flowws$_{freud}$

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Contents:

`flowws-freud` is an in-development set of modules to create reusable pipelines for scientific simulations using freud.

`flowws-freud` is being developed in conjunction with flowws and flowws-analysis. See their documentation for an overview of how to use the modules found here and other useful modules for analysis and visualization of simulation data, respectively.

CHAPTER 1

Installation

Install `flowws-freud` from PyPI:

```
pip install flowws-freud
```

Alternatively, install from source:

```
pip install git+https://github.com/klarh/flowws-freud.git#egg=flowws-freud
```

CHAPTER 2

Examples

Consult the flowws-examples project for examples using `flowws-freud` modules.

CHAPTER 3

API Documentation

Browse more detailed documentation online or build the sphinx documentation from source:

```
git clone https://github.com/klarh/flowws-freud
cd flowws-freud/doc
pip install -r requirements.txt
make html
```

3.1 Modules

class flowws_freud.**LocalDensity**(***kwargs*)
Compute the local density of particles in the system

Parameters

- **histogram_bins** – Number of bins to use in the histogram plot
- **r_max** – Maximum radial distance
- **diameter** – Smoothing diameter to use in the density calculation

run(*scope*, *storage*)
Compute and provide the local density

class flowws_freud.**RDF**(***kwargs*)
Compute and plot the radial distribution function (RDF)

Parameters

- **bins** – Number of bins to use
- **r_min** – Minimum radial distance
- **r_max** – Maximum radial distance
- **bond_max** – Render bonds that have length up to the given distance
- **bond_width** – Width of drawn bonds, if enabled

run(*scope*, *storage*)
Compute and provide the RDF

class flowws_freud.**SmoothBOD**(**args*, ***kwargs*)
Compute and display Bond Orientational Order Diagrams (BOODs)

Parameters

- **num_neighbors** – Number of neighbors to compute
- **use_distance** – Use distance, rather than num_neighbors, to find bonds
- **r_max** – Maximum radial distance if use_distance is given
- **on_surface** – Restrict the BOOD to be on the surface of a sphere
- **average** – If True, average the BOOD
- **average_keys** – List of scope keys to generate distinct series when averaging

run(*scope*, *storage*)
Compute the bonds in the system

class flowws_freud.**Steinhardt**(***kwargs*)
Compute the Steinhardt order parameter of particles in the system

Parameters

- **histogram_bins** – Number of bins to use in the histogram plot
- **l** – Spherical harmonic degree of the order parameter
- **r_max** – Maximum radial distance to consider for neighbors (if given)
- **num_neighbors** – Number of neighbors to use; overrules r_max if given
- **r_guess** – Characteristic distance for finding num_neighbors neighboring particles

run(*scope*, *storage*)
Compute and provide the Steinhardt order parameter

3.2 Indices and tables

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