Aqua-Duct Documentation

Release 0.5.9

Tomasz Magdziarz    Karolina Mitusińska
Agata Raczyńska      Artur Góra

Mar 13, 2018
AQUA-DUCT INSTALLATION GUIDE

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.

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.

1.3 Requirements

1.3.1 Software-wise requirements

aquaduct

- numpy >= 1.10.0
- scipy >= 0.17.1
- scikit-learn >= 0.16.0
- MDAnalysis[amber] >= 0.16.0, < 0.17.0
- joblib >= 0.10
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).

1.4 Installation

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
```

1.4.1.1 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.

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
```
1.4.2.1 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:

```bash
# 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
    HDF5_dir = /usr/lib
    HDF5_libdir = /usr/lib
    HDF5_incdir = /usr/include
    netCDF4_dir = /usr/lib
    netCDF4_libdir = /usr/lib
    netCDF4_incldir = /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.

1.4.2.2 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:

```bash
# 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.

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.

1.4.3.1 System native Python

```bash
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.

1.4.3.2 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.

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:

```bash
# 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:

```bash
# install scikit-learn
pip install scikit-learn
# finally, install aquaduct
pip install aquaduct
```

## 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:

```bash
# 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:

```bash
# 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:

```bash
pkg_add py-scipy
```

Install pip if it is missing:

```bash
pkg_add py-pip
```

Install netCDF4 Python:
At this point you can follow generic Python instructions, type:

```bash
pip2.7 install aquaduct
```

### 1.4.5.1 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:

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

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

```bash
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:

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

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

```bash
python2.7 setup.py build
python2.7 setup.py install
python2.7 setup2.py install
```

```bash
cp pymol /usr/local/bin
```

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

### 1.4.5.2 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.
Valve application is a driver that uses aquaduct module to perform analysis of trajectories of selected residues in Molecular Dynamics simulation.

2.1 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.

2.1.1 Usage

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

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

It should display following information:

```
usage: valve.py [-h] [--debug] [--debug-file DEBUG_FILE] 
                [--dump-template-config] [-t THREADS] [-c CONFIG_FILE] [--sps] 
                [--max-frame MAX_FRAME] [-min-frame MIN_FRAME] 
                [-step-frame STEP_FRAME] [-sandwich] [-cache-dir CACHEDIR] 
                [-cache-mem] [-version] [-license]

