$ distance at which to compute the PMFT.
- `y_max` (*float*) – Maximum $y$ distance at which to compute the PMFT.
- `bins` *(unsigned int or sequence of length 3)* – If an unsigned int, the number of bins in $x, y, \theta$. If a sequence of three integers, interpreted as `(num_bins_x, num_bins_y, num_bins_t)`.

**bin_centers**
The centers of each bin in the histogram (has the same shape as the histogram itself).

**Type** *numpy.ndarray*

**property bin_counts**
The bin counts in the histogram.

**Type** *numpy.ndarray*

**bin_edges**
The edges of each bin in the histogram (is one element larger in each dimension than the histogram because each bin has a lower and upper bound).

**Type** *numpy.ndarray*

**bounds**
A list of tuples indicating upper and lower bounds of each axis of the histogram.

**Type** *list (tuple)*

**property box**
The box object used in the last computation.

**Type** *freud.box.Box*

**compute**
Calculates the PMFT.

**Parameters**
• **system** – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.

• **orientations** \((N_{\text{points}}, 4)\) or \((N_{\text{points}},)\) `numpy.ndarray` – Orientations associated with system points that are used to calculate bonds. If the array is one-dimensional, the values are treated as angles in radians corresponding to **counterclockwise** rotations about the z axis.

• **query_points** \((N_{\text{query_points}}, 3)\) `numpy.ndarray`, optional) – Query points used to calculate the PMFT. Uses the system’s points if `None` (Default value = `None`).

• **query_orientations** \((N_{\text{query_points}}, 4)\) `numpy.ndarray`, optional) – Query orientations associated with query points that are used to calculate bonds. If the array is one-dimensional, the values are treated as angles in radians corresponding to **counterclockwise** rotations about the z axis. Uses `orientations` if `None`. (Default value = `None`).

• **neighbors** (`freud.locality.NeighborList` or dict, optional) – Either a `NeighborList` of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: `None`).

• **reset** (bool) – Whether to erase the previously computed values before adding the new computation; if `False`, will accumulate data (Default value: `True`).

**default_query_args**

The default query arguments are `{'mode': 'ball', 'r_max': self.r_max}`.

**nbins**

The number of bins in each dimension of the histogram

Type list

**property pmft**

The discrete potential of mean force and torque.

Type `np.ndarray`

**class freud.pmft.PMFTXYZ**

Bases: `freud.pmft._PMFT`

Computes the PMFT [vAKA+14][vAAS+13] in coordinates \(x, y, z\).

Since there are 6 degrees of translational and rotational freedom in 3 dimensions, this class is implicitly integrating out three of them. In particular, we are disregarding the orientational degrees of freedom in the system. The simplest parameterization of these degrees is using Euler angles. The total volume of orientations that are implicitly integrated out by this calculation can be computed by an explicit integral over the Euler angles:

\[
\int_0^{2\pi} \int_0^\pi \int_0^{2\pi} \sin \theta d\phi d\theta d\psi = 8\pi^2
\]

For more information on this calculation, see [GMS63] (the equation is also reproduced without proof at [https://en.wikipedia.org/wiki/3D_rotation_group#Spherical_harmonics](https://en.wikipedia.org/wiki/3D_rotation_group#Spherical_harmonics)). This prefactor of \(8\pi^2\) is accounted for in the Jacobian used to compute the `PMFTXYZ`.

**Parameters**

• **x_max** (`float`) – Maximum \(x\) distance at which to compute the PMFT.

• **y_max** (`float`) – Maximum \(y\) distance at which to compute the PMFT.

• **z_max** (`float`) – Maximum \(z\) distance at which to compute the PMFT.
• **bins** *(unsigned int or sequence of length 3)* – If an unsigned int, the number of bins in x, y, and z. If a sequence of three integers, interpreted as (num_bins_x, num_bins_y, num_bins_z).

• **shiftvec** *(list)* – Vector pointing from [0, 0, 0] to the center of the PMFT.

**bin centers**
The centers of each bin in the histogram (has the same shape as the histogram itself).

  Type `numpy.ndarray`

**property bin_counts**
The bin counts in the histogram.

  Type `numpy.ndarray`

**bin_edges**
The edges of each bin in the histogram (is one element larger in each dimension than the histogram because each bin has a lower and upper bound).

