Aqua-Duct Documentation

Release 1.0.5

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CHAPTER

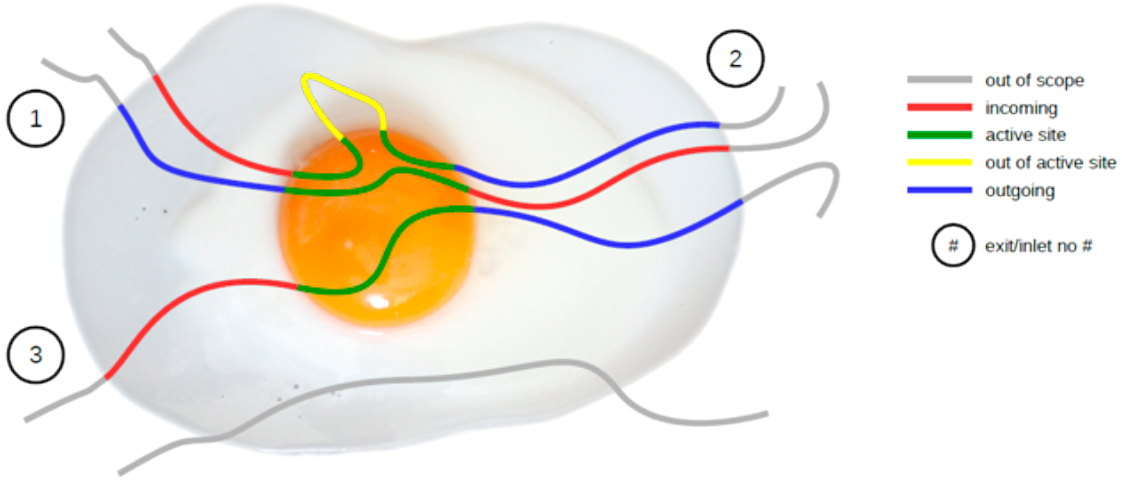
ONE

END-USER DOCUMENTATION

1.1 How does AQUA-DUCT work

AQUA-DUCT is a tool perfectly capable of tracing molecules that enter defined region of the macromolecule during MD simulation. Detailed statistics and visualization of all traced molecules are available. Moreover, AQUA-DUCT performs clustering of exits/inlets data and groups identified paths according to this clusters - inlet-exit event grouping.

Following picture illustrates the concept behind AQUA-DUCT. Molecules which flow through the active site are traced. Incoming, outgoing, and active site parts of paths are detected and visualized accordingly. Traced molecules form clusters which allow for further detailed analysis of the flow. Optionally, AQ can trace molecules which does not flow through the active site. This can be useful to ilustrate overall flow and can be also used to derive relative number of molecules visiting the active site.



AQUA-DUCT performs calculations in 6 stages:

1. Traceable residues
2. Raw paths
3. Separate paths
4. Clustering of inlets
5. Analysis
6. Visualization

Following sections briefly explain these stages, detailed description can be found in the AQ documentation.

1.1.1 Traceable residues

In the first stage of calculation AQ finds all residues that should be traced and appends them to the list of *traceable residues*. It is done in a loop over all frames. In each frame residues of interest are searched and appended to the list but only if they are not already present on the list. In *sandwich* mode this is repeated for each layer.

The search of the residues is done according to user provided definitions. Two requirements have to be met to append residue to the list:

1. The residue has to be found according to the *Object* definition.
2. The residue has to be within the *Scope* of interest.

The *Object* definition encompasses usually the active site of the protein. The *Scope* of interest defines, on the other hand, the boundaries in which residues are traced and is usually defined as protein.

Since AQUA-DUCT in its current version uses MDAnalysis Python module for reading, parsing and searching of MD trajectory data, definitions of *Object* and *Scope* have to be given as its *Selection Commands*.

1.1.1.1 Object definition

Object definition has to comprise of two elements:

1. It has to define residues to trace.
2. It has to define spatial boundaries of the *Object* site.

For example, proper Object definition could be following:

```
(resname WAT) and (sphzone 6.0 (resnum 99 or resnum 147))
```

It defines `WAT` as residues that should be traced and defines spatial constrains of the *Object* site as spherical zone within 6 Angstroms of the center of masses of residues with number 99 and 147.

1.1.1.2 Scope definition

Scope can be defined in two ways: as *Object* but with broader boundaries or as the convex hull of selected molecular object.

In the first case definition is very similar to *Object* and it has to follow the same limitations. For example, proper *Scope* definition could be following:

```
resname WAT around 2.0 protein
```

It consequently has to define `WAT` as residues of interest and defines spatial constrains: all `WAT` residues that are within 2 Angstroms of the protein.

If the *Scope* is defined as the convex hull of selected molecular object (which is **recommended**), the definition itself have to comprise of this molecular object only, for example `protein`. In that case the scope is interpreted as the interior of the convex hull of atoms from the definition. Therefore, *traceable residues* would be in the scope only if they are within the convex hull of atoms of `protein`.

1.1.2 Raw paths

The second stage of calculations uses the list of all traceable residues from the first stage and finds coordinates of center of masses for each residue in each frame. As in the first stage, it is done in a loop over all frames. For each residue in each frame AQUA-DUCT calculates or checks two things:

1. Is the residue in the *Scope* (this is always calculated according to the Scope definition).
2. Is the residue in the *Object*. This information is partially calculated in the first stage and can be reused in the second. However, it is also possible to recalculate this data according to the new *Object* definition.

For each of the *traceable residues* a special *Path* object is created which stores frames in which a residue is in *scope* or in *object*.

1.1.3 Separate paths

The third stage uses collection of *Path* objects to create *Separate Path* objects. Each *Path* comprise data for one residue. It may happen that the residue enters and leaves the *Scope* and the *Object* many times over the entire MD. Each such an event is considered by AQUA-DUCT as a separate path.

There are two types of *Separate Paths*:

- *Object Paths*
- *Passing Paths*

Object Paths are traces of molecules that visited *Object* area. *Passing Paths* are traces of molecules that entered *Scope* but did not entered *Object* area.

Passing paths comprises of one part only. Each *object path* comprises of three parts:

1. *Incoming* - Defined as a path that leads from the point in which residue enters the *Scope* and enters the object for the firs time.
2. *Object* - Defined as a path that leads from the point in which residue enters the *Object* for the first time and leaves it for the last time.
3. *Outgoing* - Defined as a path that leads from the point in which residue leaves the *Object* for the last lime and leaves the *Scope*.

It is also possible that incoming and/or outgoing part of the separate path is empty.

After the initial search of *Separate Path* objects it is possible to run special procedure, Auto Barber, which trims paths down to the approximated surface of the macromolecule or other molecular entity defined by the user.

Separate paths can be optionally smoothed for visualization purposes. AQUA-DUCT implements several smoothing methods, including Savitzky-Golay filter.

1.1.4 Clustering of inlets

Each of the separate paths has beginning and end. If they are at the boundaries of the *Scope* they are considered as *Inlets*, i.e. points that mark where the *traceable residues* enters or leaves the *Scope*. Clusters of inlets, on the other hand, mark endings of tunnels or ways in the system which was simulated in the MD.

Clustering of inlets is performed in following steps:

1. *Initial clustering*: All inlets are submitted to selected clustering method and depending on the method and settings, some of the inlets might not be arranged to any cluster and are considered as outliers.
2. [Optional] *Outliers detection*: Arrangement of inlets to clusters is sometimes far from optimal. In this step, *inlets* that do not fit to cluster are detected and annotated as outliers. This step can be executed in two modes:
    1. *Automatic mode*: Inlet is considered to be an outlier if its distance from the centroid is greater then mean distance + 4 * standard deviation of all distances within the cluster.
    2. *Defined threshold*: Inlet is considered to be an outlier if its minimal distance from any other point in the cluster is greater then the threshold.
3. [Optional] *Reclustering of outliers*: It may happen that the outliers form actually clusters but it was not recognized in initial clustering. In this step clustering is executed for outliers only and found clusters are appended to the clusters identified in the first step. Rest of the inlets are marked as outliers.

At the end of clustering stage it is possible to run procedure for *master path* generation. First, separate paths are grouped according to clusters. Paths that begin and end in particular clusters are grouped together. Next, for each group a *master path* (i.e., average path) is generated.

1.1.5 Analysis

Fifth stage of AQUA-DUCT calculations analyses results calculated in stages 1 to 4. Results of the analysis are displayed on the screen or can be save to text file. Detailed description of analysis result file can be found in the AQ documentation.

1.1.6 Visualization

Sixth stage of AQUA-DUCT calculations visualizes results calculated in stages 1 to 4. Visualization is done with PyMOL. AQUA-DUCT automatically starts PyMOL and loads visualizations in to it. Molecule is loaded as PDB file. Other objects like Inlets clusters or paths are loaded as CGO objects.

1.2 Aqua-Duct's Valve driver documentation

1.2.1 *Valve* manual

Valve application is a driver that uses `aquaduct` module to perform analysis of trajectories of selected residues in Molecular Dynamics simulation.

1.2.1.1 *Valve* invocation

Once `aquaduct` module is installed (see *Aqua-Duct installation guide*) properly on the machine, *Valve* is available as `valve.py` command line tool.

Usage

Basic help of *Valve* usage can be displayed by the following command:

```
valve.py --help
```

It should display the following information:

```
usage: valve.py [-h] [-c CONFIG_FILE] [-t THREADS] [--force-save] [--debug]
                [--debug-file DEBUG_FILE] [--version] [--license]
                [--dump-template-config]

Valve, Aquaduct driver

optional arguments:
  -h, --help            show this help message and exit
  -c CONFIG_FILE        Config file filename. (default: None)
  -t THREADS            Limit Aqua-Duct calculations to given number of
                        threads. (default: None)
  --force-save          Force saving results. (default: False)
  --debug               Prints debug info. (default: False)
  --debug-file DEBUG_FILE
                        Debug log file. (default: None)
  --version             Prints versions and exits. (default: False)
  --license             Prints short license info and exits. (default: False)
  --dump-template-config
                        Dumps template config file. Suppress all other output
                        or actions. (default: False)
```

Configuration file template

Configuration file used by *Valve* is of moderate length and complexity. It can be easily prepared with a template file that can be printed by *Valve*. Use the following command to print configuration file template on the screen:

```
valve.py --dump-template-config
```

Configuration file template can also be easily saved as a file with:

```
valve.py --dump-template-config > config.txt
```

Where config.txt is a configuration file template.

For detailed description of configuration file and available options see *Configuration file options*.

Valve calculation run

Once configuration file is ready *Valve* calculations can be run with the following simple command:

```
valve.py -c config.txt
```

Some of *Valve* calculations can be run in parallel. By default all available CPU cores are used. This is not always desired - limitation of used CPU cores can be done with `-t` option which limits number of concurrent threads used by *Valve*. If it equals 1 no parallelism is used.

Note: Specifying number of threads greater than the available CPU cores is generally not optimal.

However, in order to maximize the usage of available CPU power it is recommended to set it as the actual number of cores + 1. It is caused by the fact that *Valve* uses one thread for the main process and the more than one threads for processes of parallel calculations. When parallel calculations are executed the main thread waits for results.

Debugging

Valve can output some debug information. Use `--debug` to see all debug information on the screen or use `--debug-file` with some file name to dump all debug messages to the given file. Beside debug messages, standard messages will be saved in the file as well.

1.2.1.2 How does *Valve* work

Application starts with parsing input options. If `--help` or `--dump-template-config` options are used, appropriate messages are printed on the screen and *Valve* quits with signal `0`.

Note: In current version *Valve* does not check the validity of the config file.

If config file is provided (option `-c`) *Valve* parses it quickly and regular calculations start according to their contents. Calculations performed by *Valve* are done in six stages which are described in the next sections.

Traceable residues

In the first stage of calculations *Valve* finds all residues that should be traced and appends them to the list of *traceable residues*. It is done in a loop over all frames. In each frame residues of interest are searched and appended to the list but only proveded that they are not already present on the list. In *sandwich* mode this is repeated for each layer.

The search of *traceable residues* is done according to specifications provided by user. Two requirements have to be met to append residue to the list:

1. The residue has to be found according to the *object* definition.
2. The residue has to be within the *scope* of interest.

The *object* definition usually encompasses the active site of the protein (or other region of interest of macromolecule in question). The *scope* of interest defines, on the other hand, the boundaries in which residues are traced and is usually defined as protein.

Since `aquaduct`, in its current version, uses MDAnalysis Python module for reading, parsing and searching of MD trajectory data, definitions of *object* and *scope* have to be given as its *Selection Commands*.

Object definition

Object definition has to comprise of two elements:

1. It has to define residues to trace.
2. It has to define spatial boundaries of the *object* site.

For example, proper *object* definition could be as following:

```
(resname WAT) and (sphzone 6.0 (resnum 99 or resnum 147))
```

It defines `WAT` as residues that should be traced and defines spatial constrains of the *object* site as spherical zone within 6 Angstroms from the center of masses of residues with number 99 and 147.

Scope definition

Scope can be defined in two ways: as *object* but with broader boundaries or as the convex hull of selected molecular object.

In the first case definition is very similar to *object* and it has to follow the same limitations. For example, a proper *scope* definition could be as follows:

```
resname WAT and around 2.0 protein
```

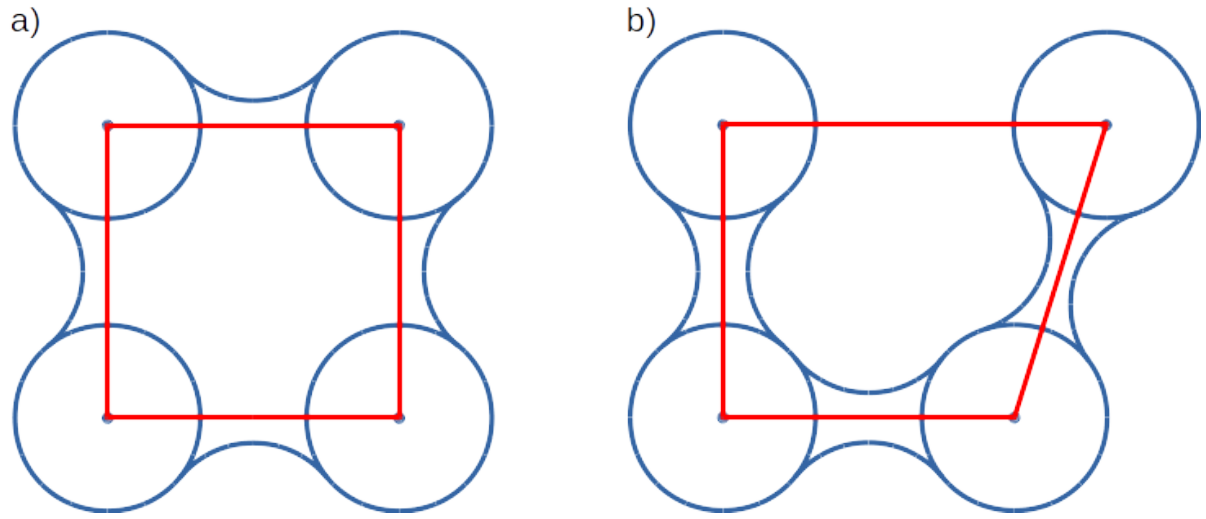
It consequently has to define `WAT` as residues of interest and defines spatial constrains: all `WAT` residues that are within 2 Angstroms of the protein.

If the *scope* is defined as the convex hull of selected molecular object (which is **recommended**), the definition itself has to comprise of this molecular object only, for example `protein`. In that case the scope is interpreted as the interior of the convex hull of atoms from the definition. Therefore, *traceable residues* would be in the scope only if they were within the convex hull of atoms of `protein`.

Convex hulls of macromolecule atoms

AQ uses quickhull algorithm for convex hull calculations (via SciPy class `scipy.spatial.ConvexHull`, see also http://www.qhull.org/ and original publication The quickhull algorithm for convex hulls).

Convex hull concept is used to check if traced molecules are inside of the macromolecule. Convex hull can be considered as rough approximation of molecular surface. The following picture shows schematic comparison of convex hull and solvent excluded surface (SES):



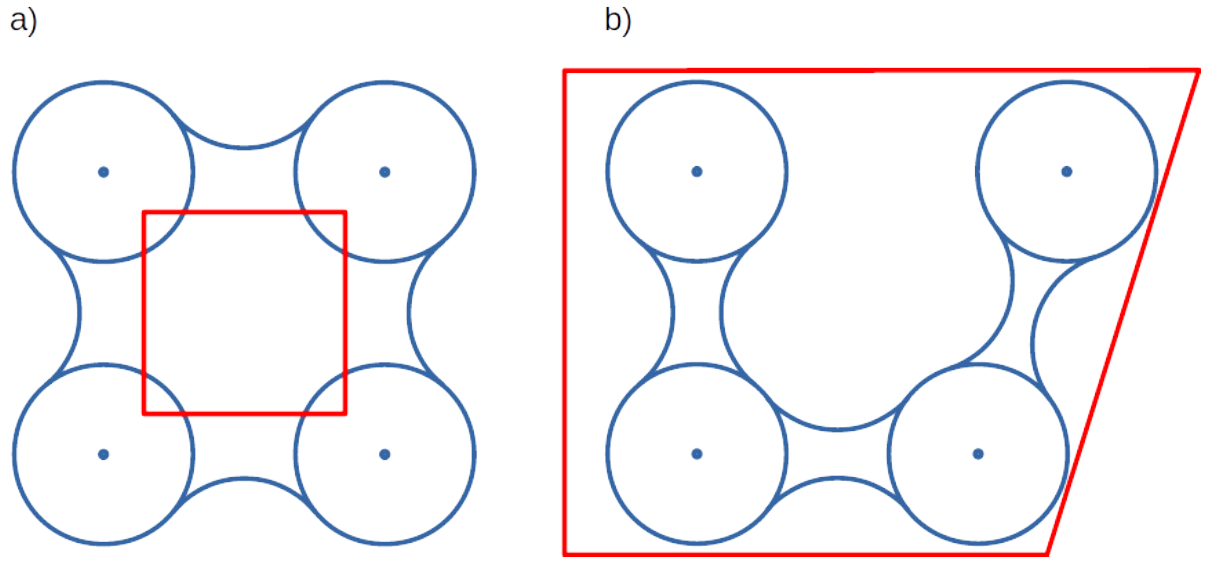
Convex hull (red shape) of atoms (blue dots with VdW spheres) and SES (blue line): **a)** convex hull and SES cover roughly the same area, convex hull approximates SES; **b)** movement of one atom dramatically changes SES, however, interior of the molecule as approximated by convex hull remains stable.

No doubts, convex hull is a very rough approximation of SES. It has, however, one very important property when it is used to approximate interior of molecules: its interior does not considerably depend on the molecular conformation of a molecule (or molecular entity) in question.

Convex hull inflation

AQ allows to alter size of the scope convex hulls by means of *inflate* options. Once *scope* is defined as convex hull of particular atoms, vertices of it can be interpreted as vectors originating in the center of geometry of the convex hull. Value of inflate option is added to such vectors and in consequence theirs leghts are increased (or decreased if added value is negative). Finally, convex hull is recalculated using points resulting from *inflated* vectors.

In reference to the previous picture, consider the following example:



On the left panel **a)** convex hull was deflated with negative value of *inflate* option, whareas on the right panel **b)** convex hull was inflated with positive value of *inflate* option.

This feautre is available in all stages where *scope* convex hull is used. For more details on configuration look for *inflate* options in the configuration file.

Raw paths

The second stage of calculations uses the list of all traceable residues from the first stage and for every residue in each frame two checks are performed:

1. Is the residue in the *scope* (this is always calculated according to the scope definition).
2. Is the residue in the *object*. This information is partially calculated in the first stage and can be reused in the second. However, it is also possible to recalculate this data according to the new *object* definition.

For each of the *traceable residues* a special *Path* object is created which stores frames in which a residue is in the *scope* or in the *object*.

Note: Residue is in the *object* only if it is also in the *scope*.

Separate paths

The third stage uses collection of *Path* objects to create *Separate Path* objects. Each *Path* comprises data for one residue. It may happen that the residue enters and leaves the *scope* and the *object* many times over the entire MD. Each such event is considered by *Valve* as a separate path.

There are two types of *Separate Paths*:

- *Object Paths*
- *Passing Paths*

Object Paths are traces of molecules that visited *Object* area. *Passing Paths* are traces of molecules that entered *Scope* but did not entered *Object* area.

Passing paths comprises of one part only. Each *object path* comprises of following parts:

1. *Incoming* - Defined as a path that leads from the point in which residue enters the *scope* and enters the object for the first time.
2. *Object* - Defined as a path that leads from the point in which residue enters the *object* for the first time and leaves it for the last time.
3. [Optional] *Out of active site* - Defined as a path between the *Object* paths that leads from the point in which residue leaves the *object* but stays within the *scope* and enters the *object* again.
4. *Outgoing* - Defined as a path that leads from the point in which residue leaves the *object* for the last time and leaves the *scope*.

It is also possible that incoming and/or outgoing part of the separate path is empty.

Note: Generation of *Passing paths* is optional and can be switched off.

Warning: Generation of *Passing paths* without redefinition of *Object* area in stage I and II may lead to false results.

Auto Barber

After the initial search of *Separate Path* objects, it is possible to run Auto Barber procedure which trims paths down to the approximated surface of the macromolecule or other molecular entity defined by the user. This trimming is done by creating collection of spheres that have centers at the ends of paths and radii equal to the distance from the center to the nearest atom of user defined molecular entity. Next, parts of raw paths that are inside these spheres are removed and separate paths are recreated.

Auto Barber procedure has several options, for example:

- **auto_barber** allows to define molecular entity which is used to calculate radii of spheres used for trimming raw paths.
- **auto_barber_mincut** allows to define minimal radius of spheres. Spheres of radius smaller than this value are not used in trimming.
- **auto_barber_maxcut** allows to define maximal radius of spheres. Spheres of radius greater than this value are not used in trimming.
- **auto_barber_tovdw** if set to *True* radii of spheres are corrected (decreased) by Van der Waals radius of the closest atom.

See also *options of separate_paths* stage.

Smoothing

Separate paths can be optionally smoothed. Current `aquaduct` version allows to perform *soft* smoothing only, i.e. smoothing is used only for visualization purposes. Raw paths cannot be replaced by the smoothed.

Available methods

Aqua-Duct implements several smoothing methods:

1. Savitzky-Golay filter - `SavgolSmooth` - see also original publication Smoothing and Differentiation of Data by Simplified Least Squares Procedures (doi:10.1021/ac60214a047).
2. Window smoothing - `WindowSmooth`
3. Distance Window smoothing - `DistanceWindowSmooth`
4. Active Window smoothing - `ActiveWindowSmooth`
5. Max Step smoothing - `MaxStepSmooth`
6. Window over Max Step smoothing - `WindowOverMaxStepSmooth`
7. Distance Window over Max Step smoothing - `DistanceWindowOverMaxStepSmooth`
8. Active Window over Max Step smoothing - `ActiveWindowOverMaxStepSmooth`

For detailed information on available configuration options see configuration file *smooth section* description.

Clustering of inlets

Each of the separate paths has the beginning and end. If they are at the boundaries of the *scope* they are considered as *Inlets*, i.e. points that mark where the *traceable residues* enter or leave the *scope*. Clusters of inlets, on the other hand, mark endings of tunnels or ways in the system which were simulated in the MD.

Clustering of inlets is performed in the following steps:

1. *Initial clustering*: All inlets are submitted to selected clustering method and depending on the method and settings, some of the inlets might not be arranged to any cluster and are considered as outliers.
2. [Optional] *Outliers detection*: Arrangement of inlets to clusters is sometimes far from optimal. In this step, *inlets* that do not fit into cluster are detected and annotated as outliers. This step can be executed in two modes:
    1. *Automatic mode*: Inlet is considered to be an outlier if its distance from the centroid is greater than the mean distance + 4 * standard deviation of all distances within the cluster.
    2. *Defined threshold*: Inlet is considered to be an outlier if its minimal distance from any other point in the cluster is greater than the threshold.
3. [Optional] *Reclustering of outliers*: It may happen that the outliers form actually clusters but it was not recognized in the initial clustering. In this step clustering is executed only for outliers and the clusters that were found are appended to the clusters identified in the first step. Rest of the inlets are marked as outliers.

