freud: A Software Suite for High Throughput Analysis of Particle Simulation Data

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Abstract

The \texttt{freud} Python package is a powerful library for analyzing simulation data. Written with modern simulation and data analysis workflows in mind, \texttt{freud} provides a Python interface to fast, parallelized C++ routines that run efficiently on laptops, workstations, and supercomputing clusters. The package provides the core tools for finding particle neighbors in periodic systems, and offers a uniform API to a wide variety of methods implemented using these tools. As such, \texttt{freud} users can access standard methods such as the radial distribution function as well as newer, more specialized methods such as the potential of mean force and torque and local crystal environment analysis with equal ease. While many comparable tools place a heavy emphasis on reading and operating on trajectory file formats, \texttt{freud} instead accepts numerical arrays of data directly as inputs. By remaining agnostic to its data source, \texttt{freud} is suitable for analyzing any coarse-grained particle simulation, regardless of the original data representation or simulation method. When used for on-the-fly analysis in conjunction with scriptable simulation software such as HOOMD-blue \cite{1, 2}, \texttt{freud} enables smart simulations that adapt to the current state of the system, allowing users to study phenomena such as nucleation and growth.

Keywords: analysis; simulation; molecular dynamics; Monte Carlo; computational materials science

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PROGRAM SUMMARY

Program Title: freud
Licensing provisions: BSD 3-Clause
Programming language: Python, C++

Nature of problem: Simulations of coarse-grained, nano-scale, and colloidal particle systems typically require analyses specialized to a particular system. Certain more standardized techniques – including correlation functions, order parameters, and clustering – are computationally intensive tasks that must be carefully implemented to scale to the larger systems common in modern simulations.

Solution method: freud performs a wide variety of particle system analyses, offering a Python API that interfaces with many other tools in computational molecular sciences via NumPy array inputs and outputs. The algorithms in freud leverage parallelized C++ to scale to large systems and enable real-time analysis. The library’s broad set of features encode few assumptions compared to other analysis packages, enabling analysis of a broader class of data ranging from biomolecular simulations to colloidal experiments.

Unusual features:

1. freud provides very fast, parallel implementations of standard analysis methods like RDFs and correlation functions.
2. freud includes the reference implementation for the potential of mean force and torque (PMFT).
3. freud provides various novel methods for characterizing particle environments, including the calculation of descriptors useful for machine learning.

Additional comments: The source code is hosted on GitHub (https://github.com/glotzerlab/freud), and documentation is available online (https://freud.readthedocs.io/). The package may be installed via pip install freud-analysis or conda install -c conda-forge freud.

1. Introduction

Molecular simulation is a crucial pillar in the investigation of scientific phenomena. Increased computational resources, better algorithms, and new
hardware architectures have made it possible to simulate complex systems over longer timescales than ever before [3–7]. The sheer volume of data necessitates computationally efficient analysis tools, while the diversity of data requires flexible tools that can be adapted for specific systems. Additionally, to support scientists with limited prior computing experience, tools must be usable without extensive knowledge of the underlying code.

Numerous software packages that satisfy these requirements have arisen in recent years. Tools such as MDTraj, MDAnalysis, LOOS, MMTK, and VMD [8–12] provide efficient implementations of various standard analysis methods. These tools generally target all-atom simulations, particularly biomolecular simulations. This focus is manifested through: a strong emphasis on trajectory management; extensive support for selecting important subsets of system topology such as atoms, residues, and protein backbones; and implementations of highly specific analyses involving, for instance, hydrogen bonding and protein secondary structure (using, e.g., DSSP [13]). In coarse-grained simulations, which have no common system representation, such selection tools are far less important. Moreover, the predominant analyses of these simulations are quite different, involving measurements like numbers of nearest neighbors, diffraction patterns, or bond-orientational order parameters. As a result, these systems require analysis toolkits that are agnostic to system representations and offer different analysis methods than most existing tools.