  Type `numpy.ndarray`

**bounds**
A list of tuples indicating upper and lower bounds of each axis of the histogram.

  Type `list(tuple)`

**property box**
The box object used in the last computation.

  Type `freud.box.Box`

**compute**
Calculates the PMFT.

**Note:** The orientations of the system points are irrelevant for this calculation because that dimension is integrated out. The provided `query_orientations` are therefore always associated with `query_points` (which are equal to the system points if no `query_points` are explicitly provided).

### Parameters

- **system** – Any object that is a valid argument to `freud.locality.NeighborQuery.from_system`.

- **query_orientations** *(N_points, 4) numpy.ndarray)* – Query orientations associated with query points that are used to calculate bonds.

- **query_points** *(N_query_points, 3) numpy.ndarray, optional)* – Query points used to calculate the PMFT. Uses the system’s points if None (Default value = None).

- **face_orientations** *(N_points, N_faces, 4) numpy.ndarray, optional)* – Orientations of particle faces to account for symmetry of the points. If not supplied by user or None, unit quaternions will be supplied. If a 2D array of shape (N_faces, 4) or a 3D array of shape (1, N_faces, 4) is supplied, the supplied quaternions will be broadcast for all points. (Default value = None).

- **neighbors** *(freud.locality.NeighborList or dict, optional)* – Either a `NeighborList` of neighbor pairs to use in the calculation, or a dictionary of query arguments (Default value: None).
• **reset** (bool) – Whether to erase the previously computed values before adding the new computation; if False, will accumulate data (Default value: True).

**default_query_args**
The default query arguments are `{mode: 'ball', 'r_max': self.r_max}`.

**nbins**
The number of bins in each dimension of the histogram

**Type** list

**property pmft**
The discrete potential of mean force and torque.

**Type** np.ndarray

## 6.20 Development Guide

Contributions to freud are highly encouraged. The pages below offer information about freud’s design goals and how to contribute new modules.

### 6.20.1 Design Principles

**Vision**

The freud library is designed to be a powerful and flexible library for the analysis of simulation output. To support a variety of analysis routines, freud places few restrictions on its components. The primary requirement for an analysis routine in freud is that it should be substantially computationally intensive so as to require coding up in C++: **all freud code should be composed of fast C++ routines operating on systems of particles in periodic boxes**. To remain easy-to-use, all C++ modules should be wrapped in Python code so they can be easily accessed from Python scripts or through a Python interpreter.

In order to achieve this goal, freud takes the following viewpoints:

- freud works directly with NumPy <http://www.numpy.org/>_ arrays to retain maximum flexibility. Integrations with other tools should be performed via the common data representations of NumPy arrays.

- For ease of maintenance, freud uses Git for version control; GitHub for code hosting and issue tracking; and the PEP 8 standard for code, stressing explicitly written code which is easy to read.

- To ensure correctness, freud employs unit testing using the Python unittest framework. In addition, freud utilizes CircleCI for continuous integration to ensure that all of its code works correctly and that any changes or new features do not break existing functionality.

**Language choices**

The freud library is written in two languages: Python and C++. C++ allows for powerful, fast code execution while Python allows for easy, flexible use. Intel Threading Building Blocks parallelism provides further power to C++ code. The C++ code is wrapped with Cython, allowing for user interaction in Python. NumPy provides the basic data structures in freud, which are commonly used in other Python plotting libraries and packages.
Unit Tests

All modules should include a set of unit tests which test the correct behavior of the module. These tests should be simple and short, testing a single function each, and completing as quickly as possible (ideally < 10 sec, but times up to a minute are acceptable if justified).

Benchmarks

Modules can be benchmarked in the following way. The following code is an example benchmark for the `freud.density.RDF` module.

```python
import numpy as np
import freud
from benchmark import Benchmark
from benchmarker import run_benchmarks

class BenchmarkDensityRDF(Benchmark):
    def __init__(self, r_max, bins, r_min):
        self.r_max = r_max
        self.bins = bins
        self.r_min = r_min

    def bench_setup(self, N):
        self.box_size = self.r_max*3.1
        np.random.seed(0)
        self.points = np.random.random_sample((N, 3)).astype(np.float32) *
                      self.box_size - self.box_size/2
        self.rdf = freud.density.RDF(self.bins, self.r_max, r_min=self.r_min)
        self.box = freud.box.Box.cube(self.box_size)

    def bench_run(self, N):
        self.rdf.compute((self.box, self.points), reset=False)
        self.rdf.compute((self.box, self.points))

def run():
    Ns = [1000, 10000]
    r_max = 10.0
    bins = 10
    r_min = 0
    number = 100
    name = 'freud.density.RDF'
    classobj = BenchmarkDensityRDF

    return run_benchmarks(name, Ns, number, classobj,
                           r_max=r_max, bins=bins, r_min=r_min)

if __name__ == '__main__':
    run()
```