Potentially recursive clustering

Both *Initial clustering* and *Reclustering* can be run in a recursive manner. If in the appropriate sections defining clustering methods option *recursive_clustering* is used, appropriate method is run for each cluster separately. Clusters of specific size can be excluded from recursive clustering (option *recursive_threshold*). It is also possible to limit maximal number of recursive levels - option *max_level*.

For additional information see *clustering sections* options.

Available methods

Aqua-Duct implements several clustering methods. The recommended method is **barber** method which bases on *Auto Barber* procedure. Rest of the methods are implemented with `sklearn.cluster` module:

1. `aquaduct.geom.cluster.BarberCluster` - default for *Initial clustering*. It gives excellent results. For more information see *barber clustering method* description.
2. `MeanShift` - see also original publication Mean shift: a robust approach toward feature space analysis (doi:10.1109/34.1000236).
3. `DBSCAN` - default for *Reclustering of outliers*, see also original publication A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise
4. `AffinityPropagation` - see also original publication Clustering by Passing Messages Between Data Points (doi:10.1126/science.1136800)
5. `KMeans` - see also k-means++: The advantages of careful seeding, Arthur, David, and Sergei Vassilvitskii in Proceedings of the eighteenth annual ACM-SIAM symposium on Discrete algorithms, Society for Industrial and Applied Mathematics (2007), pages 1027-1035.
6. `Birch` - see also Tian Zhang, Raghu Ramakrishnan, Maron Livny BIRCH: An efficient data clustering method for large databases and Roberto Perdisci JBirch - Java implementation of BIRCH clustering algorithm.

For additional information see *clustering sections* options.

Master paths

At the end of clustering stage it is possible to run procedure for *master path* generation. First, separate paths are grouped according to the clusters. Paths that begin and end in particular clusters are grouped together. Next, for each group a *master path* (i.e., average path) is generated in the following steps:

1. First, length of *master path* is determined. Lengths of each parts (incoming, object, outgoing) for each separate paths are normalized with bias towards the longest paths. These normalized lengths are then used as weights for averaging not normalized lengths. Values for all parts are summed and resulting value is the desired length of *master path*.
2. All separate paths are divided into chunks. Number of chunks is equal to the desired length of *master path* calculated in the previous step. Lengths of separate paths can be quite diverse, therefore, for different paths, chunks are of different lengths.
3. For each chunk, the averaging procedure is run:
    1. Coordinates for all separate paths for a given chunk are collected.
    2. Normalized lengths with bias toward the longest paths for all separate paths for a given chunk are collected.
    3. New coordinates are calculated as weighted average of collected coordinates. Collected normalized lengths are used as weights.
    4. In addition, width of chunk is calculated as a mean value of collected coordinates of mutual distances.
    5. Type of chunk is calculated as probability (frequency) of being in the *scope*.
4. Results for all chunks are collected, types probability are changed to types. All data is then used to create Master Path. If this fails no path is created.

More technical details on master path generation can be found in *`aquaduct.geom.master.CTypeSpathsCollection.get_master_path()`* method documentation.

Passing paths

If *Passing paths* are allowed (see `allow_passing_paths` option in *separate_paths configuration*) they will be generated using list of *traceable residues* from the first stage of calculations. In usual settings, where *Object* and *Scope* definitions are the same in both the I and II stage, this will result in relatively low number of passing paths. In particular, this will not show the real number of traced molecules that enter the *Scope* during the simulation.

To get correct picture, configuration options have to be adjusted according to one of the following suggestions:

1. Adding *passing* molecules [recommended]
    - **Stage traceable_residues**
        - `add_passing` should define all molecules to be traced. If water is traced this should be set to e.g. `resname WAT HOH TIP`.
    - **Stage separate_paths**
        - `allow_passing_paths` should be set to `True`. This allows generation of passing paths.
2. Redefinition of *scope* and *object* areas
    - **Stage traceable_residues**
        - `object` should be broad enough to encompass all molecules that should be traced. For example, if water is traced, `object` definition could be as following: `resname WAT`.
    - **Stage raw_paths**
        - In order to retain default Aqua-Duct behavior of tracing molecules that flow through *Object* area, it have to be redefined to encompass the active site only - see *Object definition* discussion.
        - `clear_in_object_info` should be set to `True`. Otherwise, traceable molecules will be limited according to the current `object` definition but *Object* boundaries from **traceable_residues** stage will be used.
    - **Stage separate_paths**
        - `allow_passing_paths` should be set to `True`. This allows generation of passing paths.

Clustering of passing paths

Additionally, in stage **inlets_clustering**, the following options could also be adjusted:

- `exclude_passing_in_clustering` could be set to `True`. This will exclude the passing paths inlets from clustering.
- If passing paths are not clustered they will be added as outliers. Option `add_passing_to_clusters` allows to add some of passing paths inlets to the already existing clusters. This is done by Auto Barber method and therefore this option should define molecular entity used in Auto Barber procedure, for example `protein`.

Analysis

Fifth stage of *Valve* calculations analyses results calculated in stages 1 to 4. Results of the analysis are displayed on the screen or can be saved to a text file and comprise of several parts.

General summary

Results start with a general summary.

- Title and data stamp.

- [Optional] Dump of configuration options.
- Frames window.
- **Names of traced molecules.**

  Note: If more than one name is on the list all consecutive sections of *Analysis* results are provided for each name separately, as well as for all names.

- Number of traceable residues.
- Number of separate paths.
- Number of inlets.
- **Number of clusters.**
  - Outliers flag, *yes* if they are present.
- Clustering history - a tree summarizing calculated clusters.

Clusters statistics

- **Clusters summary - inlets.**
  - **Summary of inlets clusters. Table with 4 columns:**
    1. **Cluster**: ID of the cluster. Outliers have 0.
    2. **Size**: Size of the cluster.
    3. **INCOMING**: Number of inlets corresponding to separate paths that enter the scope.
    4. **OUTGOING**: Number of inlets corresponding to separate paths that leave the scope.
- **Cluster statistics.**
  - **Probabilities of transfers. Table with 7 columns:**
    1. **Cluster**: ID of the cluster. Outliers have 0.
    2. **IN-OUT**: Number of separate paths that both enter and leave the scope by this cluster.
    3. **diff: Number of separate paths that:**
       * Enter the scope by this cluster but leave the scope by another cluster, or
       * Enter the scope by another cluster but leave the scope by this cluster.
    4. **N: Number of separate paths that:**
       * Enter the scope by this cluster and stays in the object, or
       * Leaves the scope by this cluster after staying in the object.
    5. **IN-OUT_prob**: Probability of **IN-OUT**.
    6. **diff_prob**: Probability of **diff**.
    7. **N_prob**: Probability of **N**.
  - **Mean lengths of transfers. Table with 8 columns:**
    1. **Cluster**: ID of the cluster. Outliers have 0.
    2. **X->Obj**: Mean length of separate paths leading from this cluster to the object.
    3. **Obj->X**: Mean length of separate paths leading from the object to this cluster.
    4. **p-value**: p-value of *ttest* of comparing **X->Obj** and **Obj->X**.

5. **X->ObjMin**: Minimal value of length of separate paths leading from this cluster to the object.
6. **X->ObjMinID**: ID of separate path for which **X->ObjMin** was calculated.
7. **Obj->XMin**: Minimal value of length of separate paths leading from the object to this cluster.
8. **Obj->XMinID**: ID of separate path for which **Obj->XMin** was calculated.

– **Mean frames numbers of transfers. Table with 8 columns:**

1. **Cluster**: ID of the cluster. Outliers have 0.
2. **X->Obj**: Mean number of frames of separate paths leading from this cluster to the object.
3. **Obj->X**: Mean number of frames of separate paths leading from the object to this cluster.
4. **p-value**: p-value of *ttest* of comparing **X->Obj** and **Obj->X**.
5. **X->ObjMin**: Minimal value of number of frames of separate paths leading from this cluster to the object.
6. **X->ObjMinID**: ID of separate path for which **X->ObjMin** was calculated.
7. **Obj->XMin**: Minimal value of number of frames of separate paths leading from the object to this cluster.
8. **Obj->XMinID**: ID of separate path for which **Obj->XMin** was calculated.

Note: Distributions of **X->Obj** and **Obj->X** might be not normal, *ttest* may result in unrealistic values. This test will be changed in the future releases.

Clusters types statistics

- **Separate paths clusters types summary. Tables with 11 columns.**
  – **Mean length of paths:**
    1. **CType**: Separate path Cluster Type.
    2. **Size**: Number of separate paths belonging to Cluster type.
    3. **Size%**: Percentage of **Size** relative to the total number of separate paths.
    4. **Tot**: Average total length of paths.
    5. **TotStd**: Standard deviation of **Tot**.
    6. **Inp**: Average length of incoming part of paths. If no incoming parts are available, NaN is printed (not a number).
    7. **InpStd**: Standard deviation of **Inp**.
    8. **Obj**: Average length of object part of paths. If no incoming parts are available, NaN is printed.
    9. **ObjStd**: Standard deviation of **Inp**.
    10. **Out**: Average length of outgoing part of paths. If no incoming parts are available, NaN is printed.
    11. **OutStd**: Standard deviation of **Inp**.
  – **Mean number of frames:**
    1. **CType**: Separate path Cluster Type.
    2. **Size**: Number of separate paths belonging to Cluster type.

3. **Size%**: Percentage of **Size** relative to the total number of separate paths.
4. **Tot**: Average total number of frames of paths.
5. **TotStd**: Standard deviation of **Tot**.
6. **Inp**: Average total number of incoming part of paths. If no incoming parts are available, NaN is printed (not a number).
7. **InpStd**: Standard deviation of **Inp**.
8. **Obj**: Average total number of object part of paths. If no incoming parts are available, NaN is printed.
9. **ObjStd**: Standard deviation of **Inp**.
10. **Out**: Average total number of outgoing part of paths. If no incoming parts are available, NaN is printed.
11. **OutStd**: Standard deviation of **Inp**.

Cluster Type of separate path

Clusters types (or CType) is a mnemonic for separate paths that leads from one cluster to another, including paths that start/end in the same cluster or start/end in the *Object* area.

Each separate path has two ends: beginning and end. Both of them either belong to one of the clusters of inlets, or are among outliers, or are inside the scope. If an end belongs to one of the clusters (including outliers) it has ID of the cluster. If it is inside the scope it has special ID of `N`. Cluster type is an ID composed of IDs of both ends of separate path separated by colon charter.

All separate paths data

- **List of separate paths and their properties. Table with 20 columns.**
    1. **ID**: - Separate path ID.
    2. **RES**: - Residue name.
    3. **BeginF**: Number of the frame in which the path begins.
    4. **InpF**: Number of the frames in which path is in Incoming part.
    5. **ObjF**: Number of the frames in which path is in Object part.
    6. **ObjFS**: Number of the frames in which path is strictly in Object part.
    7. **OutF**: Number of the frames in which path is in Outgoing part.
    8. **EndF**: Number of the frame in which the path ends.
    9. **TotL**: Total length of path.
    10. **InpL**: Length of Incoming part. If no incoming part, NaN is given.
    11. **ObjL**: Length of Object part.
    12. **OutL**: Length of Outgoing part. If no outgoing part, NaN is given.
    13. **TotS**: Average step of full path.
    14. **TotStdS**: Standard deviation of **TotS**.
    15. **InpS**: Average step of Incoming part. If no incoming part, NaN is given.
    16. **InpStdS**: Standard deviation of **InpS**.
    17. **ObjS**: Average step of Object part.
    18. **ObjStdS**: Standard deviation of **ObjS**.

19. **OutS**: Average step of Outgoing part. If no outgoing part, NaN is given.
20. **OutStdS**: Standard deviation of **OutS**.
21. **CType**: Cluster type of separate path.

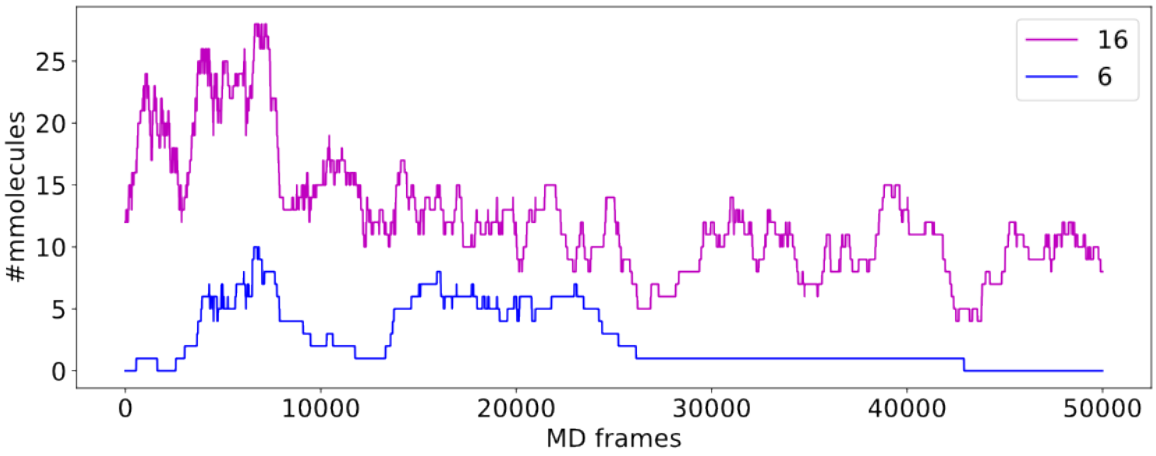
Separate path ID

Separate Path IDs are composed of three numbers separated by colon. First number is the layer number, if no *sandwich* option is used, it is set to `0`. The second number is residue number. The third number is consecutive number of the separate path made by the residue. Numeration starts with 0.

Frames dependent analysis

In addition to general summary Aqua-Duct calculates frames dependent parameters. Two types of values are calculated: number of traced paths, and *Object* and *Scope* sizes. Results are saved in the additional CSV file or are printed on the screen.

Calculated numbers of traced paths can be used to visualize behavior of the system in question. For example, one can analyze number of paths in two different clusters:



The above plot shows number of water molecules (or paths) in cluster 16 and 6 throughout the simulation. One can observe that number of molecules in cluster 6 diminishes approximately in the middle. This kind of plot can be easily generated with additional CSV data.

Number of traced paths

For each frame, numbers of traced paths are calculated for the following categories:

1. Name of traced molecules - `amol` is used for all possible names.
2. Paths types (`object` for standard paths and `passing` for passing paths) - `apaths` is used for all possible paths types.
3. Clusters and cluster types - `aclusts` is used for all possible clusters and `actypes` is used for all possible cluster types.
4. Part of paths. Possible values are: `walk`, `in`, `object`, `out`, and `in_out`. Where `walk` corresponds to any part of path and in case of passing paths only this category is used; `in`, `object`, and `out` correspond to incoming, object, and outgoing parts; `in_out` corresponds to sum of incoming and outgoing parts.

All of the above listed categories are combined together, and the final number of calculated categories may be quite big.

Size of *Object* and *Scope*

If option `calculate_scope_object_size` is set `True` and values of `scope_chull` and `object_chull` correspond to appropriate molecular entities, Aqua-Duct calculates area and volume of *Scope* and *Object*. Calculated sizes are estimated as resulting from convex hull approximations.

Visualization

Sixth stage of *Valve* calculations visualizes results calculated in stages 1 to 4. Visualization is done with PyMOL. *Valve* creates visualizations in two modes:

1. Two files are created: special Python script and archive with data. Python script can be simply started with python, it automatically opens PyMol and loads all data from the archive. Optionally, it can automatically save PyMol session.
2. PyMol is automatically started and all data is loaded directly to PyMol workspace.

Molecule is loaded as a PDB file. Other objects like Inlets clusters or paths are loaded as CGO objects.

Visualization script

By default *Valve* creates Python visualization script and archive with data files. This script is a regular Python script. It does not depend on AQUA-DUCT. To run it, python2.7 and PyMol are required. If no **save** option is used *Valve* saves visualization script as `6_visualize_results.py`. To load full visualization call:

```
python 6_visualize_results.py --help

usage: 6_visualize_results.py [-h] [--save-session SESSION]
                              [--discard DISCARD] [--keep KEEP]
                              [--force-color FC] [--fast]

Aqua-Duct visualization script

optional arguments:
  -h, --help            show this help message and exit
  --save-session SESSION
                        Pymol session file name.
  --discard DISCARD     Objects to discard.
  --keep KEEP           Objects to keep.
  --force-color FC      Force specific color.
  --fast                Hides all objects while loading.
```

Option `--save-session` allows to save PyMol session file. Once visualization is loaded session is saved and PyMol closes. Option `--fast` increases slightly loading of objects.

Option `--force-color` allows to change default color of objects. It accepts list of specifications comprised of pairs 'object name' and 'color name'. For example: `'scope_shape0 yellow cluster_1 blue'`. This will color *scope_shape0* object in yellow and *cluster_1* in blue:

```
python 6_visualize_results.py --force-color 'scope_shape0 yellow cluster_1 blue'
```

Note: List of specifications has to be given in parentheses.

Note: List of specifications has to comprise of full objects' names.

Note: Currently, `--force-color` does not allow to change color of molecules. It can be done in PyMol.

Options `--keep` and `--discard` allows to select specific objects for visualization. Both accept list of names comprising of full or partial object names. Option `--keep` instructs script to load only specified objects, whereas `--discard` instructs to skip specific objects. For example, to keep shapes of object and scope, as well as molecule and clusters only, one can call the following:

```
python 6_visualize_results.py --keep 'shape molecule cluster'
```

To discard all raw paths:

```
python 6_visualize_results.py --discard 'raw'
```

Options can be used simultaneously, order does matter:

1. If `--keep` is used first, objects are not displayed if they are not on the *keep* list. If they are on the list, visualization script checks if they are on the *discard* list. If yes, objects are not displayed.
2. If `--discard` is used first, objects are not displayed if they are on the *discard* list and are not on the *keep* list.

For example, in order to display molecule, clusters, and only raw master paths, one can use the following command:

```
python 6_visualize_results.py --keep 'molecule cluster master' --discard 'smooth'
```

Note: Options `--keep` and `--discard` accepts both full and partial object names.

Note: List of names has to be given in parentheses.

Visualization objects

The following is a list of objects created in PyMOL (all of them are optional). PyMOL object names in **bold** text and short explanation is given.

- Selected frame of the simulated system. Object name: **molecule** plus number of layer, if no *sandwich* option is used, it becomes by default **molecule0**.
- Approximate shapes of object and scope. Objects names **object_shape** and **scope_shape** plus number of layer, if no *sandwich* option is used, **0** is added by default.
- Inlets clusters, each cluster is a separate object. Object name: **cluster_** followed by cluster annotation: outliers are annotated as **out**; regular clusters by ID.
- List of cluster types, raw paths. Each cluster type is a separate object. Object name composed of cluster type (colon replaced by underline) plus **_raw**.
- List of cluster types, smooth paths. Each cluster type is a separate object. Object name composed of cluster type (colon replaced by underline) plus **_smooth**.
- All raw paths. They can be displayed as one object or separated into Incoming, Object and Outgoing part. Object name: **all_raw**, or **all_raw_in**, **all_raw_obj**, and **all_raw_out**.
- All raw paths inlets arrows. Object name: **all_raw_paths_io**.
- All smooth paths. They can be displayed as one object or separated into Incoming, Object and Outgoing part. Object name: **all_smooth**, or **all_smooth_in**, **all_smooth_obj**, and **all_smooth_out**.
- All raw paths inlets arrows. Object name: **all_raw_paths_io**.

- Raw paths displayed as separate objects or as one object with several states. Object name: **raw_paths_** plus number of path or **raw_paths** if displayed as one object.
- Smooth paths displayed as separate objects or as one object with several states. Object name: **smooth_paths_** plus number of path or **smooth_paths** if displayed as one object.
- Raw paths arrows displayed as separate objects or as one object with several states. Object name: **raw_paths_io_** plus number of path or **raw_paths_io** if displayed as one object.
- Smooth paths arrows displayed as separate objects or as one object with several states. Object name: **smooth_paths_io_** plus number of path or **smooth_paths_io** if displayed as one object.
- **CoS** center of the scope area (system).
- **CoO** center of the object area (system).

Color schemes

Inlets clusters are colored automatically. Outliers are gray.

Incoming parts of paths are red, Outgoing parts are blue. Object parts in case of smooth paths are green and in case of raw paths are green if residue is precisely in the object area or yellow if it leaved object area but it is not in the Outgoing part yet. *Passing paths* are displayed in grey.

Arrows are colored in accordance to the colors of paths.

1.2.2 Configuration file options

Valve configuration file is a simple and plain text file. It has similar structure as INI files commonly used in one of the popular operating systems and is compliant with Python module `ConfigParser`.

Configuration file comprises of several *sections*. They can be grouped into three categories. Names of sections are in **bold** text.

1. **Global settings:**
    - **global**
2. **Stages options:**
    1. **traceable_residues**
    2. **raw_paths**
    3. **separate_paths**
    4. **inlets_clustering**
    5. **analysis**
    6. **visualize**
3. **Methods options:**
    - **smooth**
    - **clustering**
    - **reclusteriation**

1.2.2.1 Section global

This section allows settings of trajectory data and is reserved for other future global options.

Option	Default value	Description
top	None	Path to topology file. Aqua-Duct supports PDB, PRMTOP, PFS topology files.
trj	None	Path to trajectory file. Aqua-Duct supports NC and DCD trajectory files.
twoway	True	Try to use *two-way* scanning in the stage II.
sand-wich	False	If set `True` trajectories are read as layers.
max_frame	None	Maximal number of frame to be read from trajectory data. If set `None` trajectory is read to the last possible frame.
min_frame	0	Minimal number of frame to be read from trajectory data.
step_frame	1	Step used in reading trajectory. Default value of 1 stands for reading every frame. If it is greater than 1, only every step-value frame is read.
sps	True	Try to store data in single precission storage.
cache_dir	None	Allows to set path to the directory for cache data.
cache_mem	False	If set `True`, all data will be cached in RAM.

Option **trj** can be used to provide list of trajectory files separated by standard path separator '`:`' on POSIX platforms and '`;`' on Windows - see `os.pathsep`.

Note: Options **top** and **trj** are mandatory.

Note: Options **min_frame**, **max_frame**, and **step_frame** can be used to limit calculations to a specific part of trajectory. For example, in order to to run calculations for 1000 frames starting from frame 5000 use the following options:

```
min_frame = 4999
max_frame = 5999
```

To run calculations for every 5th frame use:

```
step_frame = 5
```

Sandwich

Trajectory data can be provided as several files. By default these files are processed in sequential manner making one long trajectory. If option **sandwich** is used trajectory files are read as layers. For each layer, search for traceable residues is done separately (stage I and II) but processing and analysis (stage III, IV, V, and VI) are done for all paths simultaneously. Usage of **sandwich** option is further referenced as *sandwich* mode.

Cache

Storage of coordinates for all paths for very long MD trajectories requires huge amount of RAM. User can decide whether *aquaduct* should store coordinates in memory or in separated directory. Option **cache-mem** instruct *Valve* to store coordinates in RAM; **cache-dir** stores coordinates in selected directory. If neither of both options is selected, coordinates are calculated on demand.

Note: If no cache is used (memory or dir) *Master paths* cannot be calculated.

Single precision storage

Most of the calculation in *Valve* is performed by NumPy. By default, NumPy uses double precision floats. *Valve* does not change this behavior but has special option **sps** which forces to store all data (both internal data stored in RAM and on the disk) in single precision. This spares a lot of RAM and is recommended when you perform calculation for long trajectories and your amount of RAM is limited.

1.2.2.2 Common settings of stage sections

Stages 1-4 which perform calculations have some common options allowing for execution control and saving/loading data.

Option	Default value	Description
execute	runonce	Option controls stage execution. It can have one of three possible values: `run`, `runonce`, and `skip`. If it is set to `run` calculations are always performed and if **dump** is set, dump file is saved. If it is set to `runonce`, calculations are performed when there is no dump file specified by **dump** option. If it is present, calculations are skipped and data is loaded from the file. If it is set to `skip`, calculations are skipped and if **dump** is set, data is loaded from the file.
dump	[dump file name]	File name of dump data. It is used to save results of calculations or to load previously calculated data - this depends on **execute** option. Default value of this option depends on the stage and for stages 1 to 4 is one of the following (listed in order): • 1_traceable_residues_data.dump • 2_raw_paths_data.dump • 3_separate_paths_data.dump • 4_inlets_clustering_data.dump

Stages 5-6 also use **execute** option, however, since they do not perform calculations *per se*, instead of **dump** option, they use **save**.