In this paper we introduce freud, an open-source simulation analysis toolkit that addresses these needs. All inputs to and outputs from freud are numerical arrays of data, and the package makes no reference to predefined notions of atoms or molecules. As a result, freud can analyze particle-based data from both experiments or simulations regardless of the specific tools, methods, or software that were used to generate it. The package provides an easy-to-use Python Application Programming Interface (API) for accessing fast methods implemented in C++, and it implements numerous specific methods such as radial distribution functions and correlation functions that are common in the field of soft-matter physics (see fig. 1). Prior works have used freud for: computing complex correlation functions and PMFTs in two dimensions [3]; PMFTs in depletion-mediated self-assembly of hard cuboctahedra [14]; PMFTs in analysis of two-dimensional shape allophiles [15]; Steinhardt order parameters for identifying solid-like particles [16, 17]; umbrella sampling of solid-solid phase transitions using Steinhardt order parameters [18]; spherical harmonics for machine learning on crystal structures [19]; calculation of strain fields by finding neighbors of particles against a
Figure 1: The freud library is capable of computing a number of characteristics of a system of particles. Here, we demonstrate some of those features on a simple 2D Monte Carlo simulation of polygons, which exhibits hexatic ordering [3].

a) Phase separation is clearly evident in this system of $512^2$ pentagons colored by local density $\Phi$; the system is divided into denser (blue) and less dense (red) regions. b) Zooming into a particularly dense region shows that the hexatic ordering (left half) is generally uniform across the region. The Voronoi diagram of the system (right half) is also largely defect-free, with just a few pentagons having more or fewer than 6 nearest neighbors. c) The spatial correlation of the hexatic order parameter $C_{\psi_6}(r)$ is nearly constant for a nearly perfect crystal of pentagons (orange), whereas it decays very quickly in a fluid (blue). For a comparable system of hexagons, however, we see an intermediate hexatic phase between the solid and fluid phases in which the hexatic order parameter exhibits a power-law decay (green). d) The radial distribution function $g(r)$ for the system of pentagons shows the expected sequence of neighbor shells as a function of distance.

uniform grid [20]; measuring rotational degrees of freedom in entropically ordered systems [21]; pair potential optimization for designing complex crystals [22]; and more.

The paper is organized as follows. We first address the core design principles that went into building freud in section 2. Section 3 focuses more
2. Design

While most simulation analysis tools focus on calculating properties involving molecular topologies, freud is fundamentally designed for analyzing the local neighborhoods of particles, particularly where such local analyses provide global insight about the system. As such, the freud API avoids any form of trajectory object encoding system topology, instead operating directly on NumPy arrays of data. This choice makes freud equally easy to use for one-off analyses or as part of a larger pipeline, especially because NumPy arrays are the de facto standard for numerical data in Python. Basing the API around numerical data also removes any dependence on specific file formats, allowing freud to circumvent the complexities and limitations associated with tying analyses to specific system representations. Since high quality file parsers generally exist for all the common trajectory file formats (for instance, MDAnalysis supports DCD, PDB, or XYZ files), array data can easily be extracted from trajectories using other tools and passed to freud for analysis.

Most well-established tools differ from freud in this regard, placing a heavy emphasis on directly parsing files into some internal trajectory representation. Tools like VMD, PyMOL, or cpptraj, as well as the analysis methods built into simulation toolkits like LAMMPS and GROMACS, are designed around performing analyses directly on trajectory files from the command line. More recently, providing a Python interface to these functions has become a common theme; examples include VMD’s Python interpreter and the pytraj front end to the cpptraj package. However, such Python APIs are typically limited, and freud instead follows the approach of many newer tools like MDAnalysis, MDTraj, LOOS, and Pteros, which are designed around first-class Python APIs. Of these, the tools most similar to freud are LOOS and Pteros, which are specifically designed to easily enable the incorporation of custom analyses. Nonetheless, these packages

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1The code for these examples and many others is available at [https://github.com/glotzerlab/freud-examples](https://github.com/glotzerlab/freud-examples)
are still designed around simulation data acquired by parsing trajectory files, and the analyses they encode remain primarily of interest in the context of molecular topologies.

The analyses in freud typically follow a different pattern. Since the first task in characterizing local neighborhoods is often the identification of neighboring particles, freud provides efficient methods for finding neighbors in arbitrary system geometries. As it is central to nearly all functionality in freud, nearest neighbor finding is designed to be as fast and flexible as possible, supporting various algorithms optimized for different system configurations and offering different criteria for neighbor finding, including queries based on either a cutoff distance or a number of nearest neighbors. The package’s system box representation and neighbor finding tools are exposed to users in Python, enabling the easy implementation of complex custom analyses directly in Python (for an example, see section 5.3).

The analysis methods in freud are essentially independent tools that make use of these objects to efficiently perform various calculations. In general, methods are designed to support both one-shot analysis, i.e. over a single trajectory frame, or cumulative calculations over many frames to get better statistics (see section 4.1). These features are all presented with a common API easing the transition between the different types of analyses needed for different simulations. All methods in freud are accelerated through extensive parallelization.

