Auto-FOX Documentation

Release 0.7.4

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ONE

AUTOMATED FORCEFIELD OPTIMIZATION EXTENSION 0.7.4

Auto-FOX is a library for analyzing potential energy surfaces (PESs) and using the resulting PES descriptors for constructing forcefield parameters. Further details are provided in the documentation.

1.1 Currently implemented

This package is a work in progress; the following functionalities are currently implemented:

- The MultiMolecule class, a class designed for handling and processing potential energy surfaces. (1)
- A multi-XYZ reader. (2)
- A radial and angular distribution generator (RDF & ADF). (3)
- A root mean squared displacement generator (RMSD). (4)
- A root mean squared fluctuation generator (RMSF). (5)
- Tools for describing shell structures in, *e.g.*, nanocrystals or dissolved solutes. (6)
- A Monte Carlo forcefield parameter optimizer. (7)

1.2 Using Auto-FOX

- An input file with some basic examples is provided in the FOX.examples directory.
- An example MD trajectory of a CdSe quantum dot is included in the FOX.data directory.
  - The absolute path + filename of aforementioned trajectory can be retrieved as following:

```
from FOX import example_xyz
```

- Further examples and more detailed descriptions are available in the documentation.

1.3 Installation

1.3.1 Anaconda environments

- While not a strictly required, it stronly recomended to use the virtual environments of Anaconda.
  - Available as either Miniconda or the complete Anaconda package.
- Anaconda comes with a built-in installer; more detailed installation instructions are available for a wide range of OSs.
  - See the Anaconda documentation.
- Anaconda environments can be created, enabled and disabled by, respectively, typing:
  - Create environment: `conda create --name FOX python=3.7`
  - Enable environment: `conda activate FOX`
  - Disable environment: `conda deactivate`

1.3.2 Installing Auto-FOX

- If using Conda, enable the environment: `conda activate FOX`
- Install **Auto-FOX** with PyPi: `pip install git+https://github.com/nlesc-nano/auto-FOX@master --upgrade`
- Congratulations, **Auto-FOX** is now installed and ready for use!

1.3.3 Optional dependencies

- Use of the FOX.monte_carlo module requires h5py. Note: h5py is not distrbuted via PyPi:
  - Anaconda: `conda install --name FOX -y -c conda-forge h5py`
- The plotting of data produced by **Auto-FOX** requires Matplotlib. Matplotlib is distributed by both PyPi and Anaconda:
  - Anaconda: `conda install --name FOX -y -c conda-forge matplotlib`
  - PyPi: `pip install matplotlib`
- Construction of the angular distribution function in parallel requires DASK.
  - Anaconda: `conda install -name FOX -y -c conda-forge dask`

CHAPTER

TWO

AUTO-FOX DOCUMENTATION

2.1 Radial & Angular Distribution Function

Radial and angular distribution function (RDF & ADF) generators have been implemented in the *MultiMolecule* class. The radial distribution function, or pair correlation function, describes how the particale density in a system varies as a function of distance from a reference particle. The herein implemented function is designed for constructing RDFs between all possible (user-defined) atom-pairs.

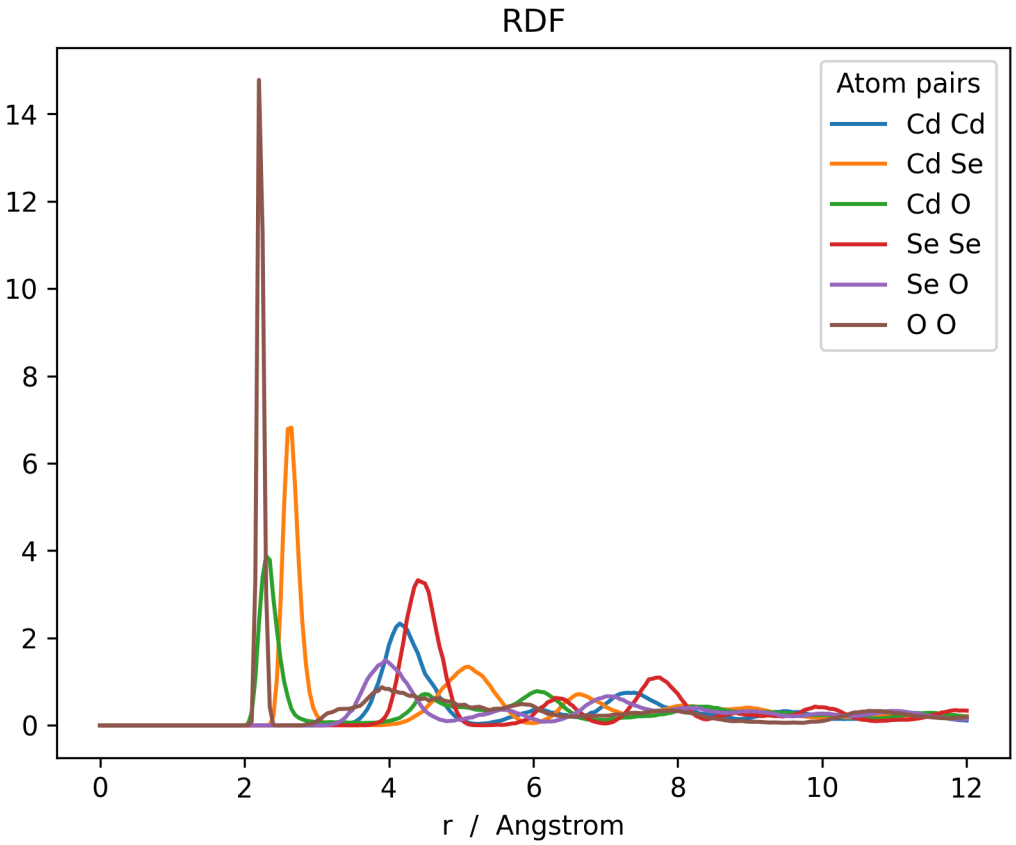
$$g(r) = \frac{V}{N_a * N_b} \sum_{i=1}^{N_a} \sum_{j=1}^{N_b} \langle *placeholder* \rangle$$

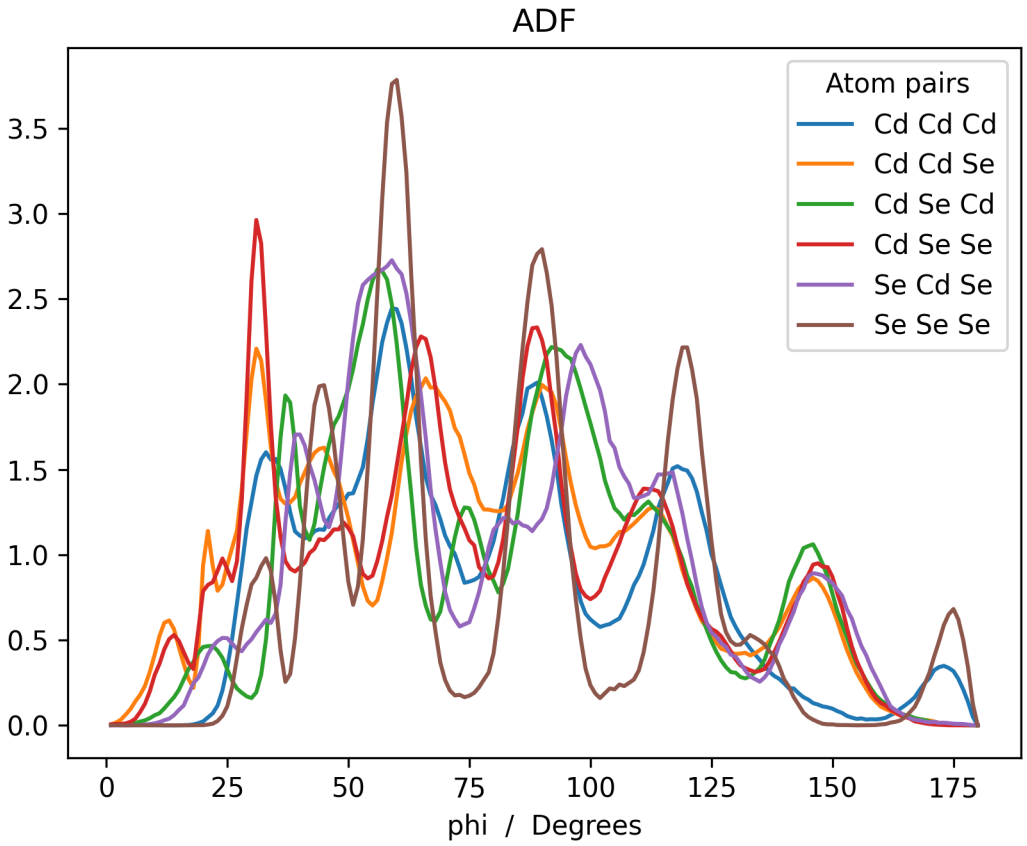
Given a trajectory, `mol`, stored as a *MultiMolecule* instance, the RDF can be calculated with the following command: `rdf = mol.init_rdf(atom_subset=None, low_mem=False)`. The resulting `rdf` is a Pandas dataframe, an object which is effectively a hybrid between a dictionary and a NumPy array.

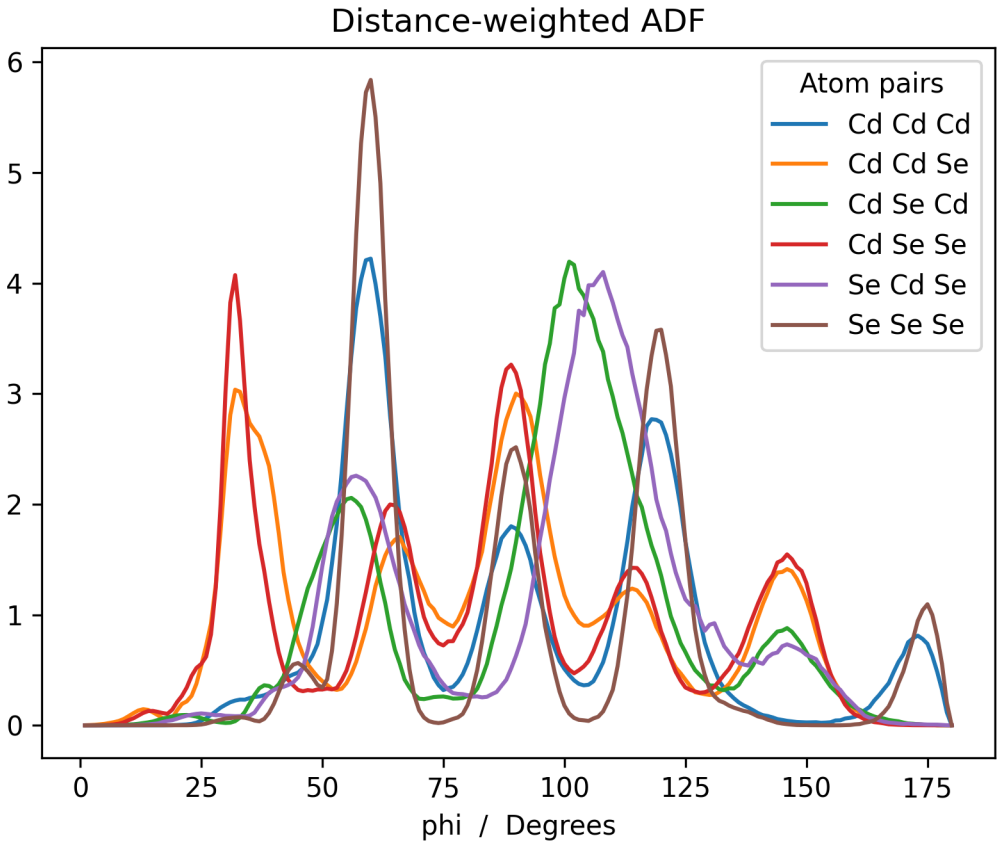
A slower, but more memory efficient, method of RDF construction can be enabled with `low_mem=True`, causing the script to only store the distance matrix of a single molecule in memory at once. If `low_mem=False`, all distance matrices are stored in memory simultaneously, speeding up the calculation but also introducing an additional linear scaling of memory with respect to the number of molecules. Note: Due to larger size of angle matrices it is recommended to use `low_mem=False` when generating ADFs.

Below is an example RDF and ADF of a CdSe quantum dot pacified with formate ligands. The RDF is printed for all possible combinations of cadmium, selenium and oxygen (Cd_Cd, Cd_Se, Cd_O, Se_Se, Se_O and O_O).

```
>>> from FOX import MultiMolecule, example_xyz

>>> mol = MultiMolecule.from_xyz(example_xyz)

# Default weight: np.exp(-r)
>>> rdf = mol.init_rdf(atom_subset=('Cd', 'Se', 'O'))
>>> adf = mol.init_adf(r_max=8, weight=None, atom_subset=('Cd', 'Se'))
>>> adf_weighted = mol.init_adf(r_max=8, atom_subset=('Cd', 'Se'))

>>> rdf.plot(title='RDF')
>>> adf.plot(title='ADF')
>>> adf_weighted.plot(title='Distance-weighted ADF')
```


RDF
Atom pairs
Cd Cd
Cd Se
Cd O
Se Se
Se O
O O
14
12
10
8
6
4
2
0
0
2
4
6
8
10
12
r / Angstrom


ADF
Atom pairs
Cd Cd Cd
Cd Cd Se
Cd Se Cd
Cd Se Se
Se Cd Se
Se Se Se
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
25
50
75
100
125
150
175
phi / Degrees


Distance-weighted ADF
Atom pairs
Cd Cd Cd
Cd Cd Se
Cd Se Cd
Cd Se Se
Se Cd Se
Se Se Se
0
1
2
3
4
5
6
0
25
50
75
100
125
150
175
phi / Degrees

2.1.1 API

`MultiMolecule.`**`init_rdf`**(*mol_subset=None*, *atom_subset=None*, *dr=0.05*, *r_max=12.0*, *mem_level=2*)

Initialize the calculation of radial distribution functions (RDFs).

RDFs are calculated for all possible atom-pairs in **atom_subset** and returned as a dataframe.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **dr** (*float*) – The integration step-size in Ångström, *i.e.* the distance between concentric spheres.
- **r_max** (*float*) – The maximum to be evaluated interatomic distance in Ångström.
- **mem_level** (*int*) – Set the level of to-be consumed memory and, by extension, the execution speed. Given a molecule subset of size m, atom subsets of (up to) size n and the resulting RDF with p points (`p = r_max / dr`), the **mem_level** values can be interpreted as following:
  - `0`: Slow; memory scaling: n^2
  - `1`: Medium; memory scaling: $n^2 + m * p$
  - `2`: Fast; memory scaling: $n^2 * m$

Returns A dataframe of radial distribution functions, averaged over all conformations in **xyz_array**. Keys are of the form: at_symbol1 + ' ' + at_symbol2 (*e.g.* `"Cd Cd"`). Radii are used as index.

Return type *pd.DataFrame*

`MultiMolecule.`**`init_adf`**(*mol_subset=None*, *atom_subset=None*, *r_max=8.0*, *weight=<function neg_exp>*)

Initialize the calculation of distance-weighted angular distribution functions (ADFs).

ADFs are calculated for all possible atom-pairs in **atom_subset** and returned as a dataframe.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **r_max** (*float* or *str*) – The maximum inter-atomic distance (in Angstrom) for which angles are constructed. The distance cuttoff can be disabled by settings this value to `np.inf`, `"np.inf"` or `"inf"`.
- **weight** (*Callable[[np.ndarray], np.ndarray], optional*) – A callable for creating a weighting factor from inter-atomic distances. The callable should take an array as input and return an array. Given an angle ϕ_{ijk}, to the distance r_{ijk} is defined as $max[r_{ij}, r_{jk}]$. Set to `None` to disable distance weighting.

Returns A dataframe of angular distribution functions, averaged over all conformations in this instance.

Return type *pd.DataFrame*

Note: Disabling the distance cuttoff is strongly recommended (*i.e.* it is faster) for large values of **r_max**. As a rough guideline, `r_max="inf"` is roughly as fast as `r_max=15.0` (though this is, of course, system dependant).

Note: The ADF construction will be conducted in parralel if the DASK package is installed. DASK can be installed, via anaconda, with the following command: `conda install -n FOX -y -c conda-forge dask`.

2.2 Root Mean Squared Displacement & Fluctuation

2.2.1 Root Mean Squared Displacement

The root mean squared displacement (RMSD) represents the average displacement of a set or subset of atoms as a function of time or, equivalently, moleculair indices in a MD trajectory.

$$\rho^{\mathrm{RMSD}}(t) = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\mathbf{r}_i(t) - \mathbf{r}_i^{\mathrm{ref}}\right)^2}$$

Given a trajectory, `mol`, stored as a *MultiMolecule* instance, the RMSD can be calculated with the *MultiMolecule.init_rmsd()* method using the following command:

```
>>> rmsd = mol.init_rmsd(atom_subset=None)
```

The resulting `rmsd` is a Pandas dataframe, an object which is effectively a hybrid between a dictionary and a NumPy array.

Below is an example RMSD of a CdSe quantum dot pacified with formate ligands. The RMSD is printed for cadmium, selenium and oxygen atoms.