Option	Default value	Description
execute	run	Option controls stage execution. It can have one of three possible values: `run`, `runonce`, and `skip`. If it is set to `run` or `runonce`, stage is executed and results are saved according to the **save** option. If it is set to `skip`, stage is skipped.
save	[save file name]	File name for saving results. Default value of this option depends on the stage and for stages 1 to 4 is one of the following (listed in order): • 5_analysis_results.txt & 5_analysis_results.txt.csv • 6_visualize_results.py & 6_visualize_results.tar.gz Stage 5 saves `.txt` file with analysis of results and, if requested, it saves additional `.csv` with various counts of traced molecules. Stage 6 can save results in two different ways: 1. As Python script - extension `.py` plus companion archive `.tar.gz`, 2. As PyMOL session - extension `.pse`.

1.2.2.3 Stage traceable_residues

Option	Default value	Description
scope	None	Definition of *Scope* of interest. See also *Scope definition*.
scope_convexhull	True	Flag to set if *Scope* is direct or convex hull definition.
scope_everyframe	False	Flag to set *Scope* evaluation mode. If set `True` *Scope* is evaluated in every frame. This makes sense if the definition is complex and depends on distances between molecular entities.
scope_convexhull_inflate	None	Increase (or if negative - decrease) size of the scope convex hull.
object	None	Definition of *Object* of interest. See also *Object definition*.
add_passing	None	Definition of molecules that should be added to traced molecules even if they were not present in *Object*.

Note: Options **scope** and **object** are mandatory.

1.2.2.4 Stage raw_paths

This stage also requires definition of the *Scope* and *Object*. If appropriate settings are not given, settings from the previous stage are used.

Option	Default value	Description
scope	None	Definition of *Scope* of interest. See also *Scope definition*. If `None`, value from previous stage is used.
scope_convexhull	None	Flag to set if the *Scope* is direct or convex hull definition.
scope_everyframe	False	Flag to set *Scope* evaluation mode. If set `True` *Scope* is evaluated in every frame. This makes sense if the definition is complex and depends on distances between molecular entities. If `None`, value from previous stage is used.
scope_convexhull_inflate	None	Increase (or if negative - decrease) size of the scope convex hull. If `None`, value from previous stage is used.
object	None	Definition of *Object* of interest. See also *Object definition*. If `None`, value from previous stage is used
clear_in_object_info	False	If it is set to `True`, information on occupation of *Object* site by traceable residues calculated in the previous stage is cleared and has to be recalculated. This is useful if definition of *Object* was changed.
discard_singletons	1	If `> 0`, discards paths of given lenght.
discard_empty_paths	True	If set to `True`, empty paths are discarded.

1.2.2.5 Stage separate_paths

Option	Default value	Description
discard_empty_paths	True	If set to `True`, empty paths are discarded.
sort_by_id	True	If set to `True`, separate paths are sorted by ID. Otherwise they are sorted in order of appearance.
discard_short_paths	20	This option allows to discard paths which are shorter than the threshold, which is defined as the total number of frames.
discard_short_object	2.0	This option allows to discard paths whose objects are shorter than the threshold, which is defined as total length in metric units.
discard_short_logic	or	If both `discard_short_paths` and `discard_short_object` options are used, this option allows to set combination logic. If it is set to `or`, a path is discarded if any of discard criterion is met. If it is set `and`, both criteria have to be met to discard path.
auto_barber	None	This option allows to select molecular entity used in Auto Barber procedure. See also *Auto Barber* and *`barber_with_spheres()`*.
auto_barber_mincut	None	Minimal radius of spheres used in Auto Barber. If a sphere has radius smaller than this value, it is not used in AutoBarber procedure. This option can be switched off by setting it to `None`.
auto_barber_maxcut	2.8	Maximal radius of spheres used in Auto Barber. If a sphere has radius greater than this value, it is not used in AutoBarber procedure. This option can be switched off by setting it to `None`.
auto_barber_mincut_level	True	If set `True`, spheres of radius smaller than **mincut** are resized to **mincut** value.
auto_barber_maxcut_level	True	If set `True`, spheres of radius greater than **maxcut** are resized to **maxcut** value.
auto_barber_tovdw	True	If set `True`, cutting of spheres is corrected by decreasing its radius by VdW radius of the closest atom.
allow_passing_paths	False	If set `True`, paths that do not enter the object are detected and added to the rest of paths as 'passing' paths.
separate_barber	True	Apply AutoBarber for each type of traced molecules separately.
calculate_coo	False	If set `True`, center of the object is calculated.

1.2.2.6 Stage inlets_clustering

Option	Default value	Description
recluster_outliers	False	If set to `True`, reclustering of outliers is executed according to the method defined in **reclustering** section.
detect_outliers	False	If set, detection of outliers is executed. It could be set as a floating point distance threshold or set to `Auto`. See *Clustering of inlets* for more details.
singletons_outliers	False	Maximal size of cluster to be considered as outliers. If set to number > 0 clusters of that size are removed and their objects are moved to outliers. See *Clustering of inlets* for more details.
max_level	5	Maximal number of recursive clustering levels.
create_master_paths	False	If set to `True`, master paths are created (fast CPU and big RAM recommended; 50k frames long simulation may need ca 20GB of memory)
master_paths_amount	None	Allows to limit number of single paths used for master paths calculations. If it is a number in range `(0,1)`, then it is interpreted as a percent number of paths to be used. It is is a integer number `>= 1` it is an absoulte number of used paths.
separate_master	False	If set to `True`, master mapths are generated for each of traced molecules' types separately.
separate_master_all	True	If **separate_master** is used and this option is set `True`, master paths will be also generated for all traced molecules' types as it is done when **separate_master** is set `False`.
exclude_passing_in_clustering	True	If set to `True`, passing paths are not clustered with normal paths.
add_passing_to_clusters	None	Allows to run procedure for adding passing paths inlets to clusters with Auto Barber method. To enable this the option should be set to molecular entity that will be used by Auto Barber.
renumber_clusters	False	If set `True`, clusters have consecutive numbers starting from 1 (or 0 if outliers are present) starting from the bigest cluster.
join_clusters	None	This option allows to join selected clusters. Clusters' IDs joined with + character lists clusters to be joined together. Several such blocks separated by space can be used. For example, if set to `1+3+4 5+6` clusters 1, 3, and 4 will be joined in one cluster and cluster 5, and 6 will be also joined in another cluster.
inlets_center	cos	Allows to choose center of inlets points. This central point is further used as a reference point in calculations of clusters' areas and contours. If set *cos* center of system calculated as average center of the scope area is used. Alternatively it can be set to *coo*, then center of the object area is used.
clustering_order	old-school	Allow to change order of clustering steps. • **old-school** order - clustering, reclustering, removing singletons, adding passing paths to clusters, join clusters, renumbering clusters, removing inlets in specified_clusters • **aquarius** order - clustering, joining clusters, renumbering clusters, outliers detection, reclustering, removing singletons, adding passing paths to clusters, removing inlets in specified_clusters

1.2.2.7 Stage analysis

Option	Default value	Description
dump_config	True	If set to `True`, configuration options, as seen by Valve, are added to the head of results.
calculate_scope_object_size	False	If set to `True`, volumes and areas of object and scope approximated by convex hulls are calculated for each of the analyzed frames and saved in output CSV file.
scope_chull	None	Scope convex hull definition used in calculating volume and area.
scope_chull_inflate	None	Increase (or if negative - decrease) size of the scope convex hull.
object_chull	None	Object convex hull definition used in calculating volume and area.
cluster_area	True	If set `True`, clusters' areas are estimated with kernel density estimation method (KDE).
cluster_area_precision	20	Precision of KDE method in clusters' areas estimation method. This options controls number of grid points per one square A as used in KDE. Higher values means better precision. Number of points can be calculated as $P^{2/3}$.
cluster_area_expand	2	Space occupied by clusters' points can be expanded before KDE calculation. This option controls amount of A by which the cluster space is expanded. Average amount of expansion can be calcualted as $E^{2/3}$.

1.2.2.8 Stage visualize

Option	Default value	Description
split_by_type	False	If `True`, visulaizations of all objects that correspond to particular types of traced molecules are splited. Appropriate molecule name is added to created objects.
retain_all_types	False	If `True` and *split_by_type* option is `True` as well, standard visualization for all types of traced moelcules will be generated as well.
all_paths_raw	False	If `True`, produces one object in PyMOL that holds all paths visualized by raw coordinates.
all_paths_smooth	False	If `True`, produces one object in PyMOL that holds all paths visualized by smooth coordinates.
all_paths_split	False	If is set `True`, objects produced by **all_paths_raw** and **all_paths_smooth** are split into Incoming, Object, and Outgoing parts and visualized as three different objects.
all_paths_raw_io	False	If set `True`, arrows pointing beginning and end of paths are displayed oriented accordingly to raw paths orientation.
all_paths_smooth_io	False	If set `True`, arrows pointing beginning and end of paths are displayed oriented accordingly to smooth paths orientation.
all_paths_amount	None	Allows to limit number of visualised paths. If it is a number in range `(0,1)`, then it is interpreted as a percent number of paths to be visualized. It is is a integer number `>= 1` it is total number of all_paths visualized.

Continued on next page

Table 1 – continued from previous page

Option	Default value	Description
simply_smooths	RecursiveVector	Option indicates linear simplification method to be used in plotting smooth paths. Simplification removes points which do not (or almost do not) change the shape of smooth path. Possible choices are: • `RecursiveVector` (*LinearizeRecursiveVector*), • `HobbitVector` (*LinearizeHobbitVector*), • `OneWayVector` (*LinearizeOneWayVector*), • `RecursiveTriangle` (*LinearizeRecursiveTriangle*), • `HobbitTriangle` (*LinearizeHobbitTriangle*), • `OneWayTriangle` (*LinearizeOneWayTriangle*). Optionally name of the method can be followed by a threshold value in parentheses, i.e. `RecursiveVector(0.05)`. For sane values of thresholds see appropriate documentation of each method. Default values work well. This option is not case sensitive. It is recommended to use default method or `HobbitVector` method.
paths_raw	False	If set `True`, raw paths are displayed as separate objects or as one object with states corresponding to number of path.
paths_smooth	False	If set `True`, smooth paths are displayed as separate objects or as one object with states corresponding to number of path.
paths_raw_io	False	If set `True`, arrows indicating beginning and end of paths, oriented accordingly to raw paths, are displayed as separate objects or as one object with states corresponding to number of paths.
paths_smooth_io	False	If set `True`, arrows indicating beginning and end of paths, oriented accordingly to smooth paths, are displayed as separate objects or as one object with states corresponding to number of paths.
paths_states	False	If set `True`, objects displayed by **paths_raw**, **paths_smooth**, **paths_raw_io**, and **paths_smooth_io** are displayed as one object with states corresponding to number of paths. Otherwise they are displayed as separate objects.
ctypes_raw	False	Displays raw paths in a similar manner as non split **all_paths_raw** but each cluster type is displayed as a separate object.
ctypes_smooth	False	Displays smooth paths in a similar manner as non split **all_paths_smooth** but each cluster type is displayed as a separate object.
ctypes_amount	None	Allows to limit number of visualised ctypes. If it is a number in range `(0,1)`, then it is interpreted as percent number of ctypes to be visualized. It is is a integer number >= `1`, it is total number of visualized ctypes.
inlets_clusters	False	If set `True`, clusters of inlets are visualized.
inlets_clusters_amount	None	Allows to limit number of visualised inlets. If it is a number in range `(0,1)` then it is interpreted as percent number of inlets to be visualized. It is is a integer number >= `1` it is total number of visualized inlets.

Continued on next page

Table 1 – continued from previous page

Option	Default value	Description
show_molecule	False	If set to selection of some molecular object in the system, for example to `protein`, this object is displayed.
show_molecule_frames	0	Allows to indicate which frames of object defined by **show_molecule** should be displayed. It is possible to set several frames. In that case frames would be displayed as states.
show_scope_chull	False	If set to selection of some molecular object in the system, for example to `protein`, convex hull of this object is displayed.
show_scope_chull_inflate	None	Increase (or if negative decrease) size of the scope convex hull.
show_scope_chull_frames	0	Allows to indicate for which frames of object defined by **show_chull** convex hull should be displayed. It is possible to set several frames. In that case frames would be displayed as states.
show_object_chull	False	If set to selection of some molecular object in the system, convex hull of this object is displayed. This works exacly the same way as **show_chull** but is meant to mark object shape. It can be achieved by using *name * and* molecular object definition plus some spatial constrains, for example those used in object definition.
show_object_chull_frames	0	Allows to indicate for which frames of object defined by **show_object** convex hull should be displayed. It is possible to set several frames. In that case frames would be displayed as states.
cluster_area	True	If set `True`, clusters' areas are estimated with kernel density estimation method (KDE) and plotted as countour.
cluster_area_precision	20	Precision of KDE method in clusters' areas estimation method. This options controls number of grid points per one square A as used in KDE. Higher values means better precision. Number of points can be calculated as $P^{2/3}$.
cluster_area_expand	2	Space occupied by clusters' points can be expanded before KDE calculation. This option controls amount of A by which the cluster space is expanded. Average amount of expansion can be calcualted as $E^{2/3}$.

Note: Possibly due to limitations of `MDAnalysis` only whole molecules can be displayed. If **show_molecule** is set to `backbone` complete protein will be displayed anyway. This may change in future version of `MDAnalysis` and or *aquaduct*.

Note: If several frames are selected, they are displayed as states which may interfere with other PyMOL objects displayed with several states.

Note: If several states are displayed, protein tertiary structure data might be lost. This seems to be limitation of either `MDAnalysis` or PyMOL.

1.2.2.9 Clustering sections

Default section for definition of clustering method is named **clustering** and default section for reclustering method definition is named **reclustering**. All clustering sections shares some common options. Other options depends on the method.

Option	Default value	Description
method	barber or dbscan	Name of clustering method. It has to be one of the following: barber, dbscan, affprop, meanshift, birch, kmeans. Default value depends whether it is **clustering** section (barber) or **reclustering** section (dbscan).
recursive_clustering	clustering or None	If set to name of some section that holds clustering method settings, this method is called in the next recursion of clusteriation. Default value for **reclustering** is None.
recursive_threshold	None	Allows to set threshold that excludes clusters of certain size from reclustering. Value of this option comprises of *operator* and *value*. Operator can be one of the following: >, >=, <=, <. Value has to be expressed as floating number and it have to be in the range of 0 to 1. One can use several definitions separated by a space character. Only clusters of size complying with all thresholds definitions are submitted to reclustering.

barber

Clustering by **barber** method bases on *Auto Barber* procedure. For each inlets a sphere is constructed according to Auto Barber **separate_paths** stage settings or according to parameters given in clustering section. Next, inlets that form coherent clouds of mutually intersecting spheres are grouped into clusters. Method **barber** supports the same settings as Auto Barber settings:

Option	Value type	Description
auto_barber	str	This option allows to select molecular entity used in Auto Barber procedure. See also *Auto Barber* and `barber_with_spheres()`.
auto_barber_mincut	float	Minimal radius of spheres used in Auto Barber. If a sphere has radius smaller than this value, it is not used to cut. This option can be switched off by setting it to `None`.
auto_barber_maxcut	float	Maximal radius of spheres used in Auto Barber. If a sphere has radius greater than this value, it is not used to cut. This option can be switched off by setting it to `None`.
auto_barber_mincut_level	bool	If set `True`, spheres of radius less than **mincut** are resized to **mincut** value.
auto_barber_maxcut_level	bool	If set `True`, spheres of radius greater than **maxcut** are resized to **maxcut** value.
auto_barber_tovdw	bool	If set `True`, cutting of spheres is corrected by decreasing its radius by VdW radius of the closest atom.

dbscan

For detailed description look at `sklearn.cluster.DBSCAN` documentation. The following table summarizes options available in *Valve* and is a copy of original documentation.

Option	Value type	Description
eps	float	The maximum distance between two samples for them to be considered as in the same neighborhood.
min_samples	int	The number of samples (or total weight) in a neighborhood for a point to be considered as a core point. This includes the point itself.
metric	str	The metric to use when calculating distance between instances in a feature array. Can be one of the following: • `euclidean`, • `cityblock`, • `cosine`, • `manhattan`.
algorithm	str	The algorithm to be used by the NearestNeighbors module to compute pointwise distances and find nearest neighbors. Can be one of the following: • `auto`, • `ball_tree`, • `kd_tree`, • `brute`.
leaf_size	int	Leaf size passed to BallTree or cKDTree.

affprop

For detailed description look at `AffinityPropagation` documentation. The following table summarizes options available in *Valve* and is a copy of original documentation.

Option	Value type	Description
damping	float	Damping factor between 0.5 and 1.
convergence_iter	int	Number of iterations with no change in the number of estimated clusters that stops the convergence.
max_iter	int	Maximum number of iterations.
preference	float	Points with larger values of preferences are more likely to be chosen as exemplars.

meanshift

For detailed description look at `MeanShift` documentation. Following table summarized options available in *Valve* and is a copy of original documentation.

Option	Value type	Description
bandwidth	Auto or float	Bandwidth used in the RBF kernel. If `Auto` or `None` automatic method for bandwidth estimation is used. See `estimate_bandwidth()`.
cluster_all	bool	If true, then all points are clustered, even those orphans that are not within any kernel.
bin_seeding	bool	If true, initial kernel locations are not locations of all points, but rather the location of the discretized version of points, where points are binned onto a grid whose coarseness corresponds to the bandwidth.
min_bin_freq	int	To speed up the algorithm, accept only those bins with at least min_bin_freq points as seeds. If not defined, set to 1.

birch

For detailed description look at `Birch` documentation. Following table summarized options available in *Valve* and is a copy of original documentation.

Option	Value type	Description
threshold	float	The radius of the subcluster obtained by merging a new sample and the closest subcluster should be smaller than the threshold. Otherwise a new subcluster is started.
branching_factor	int	Maximum number of CF subclusters in each node.
n_clusters	int	Number of clusters after the final clustering step, which treats the subclusters from the leaves as new samples. By default, this final clustering step is not performed and the subclusters are returned as they are.

kmeans

For detailed description look at `KMeans` documentation. The following table summarized options available in *Valve* and is a copy of original documentation.

Option	Value type	Description
n_clusters	int	The number of clusters to form as well as the number of centroids to generate.
max_iter	int	Maximum number of iterations of the k-means algorithm for a single run.
n_init	int	Number of times the k-means algorithm will be run with different centroid seeds. The final results will be the best output of n_init consecutive runs in terms of inertia.
init	str	Method for initialization, defaults to `k-means++`. Can be one of following: `k-means++` or `random`.
tol	float	Relative tolerance with regards to inertia to declare convergence.

1.2.2.10 Smooth section

Section **smooth** supports the following options:

Option	Value type	Description
method	str	Smoothing method. Can be one of the following: • `window`, (see *`WindowSmooth`*) • `mss`, (see *`MaxStepSmooth`*) • `window_mss`, (see *`WindowOverMaxStepSmooth`*) • `awin`, (see *`ActiveWindowSmooth`*) • `awin_mss`, (see *`ActiveWindowOverMaxStepSmooth`*) • `dwin`, (see *`DistanceWindowSmooth`*) • `dwin_mss`, (see *`DistanceWindowOverMaxStepSmooth`*) • `savgol`. (see *`SavgolSmooth`*)
recursive	int	Number of recursive runs of smoothing method.
window	int or float	In window-based method defines window size. In plain `window` it has to be an int number. In `savgol` it has to be odd integer.
step	int	In step based method defines size of the step.
function	str	In window based methods defines averaging function. Can be `mean` or `median`.
polyorder	int	In `savgol` is polynomial order.

1.2.3 *Valve* tutorial

This tutorial assumes `aquaduct` and *Valve* is already installed - see *Aqua-Duct installation guide*. It is also assumed that user is acquainted with *Valve manual* and *Valve Configuration file options*.

1.2.3.1 *Valve* invocation

Usually *Valve* is run by:

```
valve.py
```

To check if *Valve* is installed and works properly try to issue following commands:

```
valve.py --help
valve.py --version
```

1.2.3.2 Test data

Mouse!

We will use 1 ns MD simulation data of sEH protein (PDBID **1cqz**). This simulation was performed in Amber 14. Necessary files can be found at Aqua-Duct home page in section download. Required data is in the *sample data* file.

1.2.3.3 Inspect your system

Before we start any calculations let's have a look at the protein of interest. Start PyMOL and get `1cqz` PDB structure (for example by typing in PyMOL command prompt `fetch 1cqz`).

To setup *Valve* calculations we need to know the active site of the protein. More precisely we need to know IDs of residues that are in the active site. This would allow us to create *Object definition*.

But wait. Is it really the correct structure? How many chains there are? What is the numeration of residues? How does it compare with the topology file from *sample data*?

Create *Object definition*

Leti's load another structure. Open file `1cqz_sample_topology.pdb` (see *Test data*). It is a first frame of the MD simulation and it is an example of how the frame of MD looks like. In order to create *Object definition* you have to discover following things:

1. What is the name of water molecules?
2. What are numbers of residues in the active site?
3. What size the active site is of?

Note: It is also a good idea to open `.pdb` file in your favorite text editor and look at residue numbers and names.

Create *Scope definition*

Scope definition is easy to create. We will use *Convex hull* version so the scope definition could be simply `backbone`.

1.2.3.4 Prepare config file

Valve performs calculations according to the configuration (aka *config*) file.

Lets start from dumping config file template to `config.txt` file. Open it in your favorite editor and fill all options. If you have troubles look at *Configuration file options* (and *Valve manual*).

Things to remember:

1. Provide correct paths to topology and trajectory data.
2. Enter correct *Object* and *Scope* definitions.
3. Make sure visualization is switched on.

1.2.3.5 Run *Valve*

Make sure all necessary data is in place. Open terminal, go to your working directory and type in:

```
valve.py -c config.txt
```

Depending on your machine and current load it may take a while (matter of minutes) to complete all calculations.

Visual inspection

In the last stage PyMOL should pop up and *Valve* should start to feed it with visualization data. This would take a moment and if you set up `save` option a PyMOL session would be saved. Once it is done *Valve* quits and switches off PyMOL. Now, you can restart it and read saved session.

Clustering

Improve clustering of Inlets. See *Configuration file options* for more hints on available clustering options.

Analysis tables

Open `5_analysis_results.txt` file and look at summaries and tables. See also *Valve manual*.

1.2.3.6 Feedback

Give us your opinion. Send your questions, inquires, anything to developer(s): info@aquaduct.pl. There are couple of questions that might be useful to form your opinion.

1. What do you like in *Valve* and *Aqua-Duct*?
2. What do you do not like in *Valve* or *Aqua-Duct*?
3. What is missing?
4. Do you find it useful?

1.3 Aqua-Duct's Pond driver documentation

1.3.1 *Pond* manual

Pond application is a driver that uses `aquaduct` module to perform further analysis of results from *Valve* calculations.

Pond can calculate pockets present in the protein and free energy profiles of *Master paths*.

1.3.1.1 *Pond* invocation

Once `aquaduct` module is installed (see *Aqua-Duct installation guide*) properly on the machine, *Pond* is available as `pond.py` command line tool.