3. Implementation

The freud package is entirely object-oriented, with two core sets of C++ classes: the Box classes, which encapsulate all logic associated with periodicity in arbitrary triclinic boxes (boxes with 3 independent basis vectors); and the NeighborQuery classes, which define a consistent API for efficiently finding, storing, and iterating over nearest neighbors. Sets of nearest neighbors can be efficiently found using two methods, cell lists [29] or a bounding volume hierarchy (BVH) method adapted from HOOMD-blue [1] [2] [30]. The NeighborList class is a lightweight storage mechanism for NeighborQuery results that accelerates performing multiple analyses on the same query result.

The analysis methods in freud are encapsulated by compute classes, which are loosely defined as classes providing a compute method that populates class attributes after performing some computation. These classes, which also frequently offer an accumulate method to support averaged calculations over
many simulation frames, typically perform calculations using NeighborQuery results computed using some Box object. Both accumulate and compute methods operate directly on NumPy arrays for maximum flexibility. Compute objects, such as the density module’s RDF class, are usually configured with constructor arguments, after which they can be used multiple times to perform distinct calculations.

Nearly all compute classes are implemented in C++, and all parallelism is accomplished using Intel Threading Building Blocks (TBB) [31]. Python bindings for these C++ classes are generated using Cython [32], and the C++ methods are mirrored in Python using thin Cython classes that dispatch calls to the underlying C++ class instances. In general, these Cython classes have limited responsibilities: managing the memory of the underlying C++ instances, sanitizing inputs when necessary, and providing transparent access via memory views on C++ arrays. Some compute classes are implemented in pure Cython when efficient implementations of the performance-critical components of the analyses are already available with a Python interface. For example, the most expensive component of the interface class is a neighbor distance calculation that can be performed using the classes in the locality module. Similarly, the msd module calls FFTs provided by NumPy or SciPy.

Currently, freud supports any Python version greater than 3.4, as well as version 2.7 for backwards compatibility. The package is distributed through both the Python Package Index (PyPI) and the conda-forge channel of the Anaconda package manager [33], making it easy to install on any Unix-based operating system. Using freud requires NumPy and TBB libraries, which are automatically installed with freud. The library can also be compiled from source using any C++ compiler with C++11 support. Compilation requires NumPy and TBB headers as well as a Cython installation. Code documentation is written using Google-style docstrings rendered using Sphinx and hosted on ReadTheDocs. The freud library is open sourced under the BSD 3-Clause License, and the source code is available directly from the repository [34].

4. Features

The general utilities in freud are contained in two modules: box and locality. The box module contains the core Box class as well as the ParticleBuffer class used to replicate boxes beyond their periodic boundary conditions for specific analyses. The locality module contains the
NeighborQuery abstract class, which defines a standardized querying API and its concrete LinkCell and AABBQuery subclasses, which implement the cell list and BVH approaches, respectively. Both these classes use efficient algorithms for finding neighbor pairs based on a distance cutoff or a desired number of neighbors. The results of these queries can be operated on dynamically or stored in the lightweight NeighborList class provided by the locality module.

The remaining modules in freud are independent of one another and contain groups of classes that implement related features. While some of freud’s features are unique, many others are common analyses. However, implementations of these methods commonly lack support for periodicity. For example, the SciPy library [35] has functions for computing Voronoi diagrams and correlation functions, but these are restricted to aperiodic systems.

The cluster module of freud can be used to find clusters of particles—where clusters are defined by distance cutoffs—and then compute properties of these clusters such as radii of gyration. The density module contains features for calculating radial distribution functions as well as spatial correlation functions of arbitrary quantities. Additionally, the density module includes the ability to estimate local system density along with a class that interpolates particle density onto a regular grid suitable for, e.g., computing discrete Fourier transforms. The interface module provides a quick tool for identifying interfaces between two mutually exclusive sets of points (e.g. a solid and a liquid phase). The voronoi module generates Voronoi diagrams for systems of particles, an easy way to characterize the local geometric arrangements in the system. The msd module enables the calculation of mean squared displacements of particles over the course of a trajectory.

The order module is perhaps the most extensive one in freud, containing a large number of different order parameters commonly used to measure ordering and identify phase transitions in crystalline systems. Of particular note are the bond-orientational order parameters $Q_l$ and $W_l$ [37] and the cubatic order parameter $W_l$ [38] (see fig. 2). The module also contains the nematic order parameter for identifying orientationally ordered, translationally disordered phases, and a solid-liquid order parameter for identifying generic ordered phases [39].