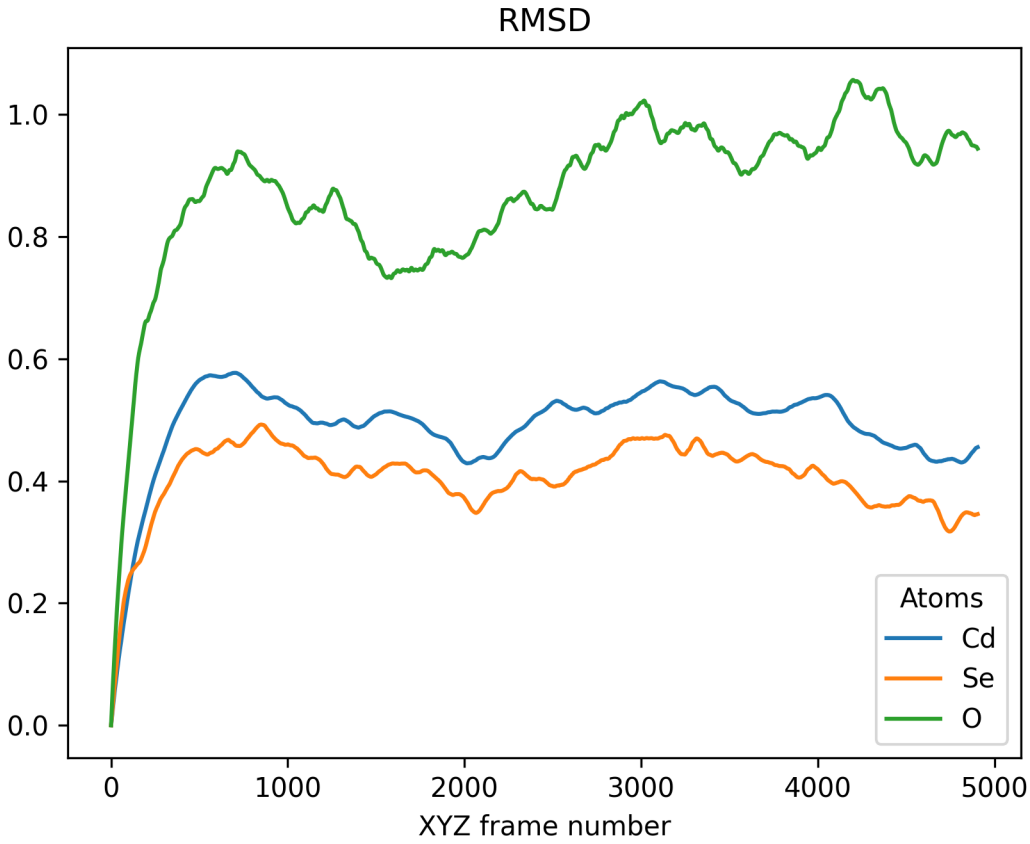
```
>>> from FOX import MultiMolecule, example_xyz

>>> mol = MultiMolecule.from_xyz(example_xyz)
>>> rmsd = mol.init_rmsd(atom_subset=('Cd', 'Se', 'O'))
>>> rmsd.plot(title='RMSD')
```

2.2.2 Root Mean Squared Fluctuation

The root mean squared fluctuation (RMSD) represents the time-averaged displacement, with respect to the time-averaged position, as a function of atomic indices.

$$\rho_i^{\mathrm{RMSF}} = \sqrt{\left\langle\left(\mathbf{r}_i - \langle\mathbf{r}_i\rangle\right)^2\right\rangle}$$

Given a trajectory, `mol`, stored as a *MultiMolecule* instance, the RMSF can be calculated with the *MultiMolecule.init_rmsf()* method using the following command:

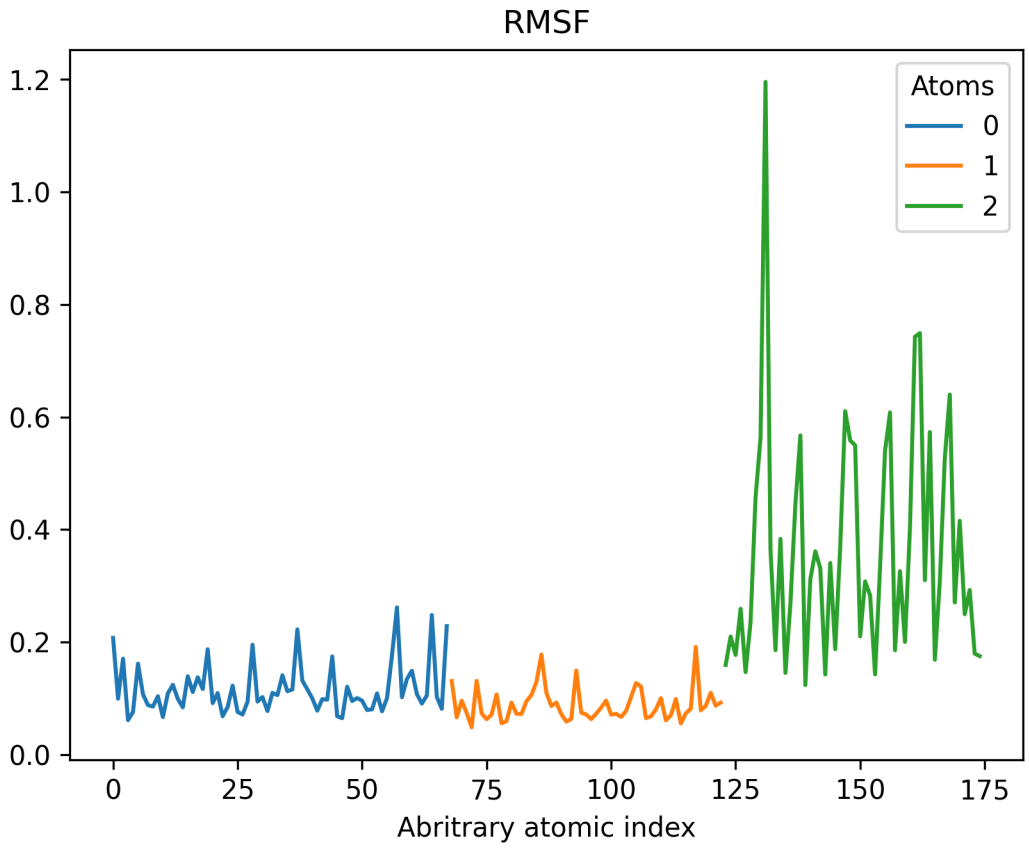

RMSD
1.0
0.8
0.6
0.4
0.2
0.0
0
1000
2000
3000
4000
5000
XYZ frame number
Atoms
Cd
Se
O

```
>>> rmsd = mol.init_rmsf(atom_subset=None)
```

The resulting `rmsf` is a Pandas dataframe, an object which is effectively a hybrid between a dictionary and a Numpy array.

Below is an example RMSF of a CdSe quantum dot pacified with formate ligands. The RMSF is printed for cadmium, selenium and oxygen atoms.

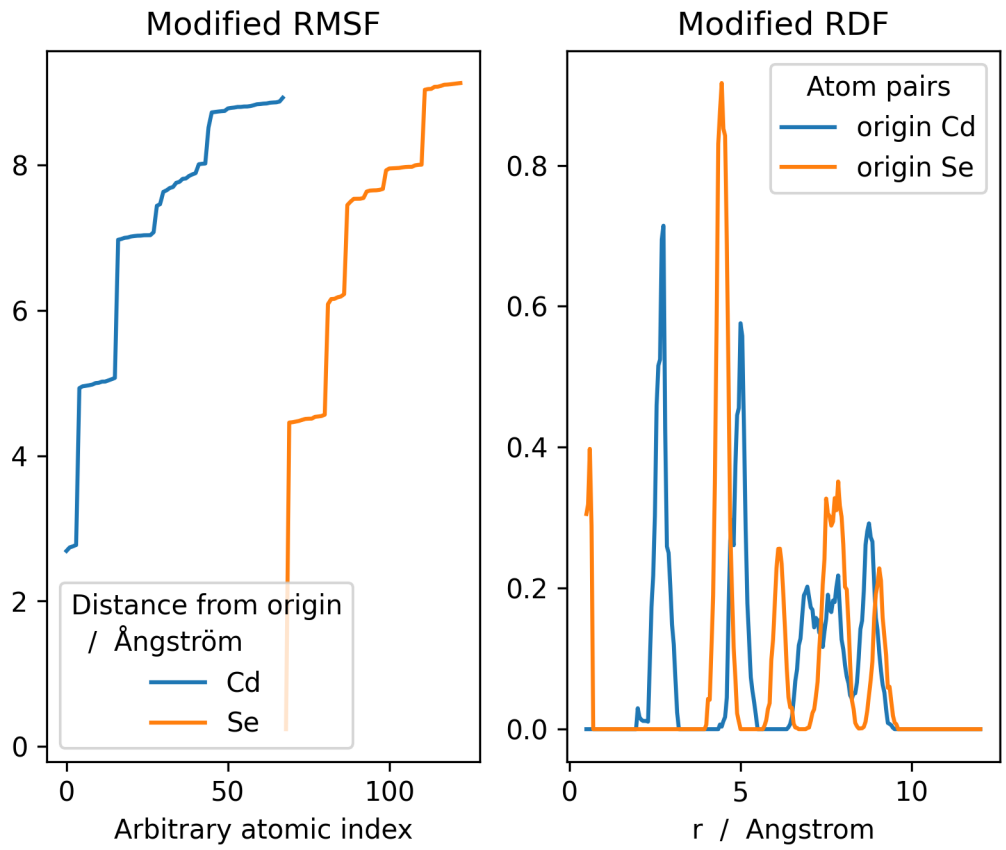
```
>>> from FOX import MultiMolecule, example_xyz

>>> mol = MultiMolecule.from_xyz(example_xyz)
>>> rmsd = mol.init_rmsf(atom_subset=('Cd', 'Se', 'O'))
>>> rmsd.plot(title='RMSF')
```



2.2.3 Discerning shell structures

See the *MultiMolecule.init_shell_search()* method.

```
>>> from FOX import MultiMolecule, example_xyz
>>> import matplotlib.pyplot as plt

>>> mol = MultiMolecule.from_xyz(example_xyz)
>>> rmsf, rmsf_idx, rdf = mol.init_shell_search(atom_subset=('Cd', 'Se'))

>>> fig, (ax, ax2) = plt.subplots(ncols=2)
>>> rmsf.plot(ax=ax, title='Modified RMSF')
>>> rdf.plot(ax=ax2, title='Modified RDF')
>>> plt.show()
```



The results above can be utilized for discerning shell structures in, *e.g.*, nanocrystals or dissolved solutes, the RDF minima representing transitions between different shells.

- There are clear minima for *Se* at ~ 2.0, 5.2, 7.0 & 8.5 Angstrom
- There are clear minima for *Cd* at ~ 4.0, 6.0 & 8.2 Angstrom

With the *MultiMolecule.get_at_idx()* method it is process the results of *MultiMolecule.init_shell_search()*, allowing you to create slices of atomic indices based on aforementioned distance ranges.

```
>>> dist_dict = {}
>>> dist_dict['Se'] = [2.0, 5.2, 7.0, 8.5]
>>> dist_dict['Cd'] = [4.0, 6.0, 8.2]
>>> idx_dict = mol.get_at_idx(rmsf, rmsf_idx, dist_dict)

>>> print(idx_dict)
{'Se_1': [27],
 'Se_2': [10, 11, 14, 22, 23, 26, 28, 31, 32, 40, 43, 44],
 'Se_3': [7, 13, 15, 39, 41, 47],
 'Se_4': [1, 3, 4, 6, 8, 9, 12, 16, 17, 19, 21, 24, 30, 33, 35, 37, 38, 42, 45, 46,␣
↪48, 50, 51, 53],
 'Se_5': [0, 2, 5, 18, 20, 25, 29, 34, 36, 49, 52, 54],
 'Cd_1': [25, 26, 30, 46],
 'Cd_2': [10, 13, 14, 22, 29, 31, 41, 42, 45, 47, 50, 51],
 'Cd_3': [3, 7, 8, 9, 11, 12, 15, 16, 17, 18, 21, 23, 24, 27, 34, 35, 38, 40, 43, 49,␣
↪52, 54, 58, 59, 60, 62, 63, 66],
 'Cd_4': [0, 1, 2, 4, 5, 6, 19, 20, 28, 32, 33, 36, 37, 39, 44, 48, 53, 55, 56, 57,␣
↪61, 64, 65, 67]
 }
```

It is even possible to use this dictionary with atom names & indices for renaming atoms in a *MultiMolecule* instance:

```
>>> print(list(mol.atoms))
['Cd', 'Se', 'C', 'H', 'O']

>>> del mol.atoms['Cd']
>>> del mol.atoms['Se']
>>> mol.atoms.update(idx_dict)
>>> print(list(mol.atoms))
['C', 'H', 'O', 'Se_1', 'Se_2', 'Se_3', 'Se_4', 'Se_5', 'Cd_1', 'Cd_2', 'Cd_3']
```

2.2.4 The atom_subset argument

In the above two examples `atom_subset=None` was used an optional keyword, one which allows one to customize for which atoms the RMSD & RMSF should be calculated and how the results are distributed over the various columns.

There are a total of four different approaches to the `atom_subset` argument:

1. `atom_subset=None`: Examine all atoms and store the results in a single column.

2. `atom_subset=int`: Examine a single atom, based on its index, and store the results in a single column.

3. `atom_subset=str` or `atom_subset=list(int)`: Examine multiple atoms, based on their atom type or indices, and store the results in a single column.

4. `atom_subset=tuple(str)` or `atom_subset=tuple(list(int))`: Examine multiple atoms, based on their atom types or indices, and store the results in multiple columns. A column is created for each string or nested list in `atoms`.

It should be noted that lists and/or tuples can be interchanged for any other iterable container (*e.g.* a Numpy array), as long as the iterables elements can be accessed by their index.

2.2.5 API

`MultiMolecule.`**`init_rmsd`**(*mol_subset=None*, *atom_subset=None*, *reset_origin=True*)
Initialize the RMSD calculation, returning a dataframe.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **reset_origin** (*bool*) – Reset the origin of each molecule in this instance by means of a partial Procrustes superimposition, translating and rotating the molecules.

Returns A dataframe of RMSDs with one column for every string or list of ints in **atom_subset**. Keys consist of atomic symbols (*e.g.* `"Cd"`) if **atom_subset** contains strings, otherwise a more generic 'series ' + str(int) scheme is adopted (*e.g.* `"series 2"`). Molecular indices are used as index.

Return type *pd.DataFrame*

`MultiMolecule.`**`init_rmsf`**(*mol_subset=None*, *atom_subset=None*, *reset_origin=True*)
Initialize the RMSF calculation, returning a dataframe.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **reset_origin** (*bool*) – Reset the origin of each molecule in this instance by means of a partial Procrustes superimposition, translating and rotating the molecules.

Returns A dataframe of RMSFs with one column for every string or list of ints in **atom_subset**. Keys consist of atomic symbols (*e.g.* `"Cd"`) if **atom_subset** contains strings, otherwise a more generic 'series ' + str(int) scheme is adopted (*e.g.* `"series 2"`). Molecular indices are used as indices.

Return type *pd.DataFrame*

`MultiMolecule.`**`init_shell_search`**(*mol_subset=None*, *atom_subset=None*, *rdf_cutoff=0.5*)
Calculate and return properties which can help determining shell structures.

The following two properties are calculated and returned:

- The mean distance (per atom) with respect to the center of mass (*i.e.* a modified RMSF).
- A series mapping abritrary atomic indices in the RMSF to the actual atomic indices.
- The radial distribution function (RDF) with respect to the center of mass.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.

- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **rdf_cutoff** (*float*) – Remove all values in the RDF below this value (Angstrom). Usefull for dealing with divergence as the "inter-atomic" distance approaches 0.0 A.

Returns

Returns the following items:

- A dataframe holding the mean distance of all atoms with respect the to center of mass.
- A series mapping the indices from 1. to the actual atomic indices.
- A dataframe holding the RDF with respect to the center of mass.

Return type *pd.DataFrame*, *pd.Series* and *pd.DataFrame*

static MultiMolecule.**get_at_idx**(*rmsf*, *idx_series*, *dist_dict*)

Create subsets of atomic indices.

The subset is created (using **rmsf** and **idx_series**) based on distance criteria in **dist_dict**.

For example, `dist_dict = {'Cd': [3.0, 6.5]}` will create and return a dictionary with three keys: One for all atoms whose RMSF is smaller than 3.0, one where the RMSF is between 3.0 and 6.5, and finally one where the RMSF is larger than 6.5.

Examples

```
>>> dist_dict = {'Cd': [3.0, 6.5]}
>>> idx_series = pd.Series(np.arange(12))
>>> rmsf = pd.DataFrame({'Cd': np.arange(12, dtype=float)})
>>> get_at_idx(rmsf, idx_series, dist_dict)

{'Cd_1': [0, 1, 2],
 'Cd_2': [3, 4, 5],
 'Cd_3': [7, 8, 9, 10, 11]
}
```

Parameters

- **rmsf** (*pd.DataFrame*) – A dataframe holding the results of an RMSF calculation.
- **idx_series** (*pd.Series*) – A series mapping the indices from **rmsf** to actual atomic indices.
- **dist_dict** (*dict [str, list [float]]*) – A dictionary with atomic symbols (see **rmsf.columns**) and a list of interatomic distances.

Returns A dictionary with atomic symbols as keys, and matching atomic indices as values.

Return type *dict* [*str*, *list* [*int*]]

Raises **KeyError** – Raised if a key in **dist_dict** is absent from **rmsf**.

2.3 The MultiMolecule Class

The API of the *MultiMolecule* class.

2.3.1 API FOX.MultiMolecule

class FOX.classes.multi_mol.**MultiMolecule**(*coords: numpy.ndarray, atoms: Optional[Dict[str, List[int]]] = None, bonds: Optional[numpy.ndarray] = None, properties: Optional[Dict[str, Any]] = None*)

A class designed for handling a and manipulating large numbers of molecules.

More specifically, different conformations of a single molecule as derived from, for example, an intrinsic reaction coordinate calculation (IRC) or a molecular dymanics trajectory (MD). The class has access to four attributes (further details are provided under parameters):

Parameters

- **coords** ($m * n * 3$ *np.ndarray* [*np.float64*]) – A 3D array with the cartesian coordinates of m molecules with n atoms.
- **atoms** (*dict [str, list [int]]*) – A dictionary with atomic symbols as keys and matching atomic indices as values. Stored in the *MultiMolecule.atoms* attribute.
- **bonds** ($k * 3$ *np.ndarray* [*np.int64*]) – A 2D array with indices of the atoms defining all k bonds (columns 1 & 2) and their respective bond orders multiplied by 10 (column 3). Stored in the *MultiMolecule.bonds* attribute.
- **properties** (*dict*) – A Settings instance for storing miscellaneous user-defined (meta-)data. Is devoid of keys by default. Stored in the *MultiMolecule.properties* attribute.

atoms

A dictionary with atomic symbols as keys and matching atomic indices as values.

Type dict [str, list [int]]

bonds

A 2D array with indices of the atoms defining all k bonds (columns 1 & 2) and their respective bond orders multiplied by 10 (column 3).

Type $k * 3$ *np.ndarray* [*np.int64*]

properties

A Settings instance for storing miscellaneous user-defined (meta-)data. Is devoid of keys by default.

Type *plams.Settings*

round(*decimals=0*, *inplace=True*)

Round the Cartesian coordinates of this instance to a given number of decimals.

Parameters

- **decimals** (*int*) – The number of decimals per element.
- **inplace** (*bool*) – Instead of returning the new coordinates, perform an inplace update of this instance.

Return type Optional[*MultiMolecule*]

delete_atoms(*atom_subset*)

Create a copy of this instance with all atoms in **atom_subset** removed.

Parameters **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A new *MultiMolecule* instance with all atoms in **atom_subset** removed.

Return type *FOX.MultiMolecule*

Raises **TypeError** – Raised if **atom_subset** is `None`.

add_atoms(*coords*, *symbols='Xx'*)

Create a copy of this instance with all atoms in **atom_subset** appended.

Examples

```
>>> import numpy as np
>>> from FOX import MultiMolecule, example_xyz

>>> mol = MultiMolecule.from_xyz(example_xyz)
>>> coords: np.ndarray = np.random.rand(73, 3)  # Add 73 new atoms with␣
↪random coords
>>> symbols = 'Br'

>>> mol_new: MultiMolecule = mol.add_atoms(coords, symbols)

>>> print(repr(mol))
MultiMolecule(..., shape=(4905, 227, 3), dtype='float64')
>>> print(repr(mol_new))
MultiMolecule(..., shape=(4905, 300, 3), dtype='float64')
```

Parameters

- **coords** (*array-like*) – A $(3,)$, $(n, 3)$, $(m, 3)$ or $(m, n, 3)$ array-like object with `m == len(self)`. Represents the Cartesian coordinates of the to-be added atoms.
- **symbols** (`str` or `Iterable` [`str`]) – One or more atomic symbols of the to-be added atoms.

Returns A new *MultiMolecule* instance with all atoms in **atom_subset** appended.

Return type *FOX.MultiMolecule*

guess_bonds(*atom_subset=None*)

Guess bonds within the molecules based on atom type and inter-atomic distances.