Valve, Aquaduct driver

optional arguments:
  -h, --help             show this help message and exit
  --debug debug          Prints debug info. (default: False)
  --debug-file DEBUG_FILE Debug log file. (default: None)
  --dump-template-config Dumps template config file. Suppress all other output or actions. (default: False)
  -t THREADS             Limit Aqua-Duct calculations to given number of threads. (default: None)
  -c CONFIG_FILE         Config file filename. (default: None)
  --sps --single-precision to store data. (default: False)
  --max-frame MAX_FRAME  Maximal number of frame. (default: None)
  --min-frame MIN_FRAME  Minimal number of frame. (default: None)
  --step-frame STEP_FRAME Frames step. (default: None)
  --sandwich Sandwich mode for multiple trajectories. (default: False)
  --cache-dir CACHEDIR   Directory for coordinates caching. (default: None)
```

2.1.2 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 following command to print configuration file template on the screen:

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

Configuration file template can also be easily saved in to 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.

2.1.3 Valve calculation run

Once configuration file is ready Valve calculations can be run with a 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 then available CPU cores is generally not optimal.

However, in order to maximize usage of available CPU power it is recommended to set it as number of cores + 1. The reason is that Valve uses one thread for the main process and the excess over one for processes for parallel calculations. When parallel calculations are executed the main thread waits for results.

**Note:** Options --min-frame, --max-frame, and --step-frame can be used to limit calculations to specific part of trajectory. For example, to run calculations for 1000 frames starting from frame 5000 use following options: --min-frame 4999 --max-frame 5999; to run calculations for every 5th frame use: --step-frame 5.

2.1.3.1 Single precision storage

Most of the calculation is 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 spare a lot of RAM and is recommended what you perform calculation for long trajectories and you have limited amount of RAM.

2.1.3.2 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.

### 2.1.3.3 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 of 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.

### 2.1.3.4 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.

## 2.2 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* parse it quickly and regular calculations starts according to its content. Calculations performed by *Valve* are done in six stages described in the next sections.

### 2.2.1 Traceable residues

In the first stage of calculation *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 if they are not already present on the list. In sandwich_option mode this is repeated for each layer.

The search of *traceable residues* is done according to user provided specifications. 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 (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](https://github.com/mdanalysis/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*.

#### 2.2.1.1 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:

\[(\text{resname WAT}) \text{ and } (\text{sphzone 6.0 (resnum 99 or resnum 147)})\]

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.

### 2.2.1.2 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:

\[\text{rename WAT and around 2.0 protein}\]

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 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.

**Convex hulls of macromolecule atoms**


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. Following picture shows schematic comparison of convex hull and solvent excluded surface (SES):

![Convex hull comparison](image.png)

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.
2.2.2 Raw paths

The second stage of calculations uses the list of all traceable residues from the first stage and for each 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 *scope* or in *object*.

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

2.2.3 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 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 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 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. *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.

2.2.3.1 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 for 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:

2.2. How does *Valve* work
• **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 then this value are not used in trimming.

• **auto_barber_maxcut** allows to define maximal radius of spheres. Spheres of radius greater then 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.

### 2.2.3.2 Smoothing

Separate paths can be optionally smoothed. Current *aquaduct* version allows 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:

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.

### 2.2.4 Clusterization 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.

Clusterization of inlets is performed in following steps:

1. **Initial clusterization**: All inlets are submitted to selected clusterization 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:
   
   (a) **Automatic mode**: Inlet is considered to be an outlier if its distance from the centroid is greater than mean distance + 4 * standard deviation of all distances within the cluster.

   (b) **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] **Reclusterization of outliers**: It may happen that the outliers form actually clusters but it was not recognized in initial clusterization. In this step clusterization 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.

### 2.2.4.1 Potentially recursive clusterization

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

For additional information see *clusterization sections* options.

### 2.2.4.2 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 clusterization*. It gives excellent results. For more information see *barber clusterization 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 *Reclusterization 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)

For additional information see *clusterization sections* options.

### 2.2.4.3 Master paths

At the end of clusterization 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 in 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 longest paths. These normalized lengths are then used for as weights in 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 averaging procedure is run:
   (a) Coordinates for all separate paths for given chunk are collected.
   (b) Normalized lengths with bias toward longest paths for all separate paths for given chunk are collected.
   (c) New coordinates are calculated as weighted average of collected coordinates. As weights collected normalized lengths are used.

### 2.2. How does Valve work

---

13
(d) In addition width of chunk is calculated as a mean value of collected coordinates mutual distances.

(e) 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.CTypePathsCollection.get_master_path() method documentation.

2.2.5 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 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 Scope during the simulation.

To get correct picture following options and settings have to be considered:

- **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 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 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.

Additionally, in stage inlets_clusterization following options could also be adjusted:

- exclude_passing_in_clusterization could be set to True. This will exclude passing paths inlets from clusterization.

- 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 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.

2.2.6 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 text file and comprise of several parts.

2.2.6.1 General summary

Results starts with 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 and, 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.

### 2.2.6.2 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.

### 2.2. How does *Valve* work
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 unrealistic values. This test will be changed in the future releases.

### 2.2.6.3 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.

#### 2.2.6.4 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 frame in which the path begins.
  4. **InpF**: Number of frame in which path begins Incoming part.
  5. **ObjF**: Number of frame in which path begins Object part.
  6. **OutF**: Number of frame in which path begins Outgoing part.
  7. **EndF**: Number of frame in which the path ends.
  8. **TotL**: Total length of path.
  9. **InpL**: Length of Incoming part. If no incoming part NaN is given.
  10. **ObjL**: Length of Object part.
  11. **OutL**: Length of Outgoing part. If no outgoing part NaN is given.
  12. **TotS**: Average step of full path.
  13. **TotStdS**: Standard deviation of **TotS**.
  14. **InpS**: Average step of Incoming part. If no incoming part NaN is given.
  15. **InpStdS**: Standard deviation of **InpS**.
  16. **ObjS**: Average step of Object part.
  17. **ObjStdS**: Standard deviation of **ObjS**.
  18. **OutS**: Average step of Outgoing part. If no outgoing part NaN is given.
  19. **OutStdS**: Standard deviation of **OutS**.
  20. **CType**: Cluster type of separate path.

### 2.2. How does Valve work
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. Third number is consecutive number of the separate path made by the residue. Numeration starts with 0.

2.2.6.5 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 is two different clusters:

![Graph showing number of water molecules in clusters 16 and 6](image)

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 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 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
2.2.7 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 PDB file. Other objects like Inlets clusters or paths are loaded as CGO objects.

2.2.7.1 Visualization script

By default Valve creates Python visualization script and archive with data files. This script is a regular Python script. It does not depends on AQUA-DUCT. To run it, python2.7 and PyMol is 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              Disable 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, molecule and clusters only one can call 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 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.

### 2.2.7.2 Visualization objects

Following is a list of objects created in PyMOL (all of them are optional). PyMOL object names given in **bold** text or 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 in to 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 in to Incoming, Object and Outgoing part. Object name: **all_smooth**, or **all_smooth_in**, **all_smooth_obj**, and **all_smooth_out**.

- All smooth 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.

2.2.7.3 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.

2.2. How does Valve work
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:**
   - (a) `traceable_residues`
   - (b) `raw_paths`
   - (c) `separate_paths`
   - (d) `inlets_clusterization`
   - (e) `analysis`
   - (f) `visualize`

3. **Methods options:**
   - `smooth`
   - `clusterization`
   - `reclusteriation`

### 3.1 Section global

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

<table>
<thead>
<tr>
<th>Option</th>
<th>Default value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>top</code></td>
<td>None</td>
<td>Path to topology file. Aqua-Duct supports PDB, PRMTOP, PFS topology files.</td>
</tr>
<tr>
<td><code>trj</code></td>
<td>None</td>
<td>Path to trajectory file. Aqua-Duct supports NC and DCD trajectory files.</td>
</tr>
</tbody>
</table>

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.
3.2 Common settings of stage sections

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

<table>
<thead>
<tr>
<th>Option</th>
<th>Default value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>execute</td>
<td>runonce</td>
<td>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 if 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 skip and if dump is set data is loaded from the file.</td>
</tr>
<tr>
<td>dump</td>
<td>[dump file name]</td>
<td>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_clusterization_data.dump</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Option</th>
<th>Default value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>execute</td>
<td>run</td>
<td>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 is saved according to save option. If it is set to skip stage is skipped.</td>
</tr>
<tr>
<td>save</td>
<td>[save file name]</td>
<td>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 &amp; 5_analysis_results.txt.csv • 6_visualize_results.py &amp; 6_visualize_results.tar.gz Stage 5 saves .txt file with analysis 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.</td>
</tr>
</tbody>
</table>

3.3 Stage traceable_residues

<table>
<thead>
<tr>
<th>Option</th>
<th>Default value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>scope</td>
<td>None</td>
<td>Definition of Scope of interest. See also Scope definition.</td>
</tr>
<tr>
<td>scope_convexhull</td>
<td>True</td>
<td>Flag to set if Scope is direct or convex hull definition.</td>
</tr>
<tr>
<td>scope_everyframe</td>
<td>False</td>
<td>Flag to set Scope evaluation mode. If set True Scope is evaluated in every frame. This make sense if the definition is complex and depends on distances between molecular entities.</td>
</tr>
<tr>
<td>object</td>
<td>None</td>
<td>Definition of Object of interest. See also Object definition.</td>
</tr>
</tbody>
</table>

Note: Options scope and object are mandatory.
3.4 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.

<table>
<thead>
<tr>
<th>Option</th>
<th>Default value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>scope</td>
<td>None</td>
<td>Definition of Scope of interest. See also Scope definition. If None value from previous stage is used.</td>
</tr>
<tr>
<td>scope_convexhull</td>
<td>None</td>
<td>Flag to set if the Scope is direct or convex hull definition.</td>
</tr>
<tr>
<td>scope_everyframe</td>
<td>False</td>
<td>Flag to set Scope evaluation mode. If set True, Scope is evaluated in every frame. This make sense if the definition is complex and depends on distances between molecular entities. If None value from previous stage is used.</td>
</tr>
<tr>
<td>object</td>
<td>None</td>
<td>Definition of Object of interest. See also Object definition. If None value from the previous stage is used</td>
</tr>
<tr>
<td>clear_in_object_info</td>
<td>False</td>
<td>If it is set to True, information on occupation of Object site by traceable residues calculated in the previous stage is cleared and have to be recalculated. This is useful if definition of Object was changed.</td>
</tr>
</tbody>
</table>
## 3.5 Stage separate_paths

<table>
<thead>
<tr>
<th>Option</th>
<th>Default value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>discard_empty_paths</td>
<td>True</td>
<td>If set to <code>True</code> empty paths are discarded.</td>
</tr>
<tr>
<td>sort_by_id</td>
<td>True</td>
<td>If set to <code>True</code> separate paths are sorted by ID. Otherwise they are sorted in order of appearance.</td>
</tr>
<tr>
<td>discard_short_paths</td>
<td>20</td>
<td>This option allows to discard paths which are shorter than the threshold which is defined as total number of frames.</td>
</tr>
<tr>
<td>discard_short_object</td>
<td>2.0</td>
<td>This option allows to discard paths which objects are shorter than the threshold which is defined as total length in metric units.</td>
</tr>
<tr>
<td>discard_short_logic</td>
<td>or</td>
<td>If both <code>discard_short_paths</code> and <code>discard_short_object</code> options are used, this option allows to set combination logic. If it is set <code>or</code> a path is discarded if any of discard criterion is met. If it is set <code>and</code> both criteria have to be met to discard path.</td>
</tr>
<tr>
<td>auto_barber</td>
<td>None</td>
<td>This option allows to select molecular entity used in Auto Barber procedure. See also Auto Barber and barber_with_spheres().</td>
</tr>
<tr>
<td>auto_barber_mincut</td>
<td>None</td>
<td>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 <code>None</code>.</td>
</tr>
<tr>
<td>auto_barber_maxcut</td>
<td>2.8</td>
<td>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 <code>None</code>.</td>
</tr>
<tr>
<td>auto_barber_mincut_level</td>
<td>True</td>
<td>If set <code>True</code> spheres of radius smaller than <code>mincut</code> are resized to <code>mincut</code> value.</td>
</tr>
<tr>
<td>auto_barber_maxcut_level</td>
<td>True</td>
<td>If set <code>True</code> spheres of radius greater than <code>maxcut</code> are resized to <code>maxcut</code> value.</td>
</tr>
<tr>
<td>auto_barber_tovdw</td>
<td>True</td>
<td>Correct cutting sphere by decreasing its radius by VdW radius of the closest atom.</td>
</tr>
<tr>
<td>allow_passing_paths</td>
<td>False</td>
<td>If set <code>True</code> paths that do not enter the object are detected and added to the rest of paths as ‘passing’ paths.</td>
</tr>
</tbody>
</table>
3.6 Stage inlets_clusterization

<table>
<thead>
<tr>
<th>Option</th>
<th>Default value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>recluster_outliers</td>
<td>False</td>
<td>If set to True reclustering of outliers is executed according to the method defined in <strong>reclusterization</strong> section.</td>
</tr>
<tr>
<td>detect_outliers</td>
<td>False</td>
<td>If set, detection of outliers is executed. It could be set as a floating point distance threshold or set to <strong>Auto</strong>. See <strong>Clusterization of inlets</strong> for more details.</td>
</tr>
<tr>
<td>singletons_outliers</td>
<td>False</td>
<td>Maximal size of cluster to be considered as outliers. If set to number &gt; 0 clusters of that size are removed and their objects are moved to outliers. See <strong>Clusterization of inlets</strong> for more details.</td>
</tr>
<tr>
<td>max_level</td>
<td>5</td>
<td>Maximal number of recursive clusterization levels.</td>
</tr>
<tr>
<td>create_master_paths</td>
<td>False</td>
<td>If set to True master paths are created (fast CPU and big RAM recommended; 50k frames long simulation may need ca 20GB of memory)</td>
</tr>
<tr>
<td>exclude_passing_in_clusterization</td>
<td>True</td>
<td>If set to True passing paths are not clustered with normal paths.</td>
</tr>
<tr>
<td>add_passing_to_clusters</td>
<td>None</td>
<td>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.</td>
</tr>
</tbody>
</table>

3.7 Stage analysis

<table>
<thead>
<tr>
<th>Option</th>
<th>Default value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>dump_config</td>
<td>True</td>
<td>If set to True configuration options, as seen by Valve, are added to the head of results.</td>
</tr>
<tr>
<td>calculate_scope_object_size</td>
<td>False</td>
<td>If set to True volumes and areas of object and scope approximated by convex hulls will be calculated for each analyzed frames and saved in output CSV file.</td>
</tr>
<tr>
<td>scope_chull</td>
<td>None</td>
<td>Scope convex hull definition used in calculating volume and area.</td>
</tr>
<tr>
<td>object_chull</td>
<td>None</td>
<td>Object convex hull definition used in calculating volume and area.</td>
</tr>
</tbody>
</table>

3.8 Stage visualize

<table>
<thead>
<tr>
<th>Option</th>
<th>Default value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>all_paths_raw</td>
<td>False</td>
<td>If True produces one object in PyMOL that holds all paths visualized by raw coordinates.</td>
</tr>
<tr>
<td>all_paths_smooth</td>
<td>False</td>
<td>If True produces one object in PyMOL that holds all paths visualized by smooth coordinates.</td>
</tr>
<tr>
<td>all_paths_split</td>
<td>False</td>
<td>If is set True objects produced by <strong>all_paths_raw</strong> and <strong>all_paths_smooth</strong> are split into Incoming, Object, and Outgoing parts and visualized as three different objects.</td>
</tr>
<tr>
<td>all_paths_raw_io</td>
<td>False</td>
<td>If set True arrows pointing beginning and end of paths are displayed oriented accordingly to raw paths orientation.</td>
</tr>
</tbody>
</table>

Continued on next page
<table>
<thead>
<tr>
<th>Option</th>
<th>Default value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>all_paths_smooth_io</td>
<td>False</td>
<td>If set True arrows pointing beginning and end of paths are displayed oriented accordingly to smooth paths orientation.</td>
</tr>
</tbody>
</table>
| 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  
  - 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 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 in separate object. |
| ctypes_smooth       | False         | Displays smooth paths in a similar manner as non split all_paths_smooth but each cluster type is displayed in separate object. |
| show_molecule       | False         | If is 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. |

Continued on next page
Table 3.1 – continued from previous page

<table>
<thead>
<tr>
<th>Option</th>
<th>Default value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>show_scope_chull</td>
<td>False</td>
<td>If is set to selection of some molecular object in the system, for example to protein, convex hull of this object is displayed.</td>
</tr>
<tr>
<td>show_scope_chull_frames</td>
<td>0</td>
<td>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.</td>
</tr>
<tr>
<td>show_object_chull</td>
<td>False</td>
<td>If is set to selection of some molecular object in the system convex hull of this object is displayed. This works exactly 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.</td>
</tr>
<tr>
<td>show_object_chull_frames</td>
<td>0</td>
<td>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.</td>
</tr>
</tbody>
</table>

**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 any way. 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.

### 3.9 Clusterization sections

Default section for definition of clusterization method is named clusterization and default section for reclustering method definition is named reclustering. All clusterization sections shares some common options. Other options depends on the method.
### 3.9.1 barber

Clusterization 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 clusterization section. Next, inlets that form coherent clouds of mutually intersecting spheres are grouped in to clusters. Method **barber** supports the same settings as Auto Barber settings:

<table>
<thead>
<tr>
<th>Option</th>
<th>Value type</th>
<th>Description</th>
</tr>
</thead>
</table>
| 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 then 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 then 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 then `mincut` are resized to `mincut` value.
| auto_barber_maxcut_level | bool | If set `True` spheres of radius greater then `maxcut` are resized to `maxcut` value.
| auto_barber_tovdw | bool      | Correct cutting sphere by decreasing its radius by VdW radius of the closest atom.

### 3.9.2 dbscan

For detailed description look at *sklearn.cluster.DBSCAN* documentation. Following table summarized options available in *Valve* and is a copy of original documentation.
<table>
<thead>
<tr>
<th>Option</th>
<th>Value type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>eps</td>
<td>float</td>
<td>The maximum distance between two samples for them to be considered as in the same neighborhood.</td>
</tr>
<tr>
<td>min_samples</td>
<td>int</td>
<td>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.</td>
</tr>
<tr>
<td>metric</td>
<td>str</td>
<td>The metric to use when calculating distance between instances in a feature array. Can be one of the following: euclidean, cityblock, cosine, manhattan.</td>
</tr>
<tr>
<td>algorithm</td>
<td>str</td>
<td>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.</td>
</tr>
<tr>
<td>leaf_size</td>
<td>int</td>
<td>Leaf size passed to BallTree or cKDTree.</td>
</tr>
</tbody>
</table>

3.9.3 affprop

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

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

3.9.4 meanshift

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

<table>
<thead>
<tr>
<th>Option</th>
<th>Value type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>bandwidth</td>
<td>Auto or float</td>
<td>Bandwidth used in the RBF kernel. If Auto or None automatic method for bandwidth estimation is used. See estimate_bandwidth().</td>
</tr>
<tr>
<td>cluster_all</td>
<td>bool</td>
<td>If true, then all points are clustered, even those orphans that are not within any kernel.</td>
</tr>
<tr>
<td>bin_seeding</td>
<td>bool</td>
<td>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.</td>
</tr>
<tr>
<td>min_bin_freq</td>
<td>int</td>
<td>To speed up the algorithm, accept only those bins with at least min_bin_freq points as seeds. If not defined, set to 1.</td>
</tr>
</tbody>
</table>

3.9. Clusterization sections

31
3.9.5 birch

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

<table>
<thead>
<tr>
<th>Option</th>
<th>Value type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>threshold</td>
<td>float</td>
<td>The radius of the subcluster obtained by merging a new sample and the closest subcluster should be lesser than the threshold. Otherwise a new subcluster is started.</td>
</tr>
<tr>
<td>branching_factor</td>
<td>int</td>
<td>Maximum number of CF subclusters in each node.</td>
</tr>
<tr>
<td>n_clusters</td>
<td>int</td>
<td>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.</td>
</tr>
</tbody>
</table>

3.9.6 kmeans

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

<table>
<thead>
<tr>
<th>Option</th>
<th>Value type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>n_clusters</td>
<td>int</td>
<td>The number of clusters to form as well as the number of centroids to generate.</td>
</tr>
<tr>
<td>max_iter</td>
<td>int</td>
<td>Maximum number of iterations of the k-means algorithm for a single run.</td>
</tr>
<tr>
<td>n_init</td>
<td>int</td>
<td>Number of time 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.</td>
</tr>
<tr>
<td>init</td>
<td>str</td>
<td>Method for initialization, defaults to k-means++. Can be one of following: k-means++ or random.</td>
</tr>
<tr>
<td>tol</td>
<td>float</td>
<td>Relative tolerance with regards to inertia to declare convergence.</td>
</tr>
</tbody>
</table>

3.10 Smooth section

Section smooth supports following options:

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

### 4.1 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
```