in a file `benchmark_density_RDF.py` in the `benchmarks` directory. More examples can be found in the `benchmarks` directory. The runtime of `BenchmarkDensityRDF.bench_run` will be timed for number of times on the input sizes of `Ns`. Its runtime with respect to the number of threads will also be measured. Benchmarks are run as a part of continuous integration, with performance comparisons between the current commit and the master branch.
Make Execution Explicit

While it is tempting to make your code do things “automatically”, such as have a calculate method find all _calc methods in a class, call them, and add their returns to a dictionary to return to the user, it is preferred in freud to execute code explicitly. This helps avoid issues with debugging and undocumented behavior:

```python
# this is bad
class SomeFreudClass(object):
    def __init__(self, **kwargs):
        for key in kwargs.keys:
            setattr(self, key, kwargs[key])

# this is good
class SomeOtherFreudClass(object):
    def __init__(self, x=None, y=None):
        self.x = x
        self.y = y
```

Code Duplication

When possible, code should not be duplicated. However, being explicit is more important. In freud this translates to many of the inner loops of functions being very similar:

```c
// somewhere deep in function_a
for (int i = 0; i < n; i++)
{
    vec3[float] pos_i = position[i];
    for (int j = 0; j < n; j++)
    {
        pos_j = = position[j];
        // more calls here
    }
}

// somewhere deep in function_b
for (int i = 0; i < n; i++)
{
    vec3[float] pos_i = position[i];
    for (int j = 0; j < n; j++)
    {
        pos_j = = position[j];
        // more calls here
    }
}
```

While it might be possible to figure out a way to create a base C++ class all such classes inherit from, run through positions, call a calculation, and return, this would be rather complicated. Additionally, any changes to the internals of the code, and may result in performance penalties, difficulty in debugging, etc. As before, being explicit is better.

However, if you have a class which has a number of methods, each of which requires the calling of a function, this function should be written as its own method (instead of being copy-pasted into each method) as is typical in object-oriented programming.
Python vs. Cython vs. C++

The `freud` library is meant to leverage the power of C++ code imbued with parallel processing power from TBB with the ease of writing Python code. The bulk of your calculations should take place in C++, as shown in the snippet below:

```python
# this is bad
def badHeavyLiftingInPython(positions):
    # check that positions are fine
    for i, pos_i in enumerate(positions):
        for j, pos_j in enumerate(positions):
            if i != j:
                r_ij = pos_j - pos_i
                # ...
                computed_array[i] += some_val
    return computed_array

# this is good
def goodHeavyLiftingInCPlusPlus(positions):
    # check that positions are fine
cplusplus_heavy_function(computed_array, positions, len(pos))
    return computed_array
```

In the C++ code, implement the heavy lifting function called above from Python:

```c++
void cplusplus_heavy_function(float* computed_array,
                              float* positions,
                              int n)
{
    for (int i = 0; i < n; i++)
    {
        for (int j = 0; j < n; j++)
        {
            if (i != j)
            {
                r_ij = pos_j - pos_i;
                // ...
                computed_array[i] += some_val;
            }
        }
    }
}
```

Some functions may be necessary to write at the Python level due to a Python library not having an equivalent C++ library, complexity of coding, etc. In this case, the code should be written in Cython and a reasonable attempt to optimize the code should be made.

### 6.20.2 Source Code Conventions

The guidelines below should be followed for any new code added to `freud`.

**Naming Conventions**

The following conventions should apply to Python, Cython, and C++ code.
• Variable names use `lower_case_with_underscores`
• Function and method names use `lowerCaseWithNoUnderscores`
• Class names use `CapWords`

### Indentation

• Spaces, not tabs, must be used for indentation
• 4 spaces are required per level of indentation and continuation lines

### Python

Code in `freud` should follow PEP 8, as well as the following guidelines. Anything listed here takes precedence over PEP 8, but try to deviate as little as possible from PEP 8. When in doubt, follow these guidelines over PEP 8.