Bonds are guessed based on the first molecule in this instance Performs an inplace modification of **self.bonds**

Parameters **atom_subset** (*Sequence*) – A tuple of atomic symbols. Bonds are guessed between all atoms whose atomic symbol is in **atom_subset**. If `None`, guess bonds for all atoms in this instance.

Return type `None`

random_slice(*start=0*, *stop=None*, *p=0.5*, *inplace=False*)

Construct a new *MultiMolecule* instance by randomly slicing this instance.

The probability of including a particular element is equivalent to **p**.

Parameters

- **start** (*int*) – Start of the interval.
- **stop** (*int*) – End of the interval.
- **p** (*float*) – The probability of including each particular molecule in this instance. Values must be between `0.0` (0%) and `1.0` (100%).
- **inplace** (*bool*) – Instead of returning the new coordinates, perform an inplace update of this instance.

Returns If **inplace** is `True`, return a new *MultiMolecule* instance.

Return type *None* or *FOX.MultiMolecule*

Raises **ValueError** – Raised if **p** is smaller than `0.0` or larger than `1.0`.

reset_origin (*mol_subset=None*, *atom_subset=None*, *inplace=True*)

Reallign all molecules in this instance.

All molecules in this instance are rotating and translating, by performing a partial partial Procrustes superimposition with respect to the first molecule in this instance.

The superimposition is carried out with respect to the first molecule in this instance.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **inplace** (*bool*) – Instead of returning the new coordinates, perform an inplace update of this instance.

Returns If **inplace** is `True`, return a new *MultiMolecule* instance.

Return type *None* or *FOX.MultiMolecule*

sort (*sort_by='symbol'*, *reverse=False*, *inplace=True*)

Sort the atoms in this instance and **self.atoms**, performing in inplace update.

Parameters

- **sort_by** (*str* or *Sequence* [*int*]) – The property which is to be used for sorting. Accepted values: `"symbol"` (*i.e.* alphabetical), `"atnum"`, `"mass"`, `"radius"` or `"connectors"`. See the plams.PeriodicTable module for more details. Alternatively, a user-specified sequence of indices can be provided for sorting.
- **reverse** (*bool*) – Sort in reversed order.
- **inplace** (*bool*) – Instead of returning the new coordinates, perform an inplace update of this instance.

Returns If **inplace** is `True`, return a new *MultiMolecule* instance.

Return type *None* or *FOX.MultiMolecule*

residue_argsort (*concatenate=True*)

Return the indices that would sort this instance by residue number.

Residues are defined based on moleculair fragments based on **self.bonds**.

Parameters **concatenate** (*bool*) – If `False`, returned a nested list with atomic indices. Each sublist contains the indices of a single residue.

Returns A 1D array of indices that would sort n atoms this instance.

Return type n *np.ndarray* [*np.int64*]

get_center_of_mass(*mol_subset=None*, *atom_subset=None*)
Get the center of mass.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A 2D array with the centres of mass of m molecules with n atoms.

Return type $m * 3$ *np.ndarray* [*np.float64*]

get_bonds_per_atom(*atom_subset=None*)
Get the number of bonds per atom in this instance.

Parameters **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A 1D array with the number of bonds per atom, for all n atoms in this instance.

Return type n *np.ndarray* [*np.int64*]

init_average_velocity(*timestep=1.0*, *rms=False*, *mol_subset=None*, *atom_subset=None*)
Calculate the average atomic velocty.

The average velocity (in fs/A) is calculated for all atoms in **atom_subset** over the course of a trajectory.

The velocity is averaged over all atoms in a particular atom subset.

Parameters

- **timestep** (*float*) – The stepsize, in femtoseconds, between subsequent frames.
- **rms** (*bool*) – Calculate the root-mean squared average velocity instead.
- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A dataframe holding $m - 1$ velocities averaged over one or more atom subsets.

Return type *pd.DataFrame*

init_time_averaged_velocity(*timestep=1.0*, *rms=False*, *mol_subset=None*, *atom_subset=None*)
Calculate the time-averaged velocty.

The time-averaged velocity (in fs/A) is calculated for all atoms in **atom_subset** over the course of a trajectory.

Parameters

- **timestep** (*float*) – The stepsize, in femtoseconds, between subsequent frames.
- **rms** (*bool*) – Calculate the root-mean squared time-averaged velocity instead.
- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A dataframe holding $m - 1$ time-averaged velocities.

Return type *pd.DataFrame*

init_rmsd(*mol_subset=None*, *atom_subset=None*, *reset_origin=True*)

Initialize the RMSD calculation, returning a dataframe.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **reset_origin** (*bool*) – Reset the origin of each molecule in this instance by means of a partial Procrustes superimposition, translating and rotating the molecules.

Returns A dataframe of RMSDs with one column for every string or list of ints in **atom_subset**. Keys consist of atomic symbols (*e.g.* `"Cd"`) if **atom_subset** contains strings, otherwise a more generic 'series ' + str(int) scheme is adopted (*e.g.* `"series 2"`). Molecular indices are used as index.

Return type *pd.DataFrame*

init_rmsf(*mol_subset=None*, *atom_subset=None*, *reset_origin=True*)

Initialize the RMSF calculation, returning a dataframe.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **reset_origin** (*bool*) – Reset the origin of each molecule in this instance by means of a partial Procrustes superimposition, translating and rotating the molecules.

Returns A dataframe of RMSFs with one column for every string or list of ints in **atom_subset**. Keys consist of atomic symbols (*e.g.* `"Cd"`) if **atom_subset** contains strings, otherwise a more generic 'series ' + str(int) scheme is adopted (*e.g.* `"series 2"`). Molecular indices are used as indices.

Return type *pd.DataFrame*

get_average_velocity(*timestep=1.0*, *rms=False*, *mol_subset=None*, *atom_subset=None*)
Return the mean or root-mean squared velocity.

Parameters

- **timestep** (*float*) – The stepsize, in femtoseconds, between subsequent frames.
- **rms** (*bool*) – Calculate the root-mean squared average velocity instead.
- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A 1D array holding $m - 1$ velocities averaged over one or more atom subsets.

Return type $m - 1$ *np.ndarray* [*np.float64*]

get_time_averaged_velocity(*timestep=1.0*, *rms=False*, *mol_subset=None*, *atom_subset=None*)
Return the mean or root-mean squared velocity (mean = time-averaged).

Parameters

- **timestep** (*float*) – The stepsize, in femtoseconds, between subsequent frames.
- **rms** (*bool*) – Calculate the root-mean squared average velocity instead.
- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A 1D array holding n time-averaged velocities.

Return type n *np.ndarray* [*np.float64*]

get_velocity(*timestep=1.0*, *norm=True*, *mol_subset=None*, *atom_subset=None*)
Return the atomic velocties.

The velocity (in fs/A) is calculated for all atoms in **atom_subset** over the course of a trajectory.

Parameters

- **timestep** (*float*) – The stepsize, in femtoseconds, between subsequent frames.
- **norm** (*bool*) – If `True` return the norm of the x, y and z velocity components.
- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A 2D or 3D array of atomic velocities, the number of dimensions depending on the value of **norm** (`True` = 2D; `False` = 3D).

Return type $m * n$ or $m * n * 3$ *np.ndarray* [*np.float64*]

get_rmsd(*mol_subset=None*, *atom_subset=None*)
Calculate the root mean square displacement (RMSD).

The RMSD is calculated with respect to the first molecule in this instance.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A dataframe with the RMSD as a function of the XYZ frame numbers.

Return type *pd.DataFrame*

get_rmsf(*mol_subset=None*, *atom_subset=None*)
Calculate the root mean square fluctuation (RMSF).

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A dataframe with the RMSF as a function of atomic indices.

Return type *pd.DataFrame*

init_shell_search(*mol_subset=None*, *atom_subset=None*, *rdf_cutoff=0.5*)
Calculate and return properties which can help determining shell structures.

The following two properties are calculated and returned:

- The mean distance (per atom) with respect to the center of mass (*i.e.* a modified RMSF).
- A series mapping abritrary atomic indices in the RMSF to the actual atomic indices.
- The radial distribution function (RDF) with respect to the center of mass.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **rdf_cutoff** (*float*) – Remove all values in the RDF below this value (Angstrom). Usefull for dealing with divergence as the "inter-atomic" distance approaches 0.0 A.

Returns

Returns the following items:

- A dataframe holding the mean distance of all atoms with respect the to center of mass.

- A series mapping the indices from 1. to the actual atomic indices.
- A dataframe holding the RDF with respect to the center of mass.

Return type *pd.DataFrame*, *pd.Series* and *pd.DataFrame*

static get_at_idx(*rmsf*, *idx_series*, *dist_dict*)

Create subsets of atomic indices.

The subset is created (using **rmsf** and **idx_series**) based on distance criteria in **dist_dict**.

For example, `dist_dict = {'Cd': [3.0, 6.5]}` will create and return a dictionary with three keys: One for all atoms whose RMSF is smaller than 3.0, one where the RMSF is between 3.0 and 6.5, and finally one where the RMSF is larger than 6.5.

Examples

```
>>> dist_dict = {'Cd': [3.0, 6.5]}
>>> idx_series = pd.Series(np.arange(12))
>>> rmsf = pd.DataFrame({'Cd': np.arange(12, dtype=float)})
>>> get_at_idx(rmsf, idx_series, dist_dict)

{'Cd_1': [0, 1, 2],
 'Cd_2': [3, 4, 5],
 'Cd_3': [7, 8, 9, 10, 11]
}
```

Parameters

- **rmsf** (*pd.DataFrame*) – A dataframe holding the results of an RMSF calculation.
- **idx_series** (*pd.Series*) – A series mapping the indices from **rmsf** to actual atomic indices.
- **dist_dict** (*dict [str, list [float]]*) – A dictionary with atomic symbols (see **rmsf.columns**) and a list of interatomic distances.

Returns A dictionary with atomic symbols as keys, and matching atomic indices as values.

Return type *dict* [*str*, *list* [*int*]]

Raises **KeyError** – Raised if a key in **dist_dict** is absent from **rmsf**.

init_rdf(*mol_subset=None*, *atom_subset=None*, *dr=0.05*, *r_max=12.0*, *mem_level=2*)

Initialize the calculation of radial distribution functions (RDFs).

RDFs are calculated for all possible atom-pairs in **atom_subset** and returned as a dataframe.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **dr** (*float*) – The integration step-size in Ångström, *i.e.* the distance between concentric spheres.

- **r_max** (*float*) – The maximum to be evaluated interatomic distance in Ångström.
- **mem_level** (*int*) – Set the level of to-be consumed memory and, by extension, the execution speed. Given a molecule subset of size m, atom subsets of (up to) size n and the resulting RDF with p points (`p = r_max / dr`), the **mem_level** values can be interpreted as following:
  - `0`: Slow; memory scaling: n^2
  - `1`: Medium; memory scaling: $n^2 + m * p$
  - `2`: Fast; memory scaling: $n^2 * m$

Returns A dataframe of radial distribution functions, averaged over all conformations in **xyz_array**. Keys are of the form: at_symbol1 + ' ' + at_symbol2 (*e.g.* `"Cd Cd"`). Radii are used as index.

Return type *pd.DataFrame*

get_dist_mat(*mol_subset=None*, *atom_subset=(None, None)*)

Create and return a distance matrix for all molecules and atoms in this instance.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A 3D distance matrix of m molecules, created out of two sets of n and k atoms.

Return type $m * n * k$ *np.ndarray* [*np.float64*]

get_pair_dict(*atom_subset*, *r=2*)

Take a subset of atoms and return a dictionary.

Parameters

- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **r** (*int*) – The length of the to-be returned subsets.

Return type `Dict[str, Tuple[ndarray, ...]]`

init_power_spectrum(*mol_subset=None*, *atom_subset=None*, *freq_max=4000*)

Calculate and return the power spectrum associated with this instance.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **freq_max** (*int*) – The maximum to be returned wavenumber (cm**-1).

Returns A DataFrame containing the power spectrum for each set of atoms in **atom_subset**.

Return type *pd.DataFrame*

get_vacf (*mol_subset=None*, *atom_subset=None*)
Calculate and return the velocity autocorrelation function (VACF).

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A DataFrame containing the power spectrum for each set of atoms in **atom_subset**.

Return type *pd.DataFrame*

init_adf (*mol_subset=None*, *atom_subset=None*, *r_max=8.0*, *weight=<function neg_exp>*)
Initialize the calculation of distance-weighted angular distribution functions (ADFs).

ADFs are calculated for all possible atom-pairs in **atom_subset** and returned as a dataframe.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **r_max** (*float* or *str*) – The maximum inter-atomic distance (in Angstrom) for which angles are constructed. The distance cuttoff can be disabled by settings this value to `np.inf`, `"np.inf"` or `"inf"`.
- **weight** (*Callable[[np.ndarray], np.ndarray], optional*) – A callable for creating a weighting factor from inter-atomic distances. The callable should take an array as input and return an array. Given an angle ϕ_{ijk}, to the distance r_{ijk} is defined as $max[r_{ij}, r_{jk}]$. Set to `None` to disable distance weighting.

Returns A dataframe of angular distribution functions, averaged over all conformations in this instance.

Return type *pd.DataFrame*

Note: Disabling the distance cuttoff is strongly recommended (*i.e.* it is faster) for large values of **r_max**. As a rough guideline, `r_max="inf"` is roughly as fast as `r_max=15.0` (though this is, of course, system dependant).

Note: The ADF construction will be conducted in parralel if the DASK package is installed. DASK can be installed, via anaconda, with the following command: `conda install -n FOX -y -c conda-forge dask`.

---

get_angle_mat (*mol_subset=0*, *atom_subset=(None, None, None)*, *get_r_max=False*)
Create and return an angle matrix for all molecules and atoms in this instance.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **get_r_max** (*bool*) – Whether or not the maximum distance should be returned or not.

Returns A 4D angle matrix of m molecules, created out of three sets of n, k and l atoms. If **get_r_max** = `True`, also return the maximum distance.

Return type $m * n * k * l$ *np.ndarray* [*np.float64*] and (optionally) *float*

as_pdb (*filename*, *mol_subset=0*)

Convert a *MultiMolecule* object into one or more Protein DataBank files (.pdb).

Utilizes the plams.Molecule.write method.

Parameters

- **filename** (*str*) – The path+filename (including extension) of the to be created file.
- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.

Return type `None`

as_mol2 (*filename*, *mol_subset=0*)

Convert a *MultiMolecule* object into one or more .mol2 files.

Utilizes the plams.Molecule.write method.

Parameters

- **filename** (*str*) – The path+filename (including extension) of the to be created file.
- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.

Return type `None`

as_mol (*filename*, *mol_subset=0*)

Convert a *MultiMolecule* object into one or more .mol files.

Utilizes the plams.Molecule.write method.

Parameters

- **filename** (*str*) – The path+filename (including extension) of the to be created file.
- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.

Return type `None`

as_xyz (*filename*, *mol_subset=None*)

Create an .xyz file out of this instance.

Comments will be constructed by iteration through `MultiMolecule.properties["comments"]` if the following two conditions are fulfilled:

- The `"comments"` key is actually present in `MultiMolecule.properties`.
- `MultiMolecule.properties["comments"]` is an iterable.

Parameters

- **filename** (*str*) – The path+filename (including extension) of the to be created file.
- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.

Return type `None`

as_mass_weighted(*mol_subset=None*, *atom_subset=None*, *inplace=False*)

Transform the Cartesian of this instance into mass-weighted Cartesian coordinates.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.
- **inplace** (*bool*) – Instead of returning the new coordinates, perform an inplace update of this instance.

Returns if **inplace** = `False` return a new *MultiMolecule* instance with the mass-weighted Cartesian coordinates of m molecules with n atoms.

Return type $m * n * 3$ *np.ndarray* [*np.float64*] or *None*

from_mass_weighted(*mol_subset=None*, *atom_subset=None*)

Transform this instance from mass-weighted Cartesian into Cartesian coordinates.

Performs an inplace update of this instance.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.
- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Return type `None`

as_Molecule(*mol_subset=None*, *atom_subset=None*)

Convert this instance into a *list* of *plams.Molecule*.

Parameters

- **mol_subset** (*slice*) – Perform the calculation on a subset of molecules in this instance, as determined by their moleculair index. Include all m molecules in this instance if `None`.

- **atom_subset** (*Sequence*) – Perform the calculation on a subset of atoms in this instance, as determined by their atomic index or atomic symbol. Include all n atoms per molecule in this instance if `None`.

Returns A list of m PLAMS molecules constructed from this instance.

Return type m *list* [*plams.Molecule*]

classmethod from_Molecule(*mol_list*, *subset='atoms'*)

Construct a *MultiMolecule* instance from one or more PLAMS molecules.

Parameters

- **mol_list** (*plams.Molecule* or *list* [*plams.Molecule*]) – A PLAMS molecule or list of PLAMS molecules.
- **subset** (*Sequence* [str]) – Transfer a subset of *plams.Molecule* attributes to this instance. If `None`, transfer all attributes. Accepts one or more of the following values as strings: `"properties"`, `"atoms"` and/or `"bonds"`.

Returns A *MultiMolecule* instance constructed from **mol_list**.

Return type *FOX.MultiMolecule*

classmethod from_xyz(*filename*, *bonds=None*, *properties=None*)

Construct a *MultiMolecule* instance from a (multi) .xyz file.

Comment lines extracted from the .xyz file are stored, as array, under `MultiMolecule.properties["comments"]`.

Parameters

- **filename** (*str*) – The path+filename of an .xyz file.
- **bonds** ($k * 3$ *np.ndarray* [*np.int64*]) – An optional 2D array with indices of the atoms defining all k bonds (columns 1 & 2) and their respective bond orders multiplied by 10 (column 3). Stored in the **MultieMolecule.bonds** attribute.
- **properties** (*dict*) – A Settings object (subclass of dictionary) intended for storing miscellaneous user-defined (meta-)data. Is devoid of keys by default. Stored in the **MultiMolecule.properties** attribute.

Returns A *MultiMolecule* instance constructed from **filename**.

Return type *FOX.MultiMolecule*

classmethod from_kf(*filename*, *bonds=None*, *properties=None*)

Construct a *MultiMolecule* instance from a KF binary file.

Parameters

- **filename** (*str*) – The path+filename of an KF binary file.
- **bonds** ($k * 3$ *np.ndarray* [*np.int64*]) – An optional 2D array with indices of the atoms defining all k bonds (columns 1 & 2) and their respective bond orders multiplied by 10 (column 3). Stored in the **MultieMolecule.bonds** attribute.
- **properties** (*dict*) – A Settings object (subclass of dictionary) intended for storing miscellaneous user-defined (meta-)data. Is devoid of keys by default. Stored in the **MultiMolecule.properties** attribute.

Returns A *MultiMolecule* instance constructed from **filename**.

Return type *FOX.MultiMolecule*

2.3.2 API FOX._MultiMolecule

class FOX.classes.multi_mol_magic.**_MultiMolecule**(*coords: numpy.ndarray*, *atoms: Optional[Dict[str, List[int]]] = None*, *bonds: Optional[numpy.ndarray] = None*, *properties: Optional[Dict[str, Any]] = None*)

Private superclass of *MultiMolecule*.

Handles all magic methods and @property decorated methods.

property loc

A getter and setter for atom-type-based slicing.

Get, set and del operations are performed using the list(s) of atomic indices associated with the provided atomic symbol(s). Accepts either one or more atomic symbols.