The most powerful features of freud are the novel analysis methods developed by researchers in our group and not implemented anywhere else. In particular, the pmft and environment modules implement features that are unique to freud. We now discuss these features in greater detail.
Figure 2: Various order parameters can be used to characterize the degree of ordering in a system. The per-particle order parameter values eventually converge to a uniform global value as the system becomes globally well-ordered. These plots show the evolution of two order parameters over the course of a Monte Carlo simulation of hard particles, which over time rearrange into an ordered phase under compression. Simulation snapshots are colored by the per-particle order parameter and rendered with fresnel [36]. a) The Steinhardt $Q_6$ order parameter is an appropriate scalar descriptor for systems forming a BCC ($cI2-W$) structure. Systems of cuboctahedra in the fluid phase show a distinctly different characteristic value of the order parameter than in the solid phase, enabling easy identification. b) The cubatic order parameter $K_{124}$ is useful for characterizing ordering in these systems of octahedra.
4.1. Potential of Mean Force and Torque

The potential of mean force and torque (PMFT) was recently developed to quantify directional entropic forces that emerge in crowded systems of hard shapes [40, 41]. Developing the concept of the PMFT proceeds naturally by first considering \( g(r) \), the radial distribution function (RDF), which indicates how far away one particle tends to be from another. The potential of mean force (PMF), which can be computed as \( w(r) = -\frac{1}{k_B T} \ln(g(r)) \), is a measure of the average energy of this configuration; more precisely, it is the potential whose derivative gives the average force experienced by two particles at a distance \( r \), where the average is taken over all configurations in which two particles sit at that distance from one another. The PMFT is a generalization of the PMF that accounts for angular coordinates and relative orientations in addition to the radial distance [41], providing crucial additional information when characterizing rotational modes as well as translational ones in systems of anisotropic particles.

The PMFT can be computed in a variety of different coordinate systems in both 2D and 3D. In practice, freud computes the PMFT by generating a histogram of relative particle positions and orientations and taking the negative logarithm of these counts. The calculation performs a highly efficient parallel binning of particles based on the appropriate coordinates. This fast implementation enables the calculation of smooth PMFTs which require the accumulation of many frames.

4.2. Local Environments

The environment module provides access to a few especially useful methods for characterizing the local environments of particles that we now illustrate in greater detail.

4.2.1. Bond-Orientational Order Diagram

The BondOrder class enables the calculation of bond-orientational order diagrams (BOODs) [43-47]. Inspired by the bond-orientational order parameters defined by Steinhardt et al. [37], BOODs characterize the local ordering of systems by calculating the vectors between all neighboring particles in a system and then projecting these onto a sphere. One example of how BOODs can be used is to identify \( n \)-fold ordering in a system; in simple crystal structures with \( n \)-fold coordination, the BOOD will show \( n \) peaks corresponding to the average location of nearest neighbors.
Figure 3: The PMFT is related to the probability of finding particles at a given position and orientation relative to one another. 

a) The PMFT of an ordered system of hexagons, where the locations of the wells indicate that particles are much more likely to sit next to the edges of their neighbors than the corners. In two dimensions, the full PMFT is 3-dimensional, since it also must account for the orientation of the second particle relative to the first; for simplicity, in this figure we have integrated out that degree of freedom.

b) A PMFT computed from a system of rhombicosidodecahedra shows distributions of neighboring particles in three dimensions (figure rendered using Mayavi). There are six degrees of freedom in 3D systems, accounting for three degrees of freedom from translation and three more from rotation. This PMFT only considers the three translational degrees of freedom for simplicity. The wells representing the deepest energy isosurfaces of the PMFT align with the largest (pentagonal) facets of the polyhedron.
In addition to the standard BOOD calculation, the class offers some additional modes of operation that can be useful in specific cases. One mode involves finding the positions of nearest neighbors in the local coordinate system of a given particle rather than the global coordinate system, which can prevent misidentifying systems with multiple grains [43]. Another mode modifies the BOOD to help identify plastic crystals, which appear crystalline due to having translational order but lack orientational ordering. In this mode, the nearest neighbor positions relative to each particle are modified by the relative orientations of these particles, creating a BOOD in which positional ordering will no longer appear except when orientational ordering is also present.