Usage

Basic help of *Pond* usage can be displayed by following command:

```
pond.py --help
```

It should display following information:

```
usage: pond.py [-h] [-c CONFIG_FILE] [-t THREADS] [-r RESULTS_DIR] [--debug]
               [--debug-file DEBUG_FILE] [--paths-types PATHS_TYPES] [--raw]
               [--raw-master] [--raw-discard-singletons RAW_SINGL]
               [--window-full] [--windows WINDOWS] [--wsize WSIZE]
               [--reference-value REF] [--reference-calc]
               [--reference-radius REF_RADIUS] [--reference-mol REF_MOL]
               [--temperature TEMP] [--gsize GRID_SIZE] [--pockets]
               [--hotspots] [--energy-profile] [--master]
               [--master-radius MASTER_RADIUS] [--master-ctypes MASTER_CTYPES]
               [--io-threshold IO_THRESHOLD] [--path-id PATH_ID]
               [--path-file PATH_FILE] [--path-radius PATH_RADIUS]
               [--path-smooth] [--raw-path] [--extract-path EXTRACT_PATH]
               [--output-file OUTPUT_FILE]

What have I got in my pocket?

optional arguments:
  -h, --help            show this help message and exit
  -c CONFIG_FILE        Config file filename. (default: None)
  -t THREADS            Limit Aqua-Duct calculations to given number of
                        threads. (default: None)
  -r RESULTS_DIR        Path to results directory (default: )
  --debug               Prints debug info. (default: False)
  --debug-file DEBUG_FILE
                        Debug log file. (default: None)
  --paths-types PATHS_TYPES
                        Limit calculations to given paths types, i.e. given
                        molecules. (default: )
  --raw                 Use raw data from paths instead of single paths.
                        (default: False)
  --raw-master          Use raw data from paths instead of single paths, only
                        in master paths calculations. (default: False)
  --raw-discard-singletons RAW_SINGL
                        Discard short scope only segments from raw data.
                        (default: 1)
  --window-full         Return full window if windows is used. (default:
                        False)
```

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```
  --windows WINDOWS     Number of windows to calculate. (default: 1)
  --wsize WSIZE         Size of window in frames. (default: None)
  --reference-value REF
                        Reference value in [kJ/mol/K]. (default: None)
  --reference-calc      Calculate reference value with scope and reference
                        molecules. (default: False)
  --reference-radius REF_RADIUS
                        Radius of reference. (default: 2.0)
  --reference-mol REF_MOL
                        Selection of reference molecules. (default: resname
                        WAT)
  --temperature TEMP    Simulation temperature. (default: 300.0)
  --gsize GRID_SIZE     Size of grid's cells. (default: 1.0)
  --pockets             Calculate pockets. (default: False)
  --hotspots            Calculates hotspots if pockets are calculated.
                        (default: False)
  --energy-profile      Calculates energy profiles for master paths. (default:
                        False)
  --master              Enables master paths calculation. (default: False)
  --master-radius MASTER_RADIUS
                        Calculate profiles for master paths with given radius.
                        (default: 2.0)
  --master-ctypes MASTER_CTYPES
                        Limit calculations to given ctypes. (default: )
  --io-threshold IO_THRESHOLD
                        Percent value of maximal density which will be used to
                        partition pocket into inner and outer instead of mean
                        value. (default: None)
  --path-id PATH_ID     Calculate profiles for specified path ID. (default:
                        None)
  --path-file PATH_FILE
                        Use coordinates from specified CSV file. (default:
                        None)
  --path-radius PATH_RADIUS
                        Calculate profiles for path with given radius.
                        (default: 2.0)
  --path-smooth         If used path coordinates will be smoothed. (default:
                        False)
  --raw-path            Use raw data from paths instead of single paths. Used
                        for path energy profiles calculations and for
                        extracting raw path. (default: False)
  --extract-path EXTRACT_PATH
                        Extract path coordinates with specified ID. (default:
                        None)
  --output-file OUTPUT_FILE
                        Output CSV filename for extracted coordinates.
                        (default: path_coords.csv)
```

Options common with *Valve*

All options related to Molecular Dynamic simulation data, configuration file, and threads have the same meaning as in *Valve*.

For detailed explanation of the following options see *Valve manual*:

- `-c CONFIG_FILE` - Configuration file name. *Pond* and *Valve* should use the same file.
- `-t THREADS` - Limits Aqua-Duct calculations to given number of threads.
- `--debug` and `--debug-file` - Allows to get debugging information.

Results directory

Pond produces many results files, especially if windows options are used. For the sake of convenience, option `-r` allows to provide output directory. If provided directory does not exist it will be created without warning. Also, *Pond* will not warn if results files overwrites existing files.

Pond calculations options

Other options are used to start or adjust *Pond* calculations:

- **Pockets** Option `--pockets` triggers pocket calculations
- **Hot-spots** Option `--hotspots` triggers hot-spot calculations but it also requires `--pockets`.
- **Energy profiles** Option `--energy-profile` triggers free energy profiles calculations for master paths.

Pond's option `--paths-types` allows to limit calculations only to paths of certain molecules. For example, `--paths-types 'WAT OXY'` loads paths of `WAT` (water molecules) and `OXY` (oxygen) molecules. All other paths (if any) will not be used.

Free energy estimation

Pond can estimate free energy by using calculated density of traced molecules. It becomes particularly useful and relevant when traced molecules include solvent.

Estimation of free energy is done according to Boltzmann inversion. Similar method was used in Rao,S. et al. (doi:10.1080/19336950.2017.1306163) paper.

Following equation relates free energy with density of molecules:

$$n(z) = C \cdot e^{\left(\frac{-E(z)}{kT}\right)}$$

Where z is point in the space, preferably along some kind of path, *n(z)* is density of molecules in point z, C is a normalization constant, E is free energy, k is Boltzmann's constant, and T is temperature.

One can easily transform the above equation to calculate energy:

$$E(z) = -kT \ln\left(n(z)\right) - kT \ln\left(C\right)$$

Term $kT \ln\left(C\right)$ does not depend on z and can be determined by assumption that free energy in the bulk of traced molecules (solvent) is zero.

Please note that option `--temperature` allows to set desired temperature in Kelvins.

Note: *Pond* returns energy in kJ/mol SI units.

Bulk reference

Value of reference correction can be directly passed to *Pond* using `--reference-value` option or can be calculated automatically by analysis of the bulk of traced molecules (solvent) using `--reference-calc` flag. Following additional options influence calculation of bulk reference:

1. **Radius of the bulk around COG.** Option `--reference-radius` allows to set the radius of the sphere within which the bulk will be scanned. The sphere is centered in COG. Radius should be selected in such a way that the sphere does not overlaps with other molecules in the simulated system. Default value is 2.0 Å.

2. **Density of reference molecules.** Once COG if the bulk and radius are setup, *Pond* scans trajectory and looks for molecules. Option `--reference-mol` allows to define molecules for which density should be calculated.

Note: If no `--reference-value` or `--reference-calc` options are used *Pond* skips estimation of free energy.

Raw data

Two types of data can by used by *Pond*:

1. Separate paths (including passing paths if any), or
2. Raw paths saved at stage II.

By default separate paths are used. Option `--raw` makes *Pond* to use raw paths in all calculations, whereas `--raw-master` makes *Pond* to use raw paths only in estimation of free energy profiles and for pockets and hot-spots separate paths are used.

Note: Best results of pockets calculation can be achieved with separate paths.

Warning: Free energy estimation with separate paths may very likely lead to false results at the borders of the scope.

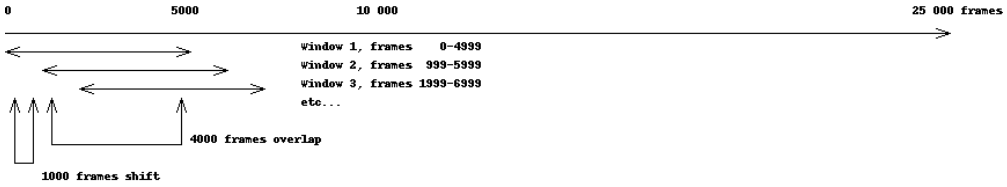
Windows

Pond performs calculations for entire trajectory and/or for user defined windows:

- `--window-full` ensures that results will be calculated for the entire trajectory.
- `--windows` allows to set number of windows.
- `--wsize` allows to change default size of windows.

By default, windows' sizes are automatically set in such a way that entire trajectory is covered and windows do not overlap to each other. Option `--wsize` allows to set size of windows (in frames), therefore, windows can also overlap with each other or can span only selected sections of the trajectory.

For example, for 25 000 snapshots long trajectory one can perform calculations in 5000 frames long windows where an overlap of a consecutive window with a next window is 4000 frames long - see following picture:



To calculate proper number of windows evenly spanning trajectory one can use following equation:

$$WINDOWS = \frac{TOTAL - WSIZE}{SHIFT} + 1$$

Where *WINDOWS* is a desired number of windows, *TOTAL* is total length of trajectory, and *SHIFT* is *WSIZE* - *OVERLAP*.

In the above example *TOTAL* = 25 000, *WSIZE* = 5 000, *SHIFT* = *WSIZE* - *OVERLAP* = 5 000 - 4 000 = 1 000. Therefore:

$$WINDOWS = \frac{25000 - 5000}{1000} + 1 = 21.$$

And *Pond* should be called with `--windows 21 --wsize 5000` options to get above described windows.

1.3.1.2 Pockets

Pockets are calculated by analysis of paths found by *Valve*. A regular grid is constructed spanning all paths. Grid size by default is 1 Å and can be altered with `--gsize` option.

Note: As for now, it is recommended that multiplicative inverse of grid size is an integer number. Therefore, grid size can be safely set to 1, 0.5, 0.25, 0.1 etc.

Next, number of paths crossing each of the grid cells is calculated over the entire trajectory and divided by the number of frames. This gives averaged density of traced molecules.

Cells with null density are removed from the grid and resulted shape corresponds to maximal area penetrated by traced molecules.

Note: If no estimation of free energy is performed values returned for pockets and hot-spots are density (of traced molecules).

Warning: Estimation of free energy for pockets calculated for non raw data may be unreliable.

Inner & outer pocket

Distribution of densities in the grid has positive skew. This suggest that pocket can be partitioned into areas of different overall distribution of traced molecules.

Indeed, *Pond* saves two types of pockets depending on the distribution of densities in the grid:

1. **Inner pocket** This is part of the pocket for which densities are greater than mean value.
2. **Outer pocket** This is counter part for **Inner pocket**, i.e. the part of the pocket for which densities are less than mean value.

Hot-spots

Further analysis of distribution of densities in the grid allows to select points of the highest densities. They are considered as **hot-spots**, i.e. points of particular importance at which traced molecules are attracted or trapped and stays for considerably long time.

Currently **hot-spots** are detected as far right tail of the distribution of densities in the grid.

1.3.1.3 Energy profiles

Pond estimates energy profiles of master paths. For each point of the master path density of paths of traced molecules is calculated within sphere of radius set by `--master-radius` option.

Option `--master-ctypes` allows to select master paths *ctypes* for which free energy estimation is calculated.

CHAPTER

TWO

TECHNICAL DOCUMENTATION

2.1 Aqua-Duct installation guide

2.1.1 Overview

Aqua-Duct software is software written in Python (CPython) and comprises of two elements:

1. aquaduct - a Python package,
2. valve - a script that uses `aquaduct` to perform calculations.

Download

You can download Aqua-Duct packages directly from Aqua-Duct homepage. This page includes older versions of Aqua-Duct as well as development version.

If you follow this installation guide you will install current release.

2.1.2 Troubleshooting

If you encounter any problems with installation do not hesitate to contact us at info@aquaduct.pl. We are **REALLY** willing to help!

Please, provide us with us much info as you can. In particular try to include following information:

- Operating system's name and version, and CPU architecture (if relevant).
- Python version.
- Command(s) you have used for installation.
- Any error/warning/info message(s) that emerged during or after installation.

2.1.3 Requirements

2.1.3.1 Software-wise requirements

- numpy >= 1.10.0
- scipy >= 0.17.1
- scikit-learn >= 0.16.0
- MDAnalysis[amber] == 0.16.2
- joblib >= 0.13

2.1.3.2 Hardware-wise requirements

Aqua-Duct should work on every machine on which you can install the above mentioned software. On computers older than 10 years it may work very slow though. We recommend 64bit SMP architecture, with at least 4GB RAM (32 GB RAM is recommended).

2.1.4 Installation

2.1.4.1 Generic Python installation

The easiest way to install Aqua-Duct is to install Python 2.7 and use following command:

```
pip install aquaduct
```

If *pip* is not available try to install it by typing:

```
easy_install pip
```

Depending on the settings of your system you can prepend the above command with *sudo* or *doas* or do *user* installation:

```
# sudo
sudo pip install aquaduct

# doas
doas pip install aquaduct

# 'user' installation
pip install aquaduct --user
```

It is also good idea to try to install Aqua-Duct using virtualenv:

```
virtualenv aquaduct_installation
cd aquaduct_installation
. bin/activate
pip install aquaduct
```

Installation of PyMOL

Under most modern GNU/Linux distributions PyMOL is available as a package in repositories. For example if you are under Ubuntu/Debian you can install it by following command:

```
sudo apt-get install pymol
```

Under Windows there are several ways to install PyMOL, for more details see PyMOL web site.

Instructions for macOS and OpenBSD are in appropriate sections below.

2.1.4.2 GNU/Linux

Installation was tested on limited number of GNU/Linux systems. On the most of modern installations you can simply follow generic instructions, for example under Ubuntu 16.04 you can type:

```
sudo pip install aquaduct
```

NetCDF4 & MDAnalysis installation Ubuntu 14.04

Other systems may require additional work, in particular installation of NetCDF4 is sometimes cumbersome. Following is an example how to install all required packages under Ubuntu 14.04:

```
# install required python packages
sudo apt-get install python-dev python-pip python-numpy python-scipy python-
↪matplotlib python-scikits-learn

# install necessary libraries and git -  all required to compile netCDF4
sudo apt-get -y install libnetcdf-dev libhdf5-dev git

# clone netcdf4 python repository
git clone https://github.com/Unidata/netcdf4-python.git
# cd to cloned repository
cd netcdf4-python
# modify setup.cfg to add paths of hdf5 and netcdf4 libraries
sed -i '/\[directories\]/a \
```

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```
HDF5_dir = /usr/lib \
HDF5_libdir = /usr/lib \
HDF5_incdir = /usr/include \
netCDF4_dir = /usr/lib \
netCDF4_libdir = /usr/lib \
netCDF4_incdir = /usr/include' setup.cfg
# run setup.py
sudo python setup.py install

# install MDAnalysis
sudo pip install "MDAnalysis[amber]==0.16.2"
```

If everything went fine you can follow generic instructions.

SciPy update and Ubuntu/Debian

Debian (and Ubuntu) uses strange approach to Python installation. To install newer version of SciPy (if required) try following procedure:

```
# install libraries required for SciPy compilation
apt-get build-dep python-scipy

# install SciPy
easy_install-2.7 --upgrade scipy
```

Warning: The above procedure will remove current SciPy from *easy-install.pth* file.

2.1.4.3 macOS

Aqua-Duct installation was tested on macOS Sierra and is quite straightforward. It can be installed either with existing system Python or with custom Python installation. In both cases one have to install Xcode for the App Store.

System native Python

```
sudo easy_install pip
sudo pip install aquaduct
```

The drawback of using system Python installation is a lack of PyMOL. It should be, however, relatively easy to compile PyMOL on your own. Try to follow compilation instruction under BSD systems.

Custom Python

This is recommended way of Aqua-Duct installation. If you do not have custom Python installation you can get it by using one of package managers available for macOS, for example homebrew. With this package manager you can do following:

```
brew install python
sudo easy_install pip
sudo pip install aquaduct
```

Next, you can install PyMOL:

```
brew install pymol
brew cask install xquartz
```

Once XQuartz is installed you should reboot. The above procedure installs PyMOL, however, PyMOL Python modules are not visible. To fix it you can issue following commands:

```
cd /usr/local/lib/python2.7/site-packages
sudo ln -s /usr/local/Cellar/pymol/*/libexec/lib/python2.7/site-packages/* ./
```

The above instruction assumes that you are using *brew* and you have only one PyMOL installation.

2.1.4.4 Windows

Installation under Windows is also possible. The limiting factor is MDAnalysis which is not officially available under Windows yet. You can, however, install Cygwin and perform Aqua-Duct installation in Cygwin.

First, start with Cygwin installation. During the setup select following packages:

- python (2.7)
- python-devel (2.7)
- python-cython
- libnetcdf-devel
- libhdf5-devel
- liblapack-devel
- libopenblas
- python-numpy
- python-six

Another key component that have to be installed is C, C++ and Fortran compilers. You can simply install **gcc-g++** and **gcc-fortran** packages as a first choice, select following packages:

- gcc-g++
- gcc-fortran

Once Cygwin is installed with all required libraries you can perform following steps:

```
# install pip
easy_install-2.7 pip
```

First, try to install SciPy:

```
# install SciPy
pip install scipy
```

If you encounter any problems related to missing **xlocale.h** header file try the following workaround:

```
# prepare fake xlocale.h
ln -s /usr/include/locale.h xlocale.h
export CFLAGS="I"$( pwd )

# install SciPy
pip install scipy
```

Note: The above procedure for SciPy installation might not be optimal. For more information please got to SciPy web page.

Now, install **scikit-learn** and then Aqua-Duct:

```
# install scikit-learn
pip install scikit-learn

# finally, install aquaduct
pip install aquaduct
```

2.1.4.5 OpenBSD

Aqua-Duct can be also installed under OpenBSD (5.9 and 6.0 amd64). NetCDF-c version 4 has to be installed as OpenBSD ships only netCDF in version 3. First, install hdf5 library and GNU make:

```
# install hdf5 and GNU make
pkg_add hdf5 gmake
```

Next, download netCDF sources. Version 4.2.1.1 works out of the box but is a bit outdated. Visit NetCDF web page and select version of your choice. Older versions are available in the FTP archive. Once netCDF is downloaded and extracted go to the source directory and try following procedure:

```
# set LD and CPP flags
export LDFLAGS=-L/usr/local/lib
export CPPFLAGS=-I/usr/local/include

# configure project
./configure --enable-shared --enable-dap --disable-doxygen --enable-netcdf-4 --
↪prefix=/path/to/netCDF4/lib

# make and install
gmake
gmake install
```

You may now install py-scipy package:

```
pkg_add py-scipy
```

Install pip if it is missing:

```
pkg_add py-pip
```

Install netCDF4 Python:

```
# define netcdf-4 installation directory
export NETCDF4_DIR=/path/to/netCDF4/lib
pip2.7 install netCDF4
```

At this point you can follow generic Python instructions, type:

```
pip2.7 install aquaduct
```

PyMOL at OpenBSD

According to our knowledge it is possible to install PyMOL 1.4.1 and it is sufficient to work with Aqua-Duct. Go to SourceForge PyMOL download page and download, save, and extract sources.

PyMOL requires Python Mega Widgets. Download, for example Pmw 1.3.3b from SourceForge Pmw download page. Extract it and install by:

```
python2.7 setup.py install
```

TKinter (2.7) and several other packages are also required:

```
pkg_add python-tkinter freeglut glew png
```

Next, go to the extracted PyMOL sources open setup.py and modify inc_dirs variable at line 129 by adding following paths:

```
"/usr/X11R6/include/freetype2",
"/usr/X11R6/include",
"/usr/local/include",
```

Now, you can build and install PyMOL by typing following commands:

```
python2.7 setup.py build
python2.7 setup.py install
python2.7 setup2.py install
cp pymol /usr/local/bin
```

PyMOL can be run by typing *pymol* or can be used as Python module.

Other BSDs

Installation on other BSDs might be easier. For example, Python netCDF4 is available in ports of FreeBSD and DragonFlyBSD. Try to install it and SciPy, then proceed to generic Python installation instructions.

If you are using NetBSD or other BSD try to follow OpenBSD instructions.

2.2 aquaduct

2.2.1 aquaduct package

2.2.1.1 Subpackages

aquaduct.apps package

Subpackages

aquaduct.apps.valve package

Submodules

aquaduct.apps.valve.clusters module

cluster_id_header()

add_cluster_id_head(*gen*)

add_cluster_id(*gen*)

clusters_inlets_header(**args*, ***kwargs*)

clusters_inlets(*cluster*, *something*, *add_id=True*, **args*, ***kwargs*)

clusters_area_header(**args*, ***kwargs*)

clusters_area(*cluster*, *something*, *add_id=True*, **args*, ***kwargs*)

clusters_stats_prob_header(**args*, ***kwargs*)

clusters_stats_prob(*cluster*, *something*, *add_id=True*, **args*, ***kwargs*)

clusters_stats_len_header(**args*, ***kwargs*)

clusters_stats_len(*cluster*, *something*, *add_id=True*, **args*, ***kwargs*)

clusters_stats_steps_header(**args*, ***kwargs*)

clusters_stats_steps(*cluster*, *something*, *add_id=True*, **args*, ***kwargs*)

aquaduct.apps.valve.core module

aquaduct.apps.valve.data module

check_version_compliance(*current*, *loaded*, *what*)

check_versions(*version_dict*)

get_vda_reader(*filename*, *mode='r'*)

class ValveDataAccess(*mode=None*, *data_file_name=None*)

Bases: object

unknown_names = 'UNK'

__init__(*mode=None*, *data_file_name=None*)

x.__init__(...) initializes x; see help(type(x)) for signature

open()

close()

__del__()

load()

dump(***kwargs*)

get_variable(*name*)

set_variable(*name*, *value*)

class ValveDataCodec
Bases: object

Class defines format of encoding AQ objects into NetCDF format. Encoding defined here can be also used to store AQ objects as NumPy arrays.

version = (0, 0, 1)
Current version of *ValveDataCodec*

static varname(*name*, **suffix*)
Name of variable made by combining base name and suffixes (if any). Base name and suffixes are joined with dot '.'.

Parameters

- **name** – Base for variable name.
- **suffix** – Optional suffixes.

Returns Name of variable made by combining base name and suffixes (if any).

Field list ends without a blank line; unexpected unindent.

Base name and suffixes are joined with dot '.'.

static encode(*name*, *value*)

static decode(*name*, *data*)

class ValveDataAccess_nc(*mode=None*, *data_file_name=None*)
Bases: *aquaduct.apps.valve.data.ValveDataAccess*

not_variable = ['version', 'aquaduct_version', 'ValveDataCodec']

open()

close()

get_variable(*name*, *copy=True*)

set_variable(*name*, *value*)

dump(***kwargs*)

load(***kwargs*)

class ValveDataAccess_numpy(*mode=None*, *data_file_name=None*)
Bases: *aquaduct.apps.valve.data.ValveDataAccess*

class ValveDataAccess_pickle(*mode=None*, *data_file_name=None*)
Bases: *aquaduct.apps.valve.data.ValveDataAccess*

mimic_old_var_name = 'aq_data_to_save'

unknown_names = 'UNK'

open()

close()

load()

dump(***kwargs*)

get_variable(*name*)

set_variable(*name*, *value*)

aquaduct.apps.valve.helpers module

aquaduct.apps.valve.spath module

class SpathIdHeader

Bases: object

name = 'ID'

format = '%9s'

__call__(*...*) <==> *x(...)*

spath_name_header()

add_path_id_head(*gen*)

add_path_id(*gen*)

size_header()

add_size_head(*gen*)

add_size(*gen*)

ctype_id_header()

add_ctype_id_head(*gen*)

add_ctype_id(*gen*)

spath_basic_info_header(**args*, ***kwargs*)

spath_basic_info(*spath*, **args*, ***kwargs*)

spath_lenght_total_info_header(**args*, ***kwargs*)

spath_lenght_total_info(*spath*, **args*, ***kwargs*)

spath_frames_total_info(*spath*, **args*, ***kwargs*)

spath_steps_info_header(**args*, ***kwargs*)

spath_steps_info(*spath*, **args*, ***kwargs*)

spath_frames_info(*spath*, **args*, ***kwargs*)

spath_ctype_header(**args*, ***kwargs*)

spath_ctype(*spath*, **args*, ***kwargs*)

spath_full_info_header(**args*, ***kwargs*)

spath_full_info(*spath*, **args*, ***kwargs*)

spaths_lenght_total_header(**args*, ***kwargs*)

spaths_length_total(*spaths*, *add_size=True*, *add_size_p100=None*, **args*, ***kwargs*)

spaths_frames_total(*spaths*, *add_size=True*, *add_size_p100=None*, **args*, ***kwargs*)

ctypes_spaths_info_header(**args*, ***kwargs*)

ctypes_spaths_info(*ctype*, *something*, *add_id=True*, **args*, ***kwargs*)

plot_spaths_traces(*spaths*, *spp=None*, *name=None*, *split=False*, *states=False*, *separate=False*, *smooth=None*)

plot_spaths_inlets(*spaths*, *spp=None*, *name=None*, *states=False*, *separate=False*, *smooth=None*)

aquaduct.apps.valve.worker module

Module contents

This module is meant to read configuration file and init some global options. It cannot import sandwich. Directly or indirectly.

class ConfigSpecialNames
Bases: object

special_names_dict = {'auto': <class aquaduct.utils.helpers.Auto>, 'false': False,

special_name(*name*)

class ValveConfig
Bases: *aquaduct.apps.valve.ConfigSpecialNames*

__init__()
x.__init__(...) initializes x; see help(type(x)) for signature

static common_config_names()

static common_traj_data_config_names()

static global_name()

static cluster_name()

static recluster_name()

static recursive_clustering_name()

static recursive_threshold_name()

static smooth_name()

stage_names(*nr=None*)

get_common_traj_data(*stage*)

get_global_options()

get_stage_options(*stage*)

get_cluster_options(*section_name=None*)

get_recluster_options()

get_smooth_options()

get_default_config()

load_config(*filename*)

save_config_stream(*fs*)

save_config(*filename*)

get_general_comment(*section*)

dump_config(*dump_template=False*)

_ValveConfig__make_options_nt(*input_options*)

valve_load_config(*filename*, *config*)

sep()

asep()

valve_begin()

valve_end()

iskeyword()
x.__contains__(y) <==> y in x.

aquaduct.apps.valveconfig package

Submodules

aquaduct.apps.valveconfig.defaults module

class longstr
Bases: str

Class used to specify type of default value.