Examples

```
>>> mol = MultiMolecule(...)
>>> mol.atoms['Cd'] = [0, 1, 2, 3, 4, 5]
>>> mol.atoms['Se'] = [6, 7, 8, 9, 10, 11]
>>> mol.atoms['O'] = [12, 13, 14]

>>> (mol.loc['Cd'] == mol[mol.atoms['Cd']]).all()
True

>>> idx = mol.atoms['Cd'] + mol.atoms['Se'] + mol.atoms['O']
>>> (mol.loc['Cd', 'Se', 'O'] == mol[idx]).all()
True

>>> mol.loc['Cd'] = 1
>>> print((mol.loc['Cd'] == 1).all())
True

>>> del mol.loc['Cd']
ValueError: cannot delete array elements
```

Parameters **mol** (MultiMolecule) – A MultiMolecule instance; see AtGetter.atoms.

mol

A MultiMolecule instance.

Type MultiMolecule

Return type LocGetter

property atom12

Get or set the indices of the atoms for all bonds in *MultiMolecule.bonds* as 2D array.

Return type *_MultiMolecule*

property atom1

Get or set the indices of the first atoms in all bonds of *MultiMolecule.bonds* as 1D array.

Return type *_MultiMolecule*

property atom2
Get or set the indices of the second atoms in all bonds of *MultiMolecule.bonds* as 1D array.

Return type ndarray

property order
Get or set the bond orders for all bonds in *MultiMolecule.bonds* as 1D array.

Return type ndarray

property x
Get or set the x coordinates for all atoms in instance as 2D array.

Return type *_MultiMolecule*

property y
Get or set the y coordinates for all atoms in this instance as 2D array.

Return type *_MultiMolecule*

property z
Get or set the z coordinates for all atoms in this instance as 2D array.

Return type *_MultiMolecule*

property symbol
Get the atomic symbols of all atoms in *MultiMolecule.atoms* as 1D array.

Return type ndarray

property atnum
Get the atomic numbers of all atoms in *MultiMolecule.atoms* as 1D array.

Return type ndarray

property mass
Get the atomic masses of all atoms in *MultiMolecule.atoms* as 1D array.

Return type ndarray

property radius
Get the atomic radii of all atoms in *MultiMolecule.atoms* as 1d array.

Return type ndarray

property connectors
Get the atomic connectors of all atoms in *MultiMolecule.atoms* as 1D array.

Return type ndarray

copy(*order='C'*, *deep=True*)
Create a copy of this instance.

Parameters

- **order** (*str*) – Controls the memory layout of the copy. See np.ndarray.copy for details.
- **copy_attr** (*bool*) – Whether or not the attributes of this instance should be returned as copies or views.

Returns A copy of this instance.

Return type *FOX.MultiMolecule*

2.4 Addaptive Rate Monte Carlo

The general idea of the MonteCarlo class, and its subclasses, is to fit a classical potential energy surface (PES) to an *ab-initio* PES by optimizing the classical forcefield parameters. This forcefield optimization is conducted using the Addaptive Rate Monte Carlo (ARMC, 1) method described by S. Cosseddu *et al* in *J. Chem. Theory Comput.*, **2017**, *13*, 297–308.

The implemented algorithm can be summarized as following:

2.4.1 The algorithm

1. A trial state, S_l, is generated by moving a random parameter retrieved from a user-specified parameter set (*e.g.* atomic charge).
2. It is checked whether or not the trial state has been previously visited.
   - If `True`, retrieve the previously calculated PES.
   - If `False`, calculate a new PES with the generated parameters S_l.

$$p(k \leftarrow l) = \begin{cases} 1, & \Delta\varepsilon_{QM-MM}(S_k) \;\; \Delta\varepsilon_{QM-MM}(S_l) \\ 0, & \Delta\varepsilon_{QM-MM}(S_k) \;\; \Delta\varepsilon_{QM-MM}(S_l) \end{cases} \tag{2.1}$$

3. The move is accepted if the new set of parameters, S_l, lowers the auxiliary error ($\Delta\varepsilon_{QM-MM}$) with respect to the previous set of accepted parameters, S_k (see (2.1)). Given a PES descriptor, r, consisting of a matrix with N elements, the auxiliary error is defined in (2.2).

$$\Delta\varepsilon_{QM-MM} = \frac{\sum_i^N \left| r_i^{QM} - r_i^{MM} \right|^2}{\sum_i^N r_i^{QM}} \tag{2.2}$$

4. The parameter history is updated. Based on whether or not the new parameter set is accepted the auxiliary error of either S_l or S_k is increased by the variable ϕ (see (2.3)). In this manner, the underlying PES is continuously modified, preventing the optimizer from getting stuck in a (local) minima in the parameter space.

$$\begin{matrix} \Delta\varepsilon_{QM-MM}(S_k) + \phi & \text{if} & \Delta\varepsilon_{QM-MM}(S_k) \;\; \Delta\varepsilon_{QM-MM}(S_l) \\ \Delta\varepsilon_{QM-MM}(S_l) + \phi & \text{if} & \Delta\varepsilon_{QM-MM}(S_k) \;\; \Delta\varepsilon_{QM-MM}(S_l) \end{matrix} \tag{2.3}$$

5. The parameter ϕ is updated at regular intervals in order to maintain a constant acceptance rate, α_t. This is illustrated in (2.4), where ϕ is updated the begining of every super-iteration κ. In this example the total number of iterations, $\kappa\omega$, is divided into κ super- and ω sub-iterations.

$$\phi_{\kappa\omega} = \phi_{(\kappa-1)\omega} * \gamma^{\text{sgn}(\alpha_t - \overline{\alpha}_{(\kappa-1)})} \quad \kappa = 1, 2, 3, ..., N \tag{2.4}$$

2.4.2 Arguments

Parameter	Default	Parameter description
param.prm_file	•	The path+filename of a CHARMM parameter file.
param.charge	•	A dictionary with atoms and matching atomic charges.
param.epsilon	•	A dictionary with atom-pairs and the matching Lennard-Jones ϵ parameter.
param.sigma	•	A dictionary with atom-pairs and the matching Lennard-Jones σ parameter.
psf.str_file	•	The path+filename to one or more stream file; used for assigning atom types and charges to ligands.
psf.rtf_file	•	The path+filename to one or more MATCH-produced rtf file; used for assigning atom types and charges to ligands.
psf.psf_file	•	The path+filename to one or more psf files; used for assigning atom types and charges to ligands.
psf.ligand_atoms	•	All atoms within a ligand, used for defining residues.
pes	•	A dictionary holding one or more functions for constructing PES descriptors.
molecule	•	A list of one or more `MultiMolecule` instances or .xyz filenames of a reference PES.
job.logfile	armc.log	The path+filename for the to-be created PLAMS logfile.
job.job_type	scm.plams.Cp2kJob	The job type, see Job.
job.name	armc	The base name of the various molecular dynamics jobs.
job.path	.	The base path for storing the various molecular dynamics jobs.
job.folder	MM_MD_workdir	The name of the to-be created directory for storing all molecular dynamics jobs.
job.keepfiles	False	Whether the raw MD results should be saved or deleted.
job.md_settings	•	A dictionary with the MD job settings. Alternativelly, the filename of YAML file can be supplied.
job.preopt_setting	•	A dictionary of geometry preoptimization job settings. Suplemented by job.md_settings.
hdf5_file	ARMC.hdf5	The filename of the to-be created HDF5 file with all ARMC results.
armc.iter_len	50000	The total number of ARMC iterations κ_{max}.
armc.sub_iter_len	100	The length of each ARMC subiteration ω.
armc.gamma	2.0	The constant γ, see (2.4).
armc.a_target	0.25	The target acceptance rate α_{target}, see

Once a the .yaml file with the ARMC settings has been sufficiently customized the parameter optimization can be started via the command prompt with: `init_armc my_settings.yaml`.

Previous caculations can be continued with `init_armc my_settings.yaml --restart True`.

2.4.3 The pes block

Potential energy surface (PES) descriptors can be descriped in the `"pes"` block. Provided below is an example where the radial dsitribution function (RDF) is used as PES descriptor, more specifically the RDF constructed from all possible combinations of cadmium, selenium and oxygen atoms.

```
pes:
    rdf:
        func: FOX.MultiMolecule.init_rdf
        kwarg:
            atom_subset: [Cd, Se, O]
```

Depending on the system of interest it might be of interest to utilize a PES descriptor other than the RDF, or potentially even multiple PES descriptors. In the latter case the the total auxiliary error is defined as the sum of the auxiliary errors of all individual PES descriptors, R (see (2.5)).

$$\Delta\varepsilon_{QM-MM} = \sum_{r}^{R} \Delta\varepsilon_{r}^{QM-MM} \tag{2.5}$$

An example is provided below where both radial and angular distribution functions (RDF and ADF, respectively) are are used as PES descriptors. In this example the RDF is construced for all combinations of cadmium, selenium and oxygen atoms (Cd, Se & O), whereas the ADF is construced for all combinations of cadmium and selenium atoms (Cd & Se).

```
pes:
    rdf:
        func: FOX.MultiMolecule.init_rdf
        args: []
        kwargs:
            atom_subset: [Cd, Se, O]

    adf:
        func: FOX.MultiMolecule.init_adf
        args: []
        kwargs:
            atom_subset: [Cd, Se]
```

In principle any function, class or method can be provided here, as type object, as long as the following requirements are fulfilled:

- The name of the block must consist of a user-specified string (`"rdf"` and `"adf"` in the example(s) above).
- The `"func"` key must contain a string representation of thee requested function, method or class. Auto-FOX will internally convert the string into a callable object.
- The supplied callable *must* be able to operate on NumPy arrays or instances of its *`MultiMolecule`* subclass.
- Arguments and keyword argument can be provided with the `"args"` and `"kwargs"` keys, respectively. The `"args"` and `"kwargs"` keys are entirely optional and can be skipped if desired.

An example of a custom, albit rather nonsensical, PES descriptor involving the numpy.sum function is provided below:

```
pes:
  numpy_sum:
      func: numpy.sum
      kwargs:
          axis: 0
```

This .yaml input, given a *MultiMolecule* instance `mol`, is equivalent to:

```
>>> import numpy

>>> func = numpy.sum
>>> args = []
>>> kwargs = {'axis': 0}

>>> func(mol, *arg, **kwarg)
```

2.4.4 The param block

```
param:
    charge:
        keys: [input, force_eval, mm, forcefield, charge]
        constraints:
            -  0 < Cs < 2
            -  1 < Pb < 3
            -  Cs == 0.5 * Br
        Cs: 1.000
        Pb: 2.000
    epsilon:
        unit: kjmol
        keys: [input, force_eval, mm, forcefield, nonbonded, lennard-jones]
        Cs Cs: 0.1882
        Cs Pb: 0.7227
        Pb Pb: 2.7740
    sigma:
        unit: nm
        keys: [input, force_eval, mm, forcefield, nonbonded, lennard-jones]
        constraints: 'Cs Cs == Pb Pb'
        Cs Cs: 0.60
        Cs Pb: 0.50
        Pb Pb: 0.60
```

The `"param"` key in the .yaml input contains all user-specified to-be optimized parameters.

There are three critical (and two optional) components to the `"param"` block:

- The key of each block (charge, epsilon & sigma).
- The `"keys"` sub-block, which points to the section path in the CP2K settings (*e.g.* ['input', 'force_eval', 'mm', 'forcefield', 'charge']).
- The sub-blocks containing either singular atoms or atom pairs.

Together, these three components point to the appropiate path of the forcefield parameter(s) of interest. As of the moment, all bonded and non-bonded potentials implemented in CP2K can be accessed via this section of the input file. For example, the following input is suitable if one wants to optimize a torsion potential (starting from $k = 10\ kcal/mol$) for all C-C-C-C bonds:

```
param:
    k:
        keys: [input, force_eval, mm, forcefield, torsion]
        unit: kcalmol
        C C C C: 10
```

Besides the three above-mentioned mandatory components, one can (optionally) supply the unit of the parameter and/or constrain its value to a certain range. When supplying units, it is the responsibility of the user to ensure the units are supported by CP2K. Furthermore, parameter constraints are, as of the moment, limited to specifying minimum and/or maximum values (*e.g.* `0 < Cs < 2`). Additional (more elaborate) constrainst are currently already available for atomic charges in the `move.charge_constraints` block (see below).

2.4.5 Parameter Guessing

```
param:
    epsilon:
        unit: kjmol
        keys: [input, force_eval, mm, forcefield, nonbonded, lennard-jones]
        Cs Cs: 0.1882
        Cs Pb: 0.7227
        Pb Pb: 2.7740
        guess: rdf
    sigma:
        unit: nm
        keys: [input, force_eval, mm, forcefield, nonbonded, lennard-jones]
        frozen:
            guess: uff
```

$$V_{LJ} = 4\varepsilon \left(\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right)$$

Non-bonded interactions (*i.e.* the Lennard-Jones ε and σ values) can be guessed if they're not explicitly by the user. There are currently two implemented guessing procedures: `"uff"` and `"rdf"`. Parameter guessing for parameters other than ε and σ is not supported as of the moment.

The `"uff"` approach simply takes all missing parameters from the Universal Force Field (UFF)[2]. Pair-wise parameters are construcetd using the standard combinatorial rules: the arithmetic mean for σ and the geometric mean for ε.

The `"rdf"` approach utilizes the radial distribution function for estimating σ and ε. σ is taken as the base of the first RDF peak, while the first minimum of the Boltzmann-inverted RDF is taken as ε.

`"crystal_radius"` and `"ion_radius"` use a similar approach to `"uff"`, the key difference being the origin of the parameters: 10.1107/S0567739476001551: R. D. Shannon, Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides, *Acta Cryst.* (1976). A32, 751-767. Note that:

- Values are averaged with respect to all charges and coordination numbers per atom type.
- These two guess-types can only be used for estimating σ parameters.

If `"guess"` is placed within the `"frozen"` block, than the guessed parameters will be treated as constants rather than to-be optimized variables.

Note

The guessing procedure requires the presence of both a .prm and .psf file. See the `"prm_file"` and `"psf"` blocks, respectively.

2.4.6 State-averaged ARMC

```
...

molecule:
    - /path/to/md_acetate.xyz
    - /path/to/md_phosphate.xyz
    - /path/to/md_sulfate.xyz

psf:
    rtf_file:
        - acetate.rtf
        - phosphate.rtf
        - sulfate.rtf
    ligand_atoms: [S, P, O, C, H]

pes:
    rdf:
        func: FOX.MultiMolecule.init_rdf
        kwargs:
            - atom_subset: [Cd, Se, O]
            - atom_subset: [Cd, Se, P, O]
            - atom_subset: [Cd, Se, S, O]

...
```

2.4.7 FOX.MonteCarlo API

class FOX.classes.monte_carlo.**MonteCarlo**(*molecule*, *param*, *md_settings*, *preopt_settings=None*, *rmsd_threshold=5.0*, *job_type=<class 'scm.plams.interfaces.thirdparty.cp2k.Cp2kJob'>*, *hdf5_file='ARMC.hdf5'*, *apply_move=<ufunc 'multiply'>*, *move_range=None*, *keep_files=False*, *logger=None*, *pes_post_process=None*)

The base *MonteCarlo* class.

property job_name

Get the (lowered) name of `MonteCarlo.job_type`.

Return type str

property molecule

Get **value** or set **value** as a tuple of MultiMolecule instances.

Return type Tuple[*MultiMolecule*, ...]

property md_settings

Get **value** or set **value** as a *plams.Settings* instance.

Return type Tuple[Settings, ...]

property preopt_settings

Get **value** or set **value** as a *plams.Settings* instance.

Return type Tuple[Settings, ...]

property move_range
Get **value** or set **value** as a *np.ndarray*.

Return type ndarray

property logger
Get or set the logger.

Return type Logger

keys()
Return a view of MonteCarlo.history_dict's keys.

Return type KeysView

items()
Return a view of MonteCarlo.history_dict's items.

Return type ItemsView

values()
Return a view of MonteCarlo.history_dict's values.

Return type ValuesView

add_pes_evaluator(*name*, *func*, *args=()*, *kwargs=mappingproxy({})*)
Add a callable to this instance for constructing PES-descriptors.

Examples

```
>>> from FOX import MonteCarlo, MultiMolecule

>>> mc = MonteCarlo(...)
>>> mol = MultiMolecule.from_xyz(...)

# Prepare arguments
>>> name = 'rdf'
>>> func = FOX.MultiMolecule.init_rdf
>>> atom_subset = ['Cd', 'Se', 'O']  # Keyword argument for func

# Add the PES-descriptor constructor
>>> mc.add_pes_evaluator(name, func, kwargs={'atom_subset': atom_subset})
```

Parameters

- **name** (*str*) – The name under which the PES-descriptor will be stored (*e.g.* "RDF").
- **func** (*Callable*) – The callable for constructing the PES-descriptor. The callable should take an array-like object as input and return a new array-like object as output.
- **args** (Sequence) – A sequence of positional arguments.
- **kwargs** (dict or Iterable [dict]) – A dictionary or an iterable of dictionaries with keyword arguments. Providing an iterable allows one to use a unique set of keyword arguments for each molecule in *MonteCarlo.molecule*.

Return type None

move()
Update a random parameter in **self.param** by a random value from **self.move.range**.

Performs in inplace update of the `'param'` column in **self.param**. By default the move is applied in a multiplicative manner. **self.job.md_settings** and **self.job.preopt_settings** are updated to reflect the change in parameters.

Examples

```
>>> print(armc.param['param'])
charge   Br      -0.731687
         Cs       0.731687
epsilon  Br Br    1.045000
         Cs Br    0.437800
         Cs Cs    0.300000
sigma    Br Br    0.421190
         Cs Br    0.369909
         Cs Cs    0.592590
Name: param, dtype: float64

>>> for _ in range(1000):  # Perform 1000 random moves
>>>     armc.move()

>>> print(armc.param['param'])
charge   Br      -0.597709
         Cs       0.444592
epsilon  Br Br    0.653053
         Cs Br    1.088848
         Cs Cs    1.025769
sigma    Br Br    0.339293
         Cs Br    0.136361
         Cs Cs    0.101097
Name: param, dtype: float64
```

Returns A tuple with the (new) values in the `'param'` column of **self.param**.

Return type *tuple* [*float*]

clip_move(*idx*, *value*)

Ensure that **value** falls within a user-specified range.

Return type `float`

run_md()

Run a geometry optimization followed by a molecular dynamics (MD) job.

Returns a new *MultiMolecule* instance constructed from the MD trajectory and the path to the MD results. If no trajectory is available (*i.e.* the job crashed) return *None* instead.

- The MD job is constructed according to the provided settings in **self.job**.

Returns A list of *MultiMolecule* instance(s) constructed from the MD trajectory & a list of paths to the PLAMS results directories. The *MultiMolecule* list is replaced with `None` if the job crashes.

Return type *FOX.MultiMolecule* and *tuple* [*str*]

clear_job_cache()

Clear `MonteCarlo.job_cache` and, optionally, delete all cp2k output files.

Return type `None`

get_pes_descriptors (*key*, *get_first_key=False*)
Check if a **key** is already present in **history_dict**.

If `True`, return the matching list of PES descriptors; If `False`, construct and return a new list of PES descriptors.

- The PES descriptors are constructed by the provided settings in **self.pes**.