### 4.2 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.

### 4.3 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*?

#### 4.3.1 Create Object definition

Let’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.

4.3.2 Create Scope definition

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

4.4 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.

4.5 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.

4.5.1 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.

4.5.2 Clusterization

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

4.5.3 Analysis tables

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

4.6 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?
5.1 aquaduct package

5.1.1 Subpackages

5.1.1.1 aquaduct.apps package

Submodules

aquaduct.apps.data module

class GlobalConfigStore
    Bases: object
    cachedir = None
    cachemem = False

class CoordsRangeIndexCache
    Bases: object
    cache = {}

get_cric_reader (mode='r')
save_cric()
load_cric()
check_version_compliance (current, loaded, what)
check_versions (version_dict)

class LoadDumpWrapper (filehandle)
    Bases: object
    This is wrapper for pickled data that provides compatibility with earlier versions of Aqua-Duct.
    Conversions in use:
    1. replace ‘aquaduct.’ by ‘aquaduct.’

__init__ (filehandle)
convert (s)
read (*args, **kwargs)
readline (*args, **kwargs)

get_vda_reader (filename)

class ValveDataAccess_pickle (mode=None, data_file_name=None, reader=None)
    Bases: aquaduct.apps.data.ValveDataAccess
mimic_old_var_name = 'aq_data_to_save'
unknown_names = 'UNK'
open(data_file_name, mode)
close()
load()
dump(**kwargs)
get_variable(name)
set_variable(name, value)
class ValveDataAccessRoots
    Bases: object
    roots = []
    open(data_file_name, mode)
    close_all()
    __del__()
get_object_name(something)
get_object_from_name(name)
class IdsOverIds
    Bases: object
    static dict2arrays(d)
    static arrays2dict(values=None, keys_lens=None)
class ValveDataAccess_nc(*args, **kwargs)
    Bases: aquaduct.apps.data.ValveDataAccess
    __init__(*args, **kwargs)
    open(data_file_name, mode)
ValveDataAccess
    alias of ValveDataAccess_pickle

aquaduct.apps.valvecore module

class ValveConfig
    Bases: object, aquaduct.apps.valvecore.ConfigSpecialNames
    __init__()
    static common_config_names()
    static common_traj_data_config_names()
    static global_name()
    static cluster_name()
    static recluster_name()
    static recursive_clusterization_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)
_valve_config__make_options_nt (input_options)

valve_begin ()
valve_end ()
valve_load_config (filename, config)

valve_exec_stage (stage, config, stage_run, no_io=False, run_status=None, **kwargs)
stage_I_run (config, options, **kwargs)
stage_II_run (config, options, all_res=None, number_frame_rid_in_object=None, **kwargs)
stage_III_run (config, options, paths=None, **kwargs)
stage_IV_run (config, options, spaths=None, center_of_system=None, **kwargs)
stage_V_run (config, options, spaths=None, paths=None, inls=None, ctypes=None, reader=None, **kwargs)
stage_VI_run (config, options, spaths=None, inls=None, ctypes=None, master_paths=None, master_paths_smooth=None, **kwargs)
aquaduct_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

Module contents

5.1.1.2 aquaduct.geom package

Submodules

aquaduct.geom.cluster module

This module provides functions for clusterization. Clusterization is done by scikit-learn module.

get_required_params (method)

class BarberClusterResult (labels_)
    Bases: object

    Helper class for results of barber clusterization.
class BarberCluster
    Bases: object
    Wrapper class that implements barber clusterization.

    fit (coords, spheres=None)
    Parameters
    • coords (Iterable) – Input coordinates of points to be clustered.
    • spheres (Iterable) – Input spheres for each point.