4.2.2. Spherical Harmonic Descriptors

The BOOD is closely related to the Steinhardt order parameters $Q_l$ and $W_l$, which measure rotational order in a system using spherical harmonics. While the BOOD is essentially a histogram of nearest neighbor bonds, the Steinhardt order parameters take this one step further, measuring $l$-fold order by constructing scalar quantities from rotationally invariant combinations of spherical harmonics of degree $l$ calculated from the locations of nearest-neighbor bonds. However, spherical harmonic representations can also be used in a variety of different ways. For example, distinguishing different grains of the same crystal structure could be done using descriptors that are not rotationally invariant. Alternatively, we can often obtain rotationally-invariant descriptions of local environments for crystal structure identification via the principal axes of the moment of inertia tensor of the environments, or by using particle orientations of anisotropic particles [19, 38, 48]. To support such spherical harmonic analyses, the LocalDescriptors class in freud computes spherical harmonics characterizing particle neighborhoods. These harmonics can then be used to compute more complex descriptors of local particle environments. These methods have proven useful in identifying multiple complex crystal structures [19] (see fig. 4). One method for identifying these structures is to use the information contained in this array of spherical harmonics as a set of per-particle features in an artificial neural network (ANN) that classifies complex crystal structures [19].

4.2.3. Environment Matching

Methods like the spherical harmonic descriptors and the BOOD characterize ordering in systems by characterizing system-averaged quantities
Figure 4: Spherical harmonic descriptors can be used to identify the nucleation and growth of tP30-CrFe (Frank-Kasper $\sigma$ phase). a–c) As time progresses, crystallites nucleate and grow. Solid-like particles (blue) are identified via a simple feedforward artificial neural network using spherical harmonic descriptors (described in more detail in [19]).

from neighbor bonds. The MatchEnv class takes a different approach by defining environments according to the nearest neighbors of each particle and performing point set registration to identify and cluster similar environments [49]. This type of analysis is particularly useful because it emphasizes local information for each particle rather than performing any sort of system-wide averaging. As a result, it can be used for tasks such as identifying different Wyckoff positions in a crystal.

4.2.4. Angular Separation

The AngularSeparation class provides a simple way to characterize typical particle orientations in a system. Orientations can be compared to a reference set of orientations (one for each particle) or a single reference value, yielding a scalar value describing orientational order relative to the reference input. The method accounts for symmetry by accepting an array of equivalent quaternions corresponding to all symmetry-preserving operations in the rotation group of interest. This metric can be used as an order parameter for measuring orientational disorder in plastic crystals, which exhibit translational order and orientational disorder [50].

5. Examples

In this section, we demonstrate the use of freud and how it can be used in conjunction with the broader scientific software ecosystem. Some file
Figure 5: Environment matching allows us to detect variations in the local environments of particles. a) The presence of grain boundaries in this system (rendered with fresnel) is clearly visible due to the different coloring according to local environments. b) The two distinct domains (blue and grey particles) are clustered separately, but we can see that they both exhibit FCC-like (cF4-Cu) ordering in their stacking pattern (upper-right). The environment matching method can also detect the different environments of the stacking faults themselves (mauve and orange), which exhibit an ABA stacking pattern instead of the expected ABC pattern (lower-right).
formats, like GSD, provide their own readers, while many other file formats are supported by toolkits such as MDAnalysis [9] and MDTraj [8]. We make use of these tools to provide data to freud, and we encourage users to make use of them as well to preprocess inputs for freud methods. The code for these examples and many others is available at [https://github.com/glotzerlab/freud-examples](https://github.com/glotzerlab/freud-examples).