Parameters

- **key** (*tuple [float]*) – A key in **history_dict**.
- **get_first_key** (*bool*) – Keep the both the files and the job_cache if this is the first ARMC iteration. Usefull for manual inspection in case cp2k hard-crashes at this point.

Returns A previous value from **history_dict** or a new value from an MD calculation & a *MultiMolecule* instance constructed from the MD simulation. Values are set to `np.inf` if the MD job crashed.

Return type *dict* [*str*, *np.ndarray* [*np.float64*]) and *FOX.MultiMolecule*

2.4.8 FOX.ARMC API

class FOX.classes.armc.**ARMC**(*iter_len=50000*, *sub_iter_len=100*, *gamma=200*, *a_target=0.25*, *phi=1.0*, *apply_phi=<ufunc 'add'>*, ***kwargs*)
The Addaptive Rate Monte Carlo class (*ARMC*).

A subclass of *MonteCarlo*.

Parameters

- **iter_len** (*int*) – The total number of ARMC iterations $\kappa\omega$.
- **sub_iter_len** (*int*) – The length of each ARMC subiteration ω.
- **gamma** (*float*) – The constant γ.
- **a_target** (*float*) – The target acceptance rate α_t.
- **phi** (*float*) – The variable ϕ.
- **apply_phi** (*Callable*) – The callable used for applying ϕ to the auxiliary error. The callable should be able to take 2 floats as argument and return a new float.
- ****kwargs** (**|Any|_**) – Keyword arguments for the `MonteCarlo` superclass.

property super_iter_len
Get `ARMC.iter_len // ARMC.sub_iter_len`.

Return type `int`

classmethod from_yaml (*filename*)
Create a *ARMC* instance from a .yaml file.

Parameters **filename** (*str*) – The path+filename of a .yaml file containing all *ARMC* settings.

Returns A new *ARMC* instance and a dictionary with keyword arguments for `run_armc()`.

Return type *FOX.ARMC* and *dict*

to_yaml (*filename*, *logfile=None*, *path=None*, *folder=None*)
Convert an *ARMC* instance into a .yaml readable by *ARMC.from_yaml*.

Parameters **filename** (str, bytes, os.pathlike or io.IOBase) – A filename or a file-like object.

Return type None

do_inner(*kappa*, *omega*, *acceptance*, *key_old*)
Run the inner loop of the ARMC.__call__() method.

Parameters

- **kappa** (*int*) – The super-iteration, κ, in ARMC.__call__().
- **omega** (*int*) – The sub-iteration, ω, in ARMC.__call__().
- **history_dict** (*dict* [*tuple* [*float*], *np.ndarray* [*np.float64*]]) – A dictionary with parameters as keys and a list of PES descriptors as values.
- **key_new** (*tuple [float]*) – A tuple with the latest set of forcefield parameters.

Returns The latest set of parameters.

Return type *tuple* [*float*]

get_aux_error(*pes_dict*)
Return the auxiliary error $\Delta\varepsilon_{QM-MM}$.

The auxiliary error is constructed using the PES descriptors in **values** with respect to **self.ref**.

The default function is equivalent to:

$$\Delta\varepsilon_{QM-MM} = \frac{\sum_i^N |r_i^{QM} - r_i^{MM}|^2}{r_i^{QM}}$$

Parameters **pes_dict** ([*dict* [str, *np.ndarray* [*np.float64*]]) – An dictionary with $m * n$ PES descriptors each.

Returns An array with $m * n$ auxilary errors

Return type $m * n$ *np.ndarray* [*np.float64*]

update_phi(*acceptance*)
Update the variable ϕ.

ϕ is updated based on the target accepatance rate, α_t, and the acceptance rate, **acceptance**, of the current super-iteration.

- The values are updated according to the provided settings in **self.armc**.

The default function is equivalent to:

$$\phi_{\kappa\omega} = \phi_{(\kappa-1)\omega} * \gamma^{\text{sgn}(\alpha_t - \overline{\alpha}_{(\kappa-1)})}$$

Parameters **acceptance** (*np.ndarray* [*bool*]) – A 1D boolean array denoting the accepted moves within a sub-iteration.

Return type None

restart()
Restart a previously started Addaptive Rate Monte Carlo procedure.

Return type None

2.5 Multi-XYZ reader

A reader of multi-xyz files has been implemented in the `FOX.io.read_xyz` module. The .xyz fileformat is designed for storing the atomic symbols and cartesian coordinates of one or more molecules. The herein implemented *FOX.io.read_xyz.read_multi_xyz()* function allows for the fast, and memory-effiecient, retrieval of the various molecular geometries stored in an .xyz file.

An .xyz file, `example_xyz_file`, can also be directly converted into a *MultiMolecule* instance.

```
>>> from FOX import MultiMolecule, example_xyz

>>> mol = MultiMolecule.from_xyz(example_xyz)

>>> print(type(mol))
<class 'FOX.classes.multi_mol.MultiMolecule'>
```

2.5.1 API

`FOX.io.read_xyz.`**`read_multi_xyz`**(*filename*, *return_comment=True*)

Read a (multi) .xyz file.

Parameters

- **filename** (*str*) – The path+filename of a (multi) .xyz file.
- **return_comment** (*bool*) – Whether or not the comment line in each Cartesian coordinate block should be returned. Returned as a 1D array of strings.

Return type `Union[Tuple[ndarray, Dict[str, List[int]]], Tuple[ndarray, Dict[str, List[int]], ndarray]]`

Returns

- $m * n * 3$ *np.ndarray* [*np.float64*], *dict* [*str*, *list* [*int*]] and
- (optional) m *np.ndarray* [*str*] –
  - A 3D array with Cartesian coordinates of m molecules with n atoms.
  - A dictionary with atomic symbols as keys and lists of matching atomic indices as values.
  - (Optional) a 1D array with m comments.

Raises **XYZError** – Raised when issues are encountered related to parsing .xyz files.

classmethod `MultiMolecule.`**`from_xyz`**(*filename*, *bonds=None*, *properties=None*)

Construct a *MultiMolecule* instance from a (multi) .xyz file.

Comment lines extracted from the .xyz file are stored, as array, under `MultiMolecule.properties["comments"]`.

Parameters

- **filename** (*str*) – The path+filename of an .xyz file.
- **bonds** ($k * 3$ *np.ndarray* [*np.int64*]) – An optional 2D array with indices of the atoms defining all k bonds (columns 1 & 2) and their respective bond orders multiplied by 10 (column 3). Stored in the **MultieMolecule.bonds** attribute.
- **properties** (*dict*) – A Settings object (subclass of dictionary) intended for storing miscellaneous user-defined (meta-)data. Is devoid of keys by default. Stored in the **MultiMolecule.properties** attribute.

Returns A *MultiMolecule* instance constructed from **filename**.

Return type *FOX.MultiMolecule*

FOX.**example_xyz: str = '/home/docs/checkouts/readthedocs.org/user_builds/auto-fox/checkout**
The path+filename of the example multi-xyz file.

2.6 FOX.ff.lj_param

A module for estimating Lennard-Jones parameters.

Examples

```
>>> import pandas as pd
>>> from FOX import MultiMolecule, example_xyz, estimate_lennard_jones

>>> xyz_file: str = example_xyz
>>> atom_subset = ['Cd', 'Se', 'O']

>>> mol = MultiMolecule.from_xyz(xyz_file)
>>> rdf: pd.DataFrame = mol.init_rdf(atom_subset=atom_subset)
>>> param: pd.DataFrame = estimate_lennard_jones(rdf)

>>> print(param)
            sigma (Angstrom)  epsilon (kj/mol)
Atom pairs
Cd Cd                   3.95          2.097554
Cd Se                   2.50          4.759017
Cd O                    2.20          3.360966
Se Se                   4.20          2.976106
Se O                    3.65          0.992538
O O                     2.15          6.676584
```

2.6.1 Index

estimate_lj(rdf[, temperature, sigma_estimate])	Estimate the Lennard-Jones σ and ε parameters using an RDF.
get_free_energy(distribution[, temperature, ...])	Convert a distribution function into a free energy function.

2.6.2 API

FOX.ff.lj_param.**estimate_lj**(*rdf*, *temperature=298.15*, *sigma_estimate='base'*)
Estimate the Lennard-Jones σ and ε parameters using an RDF.

Given a radius r, the Lennard-Jones potential $V_{LJ}(r)$ is defined as following:

$$V_{LJ}(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

The σ and ε parameters are estimated as following:

- σ: The radii at which the first inflection point or peak base occurs in **rdf**.
- ε: The minimum value in of the **rdf** ree energy multiplied by -1.
- All values are calculated per atom pair specified in **rdf**.

Parameters

- **rdf** (pandas.DataFrame) – A radial distribution function. The columns should consist of atom-pairs.
- **temperature** (float) – The temperature in Kelvin.
- **sigma_estimate** (str) – Whether σ should be estimated based on the base of the first peak or its inflection point. Accepted values are "base" and "inflection", respectively.

Returns A Pandas DataFrame with two columns, "sigma" (Angstrom) and "epsilon" (kcal/mol), holding the Lennard-Jones parameters. Atom-pairs from **rdf** are used as index.

Return type pandas.DataFrame

See also:

MultiMolecule.init_rdf() Initialize the calculation of radial distribution functions (RDFs).

get_free_energy() Convert a distribution function into a free energy function.

FOX.ff.lj_param.**get_free_energy**(*distribution*, *temperature=298.15*, *unit='kcal/mol'*, *inf_replace=nan*)

Convert a distribution function into a free energy function.

Given a distribution function $g(r)$, the free energy $F(g(r))$ can be retrieved using a Boltzmann inversion:

$$F(g(r)) = -RT * \ln(g(r))$$

Two examples of valid distribution functions would be the radial- and angular distribution functions.

Parameters

- **distribution** (*array-like*) – A distribution function (*e.g.* an RDF) as an array-like object.
- **temperature** (float) – The temperature in Kelvin.
- **inf_replace** (float, optional) – A value used for replacing all instances of infinity (np.inf).
- **unit** (str) – The to-be returned unit. See scm.plams.Units for a comprehensive overview of all allowed values.

Returns An array-like object with a free-energy function (kj/mol) of **distribution**.

Return type pandas.DataFrame

See also:

MultiMolecule.init_rdf() Initialize the calculation of radial distribution functions (RDFs).

MultiMolecule.init_adf() Initialize the calculation of distance-weighted angular distribution functions (ADFs).

2.7 PSFContainer

2.7.1 FOX.io.read_psf

A class for reading protein structure (.psf) files.

Index

PSFContainer([filename, title, atoms, ...])	A container for managing protein structure files.

API

class FOX.io.read_psf.**PSFContainer**(*filename=None*, *title=None*, *atoms=None*, *bonds=None*, *angles=None*, *dihedrals=None*, *impropers=None*, *donors=None*, *acceptors=None*, *no_nonbonded=None*)

A container for managing protein structure files.

The *PSFContainer* class has access to three general sets of methods.

Methods for reading & constructing .psf files:

- *PSFContainer.read()*
- *PSFContainer.write()*

Methods for updating atom types:

- *PSFContainer.update_atom_charge()*
- *PSFContainer.update_atom_type()*

Methods for extracting bond, angle and dihedral-pairs from *plams.Molecule* instances:

- *PSFContainer.generate_bonds()*
- *PSFContainer.generate_angles()*
- *PSFContainer.generate_dihedrals()*
- *PSFContainer.generate_impropers()*
- *PSFContainer.generate_atoms()*

Parameters

- **filename** (1 numpy.ndarray [str]) – Optional: A 1D array-like object containing a single filename. See also *PSFContainer.filename*.
- **title** (n numpy.ndarray [str]) – Optional: A 1D array of strings holding the title block. See also *PSFContainer.title*.
- **atoms** ($n * 8$ pandas.DataFrame) – Optional: A Pandas DataFrame holding the atoms block. See also *PSFContainer.atoms*.
- **bonds** ($n * 2$ numpy.ndarray [int]) – Optional: A 2D array-like object holding the indices of all atom-pairs defining bonds. See also *PSFContainer.bonds*.
- **angles** ($n * 3$ numpy.ndarray [int]) – Optional: A 2D array-like object holding the indices of all atom-triplets defining angles. See also *PSFContainer.angles*.

- **dihedrals** ($n * 4$ numpy.ndarray [int]) – Optional: A 2D array-like object holding the indices of all atom-quartets defining proper dihedral angles. See also *PSFContainer.dihedrals*.
- **impropers** ($n * 4$ numpy.ndarray [int]) – Optional: A 2D array-like object holding the indices of all atom-quartets defining improper dihedral angles. See also *PSFContainer.impropers*.
- **donors** ($n * 1$ numpy.ndarray [int]) – Optional: A 2D array-like object holding the atomic indices of all hydrogen-bond donors. See also *PSFContainer.donors*.
- **acceptors** ($n * 1$ numpy.ndarray [int]) – Optional: A 2D array-like object holding the atomic indices of all hydrogen-bond acceptors. See also *PSFContainer.acceptors*.
- **no_nonbonded** ($n * 2$ numpy.ndarray [int]) – Optional: A 2D array-like object holding the indices of all atom-pairs whose nonbonded interactions should be ignored. See also *PSFContainer.no_nonbonded*.

filename
A 1D array with a single string as filename.

Type 1 numpy.ndarray [str]

title
A 1D array of strings holding the title block.

Type n numpy.ndarray [str]

atoms
A Pandas DataFrame holding the atoms block. The DataFrame should possess the following collumn keys:

- "segment name"
- "residue ID"
- "residue name"
- "atom name"
- "atom type"
- "charge"
- "mass"
- "0"

Type $n * 8$ pandas.DataFrame

bonds
A 2D array holding the indices of all atom-pairs defining bonds. Indices are expected to be 1-based.

Type $n * 2$ numpy.ndarray [int]

angles
A 2D array holding the indices of all atom-triplets defining angles. Indices are expected to be 1-based.

Type $n * 3$ numpy.ndarray [int]

dihedrals
A 2D array holding the indices of all atom-quartets defining proper dihedral angles. Indices are expected to be 1-based.

Type $n * 4$ numpy.ndarray [int]

impropers
A 2D array holding the indices of all atom-quartets defining improper dihedral angles. Indices are expected to be 1-based.

Type $n * 4$ numpy.ndarray [int]

donors
A 2D array holding the atomic indices of all hydrogen-bond donors. Indices are expected to be 1-based.

Type $n * 1$ numpy.ndarray [int]

acceptors
A 2D array holding the atomic indices of all hydrogen-bond acceptors. Indices are expected to be 1-based.

Type $n * 1$ numpy.ndarray [int]

no_nonbonded
A 2D array holding the indices of all atom-pairs whose nonbonded interactions should be ignored. Indices are expected to be 1-based.

Type $n * 2$ numpy.ndarray [int]

np_printoptions
A mapping with Numpy print options. See np.set_printoptions.

Type Mapping [str, object]

pd_printoptions
A mapping with Pandas print options. See Options and settings.

Type Mapping [str, object]

_PRIVATE_ATTR: Set[str] = frozenset({'_np_printoptions', '_pd_printoptions'})
A from with the names of private instance attributes. These attributes will be excluded whenever calling PSF.as_dict().

_SHAPE_DICT = mappingproxy({'filename': {'shape': 1}, 'title': {'shape': 1}, 'atom
A dictionary containg array shapes among other things

_HEADER_DICT: Mapping[str, str] = mappingproxy({'!NTITLE': 'title', '!NATOM': 'atoms',
A dictionary mapping .psf headers to *PSFContainer* attribute names

__init__(*filename=None*, *title=None*, *atoms=None*, *bonds=None*, *angles=None*, *dihedrals=None*, *impropers=None*, *donors=None*, *acceptors=None*, *no_nonbonded=None*)
Initialize a *PSFContainer* instance.

static _is_dict(*value*)
Check if **value** is a dict instance; raise a TypeError if not.

Return type dict

__repr__()
Return a (machine readable) string representation of this instance.

The string representation consists of this instances' class name in addition to all (non-private) instance variables.

Returns A string representation of this instance.

Return type str

See also:

PSFContainer._PRIVATE_ATTR A set with the names of private instance variables.

PSFContainer._repr_fallback Fallback function for *PSFContainer.__repr__()* incase of recursive calls.

PSFContainer._str_iterator() Return an iterable for the iterating over this instances' attributes.

PSFContainer._str() Returns a string representation of a single **key/value** pair.

_str_iterator()
Return an iterable for the *PSFContainer.__repr__()* method.

Return type Iterable[Tuple[str, Any]]

__eq__(*value*)
Check if this instance is equivalent to **value**.

The comparison checks if the class type of this instance and **value** are identical and if all (non-private) instance variables are equivalent.

Returns Whether or not this instance and **value** are equivalent.

Return type bool

See also:

PSFContainer._PRIVATE_ATTR A set with the names of private instance variables.

PSFContainer._eq Return if **v1** and **v2** are equivalent.

PSFContainer._eq_fallback Fallback function for *PSFContainer.__eq__()* incase of recursive calls.

as_dict(*return_private=False*)
Construct a dictionary from this instance with all non-private instance variables.

The returned dictionary values are shallow copies.

Parameters **return_private** (bool) – If True, return both public and private instance variables. Private instance variables are defined in *PSFContainer._PRIVATE_ATTR*.

Returns A dictionary with keyword arguments for initializing a new instance of this class.

Return type dict [str, Any]

See also:

PSFContainer.from_dict() Construct a instance of this objects' class from a dictionary with keyword arguments.

PSFContainer._PRIVATE_ATTR A set with the names of private instance variables.

copy(*deep=True*)
Return a shallow or deep copy of this instance.

Parameters **deep** (bool) – Whether or not to return a deep or shallow copy.

Returns A new instance constructed from this instance.

Return type *PSFContainer*

__copy__()
Return a shallow copy of this instance; see *PSFContainer.copy()*.

Return type ~AT

property filename
Get *PSFContainer.filename* as string or assign an array-like object as a 1D array.

Return type str

property title
Get *PSFContainer.title* or assign an array-like object as a 1D array.

Return type ndarray

property atoms
Get *PSFContainer.atoms* or assign an a DataFrame.

Return type DataFrame

property bonds
Get *PSFContainer.bonds* or assign an array-like object as a 2D array.

Return type ndarray

property angles
Get *PSFContainer.angles* or assign an array-like object as a 2D array.

Return type ndarray

property dihedrals
Get *PSFContainer.dihedrals* or assign an array-like object as a 2D array.

Return type ndarray

property impropers
Get PSFPSFContainerimpropers or assign an array-like object as a 2D array.

Return type ndarray

property donors
Get *PSFContainer.donors* or assign an array-like object as a 2D array.

Return type ndarray

property acceptors
Get *PSFContainer.acceptors* or assign an array-like object as a 2D array.

Return type ndarray

property no_nonbonded
Get *PSFContainer.no_nonbonded* or assign an array-like object as a 2D array.

Return type ndarray

_set_nd_array(*name*, *value*, *ndmin*, *dtype*)
Assign an array-like object (**value**) to the **name** attribute as ndarray.

Performs an inplace update of this instance.

Parameters

- **name** (str) – The name of the to-be set attribute.
- **value** (array-like) – The array-like object to-be assigned to **name**. The supplied object is converted into into an array beforehand.
- **ndmin** (int) – The minimum number of dimensions of the to-be assigned array.
- **dtype** (type or numpy.dtype) – The desired datatype of the to-be assigned array.
- **Exceptions** –

- **----------** –
- **ValueError** – Raised if value array construction was unsuccessful.