Represents Text field.

class filetype
Bases: str

Class used to specify type of default value.

Represents Entry with file loading button.

class manyfiletype
Bases: str

Class used to specify type of default value.

Represents Entry with file loading button which duplicate itself when previous is loaded.

class dirtype
Bases: str

Class used to specify type of default value.

Represents Entry with dir loading button.

class DefaultSection(*config_name*, *name*, *level*, *abs_level=None*, *additional=False*)
Bases: object

__init__(*config_name*, *name*, *level*, *abs_level=None*, *additional=False*)
Contrains info about section necessary to create it.

Parameters

- **config_name** – Name of section in config.
- **name** – Brief label text, which will be displayed in Notebook tab.
- **level** – Entry level.
- **abs_level** – If specified section will be shown only when corresponding level was chosen.
- **additional** – If True values from that section wont be considered as default. Useful when section is mix of other sections.

add_entry(*entry*)
Allow to add new entry to the section or nest other section. Nested section will be showed in LabelFrame. :param entry: Entry or section :type entry DefaultEntry, DefaultSection

iter_entries()
Iterates through section entries.

__slotnames__ = []

class DefaultEntry(*config_name*, *name*, *default_values*, *help_text*, *level*, *group_label=None*, *info_text=None*, *warning_text=None*, *optionmenu_value=None*, *required=None*)

Bases: object

__init__(*config_name*, *name*, *default_values*, *help_text*, *level*, *group_label=None*, *info_text=None*, *warning_text=None*, *optionmenu_value=None*, *required=None*)

Contains info about entry necessary to create it.

Parameters

- **config_name** – Name of option in config.
- **name** – Brief label text, which will be displayed near widget.
- **default_values** – List of default values.
- **help_text** – Tooltip text.
- **level** – Entry level. Check LEVELS dict for adjust it.
- **group_label** – Used to group labels into frames. Content is a title of frame.
- **info_text** – If present information icon with content of that variable will be displayed.
- **warning_text** – If present warning icon with content of that variable will be displayed.
- **optionmenu_value** – OptionMenu value, which will cause display appropriate hiding frame.

default_value

Determines default value based on specified default values list.

Returns Entry default value.

is_menu(*section*, *option*)

Determines if option in section control hiding frames.

Returns True if option control hiding frames, otherwise False.

Return type bool

get_default_entry(*section_name*, *option_name*)

Return default entries.

Parameters

- **section_name** – Name of section where option is located.
- **option_name** – Option name which default values are demanded.

Returns DefaultEntry

get_default_section(*section_name*)

Return default section informations.

Parameters **section_name** – Name of section which informations are demaned.

Returns Default section informations.

Return type *DefaultSection*

aquaduct.apps.valveconfig.utils module

get_widget_bg(*widget*)

Return background color of specified widget.

Parameters **widget** – Ttk widget.

Returns Background color.

Return type str

widget_factory(*parent*, *default*, *state='normal'*)
Creates widget depending on default argument.

Parameters

- **parent** – Parent of new widget.
- **default** – Default widget value.
- **state** – State of widget.

Returns Widget and variable attached to it.

Return type tuple

entry_factory(*parent*, *row*, *entry_name*, *default*, *help*, *state='normal'*, *info_text=None*, *warning_text=None*)
Determines which class is used to handle specified default value.

Parameters

- **parent** – Parent of widget.
- **row** – Row number where first Entry will be grided.
- **entry_name** – Readable entry name.
- **default** – Default values of entry.
- **help** – Text which will be displayed in tooltip.
- **state** – State of widget.

Returns Entry based on default value.

class Text(*parent*, *textvariable*, ***kwargs*)
Bases: Tkinter.Text, object

__init__(*parent*, *textvariable*, ***kwargs*)

Text widget with ability to assign content to variable.

Parameters

- **parent** – Parent of widget.
- **textvariable** – String variable to which will contain Text content.
- **kwargs** – Arguments which will be passed to original tk.Text widget.

_on_update(*e*)
Text widget callback which assign its content to variable.

Parameters **e** – Event informations.

_on_var_update(**args*)
Variable callback which assign its content to Text widget.

Parameters **args** – Event informations.

class Entry(*parent*, *row*)
Bases: object

Abstract class for various Entries that manage different type of default values.

Represents single row of configuration option with Label and all input widgets.

__init__(*parent*, *row*)
x.__init__(...) initializes x; see help(type(x)) for signature

get()
Gets Entry value.

Returns Entry value.

set(*value*)
Sets Entry value.

Parameters **value** – New value of Entry.

highlight()
Changes color of input frame.

Used to highlight, which required entry is unfilled.

unhighlight()
Sets entry to default color.

class StandardEntry(*parent*, *row*, *entry_name_long*, *default*, *help*, *state*, *info_text=None*, *warning_text=None*)
Bases: *aquaduct.apps.valveconfig.utils.Entry*

__init__(*parent*, *row*, *entry_name_long*, *default*, *help*, *state*, *info_text=None*, *warning_text=None*)
Entry with standard widget.

Parameters

- **parent** – Parent of widgets.
- **row** – Row where widgets will be grided.
- **entry_name_long** – Readable entry name.
- **default** – Default values of entry.
- **help** – Text which will be displayed in tooltip.
- **state** – State of widget.

get()
Gets Entry value.

Returns Entry value.

set(*value*)
Sets Entry value.

Parameters **value** – New value of Entry.

class BoolEntry(*parent*, *row*, *entry_name_long*, *input_default*, *control_default*, *help*, *info_text=None*, *warning_text=None*)
Bases: *aquaduct.apps.valveconfig.utils.Entry*

__init__(*parent*, *row*, *entry_name_long*, *input_default*, *control_default*, *help*, *info_text=None*, *warning_text=None*)
Entry with Checkbox and Entry or text widget.

Parameters

- **parent** – Parent of widgets.
- **row** – Row where widgets will be grided.
- **entry_name_long** – Readable entry name.
- **default** – Default values of entry.
- **help** – Text which will be displayed in tooltip.
- **state** – State of widget.

get()
Get Entry value.

Returns If Checkbox is checked it return input widget value, otherwise False.

set(*value*)
Set Entry value.

Parameters **value** – Value that input widget will be set too.

Field list ends without a blank line; unexpected unindent.

If False it will set only Checkbox value to False and input widget to "". If value have str type it will set Checkbox to True and input widget to that value.

class FileEntry(*parent*, *row*, *entry_name_long*, *default*, *help*, *info_text=None*, *warning_text=None*)
Bases: *aquaduct.apps.valveconfig.utils.Entry*

__init__(*parent*, *row*, *entry_name_long*, *default*, *help*, *info_text=None*, *warning_text=None*)
Entry with Entry widget and button to load and append file name to it.

Parameters

- **parent** – Parent of widgets.
- **row** – Row where widgets will be grided.
- **entry_name_long** – Readable entry name.
- **default** – Default values of entry.
- **help** – Text which will be displayed in tooltip.
- **state** – State of widget.

callback_load_file(*e*)
Callback for selecting file.

Sets widget content to loaded file name.

get()
Gets Entry value.

Returns Entry value.

set(*value*)
Sets Entry value.

Parameters **value** – New value of Entry.

class ManyFileEntry(*parent*, *row*, *entry_name_long*, *default*, *help*, *info_text=None*, *warning_text=None*)
Bases: *aquaduct.apps.valveconfig.utils.Entry*

__init__(*parent*, *row*, *entry_name_long*, *default*, *help*, *info_text=None*, *warning_text=None*)
Entry with Text widget and button to load and append file names to it.

Parameters

- **parent** – Parent of widgets.
- **row** – Row where widgets will be grided.
- **entry_name_long** – Readable entry name.
- **default** – Default values of entry.
- **help** – Text which will be displayed in tooltip.
- **state** – State of widget.

append_entry()
Creates new entry with input widget and load button

callback_load_file(*index*)
Callback for selecting file.

Appends loaded file name at the end of Text widget.

Parameters **index** – Index of variable in self.input_vars

get()
Gets Entry value.

Returns Entry value.

set(*value*)
Sets Entry value.

If value is set to "" it deletes all input widgets, except first and sets it to ""

Parameters **value** – New value. It can be single path or paths separated by os.pathsep.

highlight()
Changes color of input frame.

Used to highlight, which required entry is unfilled.

unhighlight()
Sets entry to default color.

class DirEntry(*parent*, *row*, *entry_name_long*, *default*, *help*, *info_text=None*, *warning_text=None*)
Bases: *aquaduct.apps.valveconfig.utils.Entry*

__init__(*parent*, *row*, *entry_name_long*, *default*, *help*, *info_text=None*, *warning_text=None*)
Entry with Entry widget and button to load and append file name to it.

Parameters

- **parent** – Parent of widgets.
- **row** – Row where widgets will be grided.
- **entry_name_long** – Readable entry name.
- **default** – Default values of entry.
- **help** – Text which will be displayed in tooltip.
- **state** – State of widget.

callback_load_dir(*e*)
Callback for selecting dir.

Sets widget content to loaded dir name.

get()
Gets Entry value.

Returns Entry value.

set(*value*)
Sets Entry value.

Parameters **value** – New value of Entry.

class ParenthesedEntry(*parent*, *row*, *entry_name_long*, *input_default*, *control_default*, *help*, *info_text=None*, *warning_text=None*)
Bases: *aquaduct.apps.valveconfig.utils.Entry*

__init__(*parent*, *row*, *entry_name_long*, *input_default*, *control_default*, *help*, *info_text=None*, *warning_text=None*)
Entry with Text widget and button to load and append file names to it.

Parameters

- **parent** – Parent of widgets.
- **row** – Row where widgets will be grided.
- **entry_name_long** – Readable entry name.
- **default** – Default values of entry.
- **help** – Text which will be displayed in tooltip.
- **state** – State of widget.

get()
Gets Entry value.

Returns Value of Entry widget and value of second Entry in parentheses, eg. Value1(Value2).

set(*value*)
Sets Entry value.

Parameters **value** – First value and second value in parentheses or without second value and parentheses.

class WarningIconWidget(*parent*, *text*)
Bases: ttk.Label, object

__init__(*parent*, *text*)
Widget with waring icon and Tooltip information

Parameters

- **parent** – Parent of widget.
- **text** – Content of tooltip

class InfoIconWidget(*parent*, *text*)
Bases: ttk.Label, object

__init__(*parent*, *text*)
Widget with info icon and Tooltip information

Parameters

- **parent** – Parent of widget.
- **text** – Content of tooltip

class HidingFrame(*parent*, *row*, *text*, ***kwargs*)
Bases: ttk.Frame, object

__init__(*parent*, *row*, *text*, ***kwargs*)
Frame that remembers inner row for griding new widgets. Used to keep methods that depends on option menu value.

Parameters

- **parent** – Parent of widget.
- **row** – Row where widgets will be grided.
- **text** – Title of the Frame.
- **kwargs** – Arguments which will be passed to original ttk.Frame widget.

show()
Method to grid Frame with predefinied configuration.

class CallbackWrapper(*callback*, **args*, ***kwargs*)
Bases: object

__init__(*callback*, **args*, ***kwargs*)
Allow to use callbacks with predefined list of arguments.

__call__(*...*) <==> *x(...)*

class ToolTip(*widget*)
Bases: `object`

Code found: http://www.voidspace.org.uk/python/weblog/arch_d7_2006_07_01.shtml

__init__(*widget*)
x.__init__(...) initializes x; see help(type(x)) for signature

static create(*widget*, *text*)

showtip(*text*)

hidetip()

class VerticalScrolledFrame(*parent*, **args*, ***kw*)
Bases: `Tkinter.Frame`

A pure Tkinter scrollable frame that actually works! * Use the 'interior' attribute to place widgets inside the scrollable frame * Construct and pack/place/grid normally * This frame only allows vertical scrolling

__init__(*parent*, **args*, ***kw*)

_bind_mousewheel(*e*)

_unbind_mousewheel(*e*)

Module contents

get_img(*filename*)

Submodules

aquaduct.apps.chord module

color_gen()

hex2rgb(*color*)
Convert HEX color to RGB format. :param color: String hex color. :return: Tuple with RGB values.

polar2point(*angle*, *r*)
Transform polar coordinates to cartesian coordinates. :param angle: Angle. :param r: Radius.

generate_arc(*r*, *sa*, *ea*, *max_angle=5*, *reversed_=False*)
Generate arc vertrices with control points for quadratic Bezier curve.

Parameters

- **r** – Radius
- **sa** – Start angle.
- **ea** – End angle
- **max_angle** – Max. angle for which control point will be calculated. If > 90 curves will be significantly distorted.
- **reversed** – If True vertices will start from ea.

If *ea - sa* > *max_angle*, then *ea - sa* will be divided by *max_angle* into parts and control point will be calculated for each part.

class Node(*r*, *sa*, *ea*, *color*)
Bases: matplotlib.patches.PathPatch

__init__(*r*, *sa*, *ea*, *color*)
Represent data on Chord circle.

Parameters

- **r** – Radius.
- **sa** – Start angle.
- **ea** – End angle.
- **color** – Node color in HEX or matplotlib tuple format.

reserve_arc(*angle*)

get_arc_offset()

class Link(*r*, *sa0*, *sa1*, *ea0*, *ea1*, *color*)
Bases: matplotlib.patches.PathPatch

__init__(*r*, *sa0*, *sa1*, *ea0*, *ea1*, *color*)
Represent connection between two nodes.

Parameters

- **r** – Radius.
- **sa0** – Source start angle.
- **sa1** – Source end angle.
- **ea0** – Destination start angle.
- **ea1** – Destination end angle.
- **color** – Link color in HEX or matplotlib tuple format.

class Arrow(*r*, *sa*, *ea*, *color*, *max_angle=45*)
Bases: matplotlib.patches.PathPatch

__init__(*r*, *sa*, *ea*, *color*, *max_angle=45*)
Arrow patch for links.

Parameters

- **r** – Radius.
- **sa** – Start angle.
- **ea** – End angle.
- **color** – Arrow color in HEX or matplotlib tuple format.
- **max_angle** –

class Chord(*ax*, *r*, *nodes_sizes*, *links*, *labels*, *colors=[]*)
Bases: object

__init__(*ax*, *r*, *nodes_sizes*, *links*, *labels*, *colors=[]*)

Parameters

- **ax** –
- **r** –
- **nodes_sizes** –
- **links** –
- **labels** –

- **colors** –

aquaduct.apps.data module

class GlobalConfigStore
Bases: object

_cachedir = None

_cachemem = False

netcdf = False

nc4 = False

sandwich_import = False

cachetype = 'full'

cachedir

cachemem

class CoordsRangeIndexCache
Bases: object

cache = {}

get_frc(*number*, *rid*)

update_cric(*cric*)

setstate(*state*)

reset()

getstate()

get_cric_reader(*mode='r'*)

save_cric()

load_cric()

class FramesRangeCollection
Bases: object

__init__()
x.__init__(...) initializes x; see help(type(x)) for signature

append(*srange*)

get_ranges(*srange*)

class IterEncoder(*skipkeys=False*, *ensure_ascii=True*, *check_circular=True*, *allow_nan=True*, *sort_keys=False*, *indent=None*, *separators=None*, *encoding='utf-8'*, *default=None*)
Bases: json.encoder.JSONEncoder

default(*o*)
Implement this method in a subclass such that it returns a serializable object for o, or calls the base implementation (to raise a TypeError).

For example, to support arbitrary iterators, you could implement default like this:

```
def default(self, o):
    try:
        iterable = iter(o)
    except TypeError:
        pass
```