During continuous integration (CI), all Python and Cython code in `freud` is tested with `flake8` to ensure PEP 8 compliance. It is strongly recommended to set up a pre-commit hook to ensure code is compliant before pushing to the repository:

```bash
flake8 --install-hook git
git config --bool flake8.strict true
```

### Source

• All code should be contained in Cython files
• Python `.py` files are reserved for module level docstrings and minor miscellaneous tasks for, e.g., backwards compatibility.
• Semicolons should not be used to mark the end of lines in Python.

### Documentation Comments

• Documentation is generated using `sphinx`.
• The documentation should be written according to the Google Python Style Guide.
• A few specific notes:
  - The shapes of NumPy arrays should be documented as part of the type in the following manner:

    ```
    points ((:math:`N_{points}`, 3) :class:`numpy.ndarray`):
    ```
  - Constructors should be documented at the class level.
  - Class attributes (including properties) should be documented as class attributes within the class-level docstring.
  - Optional arguments should be documented as such within the type after the actual type, and the default value should be included within the description:
properties that are settable should be documented the same way as optional arguments: 

- `Lx (float, settable): Length in x`

- All docstrings should be contained within the Cython files.
- If you copy an existing file as a template, make sure to modify the comments to reflect the new file.
- Docstrings should demonstrate how to use the code with an example. Liberal addition of examples is encouraged.

**C++**

C++ code should follow the result of running `clang-format-6.0` with the style specified in the file `.clang-format`. Please refer to Clang Format 6 for details.

When in doubt, run `clang-format -style=file FILE_WITH_YOUR_CODE` in the top directory of the freud repository. If installing `clang-format` is not a viable option, the `check-style` step of continuous integration (CI) contains the information on the correctness of the style.

**Source**

- TBB sections should use lambdas, not functors (see this tutorial).

```cpp
void someFunction(float some_var, float other_var) {
    // code before parallel section
    parallel_for(blocked_range<size_t>(0, n), [=](const blocked_range<size_t>& r) {
        // do stuff
    });
}
```

**Documentation Comments**

- Add explanatory comments throughout your code.

**6.20.3 How to Add New Code**

This document details the process of adding new code into freud.

**Does my code belong in freud?**

The freud library is not meant to simply wrap or augment external Python libraries. A good rule of thumb is if the code I plan to write does not require C++, it does not belong in freud. There are, of course, exceptions.

**Create a new branch**

You should branch your code from master into a new branch. Do not add new code directly into the master branch.
Add a New Module

If the code you are adding is in a new module, not an existing module, you must do the following:

- Create `cpp/moduleName` folder
- Edit `freud/__init__.py`
  - Add `from . import moduleName` so that your module is imported by default.
- Edit `freud/__freud.pyx`
  - Add `include "moduleName.pxi"`. This must be done to have freud include your Python-level code.
- Create `freud/moduleName.pxi` file
  - This will house the python-level code.
  - If you have a .pxd file exposing C++ classes, make sure to import that:
    ```
cimport freud._moduleName as moduleName
    ```
- Create `freud/moduleName.py` file
  - Make sure there is an import for each C++ class in your module:
    ```
    from ._freud import MyC++Class
    ```
- Create `freud/_moduleName.pxd` file
  - This file will expose the C++ classes in your module to python.
- Edit `setup.py`
  - Add `cpp/moduleName` to the `includes` list.
  - If there are any helper cc files that will not have a corresponding Cython class, add those files to the `sources` list inside the `extensions` list.
- Add line to `doc/source/index.rst`
  - Make sure your new module is referenced in the documentation.
- Create `doc/source/moduleName.rst`

Add to an Existing Module

To add a new class to an existing module, do the following:

- Create `cpp/moduleName/SubModule.h` and `cpp/moduleName/SubModule.cc`
  - New classes should be grouped into paired .h, .cc files. There may be a few instances where new classes could be added to an existing .h, .cc pairing.
- Edit `freud/moduleName.py` file
  - Add a line for each C++ class in your module:
    ```
    from ._freud import MyC++Class
    ```
- Expose C++ class in `freud/_moduleName.pxd`
- Create Python interface in `freud/moduleName.pxi`

You must include sphinx-style documentation and unit tests.
6.21 How to cite freud

Please acknowledge the use of this software within the body of your publication for example by copying or adapting the following formulation:

_Data analysis for this publication utilized the freud library[1]_.


To cite this reference, you can use the following BibTeX entry:

```bibtex
@misc{freud,
    author = {Vyas Ramasubramani and Bradley D. Dice and Eric S. Harper and Matthew P. Spellings and Joshua A. Anderson and Sharon C. Glotzer},
    title = {freud: A Software Suite for High Throughput Analysis of Particle Simulation Data},
    year = {2019},
    eprint = {arXiv:1906.06317},
}
```

6.22 References

6.23 License

BSD 3-Clause License for freud

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6.24 Credits

6.24.1 freud Developers

The following people contributed to the development of freud.