Return type None

property segment_name
Get or set the "segment name" column in *PSFContainer.atoms*.

Return type Series

property residue_id
Get or set the "residue ID" column in *PSFContainer.atoms*.

Return type Series

__hash__(*self*)
Return the hash of this instance.

The returned hash is constructed from two components: * The hash of this instances' class type. * The hashes of all key/value pairs in this instances' (non-private) attributes.

If an unhashable instance variable is encountered, *e.g.* a list, then its id() is used for hashing.

This method will raise a TypeError if the class attribute AbstractDataClass._HASHABLE is False.

See also:

AbstractDataClass._PRIVATE_ATTR A set with the names of private instance variables.

AbstractDataClass._HASHABLE Whether or not this class is hashable.

AbstractDataClass._hash_fallback Fallback function for AbstractDataClass.__hash__() incase of recursive calls.

AbstractDataClass._hash An instance variable for caching the hash() of this instance.

Return type int

__weakref__
list of weak references to the object (if defined)

property residue_name
Get or set the "residue name" column in *PSFContainer.atoms*.

Return type Series

property atom_name
Get or set the "atom name" column in *PSFContainer.atoms*.

Return type Series

property atom_type
Get or set the "atom type" column in *PSFContainer.atoms*.

Return type Series

property charge
Get or set the "charge" column in *PSFContainer.atoms*.

Return type Series

property mass
Get or set the "mass" column in *PSFContainer.atoms*.

Return type Series

classmethod read(*filename*, *encoding=None*, ***kwargs*)

Construct a new instance from this object's class by reading the content of **filename**.

Parameters

- **filename** (str, bytes, os.PathLike or a file object) – The path+filename or a file object of the to-be read .psf file. In practice, any iterable can substitute the role of file object as long iteration returns either strings or bytes (see **encoding**).
- **encoding** (str, optional) – Encoding used to decode the input (*e.g.* "utf-8"). Only relevant when a file object is supplied to **filename** and the datastream is *not* in text mode.
- ****kwargs** (Any) – Optional keyword arguments that will be passed to both *PSFContainer._read_iterate()* and *PSFContainer._read_postprocess()*.

See also:

PSFContainer._read_iterate() An abstract method for parsing the opened file in *PSFContainer.read()*.

PSFContainer._read_postprocess() Post processing the class instance created by *PSFContainer.read()*.

Return type *PSFContainer*

classmethod _read_iterate(*iterator*)

An abstract method for parsing the opened file in read.

Parameters **iterator** (Iterator [str]) – An iterator that returns str instances upon iteration.

Return type Dict[str, Any]

Returns

- dict [str, Any] – A dictionary with keyword arguments for a new instance of this objects' class.
- ****kwargs** (Any) – Optional keyword arguments.

See also:

read() The main method for reading files.

_read_postprocess(*filename*, *encoding=None*, ***kwargs*)

Post processing the class instance created by *read()*.

Parameters

- **filename** (str, bytes, os.PathLike or a file object) – The path+filename or a file object of the to-be read .psf file. In practice, any iterable can substitute the role of file object as long iteration returns either strings or bytes (see **encoding**).
- **encoding** (str, optional) – Encoding used to decode the input (*e.g.* "utf-8"). Only relevant when a file object is supplied to **filename** and the datastream is *not* in text mode.
- ****kwargs** (Any) – Optional keyword arguments that will be passed to both *PSFContainer._read_iterate()* and *PSFContainer._read_postprocess()*.

See also:

PSFContainer.read() The main method for reading files.

Return type None

classmethod _post_process_psf(*psf_dict*)

Post-process the output of PSF.read(), casting the values into appropiat objects.

- The title block is converted into a 1D array of strings.
- The atoms block is converted into a Pandas DataFrame.
- All other blocks are converted into 2D arrays of integers.

Parameters **psf_dict** (dict [str, numpy.ndarray]) – A dictionary holding the content of a .psf file (see PSFContainer.read_psf()).

Returns The .psf output, **psf_dict**, with properly formatted values.

Return type dict [str, numpy.ndarray]

write(*filename*, *encoding=None*, ***kwargs*)

Write the content of this instance to **filename**.

Parameters

- **filename** (str, bytes, os.PathLike or a file object) – The path+filename or a file object of the to-be read .psf file. Contrary to *_read_postprocess()*, file objects can *not* be substituted for generic iterables.
- **encoding** (str, optional) – Encoding used to decode the input (*e.g.* "utf-8"). Only relevant when a file object is supplied to **filename** and the datastream is *not* in text mode.
- ****kwargs** (Any) – Optional keyword arguments that will be passed to *_write_iterate()*.

See also:

PSFContainer._write_iterate() Write the content of this instance to an opened datastream.

PSFContainer._get_writer() Take a *write()* method and ensure its first argument is properly encoded.

Return type None

_write_iterate(*write*, ***kwargs*)

Write the content of this instance to an opened datastream.

The to-be written content of this instance should be passed as str. Any (potential) encoding is handled by the **write** parameter.

Example

Basic example of a potential *_write_iterate()* implementation.

```
>>> iterator = self.as_dict().items()
>>> for key, value in iterator:
...     value: str = f'{key} = {value}'
```

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```
...     write(value)
>>> return None
```

Parameters

- **writer** (Callable) – A callable for writing the content of this instance to a file object. An example would be the `io.TextIOWrapper.write()` method.
- ****kwargs** (*optional*) – Optional keyword arguments.

See also:

PSFContainer.write() The main method for writing files.

Return type None

_write_top(*write*)

Write the top-most section of the to-be create .psf file.

The following blocks are seralized:

- `PSF.title`
- `PSF.atoms`

Parameters **write** (Callable [[AnyStr], None]) – A callable for writing the content of this instance to a file object. An example would be the `io.TextIOWrapper.write()` method.

Returns A string constructed from the above-mentioned psf blocks.

Return type str

See also:

PSFContainer.write() The main method for writing .psf files.

_write_bottom(*write*)

Write the bottom-most section of the to-be create .psf file.

The following blocks are seralized:

- `PSF.bonds`
- `PSF.angles`
- `PSF.dihedrals`
- `PSF.impropers`
- `PSF.donors`
- `PSF.acceptors`
- `PSF.no_nonbonded`

Parameters **write** (Callable [[AnyStr], None]) – A callable for writing the content of this instance to a file object. An example would be the `io.TextIOWrapper.write()` method.

See also:

PSFContainer.write() The main method for writing .psf files.

Return type None

static _serialize_array(*array*, *items_per_row=4*)
Serialize an array into a single string; used for creating .psf files.

Newlines are placed for every **items_per_row** rows in **array**.

Parameters

- **array** (numpy.ndarray) – A 2D array.
- **items_per_row** (int) – The number of values per row before switching to a new line.

Returns A serialized array.

Return type str

See also:

PSFContainer.write() The main method for writing .psf files.

update_atom_charge(*atom_type*, *charge*)
Change the charge of **atom_type** to **charge**.

Parameters

- **atom_type** (str) – An atom type in *PSFContainer.atoms* ["atom type"].
- **charge** (float) – The new atomic charge to-be assigned to **atom_type**. See *PSFContainer.atoms* ["charge"].

Raises **ValueError** – Raised if **charge** cannot be converted into a float.

Return type None

update_atom_type(*atom_type_old*, *atom_type_new*)
Change the atom type of a **atom_type_old** to **atom_type_new**.

Parameters

- **atom_type_old** (str) – An atom type in *PSFContainer.atoms* ["atom type"].
- **atom_type_new** (str) – The new atom type to-be assigned to **atom_type**. See *PSFContainer.atoms* ["atom type"].

Return type None

generate_bonds(*mol*)
Update *PSFContainer.bonds* with the indices of all bond-forming atoms from **mol**.

Parameters **mol** (*plams.Molecule*) – A PLAMS Molecule.

Return type None

generate_angles(*mol*)
Update *PSFContainer.angles* with the indices of all angle-defining atoms from **mol**.

Parameters **mol** (*plams.Molecule*) – A PLAMS Molecule.

Return type None

generate_dihedrals(*mol*)
Update *PSFContainer.dihedrals* with the indices of all proper dihedral angle-defining atoms from **mol**.

Parameters **mol** (*plams.Molecule*) – A PLAMS Molecule.

Return type None

generate_impropers(*mol*)
Update *PSFContainer.impropers* with the indices of all improper dihedral angle-defining atoms from **mol**.

Parameters **mol** (*plams.Molecule*) – A PLAMS Molecule.

Return type None

generate_atoms(*mol*, *id_map=None*)
Update *PSFContainer.atoms* with the all properties from **mol**.

DataFrame keys in *PSFContainer.atoms* are set based on the following values in **mol**:

DataFrame column	Value	Backup value(s)
"segment name"	"MOL{:d}"; See "atom type" and "residue name"	
"residue ID"	Atom.properties ["pdb_info"]["ResidueNumber"]	1
"residue name"	Atom.properties ["pdb_info"]["ResidueName"]	"COR"
"atom name"	Atom.symbol	
"atom type"	Atom.properties["symbol"]	Atom.symbol
"charge"	Atom.properties["charge_float"]	Atom.properties ["charge"] & 0.0
"mass"	Atom.mass	
"0"	0	

If a value is not available in a particular Atom.properties instance then a backup value will be set.

Parameters

- **mol** (*plams.Molecule*) – A PLAMS Molecule.
- **id_map** (Mapping[int, Hashable], optional) – A mapping of ligand residue ID's to a custom (Hashable) descriptor. Can be used for generating residue names for quantum dots with multiple different ligands.

Return type None

_construct_segment_name(*id_map=None*)
Generate a list for the PSF.atoms["segment name"] column.

Return type List[str]

to_atom_dict()
Create a dictionary of atom types and lists with their respective indices.

Returns A dictionary with atom types as keys and lists of matching atomic indices as values. The indices are 0-based.

Return type dict [str, list [int]]

write_pdb(*mol*, *pdb_file=<_io.TextIOWrapper name='<stdout>' mode='w' encoding='UTF-8'>*, *copy_mol=True*)

Construct a .pdb file from this instance and **mol**.

Parameters

- **mol** (*plams.Molecule*) – A PLAMS Molecule.
- **copy_mol** (bool) – If True, create a copy of **mol** instead of modifying it inplace.
- **pdb_file** (str ot TextIOBase) – A filename or a file-like object.

Return type None

2.8 PRMContainer

2.8.1 FOX.io.read_prm

A class for reading and generating .prm parameter files.

Index

PRMContainer([filename, atoms, bonds, ...])	A container for managing prm files.
PRMContainer.read(filename[, encoding])	Construct a new instance from this object's class by reading the content of **filename**.
PRMContainer.write([filename, encoding])	Write the content of this instance to **filename**.
PRMContainer.overlay_mapping(prm_name, param_df)	Update a set of parameters, **prm_name**, with those provided in **param_df**.
PRMContainer.overlay_cp2k_settings(cp2k_settings)	Extract forcefield information from PLAMS-style CP2K settings.

API

class FOX.io.read_prm.**PRMContainer**(*filename=None*, *atoms=None*, *bonds=None*, *angles=None*, *dihedrals=None*, *improper=None*, *impropers=None*, *nonbonded=None*, *nonbonded_header=None*, *nbfix=None*, *hbond=None*)

A container for managing prm files.

pd_printoptions

A dictionary with Pandas print options. See Options and settings.

Type dict [str, object], private

CP2K_TO_PRM

A mapping providing tools for converting CP2K settings to .prm-compatible values. See *CP2K_TO_PRM*.

Type Mapping [str, *PRMMapping*]

classmethod PRMContainer.**read**(*filename*, *encoding=None*, ***kwargs*)

Construct a new instance from this object's class by reading the content of **filename**.

Parameters

- **filename** (str, bytes, os.PathLike or a file object) – The path+filename or a file object of the to-be read .psf file. In practice, any iterable can substitute the role of file object as long iteration returns either strings or bytes (see **encoding**).
- **encoding** (str, optional) – Encoding used to decode the input (*e.g.* "utf-8"). Only relevant when a file object is supplied to **filename** and the datastream is *not* in text mode.
- ****kwargs** (Any) – Optional keyword arguments that will be passed to both *PRMContainer._read_iterate()* and *PRMContainer._read_postprocess()*.

See also:

PRMContainer._read_iterate() An abstract method for parsing the opened file in *PRMContainer.read()*.

PRMContainer._read_postprocess() Post processing the class instance created by *PRMContainer.read()*.

Return type *PRMContainer*

PRMContainer.**write**(*filename=None*, *encoding=None*, ***kwargs*)

Write the content of this instance to **filename**.

Parameters

- **filename** (str, bytes, os.PathLike or a file object) – The path+filename or a file object of the to-be read .psf file. Contrary to *_read_postprocess()*, file objects can *not* be substituted for generic iterables.
- **encoding** (str, optional) – Encoding used to decode the input (*e.g.* "utf-8"). Only relevant when a file object is supplied to **filename** and the datastream is *not* in text mode.
- ****kwargs** (Any) – Optional keyword arguments that will be passed to *_write_iterate()*.

See also:

PRMContainer._write_iterate() Write the content of this instance to an opened datastream.

PRMContainer._get_writer() Take a *write()* method and ensure its first argument is properly encoded.

Return type None

PRMContainer.**overlay_mapping**(*prm_name*, *param_df*, *units=None*)

Update a set of parameters, **prm_name**, with those provided in **param_df**.

Examples

```
>>> from FOX import PRMContainer

>>> prm = PRMContainer(...)

>>> param_dict = {}
>>> param_dict['epsilon'] = {'Cd Cd': ..., 'Cd Se': ..., 'Se Se': ...}  # epsilon
>>> param_dict['sigma'] = {'Cd Cd': ..., 'Cd Se': ..., 'Se Se': ...}  # sigma
```

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```
>>> units = ('kcal/mol', 'angstrom')  # input units for epsilon and sigma

>>> prm.overlay_mapping('nonbonded', param_dict, units=units)
```

Parameters

- **prm_name** (str) – The name of the parameter of interest. See the keys of *PRMContainer.CP2K_TO_PRM* for accepted values.
- **param_df** (pandas.DataFrame or nested Mapping) – A DataFrame or nested mapping with the to-be added parameters. The keys should be a subset of *PRMContainer.CP2K_TO_PRM[prm_name]["columns"]*. If the index/nested sub-keys consist of strings then they'll be split and turned into a pandas.MultiIndex. Note that the resulting values are *not* sorted.
- **units** (Iterable [str], optional) – An iterable with the input units of each column in **param_df**. If None, default to the defaults specified in *PRMContainer.CP2K_TO_PRM[prm_name]["unit"]*.

Return type None

PRMContainer.**overlay_cp2k_settings**(*cp2k_settings*)

Extract forcefield information from PLAMS-style CP2K settings.

Performs an inplace update of this instance.

Examples

Example input value for **cp2k_settings**. In the provided example the **cp2k_settings** are directly extracted from a CP2K .inp file.

```
>>> import cp2kparser  # https://github.com/nlesc-nano/CP2K-Parser

>>> filename = str(...)

>>> cp2k_settings: dict = cp2kparser.read_input(filename)
>>> print(cp2k_settings)
{'force_eval': {'mm': {'forcefield': {'nonbonded': {'lennard-jones': [...]}}}}}
```

Parameters **cp2k_settings** (Mapping) – A Mapping with PLAMS-style CP2K settings.

See also:

PRMMapping *PRMMapping* A mapping providing tools for converting CP2K settings to .prm-compatible values.

Return type None

2.9 Recipes

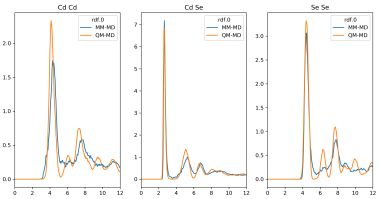
2.9.1 FOX.recipes.param

A set of functions for analyzing and plotting ARMC results.

Examples

A general overview of the functions within this module.

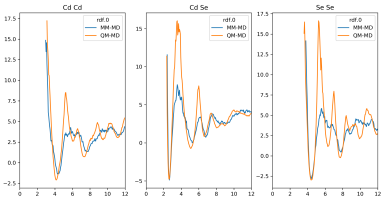
```
>>> import pandas as pd
>>> from FOX.recipes import get_best, overlay_descriptor, plot_descriptor

>>> hdf5_file: str = ...

>>> param: pd.Series = get_best(hdf5_file, name='param')  # Extract the best␣
↪parameters
>>> rdf: pd.DataFrame = get_best(hdf5_file, name='rdf')  # Extract the matching RDF

# Compare the RDF to its reference RDF and plot
>>> rdf_dict = overlay_descriptor(hdf5_file, name='rdf')
>>> plot_descriptor(rdf_dict)
```



Examples

A small workflow for calculating for calculating free energies using distribution functions such as the radial distribution function (RDF).

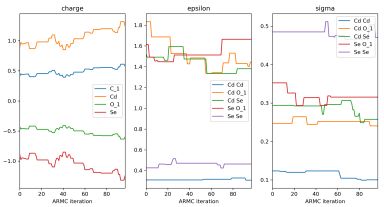
```
>>> import pandas as pd
>>> from FOX import get_free_energy
>>> from FOX.recipes import get_best, overlay_descriptor, plot_descriptor

>>> hdf5_file: str = ...

>>> rdf: pd.DataFrame = get_best(hdf5_file, name='rdf')
>>> G: pd.DataFrame = get_free_energy(rdf, unit='kcal/mol')

>>> rdf_dict = overlay_descriptor(hdf5_file, name='rdf)
>>> G_dict = {key: get_free_energy(value) for key, value in rdf_dict.items()}
>>> plot_descriptor(G_dict)
```



Examples

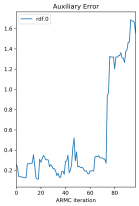
A workflow for plotting parameters as a function of ARMC iterations.

```
>>> import numpy as np
>>> import pandas as pd
>>> from FOX import from_hdf5
>>> from FOX.recipes import plot_descriptor

>>> hdf5_file: str = ...

>>> param: pd.DataFrame = from_hdf5(hdf5_file, 'param')
>>> param.index.name = 'ARMC iteration'
>>> param_dict = {key: param[key] for key in param.columns.levels[0]}

>>> plot_descriptor(param_dict)
```



This approach can also be used for the plotting of other properties such as the auxiliary error.

```
>>> ...

>>> err: pd.DataFrame = from_hdf5(hdf5_file, 'aux_error')
>>> err.index.name = 'ARMC iteration'
>>> err_dict = {'Auxiliary Error': err}

>>> plot_descriptor(err_dict)
```



On occasion it might be desirable to only print the error of, for example, accepted iterations. Given a sequence of booleans (`bool_seq`), one can slice a DataFrame or Series (`df`) using `df.loc[bool_seq]`.

```
>>> ...

>>> acceptance: np.ndarray = from_hdf5(hdf5_file, 'acceptance')  # Boolean array
>>> err_slice_dict = {key: df.loc[acceptance], value for key, df in err_dict.items()}

>>> plot_descriptor(err_slice_dict)
```

Index

get_best(hdf5_file[, name, i])	Return the PES descriptor or ARMC property which yields the lowest error.
overlay_descriptor(hdf5_file[, name, i])	Return the PES descriptor which yields the lowest error and overlay it with the reference PES descriptor.
plot_descriptor(descriptor[, show_fig, ...])	Plot a DataFrame or iterable consisting of one or more DataFrames.