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```
    else:
        return list(iterable)
    # Let the base class default method raise the TypeError
    return JSONEncoder.default(self, o)
```

get_object_name(*something*)

get_object_from_name(*name*)

Module contents

aquaduct.geom package

Submodules

aquaduct.geom.cluster module

aquaduct.geom.cluster_available_methods module

get_required_params(*method*)

aquaduct.geom.convexhull module

class SciPyConvexHull(*points*, *inflate=None*, **args*, ***kwargs*)

Bases: scipy.spatial.qhull.ConvexHull

__init__(*points*, *inflate=None*, **args*, ***kwargs*)

x.__init__(...) initializes x; see help(type(x)) for signature

vertices_ids

vertices_points

facets

edges

simplices_vertices

point_within(*point*)

is_point_within_convexhull(*point_chull*)

are_points_within_convexhull(*points*, *chull*)

aquaduct.geom.hdr module

Module performs HDR 2D calculations only with Gaussian Kerneld Density Estimator as impelemented in scipy.stats.

class HDR(*X*, *points=10*, *expand_by=1.0*, *center_of_system=None*)

Bases: object

__init__(*X*, *points=10*, *expand_by=1.0*, *center_of_system=None*)

x.__init__(...) initializes x; see help(type(x)) for signature

cell_area

cell_dimensions

_fraction2indices (*fraction=0.9*)

area_naive (*fraction=0.9*)
This is naive implementation. It calculates are in the space of prepocessed variables. Transformation to normal Cartesian space may not be trivial as details mey depends on the actual location of points.

Parameters **fraction** (*float*) – Fraction of cluster for which are should be estimated.

Return type float

Returns Area of cluster calculated in the preprocessed space.

_square_me (*position*)

area (*fraction=0.9*)

Parameters **fraction** (*float*) – Fraction of cluster for which are should be estimated.

Return type float

Returns Area of cluster calculated in the Cartesian space.

aquaduct.geom.hdr_contour module

Module performs HDR 2D calculations only with Gaussian Kerneld Density Estimator as impelemented in `scipy.stats`.

hdr2contour (*hdr*, *fraction=0.9*)

aquaduct.geom.master module

part2type_dict = {0: 9, 1: 8, 2: 9}
Part number to *GenericPathTypeCodes* dictionary.

parts = (0, 1, 2)
Parts enumerate.

class CTypeSpathsCollectionWorker (*spaths=None*, *ctype=None*, *bias_long=5*, *smooth=None*, *lock=None*)
Bases: `object`

Worker class for averaging spaths in points of master path.

__init__ (*spaths=None*, *ctype=None*, *bias_long=5*, *smooth=None*, *lock=None*)
Core method for averaging spaths in to master path.

Averaging is done in chunks.

Parameters

- **spaths** (*list*) – List of separate paths to average.
- **ctype** (`InletClusterGenericType`) – CType of spaths.
- **bias_long** (*int*) – Bias towards long paths used in `lens_norm()`.
- **smooth** (`Smooth`) – Smoothing method.

coords_types_prob_widths (*sp_slices_*)
Calculates average coordinates, type and width in given chunk.

Parameter `sp_slices_` is tuple of length equal to number of spaths. It contains slices for all spaths respectively. With these slices spaths are cut and **only** resulting chunks are used for calculations.

Therefore, this method average spaths in one point of master math. This point is defined by slices submitted as `sp_lices_` parameter.

Algorithm of averaging (within current chunks of spaths):

1. Coordinates for all spaths are collected.
2. Lengths of all spaths are collected (from cached variables) and kept as lists of lengths equal to chunks' sizes.

   Note: Lengths of collected lengths of spaths are of the same size as coordinates

3. New coordinates are calculated as weighted average of collected coordintates with `numpy.average()`. As weights collected lengths are used.

   Note: Function `numpy.average()` is called with flatten coordinates and lengths.

4. Width of average path is calculated as mean value of flatten coordinates mutual distances.
5. Type of average paths is calculated as probability (frequency) of *scope_name*.

Parameters **sp_slices** (*tuple*) – Slices that cut chunks from all paths.

Return type 3 element tuple

Returns coordinates, type (frequency), and width of averaged spaths in current point

__call__(*nr_sp_slices_*)
Callable interface.

Parameters **nr_sp_slices** (*tuple*) – Two element tuple: nr and sp_slice

class CTypeSpathsCollection(*spaths=None*, *ctype=None*, *bias_long=5*, *pbar=None*, *threads=1*)
Bases: `object`

Object for grouping separate paths that belong to the same CType. Method *get_master_path()* allows for calculation of average path.

parts = (0, 1, 2)
Enumeration of spath parts.

__init__(*spaths=None*, *ctype=None*, *bias_long=5*, *pbar=None*, *threads=1*)

Parameters

- **spaths** (*list*) – List of separate paths.
- **ctype** (`InletClusterGenericType`) – CType of spaths.
- **bias_long** (*int*) – Bias towards long paths used in *lens_norm()*.
- **pbar** – Progress bar object.
- **threads** (*int*) – Number of available threads.

beat()
Touch progress bar, if any.

update()
Update progres bar by one, if any.

lens()
Returns total lengths of all paths.

If ctype in #:# and not 0 and not None then take length of *object* part only.

Returns Total (or *object* part) lengths of all paths.

Return type numpy.ndarray

lens_norm()
Returns normalized lengths calculated by *lens()*.

Applied normalization is twofold:

1. All lengths are divided by maximal length, and
2. All lengths are subjected to pow() function with p = bias_long.

Returns Normalized total (or *object* part) lengths of all paths.

Return type numpy.ndarray

lens_real()
Returns real lengths of all paths.

Returns Sizes of all paths.

Return type list

full_size()
Returns desired size of master path.

Returns Size of master path.

Return type int

static simple_types_distribution(*types*)
Calculates normalized sizes of incoming, object, and outgoing parts of spath using generic types.

It is assumed that spath has object part.

Parameters **types** (*list*) – List of generic types.

Return type 3 element list

Returns Normalized sizes of incomin, object, and outgoing parts.

types_distribution()

Return type numpy.matrix

Returns median values of *simple_types_distribution()* for all spaths.

types_prob_to_types(*types_prob*)
Changes types probabilities as returned by *CTypeSpathsCollectionWorker.coords_types_prob_widths()* to types.

Parameters **types_prob** (*list*) – List of types probabilities.

Return type list

Returns List of *GenericPathTypeCodes*.

get_master_path(*smooth=None*, *resid=(0, 0)*)
Averages spaths into one master path.

This is done in steps:

1. Master path is an average of bunch of spaths. Its length is determined by *full_size()* method.
2. All spaths are then divided in to chunks according to *xzip_xzip()* function with N set to lenght of master path. This results in list of length equal to the length of master path. Elements of this lists are slice objects that can be used to slice spaths in appropriate chunks.
3. Next, for each element of this list *CTypeSpathsCollectionWorker.coords_types_prob_widths()* method is called. Types probabilities are changed to types wiht *types_prob_to_types()*.
4. Finally, all data are used to create appropriate MasterPath. If this fails *None* is returned.

Parameters

- **smooth** (Smooth) – Smoothing method.
- **resid** (*int*) – Residue ID of master path.

Return type *MasterPath*

Returns Average path as *MasterPath* object or *None* if creation of master path failed.

class FakeSingleResidueSelection(*resid*, *frames*, *coords*)
Bases: *aquaduct.traj.sandwich.SingleResidueSelection*

__init__(*resid*, *frames*, *coords*)
x.__init__(...) initializes x; see help(type(x)) for signature

coords(***kwargs*)

coords_smooth(*sranges*, *smooth*)

get_edges()

aquaduct.geom.pca module

class NullPrepocess
Bases: object

__init__()
x.__init__(...) initializes x; see help(type(x)) for signature

build(*X*)

__call__(*...*) <==> *x(...)*

undo(*X*)

class Center
Bases: object

__init__()
x.__init__(...) initializes x; see help(type(x)) for signature

build(*X*)

__call__(*...*) <==> *x(...)*

undo(*X*)

class Normalize
Bases: object

__init__()
x.__init__(...) initializes x; see help(type(x)) for signature

build(*X*)

__call__(*...*) <==> *x(...)*

undo(*X*)

class Standartize
Bases: object

__init__()
x.__init__(...) initializes x; see help(type(x)) for signature

test_polarize_in()

class Polarize(*center=array([0, 0, 0])*, *rvar=0.1*, *equaltf=True*)
Bases: object

__init__(*center=array([0, 0, 0])*, *rvar=0.1*, *equaltf=True*)
Prepocessing filter for 3D cartesian coordinates transformation to spherical coordinates.

Note: Component f is in range 0 - 2pi.

Parameters

- **center** – Center of the hypothetical sphere.
- **rvar** – Desired amount of variance of *r* component measured as fraction of mean *t* and *f* variance.
- **equaltf** – If set `True`, *t* range is scaled to *f*.

_mt

_Xrtf(*X*)

_circle_tf(*t*, *f*)

build(*X*)

__call__(*...*) <==> *x(...)*

undo(*X*)

class PCA(*preprocess=<aquaduct.geom.pca.NullPrepocess object>*)
Bases: `object`

__init__(*preprocess=<aquaduct.geom.pca.NullPrepocess object>*)
x.__init__(...) initializes x; see help(type(x)) for signature

build(*X*)

P

__call__(*...*) <==> *x(...)*

undo(*T*, *pc=None*)

aquaduct.geom.pocket module

get_spc(*sp*, *window=None*)

Parameters

- **sp** – Single path like object or Generic path.
- **window** (*tuple*) – Optional frames window.

Return type numpy.ndarray

Returns Coordinates of path; to be used in pocket calculation.

find_minmax(*spaths*, *pbar=None*)

Parameters

- **spaths** (*list*) – List of single like path objects.
- **pbar** – Optional progress object providing next() method.

Return type 2 element tuple of numpy.ndarray each of shape (3,)

Returns Minimal and maximal boundaries of coordinates used in pocket calulations of spaths.

find_minmax_single(*sp*)

find_minmax_map(*spaths*, *pbar=None*, *map_fun=None*)

Parameters

- **spaths** (*list*) – List of single like path objects.
- **pbar** – Optional progress object providing next() method.

Return type 2 element tuple of numpy.ndarray each of shape (3,)

Returns Minimal and maximal boundaries of coordinates used in pocket calulations of spaths.

find_edges(*spaths*, *grid_size=1.0*, *pbar=None*, *map_fun=None*)

Parameters

- **spaths** (*list*) – List of single like path objects.
- **grid_size** (*float*) – Size of grid cell in A.
- **pbar** – Optional progress object providing next() method.

Return type list of numpy.ndarrays

Returns Edges of bins of grid spanning all submited paths.

class distribution_worker(*edges=None*, *window=None*)

Bases: object

__init__(*edges=None*, *window=None*)

x.__init__(...) initializes x; see help(type(x)) for signature

__call__(*...*) <==> *x(...)*

distribution(*spaths*, *grid_size=1.0*, *edges=None*, *window=None*, *pbar=None*, *map_fun=None*)

Parameters

- **spaths** (*list*) – List of single like path objects.
- **grid_size** (*float*) – Size of grid cell in A.
- **of numpy.ndarrays edges** (*list*) – Edges of bins of grid spanning all submited paths.
- **window** (*tuple*) – Optional frames window.
- **pbar** – Optional progress object providing next() method.

Field list ends without a blank line; unexpected unindent.

:rtype tuple of numpy.ndarrays :return: Coordinates of pocket and number of points.

outer_inner(*H*, *threshold=None*)

Parameters

- **H** (*numpy.ndarray*) – Pocket distribution.
- **threshold** (*float*) – Percent value of max density which will be used to partition pocket into inner and outer.

Returns Indices of outer and inner pocket.

Return type tuple of numpy.ndarray

windows(*frames*, *windows=None*, *size=None*)

sphere_radii(*spaths*, *centers=None*, *radii=None*, *window=None*, *pbar=None*, *map_fun=None*)

class sphere_radius_worker(*window*, *centers*, *radius*)

Bases: object

__init__(*window*, *centers*, *radius*)

x.__init__(...) initializes x; see help(type(x)) for signature

__call__(*...*) <==> *x(...)*

class sphere_radius_worker_lowmem(*window*, *centers*, *radius*)
Bases: object

__init__(*window*, *centers*, *radius*)
x.__init__(...) initializes x; see help(type(x)) for signature

__call__(*...*) <==> *x(...)*

sphere_radius(*spaths*, *centers=None*, *radius=2.0*, *window=None*, *pbar=None*, *map_fun=None*)

class sphere_density_raw_worker(*pbar_queue*, *mol_name*, *radius*, *centers*, *frames*)
Bases: object

__init__(*pbar_queue*, *mol_name*, *radius*, *centers*, *frames*)
Worker used to calculate energy per each trajectory.

Parameters

- **pbar_queue** (class:*aquaduct.clui.SimpleProgressBar*) – Progress bar instance
- **mol_name** (*str*) – Name of molecule which amount will be calculated around points.
- **radius** (*float*) – Radius of selection for each point.
- **centers** (*Iterator*) – Points of path
- **frames** (*Iterator*) – Collection of frame numbers

__call__(*traj_reader*)
Worker

Parameters **traj_reader** (*Iterator*) – Trajectory reader

Returns Array with density for each point

Return type numpy.ndarray

sphere_density_raw(*trajs*, *mol_name*, *centers*, *radius*, *pool*, *window=None*, *pbar=None*)
Calculate density of sphere with specified radius and with center in each point.

Parameters

- **trajs** (class:*aquaduct.sandwich.ReaderTraj*) – Collection of trajectory readers
- **mol_name** (*str*) – Name of molecule which amount will be calculated around points.
- **radius** (*float*) – Radius of selection for each point.
- **centers** (*Iterator*) – Points of path
- **pool** (*Preconfigured Pool instance*) – Preconfigured Pool instance

Returns Density for each center.

Return type numpy.ndarray

hot_spots(*H*)

hot_spots_his(*H*, *bins=(5, 101)*)

aquaduct.geom.smooth module

Smooth module defines methods for smoothing of trajectories.

Available methods:

SavgolSmooth	Savitzky-Golay based smoothing.
WindowSmooth	Defined size window smoothing.

Continued on next page

Table 1 – continued from previous page

DistanceWindowSmooth	Distance defined size window smoothing.
ActiveWindowSmooth	Active size window smoothing.
MaxStepSmooth	Maximal step smoothing.
WindowOverMaxStepSmooth	Window smoothing over maximal step smoothing.
DistanceWindowOverMaxStepSmooth	Distance window smoothing over maximal step smoothing.
ActiveWindowOverMaxStepSmooth	Active window smoothing over maximal step smoothing.

class Smooth(*recursive=None*, ***kwargs*)

Bases: object

Base class for all smoothing methods.

__init__(*recursive=None*, ***kwargs*)

Parameters **recursive** (*int*) – Number of recursions of the method, everything evaluated to False is equivalent to 1.

smooth(*coords*)

Abstract method for smoothing method implementation.

Parameters **coords** (*Iterable*) – Input coordinates to be smoothed.

__call__(*coords*)

Call method for all smoothing methods.

Input coordinates should be iterable and each element should be numpy.ndarray. If length of coords is less then 3 smoothing method is not run and coordinates are returned unchanged.

If recursive is set smoothing method is applied appropriate number of times.

Parameters **coords** (*Iterable*) – Input coordinates to be smoothed.

Return type numpy.ndarray

Returns Smoothed coordinates.

class GeneralWindow(*fun=<function mean>*, ***kwargs*)

Bases: object

Base class for window based smoothing methods.

__init__(*fun=<function mean>*, ***kwargs*)

Parameters **fun** (*function*) – Function to be used for averaging coordinates within a window.

static max_window_at_pos(*pos*, *size*)

Method returns maximal possible window at given position of the list with given size of the list. Returned window fits in to the list of given size and is symmetrical.

Parameters

- **pos** (*int*) – Position in question.
- **size** (*int*) – Length of the list.

Return type 2 element tuple of int

Returns Lowest possible bound and highest possible bound of the window.

check_bounds_at_max_window_at_pos(*lb*, *ub*, *pos*, *size*)

Method checks if window fits in to maximal possible window calculated according to *max_window_at_pos()*. If not window is corrected.

Parameters

- **lb** (*int*) – Lower bound of the window in question.

- **ub** (*int*) – Upper bound of the window in question.
- **pos** (*int*) – Position in question.
- **size** (*int*) – Length of the list.

Return type 2 element tuple of int

Returns Lowest possible bound and highest possible bound of the window corrected to maximal possible window.

class IntWindow(*window=5*, ***kwargs*)

Bases: *aquaduct.geom.smooth.GeneralWindow*

Base class for all window smoothing methods that require integer window.

__init__(*window=5*, ***kwargs*)

Parameters **window** (*int*) – One side size of the window.

class FloatWindow(*window=5.0*, ***kwargs*)

Bases: *aquaduct.geom.smooth.GeneralWindow*

Base class for all window smoothing methods that require float window.

__init__(*window=5.0*, ***kwargs*)

Parameters **window** (*float*) – Size of the window.

class WindowSmooth(***kwargs*)

Bases: *aquaduct.geom.smooth.Smooth*, *aquaduct.geom.smooth.IntWindow*

Defined size window smoothing.

For each coordinate a symmetrical (if possible) window of size defined by `window` is created. In case of coordinates at the edges created window is truncated to the edges. Next, all coordinates within the window are averaged with a function defined by `function`. Resulting value(s) are the smoothed coordinates.

__init__(***kwargs*)

Parameters **recursive** (*int*) – Number of recursions of the method, everything evaluated to `False` is equivalent to 1.

smooth(***kwargs*)

Parameters **coords** (*Iterable*) – Input coordinates to be smoothed.

class DistanceWindowSmooth(***kwargs*)

Bases: *aquaduct.geom.smooth.Smooth*, *aquaduct.geom.smooth.FloatWindow*

Distance defined size window smoothing.

This is modification of *WindowSmooth* method. The difference is in the definition of the window size. Here, it is an average distance between points of input coordinates. Thus, before smoothing average distance between all points is calculated and this value is used to calculate actual window size.

Next, for each coordinate a symmetrical (if possible) window of size calculated in the first step is created. In case of coordinates at the edges created window is truncated to the edges. Next, all coordinates within the window are averaged with a function defined by `function`. Resulting value(s) are the smoothed coordinates.

__init__(***kwargs*)

Parameters **recursive** (*int*) – Number of recursions of the method, everything evaluated to `False` is equivalent to 1.

smooth(***kwargs*)

Parameters **coords** (*Iterable*) – Input coordinates to be smoothed.

class ActiveWindowSmooth(***kwargs*)
Bases: *aquaduct.geom.smooth.Smooth*, *aquaduct.geom.smooth.FloatWindow*

Active size window smoothing.

Similarly to *DistanceWindowSmooth* method the window size is defined as a distance. The difference is that the actual window size is calculated for each point separately. Thus, for each coordinate the window is calculated by examining the distance differences between points. In this method window is not necessarily symmetrical. Once window is calculated all coordinates within the window are averaged with a function defined by `function`. Resulting value(s) are the smoothed coordinates.

__init__(***kwargs*)

Parameters **recursive** (*int*) – Number of recursions of the method, everything evaluated to `False` is equivalent to 1.

smooth(***kwargs*)

Parameters **coords** (*Iterable*) – Input coordinates to be smoothed.

class MaxStepSmooth(*step=1.0*, ***kwargs*)
Bases: *aquaduct.geom.smooth.Smooth*

Maximal step smoothing.

This method moves thorough coordinates and calculates distance over the traversed path. If it is then `step` the coordinate is used as a "cardinal point". The beginning and the end of the path are also added to the list of cardinal points. Next, all cardinal points and points of linear interpolation between cardinal points are returned as smoothed coordinates. Number of interpolated points is in accordance to points skipped between cardinal points.

__init__(*step=1.0*, ***kwargs*)

Parameters **recursive** (*int*) – Number of recursions of the method, everything evaluated to `False` is equivalent to 1.

smooth(***kwargs*)

Parameters **coords** (*Iterable*) – Input coordinates to be smoothed.

class SavgolSmooth(*window_length=5*, *polyorder=2*, ***kwargs*)
Bases: *aquaduct.geom.smooth.Smooth*

Savitzky-Golay based smoothing.

Method uses 1D filter available in SciPy, see `savgol_filter()`. For each dimension filter is applied separately. Only `window_length` and `polyorder` attributes are used.

__init__(*window_length=5*, *polyorder=2*, ***kwargs*)

Param int window_length: Size of the window, odd number.

Param int polyorder: Polynomial order.

set_savgol_function()

smooth(***kwargs*)

Parameters **coords** (*Iterable*) – Input coordinates to be smoothed.

class WindowOverMaxStepSmooth(***kwargs*)
Bases: *aquaduct.geom.smooth.Smooth*

Window smoothing over maximal step smoothing.

First, *MaxStepSmooth* is applied, and then *WindowSmooth*.

__init__(***kwargs*)

Parameters **recursive** (*int*) – Number of recursions of the method, everything evaluated to `False` is equivalent to 1.

smooth(*coords*)

Parameters **coords** (*Iterable*) – Input coordinates to be smoothed.

class ActiveWindowOverMaxStepSmooth(***kwargs*)
Bases: *aquaduct.geom.smooth.Smooth*

Active window smoothing over maximal step smoothing.

First, *MaxStepSmooth* is applied, and then *ActiveWindowSmooth*.

__init__(***kwargs*)

Parameters **recursive** (*int*) – Number of recursions of the method, everything evaluated to `False` is equivalent to 1.

smooth(*coords*)

Parameters **coords** (*Iterable*) – Input coordinates to be smoothed.

class DistanceWindowOverMaxStepSmooth(***kwargs*)
Bases: *aquaduct.geom.smooth.Smooth*

Distance window smoothing over maximal step smoothing.

First, *MaxStepSmooth* is applied, and then *DistanceWindowSmooth*.

__init__(***kwargs*)

Parameters **recursive** (*int*) – Number of recursions of the method, everything evaluated to `False` is equivalent to 1.

smooth(*coords*)

Parameters **coords** (*Iterable*) – Input coordinates to be smoothed.

aquaduct.geom.traces module

diff(*trace*)
This function calculates the distance between 2 given points.

Parameters **trace** – coordinates in numpy array object

Returns distance between points

tracepoints(*start*, *stop*, *nr*)

Parameters

- **start** – coordinates of the first point as a numpy array object
- **stop** – coordinates of the second point as a numpy array object
- **nr** – number of elements between the first and second point

Returns two-dimentional numpy array; number of dimentions depends on nr parameter

midpoints(*paths*)

The function returns a tuple of numpy arrays extended with mid point spanning last and first element(column) of these arrays.

Parameters **paths** – a tuple of 2-dimentional np.arrays that hold 3D coordinates; each element holds one trace, all elements are supposed to make one path divided in to sections

Returns paths elements with additional mid points as a generator object

length_step_std(*trace*)
This function calculates sum, mean and standard deviation from all segments of a trace.

Parameters **trace** – coordinates of points as numpy array

Returns a tuple with basics statistics of a trace

derrivative(*values*)

vector_one(*V*)

Parameters **V** – a vector in a form of array-like object, tuple or a list

Returns vector in the same direction but of lenght 1

project_p_on_ab(*p*, *a*, *b*)

Parameters

- **p** – a point to be projected on AB line
- **a** – beginning of AB line
- **b** – end of AB line

Returns point on AB line being a projection of p

distance_p_to_ab(*p*, *a*, *b*)

Parameters

- **p** – a point of interest
- **a** – beginning of AB line
- **b** – end of AB line

Returns distance of p to AB line

is_p_above_vp0_plane(*p*, *v*, *p0*)

Parameters

- **p** – a point of interest
- **v** – vector pointing perpendicularly up from the plane perspective
- **p0** – point on the plane

Returns >0 if p point is above the plane, 0 if it is on the plane, and <0 if it is below the plane

vector_change_len(*V*, *l*)

Parameters

- **V** – a vector in a form of array-like object, tuple or a list
- **l** (*float*) – lenght by wich vectro should be increased (decreased if negative)

Returns vector in the same direction but of altered lenght

vector_norm(*V*)

Parameters **V** – a vector in a form of array-like object, tuple or a list

Returns normalized length of a vector

triangle_angles(*A*, *B*, *C*)

Parameters are coordinates of points which are tops of triangle. The function calculates angles in a triangle formed by given coordinates.

Parameters

- **A** – coordinates of the first point
- **B** – coordinates of the second point
- **C** – coordinates of the third point

Returns list of arguments where angle is given in radians , the output is as follow: [BAC,CAB,ABC]

triangle_angles_last(*A*, *B*, *C*)
Parameters are coordinates of points which are tops of triangle. The function calculates the [ABC] angle.

Parameters

- **A** – coordinates of the first point [A top]
- **B** – coordinates of the second point [B top]
- **C** – coordinates of the third point [C top]

Returns list with one value of ABC angle in radians

triangle_height(*A*, *B*, *C*)
Parameters are coordinates of points which are tops of triangle. The function calculates the ABC triangle height.

Parameters

- **A** – coordinates of the first point [A top]
- **B** – coordinates of the second point [B top]
- **C** – coordinates of the third point [C top]

Returns one value of ABC triangle height

vectors_angle(*A*, *B*)
This function calculates the angle between two given vectors (starting from the [0,0,0] to the given coordinates.

Parameters

- **A** – coordinates of the first point which is the end of the vector
- **B** – coordinates of the second point which is the end of the vector

Returns the angle between vectors in question (in radians)

vectors_angle_alt(*A*, *B*)
This function calculates the angle between two given vectors (starting from the [0,0,0] to the given coordinates

- alternative method.

Parameters

- **A** – coordinates of the first point which is the end of the vector
- **B** – coordinates of the second point which is the end of the vector

Returns the angle between vectors in question (in radians)

vectors_angle_alt_anorm(*A*, *B*, *A_norm*)

This function calculates the angle between two given vectors (starting from the [0,0,0] to the given coordinates

- alternative method with additional A_norm holding norm of A.

Parameters

- **A** – coordinates of the first point which is the end of the vector
- **B** – coordinates of the second point which is the end of the vector
- **A_norm** – additional parameter holding normalized of vector A

Returns the angle between vectors in question (in radians)

vectors_angle_anorm(*A*, *B*, *A_norm*)

This function calculates the angle between two given vectors (starting from the [0,0,0] to the given coordinates using additional A_norm holding norm of A.

Parameters

- **A** – coordinates of the first point which is the end of the vector
- **B** – coordinates of the second point which is the end of the vector
- **A_norm** – additional parameter holding normalized of vector A

Returns the angle between vectors in question (in radians)

triangle_area(*A*, *B*, *C*)