Vyas Ramasubramani - Lead developer

- Ensured PEP8 compliance.
- Added CircleCI continuous integration support.
- Created environment module and refactored order module.
- Rewrote most of freud docs, including order, density, and environment modules.
- Fixed nematic order parameter.
- Add properties for accessing class members.
- Various minor bug fixes.
- Refactored PMFT code.
- Refactored Steinhardt order parameter code.
- Wrote numerous examples of freud usage.
- Rewrote most of freud tests.
- Replaced CMake-based installation with setup.py using Cython.
- Add code coverage metrics.
- Added support for installing from PyPI, including ensuring that NumPy is installed.
- Converted all docstrings to Google format, fixed various incorrect docs.
- Debugged and added rotational autocorrelation code.
- Added MSD module.
- Wrote NeighborQuery, _QueryArgs, NeighborQueryResult classes.
- Wrote neighbor iterator infrastructure.
- Wrote PairCompute and SpatialHistogram parent classes.
- Wrote ManagedArray class.
- Wrote C++ histogram-related classes.
- Initial design of freud 2.0 API (NeighborQuery objects, neighbor computations, histograms).
• Standardized neighbor API in Python to use dictionaries of arguments or NeighborList objects for all pair computations.
• Standardized all attribute access into C++ with Python properties.
• Standardized variable naming of points/query_points across all of freud.
• Standardized vector directionality in computes.
• Enabled usage of quaternions in place of angles for orientations in 2D PMFT calculations.
• Wrote new freud 2.0 compute APIs based on neighbor_query objects and neighbors as either dictionaries or NeighborLists.
• Rewrote MatchEnv code to fit freud 2.0 API, splitting it into 3 separate calculations and rewriting internals using NeighborQuery objects.
• Wrote tutorial and reference sections of documentation.
• Unified util and common packages.
• Rewrote all docstrings in the package for freud 2.0.
• Changed Cubatic to use Mersenne Twisters for rng.
• Moved all citations into Bibtex format.
• Created data module.
• Standardized PMFT normalization.
• Enabled optional normalization of RDF.
• Changed correlation function to properly take the complex conjugate of inputs.

Bradley Dice - **Lead developer**

• Cleaned up various docstrings.
• Fixed bugs in HexOrderParameter.
• Cleaned up testing code.
• Added bumpversion support.
• Reduced all compile warnings.
• Added Python interface for box periodicity.
• Added Voronoi support for neighbor lists across periodic boundaries.
• Added Voronoi weights for 3D.
• Added Voronoi cell volume computation.
• Incorporated internal BiMap class for Boost removal.
• Wrote numerous examples of freud usage.
• Added some freud tests.
• Added ReadTheDocs support.
• Rewrote interface module into pure Cython.
• Added box duck-typing.
• Removed nose from unit testing.
• Use lambda function for parallelizing CorrelationFunction with TBB.
• Finalized boost removal.
• Wrote AABBQuery class.
• Consolidated cluster module functionality.
• Rewrote SolidLiquid order parameter class.
• Updated AngularSeparation class.
• Rewrote Voronoi implementation to leverage voro++.
• Implemented Voronoi bond weighting to enable Minkowski structure metrics.
• Refactored methods in Box and PeriodicBuffer for v2.0.
• Added checks to C++ for 2D boxes where required.
• Refactored cluster module.
• Standardized vector directionality in computes.
• NeighborQuery support to ClusterProperties, GaussianDensity, Voronoi, PeriodicBuffer, Interface.
• Standardized APIs for order parameters.
• Added radius of gyration to ClusterProperties.
• Improved Voronoi plotting code.
• Corrected number of points/query points in LocalDensity.
• Made PeriodicBuffer inherit from _Compute.
• Removed cudacpu and HOOMDMath includes.
• Added plotting functionality for Box and NeighborQuery objects.
• Added support for reading system data directly from MDAnalysis, garnett, gsd, HOOMD-blue, and OVITO.
• Revised tutorials and documentation on data inputs.
• Updated MSD to perform accumulation with `compute(., ., reset=False)`.
• Added test PyPI support to continuous integration.