API

FOX.recipes.param.**get_best**(*hdf5_file*, *name='rdf'*, *i=0*)

Return the PES descriptor or ARMC property which yields the lowest error.

Parameters

- **hdf5_file** (str) – The path+filename of the ARMC .hdf5 file.
- **name** (str) – The name of the PES descriptor, *e.g.* `"rdf"`. Alternatively one can supply an ARMC property such as `"acceptance"`, `"param"` or `"aux_error"`.
- **i** (int) – The index of the desired PES. Only relevant for PES-descriptors of state-averaged ARMCs.

Returns A DataFrame of the optimal PES descriptor or other (user-specified) ARMC property.

Return type pandas.DataFrame or pd.Series

FOX.recipes.param.**overlay_descriptor**(*hdf5_file*, *name='rdf'*, *i=0*)

Return the PES descriptor which yields the lowest error and overlay it with the reference PES descriptor.

Parameters

- **hdf5_file** (str) – The path+filename of the ARMC .hdf5 file.
- **name** (str) – The name of the PES descriptor, *e.g.* `"rdf"`.
- **i** (int) – The index of desired PES. Only relevant for state-averaged ARMCs.

Returns A dictionary of DataFrames. Values consist of DataFrames with two keys: `"MM-MD"` and `"QM-MD"`. Atom pairs, such as `"Cd Cd"`, are used as keys.

Return type dict [str, pandas.DataFrame]

FOX.recipes.param.**plot_descriptor**(*descriptor*, *show_fig=True*, *kind='line'*, *sharex=True*, *sharey=False*, ***kwargs*)

Plot a DataFrame or iterable consisting of one or more DataFrames.

Requires the matplotlib package.

Parameters

- **descriptor** (pandas.DataFrame or Iterable [pandas.DataFrame]) – A DataFrame or an iterable consisting of DataFrames.
- **show_fig** (bool) – Whether to show the figure or not.
- **kind** (str) – The plot kind to-be passed to pandas.DataFrame.plot().
- **sharex/sharey** (bool) – Whether or not the to-be created plots should share their x/y-axes.
- ****kwargs** (Any) – Further keyword arguments for the pandas.DataFrame.plot() method.

Returns A matplotlib Figure.

Return type Figure

See also:

get_best() Return the PES descriptor or ARMC property which yields the lowest error.

overlay_descriptor() Return the PES descriptor which yields the lowest error and overlay it with the reference PES descriptor.

2.9.2 FOX.recipes.psf

A set of functions for creating .psf files.

Examples

Example code for generating a .psf file. Ligand atoms within the ligand .xyz file and the qd .xyz file should be in the *exact* same order. For example, implicit hydrogen atoms added by the from_smiles functions are not guaranteed to be ordered, even when using canonical SMILES strings.

```
>>> from scm.plams import Molecule, from_smiles
>>> from FOX import PSFContainer
>>> from FOX.recipes import generate_psf

# Accepts .xyz, .pdb, .mol or .mol2 files
>>> qd = Molecule(...)
>>> ligand: Molecule = Molecule(...)
>>> rtf_file : str = ...
>>> psf_file : str = ...

>>> psf: PSFContainer = generate_psf(qd_xyz, ligand_xyz, rtf_file=rtf_file)
>>> psf.write(psf_file)
```

Examples

If no ligand .xyz is on hand, or its atoms are in the wrong order, it is possible the extract the ligand directly from the quantum dot. This is demonstrated below with oleate ($C_{18}H_{33}O_2^-$).

```
>>> from scm.plams import Molecule
>>> from FOX import PSFContainer
>>> from FOX.recipes import generate_psf, extract_ligand

>>> qd = Molecule(...)  # Accepts an .xyz, .pdb, .mol or .mol2 file
>>> rtf_file : str = ...

>>> ligand_len = 18 + 33 + 2
>>> ligand_atoms = {'C', 'H', 'O'}
>>> ligand: Molecule = extract_ligand(qd, ligand_len, ligand_atoms)

>>> psf: PSFContainer = generate_psf(qd, ligand, rtf_file=rtf_file)
>>> psf.write(...)
```

Examples

Example for multiple ligands.

```
>>> from typing import List
>>> from scm.plams import Molecule
>>> from FOX import PSFContainer
>>> from FOX.recipes import generate_psf2

>>> qd = Molecule(...)  # Accepts an .xyz, .pdb, .mol or .mol2 file
>>> ligands = ('C[O-]', 'CC[O-]', 'CCC[O-]')
>>> rtf_files = (..., ..., ...)

>>> psf: PSFContainer = generate_psf2(qd, *ligands, rtf_file=rtf_files)
>>> psf.write(...)
```

If the the psf construction with *generate_psf2()* failes to identify a particular ligand, it is possible to return all (failed) potential ligands with the **ret_failed_lig** parameter.

```
>>> ...

>>> ligands = ('CCCCCCCCC[O-]', 'CCCCBr')
>>> failed_mol_list: List[Molecule] = generate_psf2(qd, *ligands, ret_failed_lig=True)
```

Index

generate_psf(qd, ligand[, rtf_file, str_file])	Generate a `PSFContainer` instance for **qd**.
generate_psf2(qd, *ligands[, rtf_file, ...])	Generate a `PSFContainer` instance for **qd** with multiple different **ligands**.
extract_ligand(qd, ligand_len, ligand_atoms)	Extract a single ligand from **qd**.

API

FOX.recipes.psf.**generate_psf**(*qd*, *ligand*, *rtf_file=None*, *str_file=None*)
Generate a PSFContainer instance for **qd**.

Parameters

- **qd** (str or Molecule) – The ligand-pacifated quantum dot. Should be supplied as either a Molecule or .xyz file.
- **ligand** (str or Molecule) – A single ligand. Should be supplied as either a Molecule or .xyz file.
- **rtf_file** (str, optional) – The path+filename of the ligand's .rtf file. Used for assigning atom types. Alternativelly, one can supply a .str file with the **str_file** argument.
- **str_file** (str, optional) – The path+filename of the ligand's .str file. Used for assigning atom types. Alternativelly, one can supply a .rtf file with the **rtf_file** argument.

Returns A PSFContainer instance with the new .psf file.

Return type PSFContainer

FOX.recipes.psf.**generate_psf2**(*qd*, **ligands*, *rtf_file=None*, *str_file=None*, *ret_failed_lig=False*)
Generate a PSFContainer instance for **qd** with multiple different **ligands**.

Parameters

- **qd** (str or Molecule) – The ligand-pacifated quantum dot. Should be supplied as either a Molecule or .xyz file.
- ***ligands** (str, Molecule or Chem.Mol) – One or more PLAMS/RDkit Molecules and/or SMILES strings representing ligands.
- **rtf_file** (str or Iterable [str], optional) – The path+filename of the ligand's .rtf files. Filenames should be supplied in the same order as **ligands**. Used for assigning atom types. Alternativelly, one can supply a .str file with the **str_file** argument.
- **str_file** (str or Iterable [str], optional) – The path+filename of the ligand's .str files. Filenames should be supplied in the same order as **ligands**. Used for assigning atom types. Alternativelly, one can supply a .rtf file with the **rtf_file** argument.
- **ret_failed_lig** (bool) – If True, return a list of all failed (potential) ligands if the function cannot identify any ligands within a certain range. Usefull for debugging. If False, raise a MoleculeError.

Returns A single ligand Molecule.

Return type Molecule

Raises **MoleculeError** – Raised if the function fails to identify any ligands within a certain range. If ret_failed_lig = True, return a list of failed (potential) ligands instead and issue a warning.

FOX.recipes.psf.**extract_ligand**(*qd*, *ligand_len*, *ligand_atoms*)
Extract a single ligand from **qd**.

Parameters

- **qd** (str or Molecule) – The ligand-pacifated quantum dot. Should be supplied as either a Molecule or .xyz file.
- **ligand_len** (int) – The number of atoms within a single ligand.

- **ligand_atoms** (str or Iterable [str]) – One or multiple strings with the atomic symbols of all atoms within a single ligand.

Returns A single ligand Molecule.

Return type Molecule

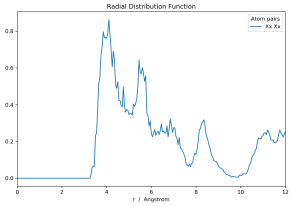
2.9.3 FOX.recipes.ligands

A set of functions for analyzing ligands.

Examples

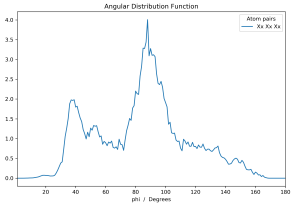
An example for generating a ligand center of mass RDF.

```
>>> import numpy as np
>>> import pandas as pd
>>> from FOX import MultiMolecule, example_xyz
>>> from FOX.recipes import get_lig_center

>>> mol = MultiMolecule.from_xyz(example_xyz)
>>> start = 123  # Start of the ligands
>>> step = 4  # Size of the ligands

# Add dummy atoms to the ligand-center of mass and calculate the RDF
>>> lig_centra: np.ndarray = get_lig_center(mol, start, step)
>>> mol_new: MultiMolecule = mol.add_atoms(lig_centra, symbols='Xx')
>>> rdf: pd.DataFrame = mol_new.init_rdf(atom_subset=['Xx'])
```



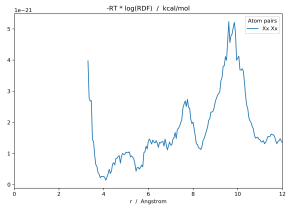
Or the ADF.

```
>>> ...

>>> adf: pd.DataFrame = mol_new.init_rdf(atom_subset=['Xx'], r_max=np.inf)
```



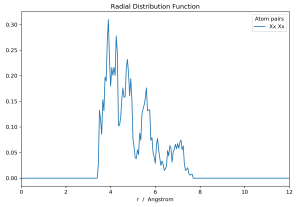
Or the potential of mean force (*i.e.* Boltzmann-inverted RDF).

```
>>> ...

>>> from scipy import constants
>>> from scm.plams import Units

>>> RT: float = 298.15 * constants.Boltzmann
>>> kj_to_kcal: float = Units.conversion_ratio('kj/mol', 'kcal/mol')

>>> with np.errstate(divide='ignore'):
>>>     rdf_invert: pd.DataFrame = -RT * np.log(rdf) * kj_to_kcal
>>>     rdf_invert[rdf_invert == np.inf] = np.nan  # Set all infinities to not-a-
↪number
```



Focus on a specific ligand subset is possible by slicing the new ligand Cartesian coordinate array.

```
>>> ...

>>> keep_lig = [0, 1, 2, 3]  # Keep these ligands; disgard the rest
>>> lig_centra_subset = lig_centra[:, keep_lig]

# Add dummy atoms to the ligand-center of mass and calculate the RDF
>>> mol_new2: MultiMolecule = mol.add_atoms(lig_centra_subset, symbols='Xx')
>>> rdf: pd.DataFrame = mol_new2.init_rdf(atom_subset=['Xx'])
```



Examples

An example for generating a ligand center of mass RDF from a quantum dot with multiple unique ligands. A .psf file will herein be used as starting point.

```
>>> import numpy as np
>>> from FOX import PSFContainer, MultiMolecule, group_by_values
>>> from FOX.recipes import get_multi_lig_center

>>> mol = MultiMolecule.from_xyz(...)
>>> psf = PSFContainer.read(...)

# Gather the indices of each ligand
>>> idx_dict: dict = group_by_values(enumerate(psf.residue_id, start=1))
>>> del idx_dict[1]  # Delete the core

# Use the .psf segment names as symbols
>>> symbols = [psf.segment_name[i].iloc[0] for i in idx_dict.values()]

# Add dummy atoms to the ligand-center of mass and calculate the RDF
>>> lig_centra: np.ndarray = get_multi_lig_center(mol, idx_dict.values())
>>> mol_new: MultiMolecule = mol.add_atoms(lig_centra, symbols=symbols)
>>> rdf = mol_new.init_rdf(atom_subset=set(symbols))
```

Index

get_lig_center(mol, start, step[, stop, ...])	Return an array with the (mass-weighted) mean position of each ligands in **mol**.
get_multi_lig_center(mol, idx_iter[, ...])	Return an array with the (mass-weighted) mean position of each ligands in **mol**.

API

FOX.recipes.ligands.**get_lig_center**(*mol*, *start*, *step*, *stop=None*, *mass_weighted=True*)

Return an array with the (mass-weighted) mean position of each ligands in **mol**.

Parameters

- **mol** (*MultiMolecule*) – A MultiMolecule instance.
- **start** (int) – The atomic index of the first ligand atoms.
- **step** (int) – The number of atoms per ligand.
- **stop** (int, optional) – Can be used for neglecting any ligands beyond a user-specified atomic index.
- **mass_weighted** (bool) – If True, return the mass-weighted mean ligand position rather than its unweighted counterpart.

Returns A new array with the ligand's centra of mass. If `mol.shape == (m, n, 3)` then, given `k` new ligands, the to-be returned array's shape is `(m, k, 3)`.

Return type numpy.ndarray

FOX.recipes.ligands.**get_multi_lig_center**(*mol*, *idx_iter*, *mass_weighted=True*)

Return an array with the (mass-weighted) mean position of each ligands in **mol**.

Contrary to *get_lig_center()*, this function can handle molecules with multiple non-unique ligands.

Parameters

- **mol** (*MultiMolecule*) – A MultiMolecule instance.
- **idx_iter** (Iterable [Sequence [int]]) – An iterable consisting of integer sequences. Each integer sequence represents a single ligand (by its atomic indices).
- **mass_weighted** (bool) – If True, return the mass-weighted mean ligand position rather than its unweighted counterpart.

Returns A new array with the ligand's centra of mass. If `mol.shape == (m, n, 3)` then, given `k` new ligands (aka the length of **idx_iter**) , the to-be returned array's shape is `(m, k, 3)`.

Return type numpy.ndarray

2.10 file_container

2.10.1 FOX.io.file_container

An abstract container for reading and writing files.

Index

AbstractFileContainer()	An abstract container for reading and writing files.

API

class FOX.io.file_container.**AbstractFileContainer**

An abstract container for reading and writing files.

Two public methods are defined within this class:

- ***AbstractFileContainer.read()*: Construct a new instance from this object's class by** reading the content to a file or file object. How the content of the to-be read file is parsed has to be defined in the *AbstractFileContainer._read_iterate()* abstract method.
- ***AbstractFileContainer.write()*: Write the content of this instance to an opened** file or file object. How the content of the to-be exported class instance is parsed has to be defined in the *AbstractFileContainer._write_iterate()*

The opening, closing and en-/decoding of files is handled by two above-mentioned methods; the parsing * *AbstractFileContainer._read_iterate()* * *AbstractFileContainer._write_iterate()*

__contains__(*value*)

Check if this instance contains **value**.

Return type bool

classmethod read(*filename*, *encoding=None*, ***kwargs*)

Construct a new instance from this object's class by reading the content of **filename**.

Parameters

- **filename** (str, bytes, os.PathLike or a file object) – The path+filename or a file object of the to-be read .psf file. In practice, any iterable can substitute the role of file object as long iteration returns either strings or bytes (see **encoding**).

- **encoding** (str, optional) – Encoding used to decode the input (*e.g.* `"utf-8"`). Only relevant when a file object is supplied to **filename** and the datastream is *not* in text mode.
- ****kwargs** (Any) – Optional keyword arguments that will be passed to both *AbstractFileContainer._read_iterate()* and *AbstractFileContainer._read_postprocess()*.

See also:

AbstractFileContainer._read_iterate() An abstract method for parsing the opened file in *AbstractFileContainer.read()*.

AbstractFileContainer._read_postprocess() Post processing the class instance created by *AbstractFileContainer.read()*.

Return type *AbstractFileContainer*

abstract classmethod _read_iterate(*iterator*, ***kwargs*)

An abstract method for parsing the opened file in `read`.

Parameters **iterator** (Iterator [str]) – An iterator that returns str instances upon iteration.

Return type Dict[str, Any]

Returns

- dict [str, Any] – A dictionary with keyword arguments for a new instance of this objects' class.
- ****kwargs** (Any) – Optional keyword arguments.

See also:

read() The main method for reading files.

_read_postprocess(*filename*, *encoding=None*, ***kwargs*)

Post processing the class instance created by *read()*.

Parameters

- **filename** (str, bytes, os.PathLike or a file object) – The path+filename or a file object of the to-be read .psf file. In practice, any iterable can substitute the role of file object as long iteration returns either strings or bytes (see **encoding**).
- **encoding** (str, optional) – Encoding used to decode the input (*e.g.* `"utf-8"`). Only relevant when a file object is supplied to **filename** and the datastream is *not* in text mode.
- ****kwargs** (Any) – Optional keyword arguments that will be passed to both *AbstractFileContainer._read_iterate()* and *AbstractFileContainer._read_postprocess()*.

See also:

AbstractFileContainer.read() The main method for reading files.

Return type None

write(*filename*, *encoding=None*, ***kwargs*)

Write the content of this instance to **filename**.

Parameters

- **filename** (str, bytes, os.PathLike or a file object) – The path+filename or a file object of the to-be read .psf file. Contrary to *_read_postprocess()*, file objects can *not* be substituted for generic iterables.
- **encoding** (str, optional) – Encoding used to decode the input (*e.g.* "utf-8"). Only relevant when a file object is supplied to **filename** and the datastream is *not* in text mode.
- ****kwargs** (Any) – Optional keyword arguments that will be passed to *_write_iterate()*.

See also:

AbstractFileContainer._write_iterate() Write the content of this instance to an opened datastream.

AbstractFileContainer._get_writer() Take a *write()* method and ensure its first argument is properly encoded.

Return type None

static _get_writer(*writer*, *encoding=None*)

Take a *write()* method and ensure its first argument is properly encoded.

Parameters

- **writer** (Callable) – A write method such as io.TextIOWrapper.write().
- **encoding** (str, optional) – Encoding used to encode the input of **writer** (*e.g.* "utf-8"). This value will be used in str.encode() for encoding the first positional argument provided to **instance_method**. If None, return **instance_method** unaltered without any encoding.

Returns A decorated **writer** parameter. The first positional argument provided to the decorated callable will be encoded using encoding. **writer** is returned unalterd if encoding=None.

Return type Callable

See also:

AbstractFileContainer.write() The main method for writing files.

abstract _write_iterate(*write*, ***kwargs*)

Write the content of this instance to an opened datastream.

The to-be written content of this instance should be passed as str. Any (potential) encoding is handled by the **write** parameter.

Example

Basic example of a potential *_write_iterate()* implementation.

```
>>> iterator = self.as_dict().items()
>>> for key, value in iterator:
...     value: str = f'{key} = {value}'
...     write(value)
>>> return None
```

Parameters

- **writer** (Callable) – A callable for writing the content of this instance to a file object. An example would be the `io.TextIOWrapper.write()` method.
- ****kwargs** (*optional*) – Optional keyword arguments.

See also:

AbstractFileContainer.write() The main method for writing files.

Return type None

classmethod inherit_annotations()

A decorator for inheriting annotations and docstrings.

Can be applied to methods of *AbstractFileContainer* subclasses to automatically inherit the docstring and annotations of identical-named functions of its superclass.