Parameters are coordinates of points which are tops of triangle. The function calculates the ABC triangle area with Heron's formula.

Parameters

- **A** – coordinates of the first point [A top]
- **B** – coordinates of the second point [B top]
- **C** – coordinates of the third point [C top]

Returns area

Return type float

square_area(*A*, *B*, *C*, *D*)

Parameters are coordinates of points which are tops of square. The function estimates the ABCD square area by calculating areas of triangles that make up the square.

Parameters

- **A** – coordinates of the first point [A top]
- **B** – coordinates of the second point [B top]
- **C** – coordinates of the third point [C top]
- **D** – coordinates of the fourth point [D top]

Returns area

Return type float

class LinearizeOneWay

Bases: object

here(*coords*)

This function simplifies the trace by removing the redundant, linear points :param coords: 3D coordinates of a trace as an array-like object :return: indices of coordinates which are a staring and ending points of linear fragments and other non-linear points of the trace

class LinearizeHobbit

Bases: *aquaduct.geom.traces.LinearizeOneWay*

and_back_again(*coords*)

__call__(*...*) <==> *x(...)*

class LinearizeRecursive

Bases: object

Base class for linearization methods classes.

It implements recursive algorithm.

here(*coords*, *depth=0*)
Core of recursive linearization argorithm.

It checks if the first, the last and the middle point are linear according to the criterion. The middle point is a selected point that is in the middle of length of the paths made by input coordinates.

If these points are linear their indices are returned. Otherwise, coordinates are split into two parts. First part spans points from the first point to the middle point (inclusive) and the second part spans points from the middle (inclusive) to the last point. Next, these two parts are submitted recursively to *here()*.

Results of these recursive calls are joined, redundant indices are removed and sorted result is returned.

Parameters

- **coords** (*numpy.ndarray*) – Input coordinates.
- **depth** (*int*) – Depth of recurence.

Returns Indices of `coords` points that can be used instead of all points in visulatization.

Return type list of int

__call__(*...*) <==> *x(...)*

class TriangleLinearize(*threshold=0.01*)
Bases: `object`

__init__(*threshold=0.01*)
x.__init__(...) initializes x; see help(type(x)) for signature

is_linear(*coords*, ***kwargs*)

class VectorLinearize(*treshold=0.05236*)
Bases: `object`

Base class for linearization methods classes.

It implements vector linearization criterion.

__init__(*treshold=0.05236*)
x.__init__(...) initializes x; see help(type(x)) for signature

is_linear_core(*coords*, *depth=None*)
Method checks if input coordinates are linear according to the threshold and depth.

It begins with calculation of the threshold. If *depth* is None it is set to 1. Current threshold is calculated with following simple equation:

$$threshold_{current} = threshold_{initial} * (2 - 0.9^{depth})$$

Next, in a loop over all points but the first and the last the angle is calculated between two vectors. The first one made by the point and the first point, and the second vector made by the last and the first point. If any of the calculated angles is bigger the the treshold methods returns False; otherwise method returns True.

Parameters

- **coords** (*numpy.ndarray*) – Coordinates for which linearization criterion is checked.
- **depth** (*int*) – Depth of recurence.

Returns True if input coordinates are linear and False otherwise.

Return type bool

is_linear(*coords*, *depth=None*, ***kwargs*)
For more detail see *is_linear_core()* which is used as the criterion of linearity in this method.

Parameters

- **coords** (*numpy.ndarray*) – Coordinates for which linearization criterion is checked.
- **depth** (*int*) – Depth of recurence.

Returns True if input coordinates are linear and False otherwise. Criterion is checked for coordinates in normal and reverse order.

Return type bool

class LinearizeRecursiveVector(*treshold=0.05236*)

Bases: *aquaduct.geom.traces.LinearizeRecursive*, *aquaduct.geom.traces.VectorLinearize*

Class provides recursive linearization of coordinates with *LinearizeRecursive* algorithm and the criterion of linearity implemented by *VectorLinearize*. This is default method.

class LinearizeRecursiveTriangle(*threshold=0.01*)

Bases: *aquaduct.geom.traces.LinearizeRecursive*, *aquaduct.geom.traces.TriangleLinearize*

Class provides recursive linearization of coordinates with *LinearizeRecursive* algorithm and the criterion of linearity implemented by *TriangleLinearize*.

class LinearizeHobbitVector(*treshold=0.05236*)

Bases: *aquaduct.geom.traces.LinearizeHobbit*, *aquaduct.geom.traces.VectorLinearize*

Class provides recursive linearization of coordinates with *LinearizeHobbit* algorithm and the criterion of linearity implemented by *VectorLinearize*.

class LinearizeHobbitTriangle(*threshold=0.01*)

Bases: *aquaduct.geom.traces.LinearizeHobbit*, *aquaduct.geom.traces.TriangleLinearize*

Class provides recursive linearization of coordinates with *LinearizeHobbit* algorithm and the criterion of linearity implemented by *TriangleLinearize*.

class LinearizeOneWayVector(*treshold=0.05236*)

Bases: *aquaduct.geom.traces.LinearizeOneWay*, *aquaduct.geom.traces.VectorLinearize*

Class provides recursive linearization of coordinates with *LinearizeOneWay* algorithm and the criterion of linearity implemented by *VectorLinearize*.

class LinearizeOneWayTriangle(*threshold=0.01*)

Bases: *aquaduct.geom.traces.LinearizeOneWay*, *aquaduct.geom.traces.TriangleLinearize*

Class provides recursive linearization of coordinates with *LinearizeOneWay* algorithm and the criterion of linearity implemented by *TriangleLinearize*.

Module contents

class Sphere

Bases: *aquaduct.geom.Sphere*

Simple sphere class.

is_point_within(*point*)

is_sphere_within(*sphere*)

is_sphere_cloud(*sphere*)

do_cut_thyself(*spheres_passed*, *progress=False*)

aquaduct.traj package

Submodules

aquaduct.traj.barber module

Module implements AutoBarber generation of spheres.

spaths2spheres(**args*, ***kwargs*)

inlets2spheres(**args*, ***kwargs*)

class WhereToCut(*spaths=None*, *inlets=None*, *expected_nr_of_spaths=None*, *selection=None*, *mincut=None*, *mincut_level=False*, *maxcut=None*, *maxcut_level=False*, *tovdw=False*, *forceempty=False*)

Bases: *aquaduct.traj.sandwich.ReaderAccess*

Class implements method for creating (optimal) set of AutoBarber spheres for a collection of spaths; access to trajectory is also required to read VdW radii.

__init__(*spaths=None*, *inlets=None*, *expected_nr_of_spaths=None*, *selection=None*, *mincut=None*, *mincut_level=False*, *maxcut=None*, *maxcut_level=False*, *tovdw=False*, *forceempty=False*)

Parameters

- **spaths** (*list*) – List of *aquaduct.traj.paths.SinglePath* objects.
- **expected_nr_of_spaths** (*int*) – Number of spaths passed. Requilred when length of spaths cannod be calculated, eg when it is a generator.
- **selection** (*str*) – Selection string of molecular object used for spheres generation.
- **mincut** (*float*) – Value of *mincut* parameter.
- **maxcut** (*float*) – Value of *maxcut* parameter.
- **mincut_level** (*bool*) – Flag of *mincut_level*.
- **maxcut_level** (*bool*) – Flag of *maxcut_level*.
- **tovdw** (*bool*) – Flag of to VdW radii correction parameter.
- **forceemtpy** (*bool*) – If set *True* spheres of radius 0 are returned if no other sphere can be generated.

check_minmaxcuts()

add_spheres_from_spaths(*spaths*)

add_spheres_from_inlets(*inlets*)

get_current_nr()

inlet2sphere(*inlet*)

spath2spheres(*sp*)

cut_thyself()

is_overlaping_with_cloud(*sphere*)

cloud_groups(*progress=False*)

barber_with_spheres(*coords*, *spheres*)

param numpy.ndarray coords: Path's coordinates subjected to barber procedure. param spheres: Spheres used to cut input coordinates. rtype: *numpy.ndarray*. return: List of indices to be kept.

barber_with_spheres_big_matrix(*coords*, *spheres*)

barber_paths(**args*, ***kwargs*)

aquaduct.traj.dumps module

class WriteMOL2(*mol2file*, *mode='w'*)
Bases: object

__init__(*mol2file*, *mode='w'*)
x.__init__(...) initializes x; see help(type(x)) for signature

print_atom_line(*xyz*, *bf*)

print_bond_line(*bid*, *ba*, *bb*, *btype='1'*)

write_scatter(*scatter*, *bf*)

write_connected(*scatter*, *bf*)

__enter__()

__exit__(*typ*, *value*, *traceback*)

__del__()

class WritePDB(*pdbfile*, *csvfile=None*, *scale_bf=1*)
Bases: object

__init__(*pdbfile*, *csvfile=None*, *scale_bf=1*)
x.__init__(...) initializes x; see help(type(x)) for signature

print_atom_line(*xyz*, *bf*)

print_conect_line(*a1*, *a2*)

write_connected(*line*, *bf*)

next_model()

write_scatter(*scatter*, *bf*)

__enter__()

__exit__(*typ*, *value*, *traceback*)

__del__()

aquaduct.traj.inlets module

class ProtoInletTypeCodes
Bases: object

surface = 'surface'

internal = 'internal'

incoming = 'inin'

outgoing = 'inout'

class InletTypeCodes
Bases: *aquaduct.traj.inlets.ProtoInletTypeCodes*

all_surface = (('surface', 'inin'), ('surface', 'inout'))

all_internal = (('internal', 'inin'), ('internal', 'inout'))

all_incoming = (('surface', 'inin'), ('internal', 'inin'))

all_outgoing = (('surface', 'inout'), ('internal', 'inout'))

surface_incoming = ('surface', 'inin')

internal_incoming = ('internal', 'inin')

internal_outgoing = ('internal', 'inout')

surface_outgoing = ('surface', 'inout')

class InletClusterGenericType(*inp*, *out*)
Bases: object

__init__(*inp*, *out*)
x.__init__(...) initializes x; see help(type(x)) for signature

input

output

static cluster2str(*cl*)

__getitem__(*item*)

__len__()

__str__() <==> *str(x)*

__repr__() <==> *repr(x)*

make_val(*base*)

__cmp__(*other*)

__hash__() <==> *hash(x)*

class InletClusterExtendedType(*surfin*, *interin*, *interout*, *surfout*)
Bases: *aquaduct.traj.inlets.InletClusterGenericType*

__init__(*surfin*, *interin*, *interout*, *surfout*)
x.__init__(...) initializes x; see help(type(x)) for signature

generic

class Inlet(*coords=None*, *inlet_type=None*, *reference=None*, *frame=None*)
Bases: object

__init__(*coords=None*, *inlet_type=None*, *reference=None*, *frame=None*)
x.__init__(...) initializes x; see help(type(x)) for signature

class Inlets(*spaths*, *center_of_system=None*, *onlytype=(('surface', 'inin'), ('surface', 'inout'))*, *passing=False*, *pbar=None*)
Bases: object

__init__(*spaths*, *center_of_system=None*, *onlytype=(('surface', 'inin'), ('surface', 'inout'))*, *passing=False*, *pbar=None*)
x.__init__(...) initializes x; see help(type(x)) for signature

__iter__()

add_leaf_wrapper(*name=None*, *message=None*, *toleaf=None*)

resize_leaf_0()

add_message_wrapper(*message=None*, *toleaf=None*)

extend_inlets(*spath*, *onlytype=None*)

add_cluster_annotations(*clusters*)

add_outliers_annotations(*new_clusters*)

add_spheres(*spheres*)

get_inlets_references()

size

coords

types

refs

refs_names

call_clustering_method(*method*, *data*, *spheres=None*)

get_flat_tree(*message=None*)

perform_clustering(*method*)

perform_reclustering(*method*, *skip_outliers=False*, *skip_size=None*)

recluster_cluster(*method*, *cluster*)

recluster_outliers(*method*)

remove_inlets(*cluster*)

small_clusters_to_outliers(*maxsize*)

renumber_clusters()

sort_clusters()

clusters_list

clusters_centers

clusters_size

join_clusters(*clusters2join*)

clusters_std

spaths2ctypes(***kwargs*)

spath2ctype(*sp*)

lim_to(*what*, *towhat*)

lim2spaths(*spaths*)

lim2rnames(*rnames*)

lim2types(*types*)

lim2clusters(*clusters*)

limspaths2(***kwargs*)

get_chull()

aquaduct.traj.paths module

class PathTypesCodes

Bases: object

__slots__ = ()

path_in_code = 1

path_object_code = 2

path_out_code = 3

path_walk_code = 0

class GenericPathTypeCodes

Bases: object

__slots__ = ()

object_name = 8

scope_name = 9

out_name = 10

class GenericPaths(*id_of_res*, *name_of_res=None*, *min_pf=None*, *max_pf=None*)

Bases: *aquaduct.traj.paths.GenericPathTypeCodes*

__slots__ = ['id', 'single_res_selection', 'name', '_types', '_frames', 'max_possibl

__init__(*id_of_res*, *name_of_res=None*, *min_pf=None*, *max_pf=None*)

x.__init__(...) initializes x; see help(type(x)) for signature

id

single_res_selection

name

_types

_frames

max_possible_frame

min_possible_frame

update_types_frames(*types*, *frames*)

__getstate__()

__setstate__(*state*)

types

types_promise

frames_of_object

frames_of_scope

frames

_frames_sr

discard_singletons(*singl=1*, *skiptype=8*)

coords

max_frame

min_frame

add_foos(*foo*, *fos*)

add_012(*os_in_frames*, *reset=False*)

add_object(*frame*)

add_scope(*frame*)

add_type(*frame*, *ftype*)

add_frames_types(*frames*, *types*)

_gpt()

_gpo(*frames_sr*)

_gpi(*frames_sr*)

find_paths (*fullonly=False*)

find_paths_types (*fullonly=False*, *passing=None*)

get_path_cont_types (*path_cont*)

get_single_path_types (*spath*)

barber_with_spheres (*spheres*)

class SinglePathID (*path_id=None*, *nr=None*, *name=None*)

Bases: object

__slots__ = ['id', 'nr', 'name']

__init__ (*path_id=None*, *nr=None*, *name=None*)

x.__init__(...) initializes x; see help(type(x)) for signature

id

nr

name

__getstate__ ()

__setstate__ (*state*)

__str__ () <==> *str(x)*

__eq__ (*other*)

x.__eq__(y) <==> x==y

yield_single_paths (**args*, ***kwargs*)

correct_spaths_ids (*spaths*, *pbar*)

yield_generic_paths (*spaths*, *progress=None*)

class MacroMolPath (*path_id*, *paths*, *types*)

Bases: *aquaduct.traj.paths.PathTypesCodes*, *aquaduct.traj.inlets.InletTypeCodes*

__slots__ = ['id', '_path_in', '_path_object', '_path_out', '_types_in', '_types_obj

empty_coords = array([], shape=(0, 3), dtype=float64)

__init__ (*path_id*, *paths*, *types*)

x.__init__(...) initializes x; see help(type(x)) for signature

id

single_res_selection

_path_in

_path_object

_path_out

_types_in

_types_object

_types_out

_object_len

__getstate__ ()

__setstate__ (*state*)

add_paths4 (*path_in*, *path_object*, *path_object_strict*, *path_out*)

_object_len_calculate ()

object_len

is_single()

is_passing()

is_frame_in(*frame*)

is_frame_object(*frame*)

is_frame_out(*frame*)

is_frame_walk(*frame*)

path_in

path_object

path_object_strict_len

path_out

types_in

types_object

types_out

coords_first_in

paths_first_in

coords_last_out

paths_last_out

coords_filo

get_inlets()

remove_inlet(*inlet_type*)

coords_in

coords_object

coords_object_strict

center_of_object

coords_out

coords

coords_cont

_paths

paths

paths_cont

types

types_cont

gtypes

gtypes_cont

etypes

etypes_cont

size

sizes

begins

ends

has_in

has_object

has_out

get_coords(***kwargs*)

_make_smooth_coords(*smooth*)

get_coords_cont(*smooth=None*)

get_distance_cont(*smooth=None*, *normalize=False*)

get_distance_rev_cont(**args*, ***kwargs*)

get_distance_both_cont(***kwargs*)

get_velocity_cont(***kwargs*)

get_acceleration_cont(***kwargs*)

class SinglePath(*path_id*, *paths*, *types*)

Bases: *aquaduct.traj.paths.MacroMolPath*

is_single()

is_passing()

class PassingPath(*path_id*, *paths*, *types*)

Bases: *aquaduct.traj.paths.MacroMolPath*

__slots__ = ['_has_in_flag', '_has_out_flag']

__init__(*path_id*, *paths*, *types*)

x.__init__(...) initializes x; see help(type(x)) for signature

_has_in_flag

_has_out_flag

__getstate__()

__setstate__(*state*)

is_single()

is_passing()

has_in

has_out

coords_first_in

paths_first_in

coords_last_out

paths_last_out

types

get_inlets()

remove_inlet(*inlet_type*)

class MasterPath(*sp*, *single_res_selection=None*)

Bases: *aquaduct.traj.paths.MacroMolPath*

__slots__ = ['width_cont']

__init__(*sp*, *single_res_selection=None*)
x.__init__(...) initializes x; see help(type(x)) for signature

width_cont

add_width(*width*)

__getstate__()

__setstate__(*state*)

aquaduct.traj.sandwich module

mda_ver()

class Window(*start*, *stop*, *step*)
Bases: object

__init__(*start*, *stop*, *step*)
x.__init__(...) initializes x; see help(type(x)) for signature

static _none_or_int(*nr*)

__repr__() <==> *repr(x)*

correct(*real_frame_no*)

range(*reverse=False*)

get_real(*frame*)

len()

split(*slices=None*)

class OpenReaderTraj
Bases: *aquaduct.traj.sandwich.OpenReaderTraj*

open()

class MasterReader
Bases: object

open_reader_traj = {}

topology = ['']

trajectory = ['']

window = None

sandwich_mode = None

engine_name = 'mda'

threads = 1

threads_multiply = 1

edges = []

__del__()

__call__(*topology*, *trajectory*, *window=None*, *sandwich=False*, *threads=1*)

Parameters

- **topology** (*list*) – List of topologies. Each element is a file name.
- **trajectory** (*list*) – List of trajectories. Each element is a file name.
- **window** (Window) – Frames window to read.

- **sandwich** (*bool*) – Flag for setting sandwitch mode.

If no sandiwch mode is used, number of topologies has to be precisely 1. In sandwich mode it can be either 1 or equal to the nuber of trajectory files.

reset()

__getstate__()

__setstate__(*state*)

engine(*topology*, *trajectory*, *number*, *window*)

Parameters

- **topology** (*str*) – Topology file name.
- **trajectory** (*list*) – List of trajectories. Each element is a file name. Alternatively, trajectory file name.
- **number** (*int*) – Number of the layer.
- **window** (Window) – Frames window.

Returns

__repr__(*) <==> *repr(x)*

sandwich(*number=False*)

baguette(*number=False*)

strata(*number=False*)

iterate(*number=False*, *threads=True*)

get_single_raw_reader_per_trajectory(*number*)

get_single_reader(*number*)

get_reader_by_id(*someid*)

real_number_of_frames()

get_edges()

number_of_frames(*onelayer=False*)

number_of_layers()

open_traj_reader_engine(*ort*)

open_traj_reader(*ort*)

class ReaderAccess

Bases: object

get_reader(*number*)

get_reader_by_id(*someid*)

get_edges()

VdW_radii = {'ac': 2.47, 'ag': 2.11, 'al': 1.84, 'am': 2.44, 'ar': 1.88, 'as': 1.8

Dictionary of VdW radii.

Data taken from L. M. Mentel, mendeleev, 2014. Available at: https://bitbucket.org/lukaszmentel/mendeleev. Package **mendeleev** is not used because it depends on too many other libraries.

class ReaderTraj(*topology*, *trajectory*, *number=None*, *window=None*)

Bases: object

__init__(*topology*, *trajectory*, *number=None*, *window=None*)

Parameters

- **topology** (*str*) – Topology file name.
- **trajectory** (*list*) – Trajectory file name.
- **number** (*int*) – Number of trajectory file.
- **window** (Window) – Frames window to read.
- **reader** (*Reader*) – Parent reader object.

This is base class for MD data access engines.

__repr__(*) <==> *repr(x)*

iterate_over_frames(*reverse=False*)

iterate(*reverse=False*)

set_frame(*frame*)

dump_frames(*frames*, *selection=None*, *filename=None*)

__del__()

number_of_frames()

open_trajectory()

close_trajectory()

set_real_frame(*real_frame*)

real_number_of_frames()

parse_selection(*selection*)

select_all()

atom_vdw(*atomid*)

atom2residue(*atomid*)

atoms_positions(*atomids*)

residues_positions(*resids*)

residues_names(*resids*)

atoms_masses(*atomids*)

dump_frames_to_file(*frames*, *selection*, *filename*)

class ReaderTrajViaMDA(*topology*, *trajectory*, *number=None*, *window=None*)

Bases: *aquaduct.traj.sandwich.ReaderTraj*

open_trajectory()

close_trajectory()

set_real_frame(*real_frame*)

parse_selection(*selection*)

select_all()

atom2residue(*atomid*)

atoms_positions(*atomids*)

residues_positions(*resids*)

residues_names(*resids*)

real_number_of_frames()

atoms_masses(*atomids*)

atom_vdw(*atomid*)

dump_frames_to_file(*frames*, *selection*, *filename*)

class Selection(*selected*)
Bases: *aquaduct.traj.sandwich.ReaderAccess*

__init__(*selected*)
x.__init__(...) initializes x; see help(type(x)) for signature

layer(*number*)

numbers()

ix(*ix*)

single(*selection_id*)

len()

__len__()

add(*other*)

remove(*other*)
Remove all items that exist in other selection.

Parameters **other** – Other selection.

uniquify()

ids()

coords()

center_of_mass()

class AtomSelection(*selected*)
Bases: *aquaduct.traj.sandwich.Selection*

vdw()

residues()

coords()

center_of_mass()

contains_residues(*other_residues*, *convex_hull=False*, *convex_hull_inflate=None*, *map_fun=None*, *known_true=None*)

containing_residues(*other_residues*, **args*, ***kwargs*)

chull(*inflate=None*)

class ResidueSelection(*selected*)
Bases: *aquaduct.traj.sandwich.Selection*

coords()

names()

single_residues()

coords_range_core(**args*, ***kwargs*)

coords_range(**args*, ***kwargs*)

smooth_coords_ranges(**args*, ***kwargs*)

class SingleResidueSelection(*resid*)
Bases: *aquaduct.traj.sandwich.ReaderAccess*

__init__(*resid*)
x.__init__(...) initializes x; see help(type(x)) for signature

coords (*frames*)

_coords (***kwargs*)

coords_smooth (*sranges*, *smooth*)

Module contents

aquaduct.utils package

Submodules

aquaduct.utils.clui module

Module comprises convieniences functions and definitios for different operations related to command line user interface.

bold (*mess*)

class roman_emulation
Bases: object

toRoman (*nr*)

emit_message_to_file_in_root_logger (*mess*)

emit_tvtb_to_file_in_root_logger (*tvtb*)

message_special (*mess*)

message (*mess*, *cont=False*)
Prints message to standard error. If FileHandler is present in the root_logger the same message is appended to the log file.

Parameters

- **mess** (*str*) – message to print
- **cont** (*bool*) – if set True no new line is printed

class fbm (*info*, *cont=True*)
Bases: object

__init__ (*info*, *cont=True*)
x.__init__(...) initializes x; see help(type(x)) for signature

__enter__ ()

__exit__ (*typ*, *value*, *traceback*)

__call__ (*...*) <==> *x(...)*

class tictoc (*mess*, *stdout=False*)
Bases: object

__init__ (*mess*, *stdout=False*)
x.__init__(...) initializes x; see help(type(x)) for signature

__enter__ ()

__exit__ (*typ*, *value*, *traceback*)

duration

gregorian_year_in_days = 365.2425
Length of Gregorian year in days. Average value. Source: https://en.wikipedia.org/wiki/Year

smart_time_string(*s*, *rl=0*, *t=1.1*, *maximal_length=None*, *maximal_units=5*)

Function transforms time in seconds to nicely formatted string of length defined by `maximal_length`. Depending on number of seconds time is represented with one or more of the following units:

Unit name	Unit abbreviation
seconds	s
minutes	m
hours	h
days	d
years	y

Maximal number of units used in time string can be set with `maximal_units`.

Parameters

- **s** (*int*) – Input time in seconds.
- **rl** (*int*) – Number of units already used for representing time.
- **t** (*float*) – Exces above standard number of current time units.
- **maximal_length** (*int*) – Maximal length of the output string. Must be greater then 0.
- **maximal_units** (*int*) – Maximal number of units used in the output string. Must be greater then 0 and lower then 6.

Returns string of nicely formated time

Return type str

gsep(*sep='-'*, *times=72*, *length=None*)

Generic separator.

Parameters

- **sep** (*str*) – Element(s) of separator.
- **times** (*int*) – Number of times `sep` is printed.
- **length** (*int*) – Optional maximal length of output.

Returns String separator.

Return type str

tsep(*line*)

Parameters **line** (*str*) – Input line.

Returns Returns default *gsep()* of length of `line`.

underline(*line*)

Parameters **line** (*str*) – Input line.

Returns String made by concatenation of `line`, `os.linesep`, and output of *tsep()* called with `line`.

Return type str

thead(*line*)

Parameters **line** (*str*) – Input line.

Returns String made by concatenation of output of *tsep()* called with `line`, `line`, `os.linesep`, and again output of *tsep()* called with `line`.

Return type str

class SimpleProgressBar(*maxval=None*, *mess=None*, *iterable=None*)

Bases: object

Simple progress bar displaying progress with percent indicator, progress bar and ETA. Progress is measured by iterations.

Variables

- ***rotate*** (*str*) – String comprising characters with frames of a rotating toy.
- ***barlenght*** (*int*) – Length of progress bar.
- **maxval** (*int*) – maximal number of iterations
- **current** (*int*) – current number of iterations
- **overrun_notice** (*bool*) – if True, overrun above maxval iterations causes insert of newline
- **overrun** (*bool*) – flag of overrun
- **begin** (*int*) – time in seconds at the initialization of the *SimpleProgressBar* class.
- **tcurrent** (*int*) – time in seconds of current iteration

rotate = '\\|/-'

barlenght = 24

__init__(*maxval=None*, *mess=None*, *iterable=None*)

Parameters

- **maxval** (*int*) – Maximal number of iterations stored to maxval.
- **mess** (*str*) – Optional message displayed at progress bar initialization.

__enter__()

__exit__(*typ*, *value*, *traceback*)

iter(*finish=False*)

bar()

ETA()

Returns ETA calculated on the basis of current number of iterations current and current time tcurrent. If number of iterations is 0 returns ?. Time is formated wiht *smart_time_string()*.

Returns ETA as string.

Return type str

percent()

Returns float number of precent progress calculated in the basis of current number of iterations current. Should return number between 0 and 100.

Returns percent progress number

Return type float

show()

Shows current progress.

If value returned by *percent()* is =< 100 then progres is printed as percent indicator leaded by ETA calculated by *ETA()*.

If value returned by *percent()* is > 100 then progress is printed as number of iterations and total time.

Progress bar is writen to standard error.

heartbeat()

next (*step=None*)

update (*step*)
Updates number of current iterations `current` by one if `step` is > 0. Otherwise number of current iterations is not updated. In boths cases time of current iteration `tcurrent` is updated and *show()* is called.

Parameters **step** (*int*) – update step

ttime ()
Calculates and returns total time string formated with *smart_time_string()*.

Returns string of total time

Return type str

finish ()
Finishes progress bar. First, *update()* is called with `step` = 0. Next message of total time is writen to standard error.

pbar
alias of *aquaduct.utils.clui.SimpleProgressBar*

get_str_timestamp ()

class SimpleTree (*name=None*, *message=None*, *treestr=None*)
Bases: object

__init__ (*name=None*, *message=None*, *treestr=None*)
x.__init__(...) initializes x; see help(type(x)) for signature

_init_str (*s*)

__repr__ (*) <==> repr(x)*

__str__ (*) <==> str(x)*

is_leaf ()

leafs_names

get_leaf (*name*)

add_message (*message=None*, *toleaf=None*, *replace=False*)

add_message_to_leaf (*message=None*, *toleaf=None*, *replace=False*)

add_leaf (*name=None*, *message=None*, *toleaf=None*)

add_leaf_to_leaf (*name=None*, *message=None*, *toleaf=None*)

print_simple_tree (*st*, *prefix=None*, *multiple=False*, *concise=True*)

aquaduct.utils.filecache module

Module used for caching results of specific function using database to store data

class DBCache (*db_dir*)
Bases: object

__init__ (*db_dir*)
x.__init__(...) initializes x; see help(type(x)) for signature

__call__ (*...) <==> x(...)*

aquaduct.utils.helpers module

Collection of helpers - functions and decorators.

combine(*seqin*)

This is an alien function. It is not extensively used.

Directly taken form http://aspn.activestate.com/ASPN/Cookbook/Python/Recipe/302478/index_txt

Returns a list of all combinations of argument sequences. For example, following call:

```
combine(((1,2),(3,4)))
```

gives following list of combinations:

```
[[1, 3], [1, 4], [2, 3], [2, 4]]
```

Parameters **seqin** (*tuple*) – Tuple of sequences to combine.

Returns All possible combinations of all input sequences.

Return type list of lists

are_rows_uniq(*some_array*)

robust_and(*a*, *b*)

robust_or(*a*, *b*)

is_number(*s*)

is_float(*s*)

lind(*l*, *ind*)

Indexes lists using lists of integers as identificators. For example:

```
lind(['a','b','c','d','e'],[1,4,2])
```

returns:

```
['b', 'e', 'c']
```

Parameters

- **l** (*list*) – List to be indexed.
- **ind** (*list*) – Integer indexes.

Returns Reindexed list.

Return type list

glind(*l*, *ind*)

Indexes lists using iterable of integers as identificators. For example:

```
glind(['a','b','c','d','e'],[1,4,2])
```

returns:

```
['b', 'e', 'c']
```

Parameters

- **l** (*list*) – List to be indexed.
- **ind** (*list*) – Integer indexes.

Returns Reindexed list.

Return type list

class Auto

Auto type definition. The class is used as an alternative value for options (if particular option supports it). If options (or variables/parameters etc.) have value of *Auto* it means that an automatic process for parametrization should be performed.

For example, if the input parameter is set to *Auto* it is supposed that its value is calculated on the basis of input data or other parameters.

__repr__()

Returns String Auto.

Return type str

__str__()

Calls *__repr__()*.

create_tmpfile(*ext=None*, *dir=None*)

Creates temporary file. File is created, closed and its file name is returned.

Note: It is responsibility of the caller to delete the file.

Parameters

- **ext** (*str*) – Optional extension of the file.
- **dir** (*str*) – Optional path to the directory where the file should be created.

Returns File name of created temporary file.

Return type str

range2int(*r*, *uniq=True*)

Transforms a string range in to a list of integers (with added missing elements from given ranges).

For example, a following string:

```
'0:2 4:5 7 9'
```

is transformed into:

```
[0,1,2,4,5,7,9]
```

Parameters

- **r** (*str*) – String of input range.
- **uniq** (*bool*) – Optional parameter, if set to *True* only unique and sorted integers are returned.

Returns List of integers.

Return type list of int

int2range(*l*)

Transforms a list of integers in to a string of ranges.

For example, a following list:

```
[0,1,2,4,5,7,9]
```

is transformed into:

```
0:2 4:5 7 9
```

Parameters **l** (*list*) – input list of int

Returns String of ranges.

Return type str

fractionof(*l*, *f=None*)

Parameters

- **l** (*list*) – input list
- **f** (*float*) – fraction

Returns Fraction of input list.

Return type generator

make_fraction(*frac*, *size*)

Parameters **frac** (*float*) – Fraction to make, can be also *None*. In that case, returned value is *None* as well.

Size int size Size of set for which fraction is made.

Returns Fracion in range (0,1).

make_fractionof(*l*, *f=None*)

Wrapper of make_fraction and fractionof functions.

chop(*l*, *n=1*)

Parameters **l** (*list*) – input list

Returns Chunks of input list, each chunk is of maximal size of n.

Return type generator

chunk(*l*, *n=1*)

Parameters **l** (*list*) – input list

Returns n chunks of input list.

Return type generator

is_iterable(*l*)

Checks if provided object is iterable. Returns True is it is iterable, otherwise returns False.

Parameters **l** (*list*) – input object

Returns True if submitted object is iterable otherwise returns False.

Return type bool

sortify(*gen*)

Decorator to convert functions' outputs into a sorted list. If the output is iterable it is converted in to a list of appropriate length. If the output is not iterable it is converted in to a list of length 1.

Written on the basis of *listify()*.

Returns Output of decorated function converted to a sorted list.

Return type list

uniqify(*gen*)
Decorator to convert functions' outputs into a sorted list of unique objects. If the output is iterable it is converted in to a list of appropriate length. If the output is not iterable it is converted in to a list of length 1.

Written on the basis of *listify()*.

Returns Output of decorated function converted to a sorted list of unique objects.

Return type list

noaction(*gen*)

listify(*gen*)
Decorator to convert functions' outputs into a list. If the output is iterable it is converted in to a list of appropriate length. If the output is not iterable it is converted in to a list of length 1.

This function was copied from:

http://argandgahandapandpa.wordpress.com/2009/03/29/python-generator-to-list-decorator/

and further improved by tljm@wp.pl.

Returns Output of decorated function converted to a list.

Return type list

tupleify(*gen*)
Decorator to convert functions' outputs into a tuple. If the output is iterable it is converted in to a tuple of apropriate length. If the output is not iterable it is converted in to a tuple of length 1.

Written on the basis of *listify()*.

Returns Output of decorated function converted to a tuple.

Return type tuple

dictify(*gen*)
Decorator to convert functions' outputs into a tuple. If the output is iterable it is converted in to a tuple of apropriate length. If the output is not iterable it is converted in to a tuple of length 1.

Written on the basis of *listify()*.

Returns Output of decorated function converted to a tuple.

Return type tuple

class arrayify(*shape=None*)
Bases: object

__init__(*shape=None*)
x.__init__(...) initializes x; see help(type(x)) for signature

__call__(*gen*)
Decorator to convert functions' outputs into a 2D numpy array. If the output is iterable it is converted in to a 2D numpy array of appropriate shape. If the output is not iterable it is converted in to a 2D numpy array of shape 1x1.

Written on the basis of *listify()*.

Returns Output of decorated function converted to a 2D numpy array.

Return type numpy.ndarray

arrayify1(*gen*)
Decorator to convert functions' outputs into a 1D numpy array. If the output is iterable it is converted in to a 2D numpy array of appropriate shape. If the output is not iterable it is converted in to a 2D numpy array of shape 1x1.

Written on the basis of *listify()*.

Returns Output of decorated function converted to a 1D numpy array.

Return type numpy.ndarray

list_blocks_to_slices(*l*)
Slices list in to block according to its elements identity. Resulting slices correspond to blocks of identical elements.

Parameters **l** (*list*) – List of any objects.

Returns Generator of slices.

Return type generator

split_list(*l*, *s*)

what2what(*what*, *towhat*)
This function search if elements of the one list (:attr: 'what') are present in the other list (:attr: 'towhat') and returns indices of elements form :attr:'what' list as a tuple. If elements from the first list are not present in the second list the tuple is empty. :param list what: Input list for which indices of elements present in `towhat` are returned. :param list towhat: List of elements which input list is indexed to. :return: Indices of `what` list that are present in `towhat` list. :rtype: tuple

make_iterable(*something*)
If input object is not iterable returns it as one element list. Otherwise returns the object.

Parameters **something** (*object*) – Input object.

Returns Iterable object.

Return type iterable or list

iterate_or_die(*something*, *times=None*, *reverse=False*)

strech_zip(**args*)

compress_zip(**args*)

zip_zip(**args*, ***kwargs*)

xzip_xzip(**args*, ***kwargs*)

concatenate(**args*)
Concatenates input iterable arguments in to one generator.

class Bunch(***kwds*)
Bases: object

http://code.activestate.com/recipes/52308 foo=Bunch(a=1,b=2)

__init__(***kwds*)
x.__init__(...) initializes x; see help(type(x)) for signature

class SmartRangeFunction(*element*, *times*)
Bases: object

Base class for all *SmartRangeFunction* based classes.

__slots__ = ['element', 'times']

__init__(*element*, *times*)
x.__init__(...) initializes x; see help(type(x)) for signature

element

times

__str__() <==> *str(x)*

__repr__() <==> *repr(x)*

__len__()

__getstate__()

__setstate__(*state*)

__eq__(*other*)
x.__eq__(y) <==> x==y

__hash__() <==> *hash(x)*

get()

rev()

isin(*element*)

first_element()

last_element()

overlaps(*srange*)

overlaps_mutual(*srange*)

contains(*srange*)

class SmartRangeEqual(*element*, *times*)
Bases: *aquaduct.utils.helpers.SmartRangeFunction*

get()

rev()

isin(*element*)

last_element()

class SmartRangeIncrement(*element*, *times*)
Bases: *aquaduct.utils.helpers.SmartRangeFunction*

get()

rev()

isin(*element*)

last_element()

class SmartRangeDecrement(*element*, *times*)
Bases: *aquaduct.utils.helpers.SmartRangeFunction*

get()

rev()

isin(*element*)

last_element()

class SmartRange(*iterable=None*, *fast_raw=None*, *fast_array=None*, *fast_minc_pairs=None*, *fast_minc_seq=None*)
Bases: object

__slots__ = ['_elements', '_len', '_min', '_max']

__init__(*iterable=None*, *fast_raw=None*, *fast_array=None*, *fast_minc_pairs=None*, *fast_minc_seq=None*)
x.__init__(...) initializes x; see help(type(x)) for signature

_elements

_len

_min

_max

static _a2e(*a*)

__getstate__()

__setstate__(*state*)

__str__() <==> *str(x)*

__repr__() <==> *repr(x)*

first_element()

last_element()

last_times()

static raw2pairs(*raw*)

static raw2sequence(*raw*)

raw

raw_equal

raw_increment

append(*element*)

get()

rev()

__len__()

__iter__()

min()

max()

isin(*element*)

aquaduct.utils.maths module

class NumpyDefaultsStorageTypes

Bases: `object`

Default types that are enforced in `numpy.ndarray` objects.

Note: It is used only througt *`defaults`* instance.

---

float_default
alias of `numpy.float64`

int_default
alias of `numpy.int64`

int_type
alias of `numpy.int8`

defaults = <aquaduct.utils.maths.NumpyDefaultsStorageTypes object>

Instance of *`NumpyDefaultsStorageTypes`* to store default values.

make_default_array(*array_like*)

Parameters **array_like** – Array like object

Returns Array with dtype set to *`NumpyDefaultsStorageTypes.float_default`*.

class MemMap
Bases: *aquaduct.utils.maths.MemMap*

Provides simple convenience wrapper for `numpy.memmap()`.

readonly()

Returns Memory map object in 'r' mode.

Return type numpy.core.memmap.memmap

readwrite()

Returns Memory map object in 'r+' mode.

Return type numpy.core.memmap.memmap

class ArrayOrArray(*filename=None*, *dtype=None*, *shape=None*)
Bases: `object`

Convenience class for handling `numpy.ndarray` and `numpy.core.memmap.memmap` objects in a transparent way.

__init__(*filename=None*, *dtype=None*, *shape=None*)

Parameters

- **str** (*filename*) – Optional name of the file to store memory mapped object.
- **dtype** – Optional dtype of array, if *None* default value of *NumpyDefaultsStorageTypes.float_default* is used.
- **shape** – Shape of the array.

If no *filename* is given then regular `numpy.ndarray` is created with `numpy.zeros()`. Otherwise *MemMap* object is created.

isndarray

Returns *True* if underlaying object is of `numpy.ndarray` type.

Return type bool

readwrite()

Returns Array with read-write access.

readonly()

Returns Array with read only access, if possible

__call__()
By default this calls *readwrite()*.

Returns Array with read-write access.

aquaduct.utils.multip module

class CpuThreadsCount
Bases: `object`

cpu_count = 2

threads_count = None

aquaduct.utils.sets module

presort(*a*, *b*)

intersection_simple(*a*, *b*)

intersection_full(*a*, *b*)

intersection_smartr(*a*, *b*)

intersection_set(*a*, *b*)

glue(*a*, *b*)

glue_simple(*a*, *b*)

xor_full(**args*, ***kwargs*)

xor_smartr(**args*, ***kwargs*)

xor_set(*a*, *b*)

xor_simple(*a*, *b*)

left_full(*a*, *b*)

left_smartr(*a*, *b*)

left_set(*a*, *b*)

left_simple(*a*, *b*)

right_full(*a*, *b*)

right_smartr(*a*, *b*)

right_set(*a*, *b*)

right_simple(*a*, *b*)

intersection(*a*, *b*)

left(*a*, *b*)

right(*a*, *b*)

aquaduct.utils.sr module

Module contents

aquaduct.visual package

Submodules

aquaduct.visual.cmaps module

aquaduct.visual.helpers module

euclidean(*A*, *B*)

cityblock(*A*, *B*)

cc_safe(*c*)

cc(*c*)

color_codes(*code*, *custom_codes=None*)

get_cmap(*size*)

class ColorMapDistMap
Bases: object

grey = (0.5, 0.5, 0.5, 1)

__init__()
x.__init__(...) initializes x; see help(type(x)) for signature

distance(*E1*, *E2*)

static color_distance(*e1*, *e2*)

__call__(*...*) <==> *x(...)*

_ColorMapDistMap__do_cadex()

f_like(*n*)

aquaduct.visual.pymol_cgo module

aquaduct.visual.pymol_connector module

class BasicPymolCGO
Bases: object

cgo_entity_begin = []

cgo_entity_end = []

__init__()
x.__init__(...) initializes x; see help(type(x)) for signature

clean(*empty=False*)

new()

get()

static make_color_triple(*color_definition*)

class BasicPymolCGOLines
Bases: *aquaduct.visual.pymol_connector.BasicPymolCGO*

cgo_entity_begin = [2.0, 1.0]

cgo_entity_end = [3.0]

add(*coords=None*, *color=None*)

class BasicPymolCGOSpheres
Bases: *aquaduct.visual.pymol_connector.BasicPymolCGO*

cgo_entity_begin = []

cgo_entity_end = []

add(*coords=None*, *radius=None*, *color=None*)

class BasicPymolCGOPointers
Bases: *aquaduct.visual.pymol_connector.BasicPymolCGO*

cgo_entity_begin = []

cgo_entity_end = []

add_cone(*coords1=None*, *coords2=None*, *radius1=None*, *radius2=None*, *color1=None*, *color2=None*)

add_pointer(*point=None*, *direction=None*, *length=None*, *color=None*, *reverse=False*)

class SimpleTarWriteHelper
Bases: object

__init__()
x.__init__(...) initializes x; see help(type(x)) for signature

open(*filename*)

save_object2tar(*obj*, *name*)

save_file2tar(*filename*, *name*)

__del__()

class ConnectToPymol
Bases: object

cgo_line_width = 2.0

ct_pymol = 'pymol'

ct_file = 'file'

__init__()
x.__init__(...) initializes x; see help(type(x)) for signature

decode_color(***kwargs*)

init_pymol()

init_script(*filename*)

add_cgo_object(*name*, *cgo_object*, *state=None*)

del_cgo_object(*name*, *state=None*)

load_pdb(*name*, *filename*, *state=None*)

orient_on(*name*)

__del__()

class SinglePathPlotter(*pymol_connector*, *linearize=None*)
Bases: object

__init__(*pymol_connector*, *linearize=None*)
x.__init__(...) initializes x; see help(type(x)) for signature

add_single_path_continous_trace(*spath*, *smooth=None*, *plot_in=True*, *plot_object=True*, *plot_out=True*, *plot_walk=True*, ***kwargs*)

paths_trace(*spaths*, *smooth=None*, *name='paths'*, *state=None*, ***kwargs*)

paths_inlets(*spaths*, *smooth=None*, *color=None*, *plot_in=True*, *plot_out=True*, *name='in-outlet'*, *state=None*, ***kwargs*)

scatter(*coords*, *radius=0.4*, *color='r'*, *name='scatter'*, *state=None*)

line(*coords*, *color='r'*, *name='line'*, *state=None*)

multiline_begin()

multiline_add(*coords*, *color='r'*)

multiline_end(*name=<function line>*, *state=None*)

convexhull(*chull*, *color='m'*, *name='convexhull'*, *state=None*)

aquaduct.visual.quickplot module

yield_spath_len_and_smooth_diff_in_types_slices(*sp*, *smooth=None*, *smooth_len=None*, *smooth_diff=None*, *types='etypes'*)

plot_colorful_lines(*x*, *y*, *c*, ***kwargs*)

spaths_spectra(*spaths*, ***kwargs*)

plot_spath_spectrum(*sp*, ***kwargs*)

spath_spectrum(*sp*, ***kwargs*)

showit(*gen*)

get_ax3d(*fig*, *sub=111*)

class SimpleTracePlotter

Bases: object

plot_line(*coords*, *color*, ***kwargs*)

single_trace(*coords*, *color='r'*, ***kwargs*)

path_trace(*path*, *color=('r'*, *'g'*, *'b')*, *plot_in=True*, *plot_object=True*, *plot_out=True*, ***kwargs*)

class SimpleProteinPlotter

Bases: *aquaduct.visual.quickplot.SimpleTracePlotter*

protein_trace(*protein*, *smooth=None*, *color=('c'*, *'m'*, *'y')*, ***kwargs*)

class SimplePathPlotter

Bases: *aquaduct.visual.quickplot.SimpleTracePlotter*

single_path_traces(*spaths*, *smooth=None*, *color=('r'*, *'g'*, *'b')*, ***kwargs*)

class MPLTracePlotter

Bases: *aquaduct.visual.quickplot.SimplePathPlotter*, *aquaduct.visual.quickplot.SimpleProteinPlotter*

init_ax(***kwargs*)

plot_line(***kwargs*)

scatter(***kwargs*)

Module contents

2.2.1.2 Module contents

Aqua-Duct - a collection of tools to trace residues in MD simulation.

version()

Returns *aquaduct* version number.

Returns 3 element tuple of int numbers

Return type tuple

version_nice()

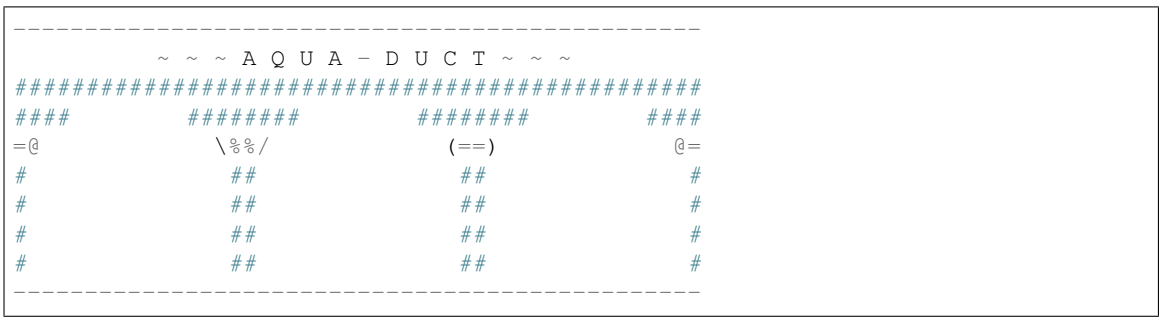
Returns *aquaduct* version number as nicely formatted string.

Returns string composed on the basis of the number returned by *version()*.

Return type str

greetings()

Returns fancy greetings of *aquaduct*. It has a form of ASCII-like graphic. Currently it returns following string:



Returns *aquaduct* fancy greetings.

Return type str

2.3 Aqua-Duct changelog

- **1.0.2 (29.07.2019)**
  - Improvements in GUI configured.
  - Fixed problems with waterfall mode.
- **1.0.0 (21.07.2019) Aqua-Duct version 1**
  - Assorted minor fixes and improvements.
- **1.0.0b1 (13.07.2019) beta**
  - New Waterfall option for analysis of custom sampled simulations.
  - New Kraken GUI tool for facilitating analysis of results.
  - RAM usage optimization in AutoBarber and other procedures.
  - Center of Object and Center of System calculation.
  - Cluster shapes KDE estimation and visualization.
  - New GUI tool for preparing configuration files.
  - Possibility to join clusters by ID and to sort and renumber cluster IDs.
  - Inlets in seleced clusters can be removed.
  - Order of clustering procedures can be altered by user.
  - AutoBarber can be run for different types of traced molecules separately.
  - New driver Pond allows to calculate pockets and master paths energy profiles.
  - Assorted improvements allowing better handling of passing paths.
  - GREAT speedup of Stage I, II, and III calculations: they run in parallel; IO can be a bottleneck though.
  - Substantial speedup of SinglePaths generation: it runs in parallel and uses fastest routines.
  - Substantial speedup of AutoBarber procedures: it runs in parallel; IO can be a bottleneck though.
  - Improvements in analysis stage. Additional info displayed in tables and added progress bar.
  - portal.py script for calculating sizes of selection(s) using convex hull approximation.
  - Improvements in dir-cache handling.
  - Some speedup of master paths calculations, more to come.
  - Paths, SinglePaths and other objects use less memory.
  - Newest MDAnalysis can be used (ie 0.17, 0.18, 0.19) however it is recommended to stay with 0.16.2.
  - Many other minor improvements and bug fixes.
- **0.5.15 (05.05.2019)**
  - Topology residue ID are printed in the analysis files.
- **0.5.14 (26.09.2018)**
  - Recommended MDAnalysis is set to >=0.16 and <0.17. Versions >=0.17 are fully supported.
  - Docs update.
  - Various performance improvements and few minor bug fixes.
- **0.5.9 (12.03.2018)**
  - Rewritten module for MD data access. Sandwich mode added.

  - Coordinates can be stored in cache directory, in memory or generated on demand.
  - Support for long trajectories.
  - Passing through paths are supported.
  - Improvements in visualization script.
  - Coordinates of residues are calculated as center of geometry.
  - Recommended MDAnalysis is set to >=0.16 and <0.17. Version 0.17 is supported but not recommended.
  - Bug fixes and code cleanup.
- **0.4.0 - 0.4.14 (20.11.2017) unofficial**
  - Uses newest MDAnalysis (0.16.2).
  - Steady improvement of documentation (including API).
  - Names of traced molecules are returned in the result file and tables are split appropriately.
  - Tables in the result file are split in regard to Object and Passing paths.
  - Passing through paths are being introduced, WIP.
  - Additional tables in the result file.
  - CRD is enabled as topology/trajectory format.
  - Traced residues are identified by resindices instead of resids; this allows to use weak topologies such as PDB.
  - Removed roman dependency.
  - In addition to histograms approximate (ConvexHull approximation) areas and volumes of the scope and object can be calculated.
  - Bug fixes and reliability fixes.
- **0.3.7 (18.07.2017)**
  - Enable XTC trajectory format.
  - Reliability fix in progress bar display.
- **0.3.6 (28.06.2017)**
  - AQ can be run for given part of trajectory.
  - Fixed bug in passing options to Barber clustering method.
  - Recursive threshold can be defined as range; no disjoint ranges are supported.
- **0.3.5 (18.04.2017)**
  - As for now, the only supported version of MDAnalysis is 0.15.
- **0.3.4 (14.04.2017)**
  - Fixed bug in progress bar updating method causing critical error in some specific circumstances.
- **0.3.3 (20.03.2017)**
  - AutoBarber default values of maxcut_level and mincut_level changed to True.
  - Improved template configuration file.
  - Number of small improvements in documentation.
- **0.3.2 (24.02.2017)**
  - Major improvement: new auto_barber based clustering method.
  - Clustering history displayed as simple ascii tree.

  - AutoBarber min and max cut level options added.
  - Barber moved to separate module.
  - Fixed bug in visualization script; if no molecule is kept do not set style and color.

- **0.3.1 (04.02.2017)**
  - AutoBarber tovdw option.
  - AutoBarber minimal and maximal cut options.
  - Fixed bug in AutoBarber: some areas were sometimes not cut.
  - Documentation improvements.
  - Valve driver simplified. Most of the functionality moved to separate module.
  - Option for single precision storage.
  - Added Savitzky-Golay smoothing; AQ requires SciPy >= 0.14 now.
  - Improved sorting of CTypes.
  - Raw and Separate paths uses SmartRanges. This allowed for excellent performance improvement of Separate paths calculation.
  - Default display of molecule changed to silver cartoon.
  - Object shape displayed in orange.
  - Fixed several small bugs.
- **0.2.26 (21.01.2017)**
  - Stage execution time debug messages.
  - Total execution time debug message.
- **0.2.25 (18.01.2017)**
  - initial public release

PDF version of the documentation is also available.

CHAPTER

THREE

DOCUMENTATION OF OLDER AQUA-DUCT VERSIONS

- Aqua-Duct v0.5
- Aqua-Duct v0.3
- Aqua-Duct v0.2

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