MeanShiftBandwidth (X, **kwargs)
    Helper function for automatic calculation of a bandwidth for MeanShift method.
    Parameters X (Iterable) – Coordinates of points to be clustered.

class PerformClustering (method, **kwargs)
    Bases: object
    Helper class for clusterization.

    __init__ (method, **kwargs)
    Parameters method (object) – Class that implements clustering via fit method.

    __str__ ()

    __call__ (coords, spheres=None)

    _get_noclusters (n)

    fit (coords, spheres=None)
    Parameters
    • coords (Iterable) – Input coordinates of points to be clustered.
    • spheres (Iterable) – Input spheres for each point. Optional, important only if method is BarberCluster.
    Returns Clusters numbers.
    Return type list of int

    centers ()
    Returns Centers of clusters.

aquaduct.geom.convexhull module

    _vertices_ids (convexhull)

    _vertices_points (convexhull)

    _point_within_convexhull (convexhull, point)

    _facets (convexhull)

    _edges (*args, **kwargs)

    is_point_within_convexhull (point_chull)
aquaduct.geom.master module

part2type_dict = {0: 's', 1: 'c', 2: 's'}

Part number to GenericPathTypeCodes dictionary.

parts = (0, 1, 2)

Parts enumerate.

class CTypeSpathsCollectionWorker (spaths=None, ctype=None, bias_long=5, smooth=None, lock=None)

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_slices_ 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 coordinates 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 CTypePathsCollection

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 progress bar by one, if any.

```
len ()
```

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 `len()`.

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 incoming, 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 CTypeSpansCollectionWorker.
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 into chunks according to xzip_xzip() function with N set to length 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 CTypeSpansCollectionWorker.
coords_types_prob_widths() method is called. Types probabilities are changed to types with types_prob_to_types() method.

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)

decoords(*args, **kwargs)

decoords_smooth(sranges, smooth)

aquaduct.geom.pca module

class Center(X)

Bases: object

__init__(X)

__call__(X)

undo(X)

class Normalize(X)

Bases: object
__init__(X)
__call__(X)
undo(X)

class Standartize(X)
    Bases: aquaduct.geom.pca.Center, aquaduct.geom.pca.Normalize
    __init__(X)
    __call__(X)
    undo(X)

class PCA(X, prepro=None)
    Bases: object
    __init__(X, prepro=None)
    P
    preprocess(X)
    preprocess_undo(X)
    __call__(X)
    undo(T)

aquaduct.geom.smooth module

Smooth module defines methods for smoothing of trajectories.

Available methods:

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SavgolSmooth</td>
<td>Savitzky-Golay based smoothing.</td>
</tr>
<tr>
<td>WindowSmooth</td>
<td>Defined size window smoothing.</td>
</tr>
<tr>
<td>DistanceWindowSmooth</td>
<td>Distance defined size window smoothing.</td>
</tr>
<tr>
<td>ActiveWindowSmooth</td>
<td>Active size window smoothing.</td>
</tr>
<tr>
<td>MaxStepSmooth</td>
<td>Maximal step smoothing.</td>
</tr>
<tr>
<td>WindowOverMaxStepSmooth</td>
<td>Window smoothing over maximal step smoothing.</td>
</tr>
<tr>
<td>DistanceWindowOverMaxStepSmooth</td>
<td>Distance window smoothing over maximal step smoothing.</td>
</tr>
<tr>
<td>ActiveWindowOverMaxStepSmooth</td>
<td>Active window smoothing over maximal step smoothing.</td>
</tr>
</tbody>
</table>

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.
- `Returns` Smoothed coordinates.

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

Base class for window based smoothing methods.

```python
__init__ (function=<function mean>, **kwargs)
```

**Parameters**

- `function (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.

```python
Parameters

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

Returns 2 element tuple of int
```

**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.

```python
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.

Returns 2 element tuple of int
```

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

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

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

**Parameters**

- `window (int)` – One side size of the window.

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

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

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

**Parameters**

- `window (float)` – Size of the window.

**class WindowSmooth (**kwargs)**

Base class for all window smoothing methods.

```python
Defined size window smoothing.
```

---

### 5.1. aquaduct package

---
For each coordinate a symmetrical (if possible) window of size defined by \texttt{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 \texttt{function}. Resulting value(s) are the smoothed coordinates.

\begin{verbatim}
__init__(**kwargs)
smooth(*args, **kwargs)

Parameters coords (Iterable) – Input coordinates to be smoothed.
\end{verbatim}

class DistanceWindowSmooth(**kwargs)
Bases: aquaduct.geom.smooth.Smooth, aquaduct.geom.smooth.FloatWindow
Distance defined size window smoothing.

This is modification of \texttt{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 \texttt{function}. Resulting value(s) are the smoothed coordinates.

\begin{verbatim}
__init__(**kwargs)
smooth(*args, **kwargs)

Parameters coords (Iterable) – Input coordinates to be smoothed.
\end{verbatim}

class ActiveWindowSmooth(**kwargs)
Bases: aquaduct.geom.smooth.Smooth, aquaduct.geom.smooth.FloatWindow
Active size window smoothing.

Similarly to \texttt{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 \texttt{function}. Resulting value(s) are the smoothed coordinates.

\begin{verbatim}
__init__(**kwargs)
smooth(*args, **kwargs)

Parameters coords (Iterable) – Input coordinates to be smoothed.
\end{verbatim}

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 \texttt{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.

\begin{verbatim}
__init__(step=1.0, **kwargs)
smooth(*args, **kwargs)

Parameters coords (Iterable) – Input coordinates to be smoothed.
\end{verbatim}

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 \texttt{savgol_filter()}. For each dimension filter is applied separately. Only \texttt{window_length} and \texttt{polyorder} attributes are used.
__init__(window_length=5, polyorder=2, **kwargs)

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

int polyorder: Polynomial order.

set_savgol_function()

smooth(*args, **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)

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)

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)

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 dimensions 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

**derivivative** *(values)*

**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

• alternative method 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)

**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__**(coords)

**class LinearizeRecursive**

**Bases:** object

Base class for linearization methods classes.
It implements recursive algorithm.

**here**(coords, depth=0)

Core of recursive linearization algorithm.

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 recurrence.

**Returns**  Indices of coords points that can be used instead of all points in visualization.

**Return type**  list of int

---

**class** TriangleLinearize**(threshold=0.01)**

**Bases:** object

**__init__**(threshold=0.01)

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

**class** VectorLinearize**(threshold=0.05236)**

**Bases:** object

Base class for linearization methods classes.

It implements vector linearization criterion.

**__init__**(threshold=0.05236)

**is_linear_core**(coords, depth=None, **kwargs)

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:

\[
\text{threshold}_{\text{current}} = \text{threshold}_{\text{initial}} \times (2 - 0.9^\text{depth})
\]

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 threshold methods returns False; otherwise method returns True.

**Parameters**

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

**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 recurrence.

**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 (*threshhold=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 (*threshhold=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 (*threshhold=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**

5.1.3  `aquaduct.traj` package

**Submodules**

`aquaduct.traj.barber` module

Module implements AutoBarber generation of spheres.

class Sphere

Bases: `aquaduct.traj.barber.Sphere`
Simple sphere class.

```python
is_point_within(point)
is_sphere_within(sphere)
is_sphere_cloud(sphere)
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.

```python
__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. Required 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.
- `forceempty (bool)` – If set True spheres of radius 0 are returned if no other sphere can be generated.

```python
check_minmaxcuts()
add_spheres_from_spaths(spaths)
add_spheres_from_inlets(inlets)
get_current_nr()
inlet2sphere(inlet)
spath2spheres(sp)
_cut_thyself(spheres_passed, progress=False)
cut_thyself()
is_overlapping_with_cloud(sphere)
cloud_groups(progress=False)
```

---

**aquaduct.traj.dumps module**

```python
class TmpDumpWriterOfMDA
Bases: object
__init__()
dump_frames(reader, frames, selection='protein')
```
Aqua-Duct Documentation, Release 0.5.9

import close
__del__()

aquaduct.traj.inlets module

class ProtoInletTypeCodes

    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')

    itype = 'internal'

class InletClusterGenericType
    Bases: object

    __init__ (inp, out)

    input
    output

    static cluster2str (cl)

    __getitem__ (item)
    __len__ ()
    __str__ ()
    __repr__ ()

    make_val (base)

    __cmp__ (other)
    __hash__ ()

class InletClusterExtendedType (surf in, inter in, inter out, surf out)
    Bases: aquaduct.traj.inlets.InletClusterGenericType

    __init__ (surf in, inter in, inter out, surf out)

    generic

class Inlet (coords=None, type=None, reference=None, frame=None)
    Bases: object
__init__ (coords=None, type=None, reference=None, frame=None)