5.1. RDF and MSD from LAMMPS simulation

Here, we consider the simple problem of calculating the RDF and the MSD of a system simulated using LAMMPS [20]. LAMMPS is a standard tool for particle simulation used in many fields, and it supports multiple output formats, including those used by other simulation codes (e.g., the DCD format from CHARMM [51] and the XTC format from GROMACS [27]). In this case, we demonstrate the simple case of using the output of a custom dump format in LAMMPS, which allows users to dump whatever quantities they want into a text file. Although the default XYZ file format lacks sufficient information to calculate an MSD, it can be easily augmented with the necessary particle image information as shown.

```
import numpy as np
import freud

# For the MSD we also need images, which can be dumped using
# the LAMMPS dump custom command as follows:
# dump 2 all custom 100 output_custom.xyz x y z ix iy iz

# 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)

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

dfd = freud.density.RDF(rmax=4, dr=0.03, rmin=1)

for frame in data:
    rdf.accumulate(box, frame[:, :3])

msd = freud.msd.MSD(box)

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

# The object contains all the data we need to plot the RDF

from matplotlib import pyplot as plt

plt.plot(rdf.R, rdf.RDF)
plt.show()

If our trajectory was instead in a DCD file, we could modify our code  
above to read the input data using MDAnalysis:

reader = MDAnalysis.coordinates.DCD.DCDReader('output.dcd')

dfd = freud.density.RDF(rmax=4, dr=0.03, rmin=1)

for frame in reader:
    rdf.accumulate(  
        box=freud.box.Box.from_matrix(frame.triclinic_dimensions),  
        positions=frame.positions)

5.2. On-the-fly analysis with HOOMD-blue

A major strength of freud is that it can also be used for on-the-fly analysis  
mid-simulation. This type of code can be used to, for example, terminate a
simulation based on some additional condition, or log a quantity at a higher frequency than we want to save the full system trajectory. In our previous example, we demonstrated the calculation of an RDF using freud. An RDF can be noisy when calculated with limited data, so we would like to build it over a large number of simulation frames; however, storing many frames can lead to unreasonably large simulation trajectory files. As an alternative, we can accumulate RDF data during a simulation without storing the entire output. Additionally, we can log an order parameter over the course of the simulation:

```python
import hoomd
from hoomd import hpmc
import freud
import numpy as np

hoomd.context.initialize('--mode=cpu')
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(rmax=4, dr=0.1)

box = freud.box.Box.from_box(system.box)
w6 = freud.order.LocalWlNear(box, 4, 6, 12)

def calc_rdf(timestep):
    snap = system.take_snapshot()
    rdf.accumulate(box, snap.particles.position)

def calc_W6(timestep):
    snap = system.take_snapshot()
    w6.compute(snap.particles.position)
    return np.mean(np.real(w6.Wl))

# Equilibrate the system before accumulating the RDF.
hoomd.run(1e4)
```
Common Neighbor Analysis (CNA) is a standard technique for analyzing the local neighborhoods of particles in a crystal. The method involves a complex classification of local neighborhoods based on a number of features. Using freud’s neighbor lists, however, the method is straightforward to implement in Python.

We first consider the simpler problem of identifying all common neighbors between any pair of points. This is equivalent to searching for the second-nearest neighbor pairs, which can be done using freud as follows (note that this code is primarily written for clarity and could easily be optimized):

```python
# For simplicity, use a randomly generated set of points
box = freud.box.Box.cube(1)
points = box.wrap(np.random.rand(20, 3))
nl = freud.locality.LinkCell(
    box, 0.5).compute(box, points).nlist

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

Our dictionary common_neighbors now contains lists of common neighbors j for every pair of points (i, k). This information could itself be useful for performing some analysis on the system. If we are interested in actually implementing CNA, then we need to use this information to build local graphs, which we can do with the networkx Python package. Combined with the code above, the CNA algorithm can be implemented as follows:

import networkx as nx
diagrams = defaultdict(list)
for (a, b), neighbors in common_neighbors.items():
    # Build up the graph of connections between the common neighbors of a and b.
    g = nx.Graph()
    for i in neighbors:
        for j in set(nl.index_j[nl.index_i == i]).intersection(neighbors):
            g.add_edge(i, j)

    # Define the first 3 identifiers for a CNA diagram.
    are_neighbors = b in nl.index_j[nl.index_i == a]
    key = (are_neighbors, len(neighbors), g.number_of_edges())
    # If we've seen any neighborhood graphs with this signature, we explicitly check if the two graphs are identical to determine whether to save this one. Otherwise, we add the new graph immediately.
    if key in diagrams:
        if all([not nx.is_isomorphic(g, h) for h in diagrams[key]]):
            diagrams[key].append(g)
In this code, we are looping over all pairs of previously identified second neighbor shells, and finding bonds between the common neighbors of these pairs. The graph of these bonds then uniquely identifies a new environment.

6. Conclusion

The freud package is unique among simulation analysis packages due to its emphasis on coarse-grained simulations and its extensibility. This extensibility ensures that new analysis methods are frequently incorporated as they are developed, and the intuitive design of freud makes it easy for users to translate their analyses from high-level languages like Python into freud C++ code. Its uniform Python API and high-performance C++ back-end make freud a suitable solution for large-scale, high-throughput simulation analysis. Additionally, its simple, compact API is highly amenable to usage with other tools for, e.g., machine learning applications. Contributions to this open-source toolkit are highly encouraged as new methods are developed in future research applications.

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