Examples

```
>>> class sub_class(AbstractFileContainer)
...
...     @AbstractFileContainer.inherit_annotations()
...     def write(filename, encoding=None, **kwargs):
...         pass

>>> sub_class.write.__doc__ == AbstractFileContainer.write.__doc__
True

>>> sub_class.write.__annotations__ == AbstractFileContainer.write.__
↪annotations__
True
```

Return type type

__weakref__

list of weak references to the object (if defined)

2.11 FOX.io.read_prm

An abstract container for reading and writing files.

2.11.1 Index

PRMContainer([filename, atoms, bonds, ...])	A container for managing prm files.

2.11.2 API

class FOX.io.read_prm.**PRMContainer**(*filename=None*, *atoms=None*, *bonds=None*, *angles=None*, *dihedrals=None*, *improper=None*, *impropers=None*, *nonbonded=None*, *nonbonded_header=None*, *nbfix=None*, *hbond=None*)

A container for managing prm files.

pd_printoptions

A dictionary with Pandas print options. See Options and settings.

Type dict [str, object], private

CP2K_TO_PRM

A mapping providing tools for converting CP2K settings to .prm-compatible values. See *CP2K_TO_PRM*.

Type Mapping [str, *PRMMapping*]

_PRIVATE_ATTR: ClassVar[FrozenSet[str]] = frozenset({'_pd_printoptions'})

A frozenset with the names of private instance attributes. These attributes will be excluded whenever calling PRMContainer.as_dict().

HEADERS: Tuple[str, ...] = ('ATOMS', 'BONDS', 'ANGLES', 'DIHEDRALS', 'NBFIX', 'HBOND'

A tuple of supported .psf headers.

INDEX: Mapping[str, List[int]] = mappingproxy({'atoms': [2], 'bonds': [0, 1], 'angle

Define the columns for each DataFrame which hold its index

COLUMNS: Mapping[str, Tuple[Union[None, int, float], ...]] = mappingproxy({'atoms':

Placeholder values for DataFrame columns

__init__(*filename=None*, *atoms=None*, *bonds=None*, *angles=None*, *dihedrals=None*, *improper=None*, *impropers=None*, *nonbonded=None*, *nonbonded_header=None*, *nbfix=None*, *hbond=None*)

Initialize a *PRMContainer* instance.

property improper

Alias for PRMContainer.impropers.

Return type Optional[DataFrame]

static _is_mapping(*value*)

Check if **value** is a dict instance; raise a TypeError if not.

Return type dict

__repr__()

Return a (machine readable) string representation of this instance.

The string representation consists of this instances' class name in addition to all (non-private) instance variables.

Returns A string representation of this instance.

Return type str

See also:

PRMContainer._PRIVATE_ATTR A set with the names of private instance variables.

PRMContainer._repr_fallback Fallback function for *PRMContainer.__repr__()* incase of recursive calls.

PRMContainer._str_iterator() Return an iterable for the iterating over this instances' attributes.

PRMContainer._str() Returns a string representation of a single **key/value** pair.

__eq__(*value*)

Check if this instance is equivalent to **value**.

The comparison checks if the class type of this instance and **value** are identical and if all (non-private) instance variables are equivalent.

Returns Whether or not this instance and **value** are equivalent.

Return type bool

See also:

PRMContainer._PRIVATE_ATTR A set with the names of private instance variables.

PRMContainer._eq Return if **v1** and **v2** are equivalent.

PRMContainer._eq_fallback Fallback function for *PRMContainer.__eq__()* incase of recursive calls.

copy(*deep=True*)

Return a shallow or deep copy of this instance.

Parameters **deep** (bool) – Whether or not to return a deep or shallow copy.

Returns A new instance constructed from this instance.

Return type *PRMContainer*

__copy__()

Return a shallow copy of this instance; see *PRMContainer.copy()*.

Return type ~AT

classmethod read(*filename*, *encoding=None*, ***kwargs*)

Construct a new instance from this object's class by reading the content of **filename**.

Parameters

- **filename** (str, bytes, os.PathLike or a file object) – The path+filename or a file object of the to-be read .psf file. In practice, any iterable can substitute the role of file object as long iteration returns either strings or bytes (see **encoding**).
- **encoding** (str, optional) – Encoding used to decode the input (*e.g.* "utf-8"). Only relevant when a file object is supplied to **filename** and the datastream is *not* in text mode.
- ****kwargs** (Any) – Optional keyword arguments that will be passed to both *PRMContainer._read_iterate()* and *PRMContainer._read_postprocess()*.

See also:

PRMContainer._read_iterate() An abstract method for parsing the opened file in *PRMContainer.read()*.

PRMContainer._read_postprocess() Post processing the class instance created by *PRMContainer.read()*.

Return type *PRMContainer*

classmethod _read_iterate(*iterator*)
An abstract method for parsing the opened file in `read`.

Parameters **iterator** (`Iterator` [`str`]) – An iterator that returns `str` instances upon iteration.

Return type `Dict`[`str`, `Any`]

Returns

- `dict` [`str`, `Any`] – A dictionary with keyword arguments for a new instance of this objects' class.
- ****kwargs** (`Any`) – Optional keyword arguments.

See also:

read() The main method for reading files.

classmethod _read_post_iterate(*kwargs*)
Post process the dictionary produced by *PRMContainer._read_iterate()*.

Return type `None`

_read_postprocess(*filename*, *encoding=None*, ***kwargs*)
Post processing the class instance created by *read()*.

Parameters

- **filename** (`str`, `bytes`, `os.PathLike` or a file object) – The path+filename or a file object of the to-be read .psf file. In practice, any iterable can substitute the role of file object as long iteration returns either strings or bytes (see **encoding**).
- **encoding** (`str`, optional) – Encoding used to decode the input (*e.g.* `"utf-8"`). Only relevant when a file object is supplied to **filename** and the datastream is *not* in text mode.
- ****kwargs** (`Any`) – Optional keyword arguments that will be passed to both *PRMContainer._read_iterate()* and *PRMContainer._read_postprocess()*.

See also:

PRMContainer.read() The main method for reading files.

Return type `None`

write(*filename=None*, *encoding=None*, ***kwargs*)
Write the content of this instance to **filename**.

Parameters

- **filename** (`str`, `bytes`, `os.PathLike` or a file object) – The path+filename or a file object of the to-be read .psf file. Contrary to *_read_postprocess()*, file objects can *not* be substituted for generic iterables.
- **encoding** (`str`, optional) – Encoding used to decode the input (*e.g.* `"utf-8"`). Only relevant when a file object is supplied to **filename** and the datastream is *not* in text mode.

- ****kwargs** (Any) – Optional keyword arguments that will be passed to *_write_iterate()*.

See also:

PRMContainer._write_iterate() Write the content of this instance to an opened datastream.

PRMContainer._get_writer() Take a *write()* method and ensure its first argument is properly encoded.

Return type None

__hash__(*self*)

Return the hash of this instance.

The returned hash is constructed from two components: * The hash of this instances' class type. * The hashes of all key/value pairs in this instances' (non-private) attributes.

If an unhashable instance variable is encountered, *e.g.* a list, then its id() is used for hashing.

This method will raise a TypeError if the class attribute AbstractDataClass._HASHABLE is False.

See also:

AbstractDataClass._PRIVATE_ATTR A set with the names of private instance variables.

AbstractDataClass._HASHABLE Whether or not this class is hashable.

AbstractDataClass._hash_fallback Fallback function for AbstractDataClass.__hash__() incase of recursive calls.

AbstractDataClass._hash An instance variable for caching the hash() of this instance.

Return type int

__weakref__

list of weak references to the object (if defined)

_write_iterate(*write*, ***kwargs*)

Write the content of this instance to an opened datastream.

The to-be written content of this instance should be passed as str. Any (potential) encoding is handled by the **write** parameter.

Example

Basic example of a potential *_write_iterate()* implementation.

```
>>> iterator = self.as_dict().items()
>>> for key, value in iterator:
...     value: str = f'{key} = {value}'
...     write(value)
>>> return None
```

Parameters

- **writer** (Callable) – A callable for writing the content of this instance to a file object. An example would be the io.TextIOWrapper.write() method.

- ****kwargs** (*optional*) – Optional keyword arguments.

See also:

PRMContainer.write() The main method for writing files.

Return type None

overlay_mapping(*prm_name*, *param_df*, *units=None*)

Update a set of parameters, **prm_name**, with those provided in **param_df**.

Examples

```
>>> from FOX import PRMContainer

>>> prm = PRMContainer(...)

>>> param_dict = {}
>>> param_dict['epsilon'] = {'Cd Cd': ..., 'Cd Se': ..., 'Se Se': ...}  #␣
↪epsilon
>>> param_dict['sigma'] = {'Cd Cd': ..., 'Cd Se': ..., 'Se Se': ...}  # sigma

>>> units = ('kcal/mol', 'angstrom')  # input units for epsilon and sigma

>>> prm.overlay_mapping('nonbonded', param_dict, units=units)
```

Parameters

- **prm_name** (str) – The name of the parameter of interest. See the keys of *PRMContainer.CP2K_TO_PRM* for accepted values.
- **param_df** (pandas.DataFrame or nested Mapping) – A DataFrame or nested mapping with the to-be added parameters. The keys should be a subset of *PRMContainer.CP2K_TO_PRM[prm_name]["columns"]*. If the index/nested sub-keys consist of strings then they'll be split and turned into a pandas.MultiIndex. Note that the resulting values are *not* sorted.
- **units** (Iterable [str], optional) – An iterable with the input units of each column in **param_df**. If None, default to the defaults specified in *PRMContainer.CP2K_TO_PRM[prm_name]["unit"]*.

Return type None

overlay_cp2k_settings(*cp2k_settings*)

Extract forcefield information from PLAMS-style CP2K settings.

Performs an inplace update of this instance.

Examples

Example input value for **cp2k_settings**. In the provided example the **cp2k_settings** are directly extracted from a CP2K .inp file.

```
>>> import cp2kparser  # https://github.com/nlesc-nano/CP2K-Parser

>>> filename = str(...)

>>> cp2k_settings: dict = cp2kparser.read_input(filename)
>>> print(cp2k_settings)
{'force_eval': {'mm': {'forcefield': {'nonbonded': {'lennard-jones': [...]}}}}
↪}
```

Parameters **cp2k_settings** (Mapping) – A Mapping with PLAMS-style CP2K settings.

See also:

PRMMapping *PRMMapping* A mapping providing tools for converting CP2K settings to .prm-compatible values.

Return type None

_overlay_cp2k_settings(*cp2k_settings*, *name*, *columns*, *key_path*, *key*, *unit*, *default_unit*, *post_process*)

Helper function for *PRMContainer.overlay_cp2k_settings()*.

Return type None

2.12 cp2k_to_prm

2.12.1 FOX.io.cp2k_to_prm

A *TypedMapping* subclass converting CP2K settings to .prm-compatible values.

Index

PRMMapping(name, key, columns, key_path, ...)	A *TypedMapping* providing tools for converting CP2K settings to .prm-compatible values.
CP2K_TO_PRM	

API

class FOX.io.cp2k_to_prm.**PRMMapping**(*name*, *key*, *columns*, *key_path*, *unit*, *default_unit*, *post_process*)

A *TypedMapping* providing tools for converting CP2K settings to .prm-compatible values.

Parameters

- **name** (str) – The name of the *PRMContainer* attribute. See *PRMMapping.name*.
- **columns** (int or Iterable [int]) – The names relevant *PRMContainer* DataFrame columns. See *PRMMapping.columns*.
- **key_path** (str or Iterable [str]) – The path of CP2K Settings keys leading to the property of interest. See *PRMMapping.key_path*.

- **key** (str or Iterable [str]) – The key(s) within *PRMMapping.key_path* containg the actual properties of interest, *e.g.* "epsilon" and "sigma". See *PRMMapping.key*.
- **unit** (str or Iterable [str]) – The desired output unit. See *PRMMapping.unit*.
- **default_unit** (str or Iterable [str, optional]) – The default unit as utilized by CP2K. See *PRMMapping.default_unit*.
- **post_process** (Callable or Iterable [Callable]) – Callables for post-processing the value of interest. Set a particular callable to None to disable post-processing. See *PRMMapping.post_process*.

name
The name of the *PRMContainer* attribute.

Type str

columns
The names relevant *PRMContainer* DataFrame columns.

Type tuple [int]

key_path
The path of CP2K Settings keys leading to the property of interest.

Type tuple [str]

key
The key(s) within *PRMMapping.key_path* containg the actual properties of interest, *e.g.* "epsilon" and "sigma".

Type tuple [str]

unit
The desired output unit.

Type tuple [str]

default_unit
The default unit as utilized by CP2K.

Type tuple [str, optional]

post_process
Callables for post-processing the value of interest. Set a particular callable to None to disable post-processing.

Type tuple [Callable, optional]

FOX.io.cp2k_to_prm.**CP2K_TO_PRM : MappingProxyType[str, PRMMapping]**
A Mapping containing *PRMMapping* instances.

```
MappingProxyType({
    'nonbonded':
        PRMMapping(name='nbfix', columns=[2, 3],
                   key_path=('input', 'force_eval', 'mm', 'forcefield', 'nonbonded
↪', 'lennard-jones'),
                   key=('epsilon', 'sigma'),
                   unit=('kcal/mol', 'angstrom'),
                   default_unit=('kcal/mol', 'kelvin'),
                   post_process=(None, sigma_to_r2)),
```

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```
    'nonbonded14':
        PRMMapping(name='nbfix', columns=[4, 5],
                   key_path=('input', 'force_eval', 'mm', 'forcefield',
↪'nonbonded14', 'lennard-jones'),
                   key=('epsilon', 'sigma'),
                   unit=('kcal/mol', 'angstrom'),
                   default_unit=('kcal/mol', 'kelvin'),
                   post_process=(None, sigma_to_r2)),

    'bonds':
        PRMMapping(name='bonds', columns=[2, 3],
                   key_path=('input', 'force_eval', 'mm', 'forcefield', 'bond'),
                   key=('k', 'r0'),
                   unit=('kcal/mol/A**2', 'angstrom'),
                   default_unit=('internal_cp2k', 'bohr'),  # TODO: internal_cp2k␣
↪????????
                   post_process=(None, None)),

    'angles':
        PRMMapping(name='angles', columns=[3, 4],
                   key_path=('input', 'force_eval', 'mm', 'forcefield', 'bend'),
                   key=('k', 'theta0'),
                   unit=('kcal/mol', 'degree'),
                   default_unit=('hartree', 'radian'),
                   post_process=(None, None)),

    'urrey-bradley':
        PRMMapping(name='angles', columns=[5, 6],
                   key_path=('input', 'force_eval', 'mm', 'forcefield', 'bend',
↪'ub'),
                   key=('k', 'r0'),
                   unit=('kcal/mol/A**2', 'angstrom'),
                   default_unit=('internal_cp2k', 'bohr'),  # TODO: internal_cp2k␣
↪????????
                   post_process=(None, None)),

    'dihedrals':
        PRMMapping(name='dihedrals', columns=[4, 5, 6],
                   key_path=('input', 'force_eval', 'mm', 'forcefield', 'torsion
↪'),
                   key=('k', 'm', 'phi0'),
                   unit=('kcal/mol', 'hartree', 'degree'),
                   default_unit=('hartree', 'hartree', 'radian'),
                   post_process=(None, None, None)),

    'improper':
        PRMMapping(name='improper', columns=[4, 5, 6],
                   key_path=('input', 'force_eval', 'mm', 'forcefield', 'improper
↪'),
                   key=('k', 'k', 'phi0'),
                   unit=('kcal/mol', 'hartree', 'degree'),
                   default_unit=('hartree', 'hartree', 'radian'),
                   post_process=(None, return_zero, None)),
})
```

2.13 typed_mapping

2.13.1 FOX.typed_mapping

A module which adds the *TypedMapping* class.

Index

TypedMapping()	A Mapping type which only allows a specific set of keys.
TypedMapping.__setattr__(name, value)	Implement setattr(self, name, value).
TypedMapping.__delattr__(name)	Implement delattr(self, name).
TypedMapping.__setitem__(name, value)	Implement self[name] = value.
TypedMapping.__bool__	Get the __bool__() method of *TypedMapping.view*.
TypedMapping.__getitem__	Get the __getitem__() method of *TypedMapping.view*.
TypedMapping.__iter__	Get the __iter__() method of *TypedMapping.view*.
TypedMapping.__len__	Get the __len__() method of *TypedMapping.view*.
TypedMapping.__contains__	Get the __contains__() method of *TypedMapping.view*.
TypedMapping.get	Get the get() method of *TypedMapping.view*.
TypedMapping.keys	Get the keys() method of *TypedMapping.view*.
TypedMapping.items	Get the items() method of *TypedMapping.view*.
TypedMapping.values	Get the values() method of *TypedMapping.view*.

API

class FOX.typed_mapping.**TypedMapping**

A Mapping type which only allows a specific set of keys.

Values cannot be altered after their assignment.

_PRIVATE_ATTR

A frozenset defining all private instance variables.

Type frozenset [str], classvar

_ATTR

A frozenset containing all allowed keys. Should be defined at the class level.

Type frozenset [str], classvar

view

Return a read-only view of all items specified in *TypedMapping._ATTR*.

Type MappingProxyType [str, Any]

TypedMapping.**__setattr__**(*name*, *value*)

Implement setattr(self, name, value).

Attributes specified in *TypedMapping._PRIVATE_ATTR* can freely modified. Attributes specified in *TypedMapping._ATTR* can only be modified when the previous value is `None`. All other attribute cannot be modified any further.

Return type `None`

`TypedMapping.__delattr__`(*name*)
Implement `delattr(self, name)`.

Raises an `AttributeError`, instance variables cannot be deleted.

Return type `NoReturn`

`TypedMapping.__setitem__`(*name*, *value*)
Implement `self[name] = value`.

Serves as an alias for *TypedMapping.__setattr__()* when **name** is in *TypedMapping._ATTR()*.

Return type `None`

`TypedMapping.__bool__`()
Get the `__bool__()` method of *TypedMapping.view*.

Return type `Callable`[[], `bool`]

`TypedMapping.__getitem__`()
Get the `__getitem__()` method of *TypedMapping.view*.

Return type `Callable`[[~KT], ~KV]

`TypedMapping.__iter__`()
Get the `__iter__()` method of *TypedMapping.view*.

Return type `Callable`[[], `Iterator`[~KT]]

`TypedMapping.__len__`()
Get the `__len__()` method of *TypedMapping.view*.

Return type `Callable`[[], `int`]

`TypedMapping.__contains__`()
Get the `__contains__()` method of *TypedMapping.view*.

Return type `Callable`[[~KT], `bool`]

`TypedMapping.get`()
Get the `get()` method of *TypedMapping.view*.

Return type `Callable`[[~KT, `Optional`[`Any`]], ~KV]

`TypedMapping.keys`()
Get the `keys()` method of *TypedMapping.view*.

Return type `Callable`[[], `KeysView`[~KT]]

`TypedMapping.items`()
Get the `items()` method of *TypedMapping.view*.

Return type `Callable`[[], `ItemsView`[~KT, ~KV]]

`TypedMapping.values`()
Get the `values()` method of *TypedMapping.view*.

Return type `Callable`[[], `ValuesView`[~KV]]

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