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)
    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_clusterization_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)
    small_clusters_to_outliers (maxsize)
    renumber_clusters ()
    sort_clusters ()
    clusters_list
    clusters_centers
    clusters_size
    clusters_std
    spaths2ctypes (*args, **kwargs)
    spath2ctype (sp)
    lim_to (what, towhat)
    lim2spaths (spaths)
    lim2rnames (rnames)
    lim2types (types)
    lim2clusters (clusters)
    limspaths2 (*args, **kwargs)
get_chull()

aquaduct.traj.paths module

union_full (a, b)
union_smartr (a, b)
union (a, b, smartr=True)
glue (a, b)
xor_full (*args, **kwargs)
xor_smartr (*args, **kwargs)
xor (a, b, smartr=True)
left (a, b, smartr=True)
right (a, b, smartr=True)

class PathTypesCodes

    path_in_code = 'i'
    path_object_code = 'c'
    path_out_code = 'o'
    path_walk_code = 'w'

class GenericPathTypeCodes

    object_name = 'c'
    scope_name = 's'
    out_name = 'n'

class GenericPaths (id_of_res, name_of_res=None, single_res_selection=None, min_pf=None, max_pf=None)
Bases: object, aquaduct.traj.paths.GenericPathTypeCodes

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

    types
    frames
    coords
    max_frame
    min_frame
    add_012 (os_in_frames)
    add_object (frame)
    add_scope (frame)
    add_type (frame, ftype)

    _gpt()
    _gpo()
    _gpi()

    get_paths_in()
get_paths_out()
find_paths(fullonly=False, smartr=True)
find_paths_types(fullonly=False)
get_single_path_types(spath)
barber_with_spheres(spheres)

class SinglePathID(path_id=None, nr=None, name=None)
    Bases: object
    __init__(path_id=None, nr=None, name=None)
    __str__()
    __eq__(other)
yield_single_paths(gps, fullonly=None, progress=None, passing=None)

yield_generic_paths(spaths, progress=None)

class MacroMolPath(path_id, paths, types, single_res_selection=None)
    Bases: object, aquaduct.traj.paths.PathTypesCodes, aquaduct.traj.inlets.InletTypeCodes
    empty_coords = array([], shape=(0, 3), dtype=float64)
    __init__(path_id, paths, types, single_res_selection=None)
    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_out
    types_in
    types_object
    types_out
    coords_first_in
    paths_first_in
    coords_last_out
    paths_last_out
    coords_filo
    get_inlets()
    coords_in
    coords_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(*args, **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(*args, **kwargs)
get_velocity_cont(*args, **kwargs)
get_acceleration_cont(*args, **kwargs)
_MacroMolPath__object_len_calculate()

class SinglePath(path_id, paths, types, single_res_selection=None)
Bases: aquaduct.traj.paths.MacroMolPath
is_single()
is_passing()

class PassingPath(path_id, paths, types, single_res_selection=None)
Bases: aquaduct.traj.paths.MacroMolPath
__init__(path_id, paths, types, single_res_selection=None)
__has_out = None
    self.has_in = True self.has_out = True
object_len
has_in
has_out
is_single()
is_passing()
```python
is_frame_walk(frame)
types
gtypes
sizes
_paths
coords
path
paths
coords_first_in
paths_first_in
coords_last_out
paths_last_out
get_coords(smooth=None)
get_inlets()
_PassingPath__object_len_calculate()

class MasterPath(sp)
    Bases: aquaduct.traj.paths.MacroMolPath
    __init__(sp)
    add_width(width)

aquaduct.traj.sandwich module

class Window(start, stop, step)
    Bases: object
    __init__(start, stop, step)
    __repr__()
    range()
    get_real(frame)
    len()

class MasterReader
    Bases: object
    open_reader_traj = {}
    topology = ''
    trajectory = ['']
    window = None
    sandwich_mode = None
    engine_name = 'mda'
    __call__(topology, trajectory, window=None, sandwich=False)

    Parameters
    * topology (str) – Topology file name.
    * trajectory (list) – List of trajectories. Each element is a fine name.
```
• window (Window) – Frames window to read.
• sandwich (bool) – Flag for setting sandwich mode.

```python
__getstate__()  
__setstate__(state)  
engine  
correct_window()  
__repr__()  
sandwich (number=False)  
baguette (number=False)  
iterate (number=False)  
get_single_reader (number)  
get_reader_by_id (someid)  
real_number_of_frames()  
number_of_frames (onelayer=False)  
number_of_layers()  
```

class ReaderAccess
Bases: object

reader

VdW_radii = {'ge': 2.11, 'gd': 2.34, 'ga': 1.87, 'la': 2.43, 'li': 1.82, 'tl': 1.96, 'lu': 2.24, 'lr': 2.46, 'th': 2.45, ...

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: aquaduct.traj.sandwich.ReaderAccess

```python
__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.

```
real_number_of_frames()
parse_selection(selection)
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)
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)
layer(number)
numbers()
ix(ix)
len()
get_reader(number)
add(other)
uniquify()
ids()
coords()
center_of_mass()

class AtomSelection(selected)
Bases: aquaduct.traj.sandwich.Selection
vdw()
residues()
coors()

center_of_mass()

contains_residues( other_residues, convex_hull=False, map_fun=None, known_true=None)

containing_residues( other_residues, *args, **kwargs)

chull()

class ResidueSelection(selected)
    Bases: aquaduct.traj.sandwich.Selection

    coords()

    names()

    single_residues()

    coords_range_core( *args, **kwargs)

    coords_range( srange, number, rid)

class FramesRangeCollection
    Bases: object

    __init__( )

    append( srange)

    get_ranges( srange)

    smooth_coords_ranges( *args, **kwargs)

class SingleResidueSelection( resid)
    Bases: aquaduct.traj.sandwich.ReaderAccess

    __init__( resid)

    get_reader()

    coords( frames)

    _coors( *args, **kwargs)

    coords_smooth( sranges, smooth)

Module contents

5.1.1.4 aquaduct.utils package

Submodules

aquaduct.utils.clui module

Module comprises convieniences functions and definitios for different operations related to command line user interface.

class roman_emulation
    Bases: object

    toRoman( nr)

emit_message_to_file_in_root_logger( mess)

message_special( mess)

5.1. aquaduct package
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)
__enter__ ()
__exit__ (typ, value, traceback)
__call__ (info)
class tictoc(mess)
Bases: object
__init__ (mess)
__enter__ ()
__exit__ (typ, value, traceback)
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:

<table>
<thead>
<tr>
<th>Unit name</th>
<th>Unit abbreviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>seconds</td>
<td>s</td>
</tr>
<tr>
<td>minutes</td>
<td>m</td>
</tr>
<tr>
<td>hours</td>
<td>h</td>
</tr>
<tr>
<td>days</td>
<td>d</td>
</tr>
<tr>
<td>years</td>
<td>y</td>
</tr>
</tbody>
</table>

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) – Excess above standard number of current time units.
- maximal_length (int) – Maximal length of the output string. Must be greater than 0.
- maximal_units (int) – Maximal number of units used in the output string. Must be greater than 0 and lower than 6.

Returns string of nicely formatted 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`

```python
class SimpleProgressBar(maxval=None, mess=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)

**Parameters**

• **maxval** *(int)* – Maximal number of iterations stored to `maxval`.
• **mess** *(str)* – Optional message displayed at progress bar initialization.

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 with `smart_time_string()`.

---

5.1. aquaduct package 63
Returns ETA as string.

Return type str

percent()
Returns float number of percent 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 progress 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 written to standard error.

heartbeat()

next()

update(step)
Updates number of current iterations current by one if step is > 0. Otherwise number of current iterations is not updated. In both cases time of current iteration tcurrent is updated and show() is called.

Parameters step(int) – update step

ttime()
Calculates and returns total time string formatted 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 written to standard error.

pbar
alias of SimpleProgressBar

get_str_timestamp()

class SimpleTree(name=None, message=None)
    Bases: object
    __init__(name=None, message=None)
    __repr__()
    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.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)*

**lind** *(l, ind)*

Indexes lists using lists of integers as identifiers. 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

**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*)

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.

**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

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 appropriate 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

```python
class arrayify(shape=None):
    Bases: object
    __init__(shape=None)
    __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)

**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**)

**class** SmartRangeFunction(element, times)

    Bases: object
    __init__(element, times)

    __str__()

    __repr__()

    __len__()

    get()

    rev()

    isin(element)

    first_element()

    last_element()

    overlaps(srange)

    overlaps_mutual(srange)

    contains(srange)

**class** SmartRangeEqual(element, times)

    Bases: aquaduct.utils.helpers.SmartRangeFunction

    type = 'e'
get()
rev()
isin(element)
last_element()

class SmartRangeIncrement (element, times)
    Bases: aquaduct.utils.helpers.SmartRangeFunction
    type = 'i'
    get()
    rev()
    isin(element)
    last_element()

class SmartRangeDecrement (element, times)
    Bases: aquaduct.utils.helpers.SmartRangeFunction
    type = 'd'
    get()
    rev()
    isin(element)
    last_element()

class SmartRange (iterable=None)
    Bases: object
    __init__ (iterable=None)
    __str__ ()
    __repr__ ()
    first_element ()
    last_element ()
    last_times ()
    raw
    append(element)
    get()
    rev()
    __len__ ()
    __iter__ ()
    min()
    max()
    isin(element)

aquaduct.utils.maths module

class NumpyDefaultsStorageTypes
    Bases: object

5.1. aquaduct package
float_default
   alias of float64

int_default
   alias of int64

make_default_array(array_like)

aquaduct.utils.multip module

class CpuThreadsCount
   Bases: object
   cpu_count = 2
   threads_count = None

Module contents

5.1.1.5 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__()
   distance(E1, E2)
   static color_distance(e1, e2)
   __call__(node)
   _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__()
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__()
open(filename)
save_object2tar(obj, name)
save_file2tar(filename, name)
__del__()
class ConnectToPymol
Bases: object
cgo_line_width = 2.0
cpymol = 'pymol'
ct_file = 'file'
__init__()
decode_color(*args, **kwargs)
init_pymol()
init_script(filename)
add_cgo_object(name, cgo_object, state=None)

5.1. aquaduct package
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)
add_single_path_continuous_trace (spath, smooth=None, plot_in=38161.0, 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)
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)
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 (*args, **kwargs)
Module contents

5.1.2 Module contents

Aqua-Duct - a collection of tools to trace residues in MD simulation.

version()  
Returns aqueduct version number.