Eric Harper, University of Michigan - Former lead developer
• Added TBB parallelism.
• Wrote PMFT module.
• Added NearestNeighbors (since removed).
• Wrote RDF.
• Added bonding module (since removed).
• Added cubatic order parameter.
• Added hexatic order parameter.
• Added Pairing2D (since removed).
• Created common array conversion logic.

Joshua A. Anderson, University of Michigan - Creator and former lead developer
• Initial design and implementation.
• Wrote LinkCell and IteratorLinkCell.
• Wrote GaussianDensity, LocalDensity.
• Added parallel module.
• Added indexing modules (since removed).
• Wrote Cluster and ClusterProperties modules.

Matthew Spellings - Former lead developer
• Added generic neighbor list.
• Enabled neighbor list usage across freud modules.
• Added correlation functions.
• Added LocalDescriptors class.
• Added interface module.

Erin Teich
• Wrote environment matching (MatchEnv) class.
• Wrote BondOrder class (with Julia Dshemuchadse).
• Wrote AngularSeparation class (with Andrew Karas).
• Contributed to LocalQl development.
• Wrote LocalBondProjection class.

M. Eric Irrgang
• Authored kspace module (since removed).
• Fixed numerous bugs.
• Contributed to freud.shape (since removed).

Chrisy Du
• Authored Steinhardt order parameter classes.
• Fixed support for triclinic boxes.

Antonio Osorio
• Developed TrajectoryXML class.
• Various bug fixes.
• OpenMP support.

Richmond Newman
• Developed the freud box.
• Solid liquid order parameter.

Carl Simon Adorf
• Developed the Python box module.

Jens Glaser
• Wrote kspace front-end (since removed).
• Modified kspace module (since removed).
• Wrote Nematic order parameter class.
Benjamin Schultz
- Wrote Voronoi class.
- Fix normalization in GaussianDensity.
- Bug fixes in shape module (since removed).

Bryan VanSaders
- Make Cython catch C++ exceptions.
- Add shiftvec option to PMFT.

Ryan Marson
- Various GaussianDensity bugfixes.

Yina Geng
- Co-wrote Voronoi neighbor list module.
- Add properties for accessing class members.

Carolyn Phillips
- Initial design and implementation.
- Package name.

Ben Swerdlow
- Documentation and installation improvements.

James Antonaglia
- Added number of neighbors as an argument to HexOrderParameter.
- Bugfixes.
- Analysis of deprecated kspace module.

Mayank Agrawal
- Co-wrote Voronoi neighbor list module.

William Zygmunt
- Helped with Boost removal.

Greg van Anders
- Bugfixes for CMake and SSE2 installation instructions.

James Proctor
- Cythonization of the cluster module.

Rose Cersonsky
- Enabled TBB-parallelism in density module.
- Fixed how C++ arrays were pulled into Cython.

Wenbo Shen
- Translational order parameter.

Andrew Karas
- Angular separation.
• Wrote reference implementation for rotational autocorrelation.

Paul Dodd
• Fixed CorrelationFunction namespace, added ComputeOCF class for TBB parallelization.

Tim Moore
• Added optional rmin argument to density.RDF.
• Enabled NeighborList indexing.

Alex Dutton
• BiMap class for MatchEnv.

Matthew Palathingal
• Replaced use of boost shared arrays with shared ptr in Cython.
• Helped incorporate BiMap class into MatchEnv.

Kelly Wang
• Enabled NeighborList indexing.

Yezhi Jin
• Added support for 2D arrays in the Python interface to Box functions.
• Rewrote Voronoi implementation to leverage voro++.
• Implemented Voronoi bond weighting to enable Minkowski structure metrics.

Brandon Butler
• Rewrote Steinhardt order parameter.

Jin Soo Ihm
• Added benchmarks.
• Contributed to NeighborQuery classes.
• Refactored C++ to perform neighbor queries on-the-fly.
• Added plotting functions to analysis classes.
• Wrote RawPoints class.
• Created Compute parent class with decorators to ensure properties have been computed.
• Updated common array conversion logic.
• Added many validation tests.

6.24.2 Source code

Eigen (http://eigen.tuxfamily.org) is included as a git submodule in freud. Eigen is made available under the Mozilla Public License v2.0 (http://mozilla.org/MPL/2.0/). Its linear algebra routines are used for various tasks including the computation of eigenvalues and eigenvectors.

fsph (https://github.com/glotzerlab/fsph) is included as a git submodule in freud. It is used for the calculation of spherical harmonics. fsph is made available under the MIT license:
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