Returns 3 element tuple of int numbers  
Return type tuple

version_nice()  
Returns aqueduct 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 aqueduct. It has a form of ASCII-like graphic. Currently it returns following string:

```
-----------------------------------------------
~ ~ ~ A Q U A - D U C T ~ ~ ~
################################################
#### ######## ######## ####
## #### #### ##
# ## ## #
# ## ## #
# ## ## #
-----------------------------------------------
```

Returns aqueduct fancy greetings.  
Return type str
AQUA-DUCT CHANGELOG

**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 clusterization 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.
  – Clusterization 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
aquaduct, 73
aquaduct.apps, 39
aquaduct.apps.data, 37
aquaduct.apps.valvecore, 38
aquaduct.geom, 51
aquaduct.geom.cluster, 39
aquaduct.geom.convexhull, 40
aquaduct.geom.master, 41
aquaduct.geom.pca, 43
aquaduct.geom.smooth, 44
aquaduct.geom.traces, 47
aquaduct.traj, 61
aquaduct.traj.barber, 51
aquaduct.traj.dumps, 52
aquaduct.traj.inlets, 53
aquaduct.traj.paths, 55
aquaduct.traj.sandwich, 58
aquaduct.utils, 70
aquaduct.utils.clui, 61
aquaduct.utils.helpers, 65
aquaduct.utils.maths, 69
aquaduct.utils.multip, 70
aquaduct.visual, 73
aquaduct.visual.cmaps, 70
aquaduct.visual.helpers, 70
aquaduct.visual.pymol_cgo, 70
aquaduct.visual.pymol_connector, 70
aquaduct.visual.quickplot, 72
Symbols

_ColorMapDistMap__do_cadex() (ColorMapDistMap method), 70
_MacroMolPath__object_len_calculate() (MacroMolPath method), 57
_PassingPath__object_len_calculate() (PassingPath method), 58
_ValveConfig__make_options_nt() (ValveConfig method), 39
__call__() (CTypeSpathsCollectionWorker method), 41
__call__() (Center method), 43
__call__() (ColorMapDistMap method), 70
__call__() (ConnectToPymol method), 71
__call__() (DistanceWindowOverMaxStepSmooth method), 47
__call__() (DistanceWindowSmooth method), 46
__call__() (FakeSingleResidueSelection method), 43
__call__() (FloatWindow method), 45
__call__() (FramesRangeCollection method), 61
__call__() (GeneralWindow method), 45
__call__() (GenericPaths method), 55
__call__() (Inlet method), 53
__call__() (InletClusterExtendedType method), 53
__call__() (InletClusterGenericType method), 53
__call__() (Inlets method), 54
__call__() (IntWindow method), 45
__call__() (LoadDumpWrapper method), 37
__call__() (MacroMolPath method), 56
__call__() (MasterPath method), 58
__call__() (MaxStepSmooth method), 46
__call__() (Normalize method), 43
__call__() (PCA method), 44
__call__() (PerformClustering method), 40
__call__() (Smooth method), 44
__call__() (Standartize method), 44
__call__() (arrayify method), 67
__call__() (fbm method), 62
__cmp__ (InletClusterGenericType method), 53
__del__() (ConnectToPymol method), 72
__del__() (ReaderTraj method), 59
__del__() (SimpleTarWriteHelper method), 71
__del__() (TmpDumpWriterOfMDA method), 53
__del__() (ValveDataAccessRoots method), 38
__enter__() (fbm method), 62
__enter__() (tictoc method), 62
__eq__() (SinglePathID method), 56
__exit__() (fbm method), 62
__exit__() (tictoc method), 62
__getitem__() (InletClusterGenericType method), 53
__getstate__() (MasterReader method), 59
__has_out (PassingPath attribute), 57
__hash__() (InletClusterGenericType method), 53
__init__() (ActiveWindowOverMaxStepSmooth method), 47
__init__() (ActiveWindowSmooth method), 46
__init__() (BarberClusterResult method), 39
__init__() (BasicPymolCGO method), 71
__init__() (Bunch method), 68
__init__() (CTypeSpathsCollection method), 42
__init__() (CTypeSpathsCollectionWorker method), 41
__init__() (Center method), 43
__init__() (ColorMapDistMap method), 70
__init__() (ConnectToPymol method), 71
__init__() (DistanceWindowOverMaxStepSmooth method), 47
__init__() (DistanceWindowSmooth method), 46
__init__() (FakeSingleResidueSelection method), 43
__init__() (FloatWindow method), 45
__init__() (FramesRangeCollection method), 61
__init__() (GeneralWindow method), 45
__init__() (GenericPaths method), 55
__init__() (Inlet method), 53
__init__() (InletClusterExtendedType method), 53
__init__() (InletClusterGenericType method), 53
__init__() (Inlets method), 54
__init__() (IntWindow method), 45
__init__() (LoadDumpWrapper method), 37
__init__() (MacroMolPath method), 56
__init__() (MasterPath method), 58
__init__() (MaxStepSmooth method), 46
__init__() (Normalize method), 43
__init__() (PCA method), 44
__init__() (PassingPath method), 57
__init__() (PerformClustering method), 40
__init__() (ReaderTraj method), 59
__init__() (SavgoSmooth method), 46
__init__() (Selection method), 60
__init__() (SimpleProgressBar method), 63
__init__() (SimpleTarWriteHelper method), 71
__init__() (SimpleTree method), 64
__init__() (SinglePathID method), 56
__init__() (SinglePathPlotter method), 72
__init__() (SingleResidueSelection method), 61
__init__() (SmartRange method), 69
__init__() (SmartRangeFunction method), 68
__init__() (Smooth method), 44
__init__() (Standartize method), 44
__init__() (TmpDumpWriterOfMDA method), 52
__init__() (TriangleLinearize method), 50
__init__() (ValveConfig method), 38
__init__() (ValveDataAccess_nc method), 38
__init__() (VectorLinearize method), 50
__init__() (WhereToCut method), 52
__init__() (Window method), 58
__init__() (WindowOverMaxStepSmooth method), 47
__init__() (WindowSmooth method), 46
__init__() (arrayify method), 67

79
Aqua-Duct Documentation, Release 0.5.9

__init__() (fbm method), 62
__init__() (tictoc method), 62
__iter__() (SmartRange method), 69
__len__() (InletClusterGenericType method), 53
__len__() (SmartRange method), 69
__len__() (SmartRangeFunction method), 68
__repr__() (Auto method), 65
__repr__() (InletClusterGenericType method), 53
__repr__() (MasterReader method), 59
__repr__() (ReaderTraj method), 59
__repr__() (SimpleTree method), 64
__repr__() (SmartRange method), 69
__repr__() (SmartRangeFunction method), 68
__repr__() (Window method), 58
_setstate__() (MasterReader method), 59
__str__() (Auto method), 65
__str__() (InletClusterGenericType method), 53
__str__() (PerformClustering method), 40
__str__() (SinglePathID method), 56
__str__() (SmartRange method), 69
__str__() (SmartRangeFunction method), 68
__str__() (Window method), 58
_coords() (SingleResidueSelection method), 61
_cut_thyself() (WhereToCut method), 52
_edges() (in module aquaduct.geom.convexhull), 40
_faces() (in module aquaduct.geom.convexhull), 40
_get_noclusters() (PerformClustering method), 40
_gpi() (GenericPaths method), 55
_gpo() (GenericPaths method), 55
_gpt() (GenericPaths method), 55
_make_smooth_coords() (MacroMolPath method), 57
_paths (MacroMolPath attribute), 57
_paths (PassingPath attribute), 58
_point_within_convexhull() (in module aquaduct.geom.convexhull), 40
_vertices_ids() (in module aquaduct.geom.convexhull), 40
_vertices_points() (in module aquaduct.geom.convexhull), 40

A
ActiveWindowOverMaxStepSmooth (class in aquaduct.geom.smooth), 47
ActiveWindowSmooth (class in aquaduct.geom.smooth), 46
add() (BasicPymolCGOLines method), 71
add() (BasicPymolCGOSpheres method), 71
add() (Selection method), 60
add_012() (GenericPaths method), 55
add_cgo_object() (ConnectToPymol method), 71
add_cluster_annotations() (Inlets method), 54
add_cone() (BasicPymolCGOPointers method), 71
add_cone() (ReaderTraj method), 54
add_cone() (SimpleTree method), 64
add_leaf() (SimpleTree method), 64
add_leaf_to_leaf() (SimpleTree method), 64
add_leaf_wrapper() (Inlets method), 54
add_message() (SimpleTree method), 64
add_message_to_leaf() (SimpleTree method), 64
add_object() (GenericPaths method), 55
add_outliers_annotations() (Inlets method), 54
add_pointer() (BasicPymolCGOPointers method), 71
add_scope() (GenericPaths method), 55
add_single_path_continuous_trace() (SinglePathPlotter method), 72
add_spheres() (Inlets method), 54
add_spheres_from_inlets() (WhereToCut method), 52
add_spheres_from_spaths() (WhereToCut method), 52
add_type() (GenericPaths method), 55
add_width() (MasterPath method), 58
all_incoming (InletTypeCodes attribute), 53
all_internal (InletTypeCodes attribute), 53
all_outgoing (InletTypeCodes attribute), 53
all_surface (InletTypeCodes attribute), 53
and_back_again() (LinearizeHobbit method), 49
append() (FramesRangeCollection method), 61
append() (SmartRange method), 69
aquaduct (module), 73
aquaduct.apps (module), 39
aquaduct.apps.data (module), 37
aquaduct.apps.valvecore (module), 38
aquaduct.geom (module), 51
aquaduct.geom.cluster (module), 39
aquaduct.geom.convexhull (module), 40
aquaduct.geom.master (module), 41
aquaduct.geom.pca (module), 43
aquaduct.geom.smooth (module), 44
aquaduct.geom.traces (module), 47
aquaduct.traj (module), 61
aquaduct.traj.barber (module), 51
aquaduct.traj.dumps (module), 52
aquaduct.traj.inlets (module), 53
aquaduct.traj.paths (module), 55
aquaduct.traj.sandwich (module), 58
aquaduct.utils (module), 70
aquaduct.utils.clui (module), 61
aquaduct.utils.helpers (module), 65
aquaduct.utils.maths (module), 69
aquaduct.utils.multip (module), 70
aquaduct.visual (module), 73
aquaduct.visual.cmaps (module), 70
aquaduct.visual.helpers (module), 70
aquaduct.visual.pymol_ego (module), 70
aquaduct.visual.pymol_connector (module), 70
aquaduct.visual.quickplot (module), 72
aquaduct_version_nice() (in module aquaduct.apps.valvecore), 39
are_rows_uniq() (in module aquaduct.utils.helpers), 65
arrayify (class in aquaduct.geom.smooth), 47
arrayify (class in aquaduct.geom.smooth), 46
arrays2dict() (IdsOverIds static method), 38
atom2residue() (ReaderTraj method), 54
atom2residue() (ReaderTrajViaMDA method), 54
atom2residue() (ReaderTrajViaMDA method), 54
atom_vdw() (ReaderTraj method), 60
atom_vdw() (ReaderTrajViaMDA method), 60
atoms_masses() (ReaderTrajViaMDA method), 60
atoms_masses() (ReaderTrajViaMDA method), 60
atoms_positions() (ReaderTraj method), 60

Index
Index
Aqua-Duct Documentation, Release 0.5.9

cpu_count (CpuThreadsCount attribute), 70
CpuThreadsCount (class in aquaduct.utils.multip), 70
create_tmpfile() (in module aquaduct.utils.helpers), 65
cp_file (ConnectToPymol attribute), 71
cp_pymol (ConnectToPymol attribute), 71
CTypeSpathsCollection (class in aquaduct.geom.master), 41
CTypeSpathsCollectionWorker (class in aquaduct.geom.master), 41
cut_thyself() (WhereToCut method), 52
decode_color() (ConnectToPymol method), 71
del_cgo_object() (ConnectToPymol method), 71
derrivative() (in module aquaduct.geom.traces), 48
dict2arrays() (IdsOverIds static method), 38
diff() (in module aquaduct.geom.traces), 47
distance() (ColorMapDistMap method), 70
DistanceWindowOverMaxStepSmooth (class in aquaduct.geom.smooth), 47
DistanceWindowSmooth (class in aquadect.geom.smooth), 46
dump() (ValveDataAccess_pickie method), 38
dump_config() (ValveConfig method), 39
dump_frames() (ReaderTraj method), 59
dump_frames () (TmpDumpWriterOfMDA method), 52
dump_frames_to_file() (ReaderTrajViaMDA method), 60
emit_message_to_file_in_root_logger() (in module aquaduct.utils.clui), 61
empty_coords (MacroMolPath attribute), 56
ends (MacroMolPath attribute), 57
engine (MasterReader attribute), 59
engine_name (MasterReader attribute), 58
ETAF() (SimpleProgressBar method), 63
etypes (MacroMolPath attribute), 57
etypes_cont (MacroMolPath attribute), 57
euclidean() (in module aquaduct.visual.helpers), 70
extend_inlets() (Inlets method), 54
f_like() (in module aquaduct.visual.helpers), 70
FakeSingleResidueSelection (class in aquaduct.geom.master), 43
fbm (class in aquaduct.utils.clui), 62
find_paths() (GenericPaths method), 56
find_paths_types() (GenericPaths method), 56
finish() (SimpleProgressBar method), 64
first_element() (SmartRange method), 69
first_element() (SmartRangeFunction method), 68
fit() (BarberCluster method), 40
fit() (PerformClustering method), 40
float_default (NumpyDefaultsStorageTypes attribute), 69
FloatWindow (class in aquaduct.geom.smooth), 45
frames (GenericPaths attribute), 55
FramesRangeCollection (class in aquaduct.traj.sandwich), 61
full_size() (CTypeSpathsCollection method), 42
G
GeneralWindow (class in aquaduct.geom.smooth), 45
generic (InletClusterExtendedType attribute), 53
GenericPaths (class in aquaduct.traj.paths), 55
GenericPathTypeCodes (class in aquaduct.traj.paths), 55
get() (BasicPymolCGO method), 71
get() (SmartRange method), 69
get() (SmartRangeDecrement method), 69
get() (SmartRangeEqual method), 68
get() (SmartRangeFunction method), 68
get() (SmartRangeIncrement method), 69
get_acceleration_cont() (MacroMolPath method), 57
get_ax3d() (in module aquaduct.visual.quickplot), 72
get_chull() (Inlets method), 54
get_cluster_options() (ValveConfig method), 39
cmap() (in module aquaduct.visual.helpers), 70
cmap() (ValveDataAccess_pickie method), 38
coodrs() (MacroMolPath method), 57
coodrs() (PassingPath method), 58
coodrs_cont() (MacroMolPath method), 57
cric_reader() (in module aquaduct.apps.data), 37
current_nr() (WhereToCut method), 52
default_config() (ValveConfig method), 39
distance_both_cont() (MacroMolPath method), 57
distance_cont() (MacroMolPath method), 57
distance_rev_cont() (MacroMolPath method), 57
flat_tree() (Inlets method), 54
general_comment() (ValveConfig method), 39
global_options() (ValveConfig method), 39
inlets() (MacroMolPath method), 56
inlets() (PassingPath method), 58
inlets() (Inlets method), 54
leaf() (SimpleTree method), 64
master_path() (CTypeSpathsCollection method), 43
object_from_name() (in module aquaduct.apps.data), 38
object_name() (in module aquaduct.apps.data), 38
paths() (GenericPaths method), 55
paths_out() (GenericPaths method), 56
ranges() (FramesRangeCollection method), 61
reader() (Selection method), 60
test() (SingleResidueSelection method), 61
reader_by_id() (MasterReader method), 61
real() (Window method), 58
recluster_options() (ValveConfig method), 39
required_params() (in module aquaduct.geom.cluster), 39
single_path_types() (GenericPaths method), 56
single_reader() (MasterReader method), 59
smooth_options() (ValveConfig method), 39
stage_options() (ValveConfig method), 39

82 Index
get_str_timestamp() (in module aquaduct.utils.cli), 64
get_variable() (ValveDataAccess_pickle method), 38
get_vda_reader() (in module aquaduct.apps.data), 37
global_name() (ValveConfig static method), 38
GlobalConfigStore (class in aquaduct.apps.data), 37
glue() (in module aquaduct.traj.paths), 55
greetings() (in module aquaduct), 55
gregorian_year_in_days (in module aquaduct.utils.clui), 62
grey (ColorMapDistMap attribute), 70
gsep() (in module aquaduct.utils.clui), 62
gtypes (MacroMolPath attribute), 57
gtypes (PassingPath attribute), 58
gtypes_cont (MacroMolPath attribute), 57
has_in (MacroMolPath attribute), 57
has_in (PassingPath attribute), 57
has_object (MacroMolPath attribute), 57
has_out (MacroMolPath attribute), 57
has_out (PassingPath attribute), 57
heartbeat() (SimpleProgressBar method), 64
here() (LinearizeOneWay method), 49
here() (LinearizeRecursive method), 50
ids() (Selection method), 60
IdsOverIds (class in aquaduct.apps.data), 38
incoming (ProtoInletTypeCodes attribute), 53
init_ax() (MPLTracePlotter method), 72
init_pymol() (ConnectToPymol method), 71
init_script() (ConnectToPymol method), 71
Inlet (class in aquaduct.traj.inlets), 53
inlet2sphere() (WhereToCut method), 52
InletClusterExtendedType (class in aquaduct.traj.inlets), 53
InletClusterGenericType (class in aquaduct.traj.inlets), 53
InletTypeCodes (class in aquaduct.traj.inlets), 54
input (InletClusterGenericType attribute), 53
is_number() (in module aquaduct.utils.helpers), 65
is_overlapping_with_cloud() (WhereToCut method), 52
is_passing() (MacroMolPath method), 56
is_passing() (PassingPath method), 57
is_passing() (SinglePath method), 57
is_point_within() (Sphere method), 52
is_point_within_convexhull() (in module aquaduct.geom.convexhull), 40
is_single() (MacroMolPath method), 56
is_single() (PassingPath method), 57
is_single() (SinglePath method), 57
is_sphere_cloud() (Sphere method), 52
is_sphere_within() (Sphere method), 52
isin() (SmartRange method), 69
isin() (SmartRangeDecrement method), 69
isin() (SmartRangeFunction method), 69
isin() (SmartRangeEqual method), 69
isin() (SmartRangeIncrement method), 69
iterate() (MasterReader method), 59
iterate_or_die() (in module aquaduct.utils.helpers), 68
iterate_over_frames() (ReaderTraj method), 59
itype (InletTypeCodes attribute), 53
ix() (Selection method), 60
last_element() (SmartRange method), 69
last_element() (SmartRangeDecrement method), 69
last_element() (SmartRangeEqual method), 69
last_element() (SmartRangeFunction method), 68
last_element() (SmartRangeIncrement method), 69
last_times() (SmartRange method), 69
layer() (Selection method), 60
leafs_names (SimpleTree attribute), 64
left() (in module aquaduct.traj.paths), 55
len() (Selection method), 60
len() (Window method), 58
length_step_std() (in module aquaduct.geom.traces), 48
lens() (CTypeSpathsCollection method), 42
lens_norm() (CTypeSpathsCollection method), 42
lens_real() (CTypeSpathsCollection method), 42
lim2clusters() (Inlets method), 54
lim2names() (Inlets method), 54
lim2spaths() (Inlets method), 54
lim2types() (Inlets method), 54
lim_to() (Inlets method), 54
limspaths2() (Inlets method), 54
lind() (in module aquaduct.utils.helpers), 65
LinearizeHobbit (class in aquaduct.geom.traces), 49
LinearizeHobbitTriangle (class in aquaduct.geom.traces), 51
LinearizeHobbitVector (class in aquaduct.geom.traces), 51
LinearizeOneWay (class in aquaduct.geom.traces), 49
LinearizeOneWayTriangle (class in aquaduct.geom.traces), 51
LinearizeOneWayVector (class in aquaduct.geom.traces), 51
LinearizeRecursive (class in aquaduct.geom.traces), 49
Index

Aqua-Duct Documentation, Release 0.5.9

LinearizeRecursiveTriangle (class in aquaduct.geom.traces), 51
LinearizeRecursiveVector (class in aquaduct.geom.traces), 51
list_blocks_to_slices() (in module aquaduct.utils.helpers), 67
listify() (in module aquaduct.utils.helpers), 67
load() (ValveDataAccess_pickle method), 38
load_config() (ValveConfig method), 39
load_cric() (in module aquaduct.apps.data), 37
load_pdb() (ConnectToPymol method), 72
LoadDumpWrapper (class in aquaduct.apps.data), 37
MacroMolPath (class in aquaduct.traj.paths), 56
make_color_triple() (BasicPymolCGO static method), 71
make_default_array() (in module aquaduct.utils.maths), 70
make_iterable() (in module aquaduct.utils.helpers), 68
MasterPath (class in aquaduct.traj.paths), 58
MasterReader (class in aquaduct.traj.sandwich), 58
max() (SmartRange method), 69
max_frame (GenericPaths attribute), 55
max_window_at_pos() (GeneralWindow static method), 45
MaxStepSmooth (class in aquaduct.geom.smooth), 46
MeanShiftBandwidth() (in module aquaduct.geom.cluster), 40
Message() (ValveDataAccess.pickle method), 38
MonteCarloSmooth (class in aquaduct.geom.smooth), 46
MessageSpecial() (ValveDataAccess.pickle method), 38
message() (ValveDataAccess_root method), 38
message() (ValveDataAccess nc method), 38
message() (ValveDataAccess_pickle method), 38
message() (ValveDataAccessRoots method), 38
Number() (ValveDataAccess_root method), 38
number_of_frames() (MasterReader method), 59
number_of_layers() (MasterReader method), 59
numbers() (Selection method), 60
NumpyDefaultsStorageTypes (class in aquaduct.utils.maths), 69
object_len (MacroMolPath attribute), 56
object_len (PassingPath attribute), 57
object_name (GenericPathTypeCodes attribute), 55
object_name (GenericPathTypeCodes attribute), 55
open() (ValveDataAccess_pickle method), 38
open() (ValveDataAccessRoots method), 38
open_reader_traj (MasterReader attribute), 58
open_trajectory() (ReaderTraj method), 59
open_trajectory() (ReaderTrajViaMDA method), 60
orient_on() (ConnectToPymol method), 72
out_name (GenericPathTypeCodes attribute), 55
output (InletClusterGenericType attribute), 53
overlaps() (SmartRangeFunction method), 68
overlaps_mutual() (SmartRangeFunction method), 68
P
P (PCA attribute), 44
parse_selection() (ReaderTraj method), 60
parse_selection() (ReaderTrajViaMDA method), 60
part2type_dict (in module aquaduct.geom.master), 41
parts (CTypeSpathsCollection attribute), 42
parts (in module aquaduct.geom.master), 41
PassingPath (class in aquaduct.traj.paths), 57
path (PassingPath attribute), 58
path_in (MacroMolPath attribute), 56
path_in_code (PathTypesCodes attribute), 55
path_object (MacroMolPath attribute), 56
path_object_code (PathTypesCodes attribute), 55
path_out (MacroMolPath attribute), 56
path_out_code (PathTypesCodes attribute), 55
path_trace() (SimpleTracePlotter method), 72
PathTypesCodes (class in aquaduct.traj.paths), 55
PathTypesCodes (class in aquaduct.traj.paths), 55
PathTypesCodes (class in aquaduct.traj.paths), 55
PCA (class in aquaduct.geom.pca), 44
percent() (SimpleProgressBar method), 64
perform_clustering() (Inlets method), 54
perform_reclustering() (Inlets method), 54
PerformClustering (class in aquaduct.geom.cluster), 40
plot_colorful_lines() (in module aquaduct.visual.quickplot), 72
plot_line() (MPLTracePlotter method), 72
plot_line() (SimpleTracePlotter method), 72
plot_spath_spectrum() (in module aquaduct.visual.quickplot), 72
plot_spath_spectrum() (in module aquaduct.visual.quickplot), 72
preprocess() (PCA method), 44
preprocess_undo() (PCA method), 44
print_simple_tree() (in module aquaduct.utils.clui), 64
protein_trace() (SimpleProteinPlotter method), 72
ProtoInletTypeCodes (class in aquaduct.traj.inlets), 53
Aqua-Duct Documentation, Release 0.5.9

**R**

range() (Window method), 58
range2int() (in module aquaduct.utils.helpers), 66
raw (SmartRange attribute), 69
read() (LoadDumpWrapper method), 37
reader (ReaderAccess attribute), 59
ReaderAccess (class in aquaduct.traj.sandwich), 59
ReaderTraj (class in aquaduct.traj.sandwich), 59
ReaderTrajViaMDA (class in aquaduct.traj.sandwich), 60
readline() (LoadDumpWrapper method), 37
real_number_of_frames() (MasterReader method), 59
real_number_of_frames() (ReaderTraj method), 59
real_number_of_frames() (ReaderTrajViaMDA method), 60
recluster_cluster() (Inlets method), 54
recluster_name() (ValveConfig static method), 38
recluster_outliers() (Inlets method), 54
recursive_clusterization_name() (ValveConfig static method), 38
recursive_threshold_name() (ValveConfig static method), 38
refs (Inlets attribute), 54
refs_names (Inlets attribute), 54
renumber_clusters() (Inlets method), 54
residues() (AtomSelection method), 60
residues_names() (ReaderTraj method), 60
residues_names() (ReaderTrajViaMDA method), 60
residues_positions() (ReaderTraj method), 60
residues_positions() (ReaderTrajViaMDA method), 60
ResidueSelection (class in aquaduct.traj.sandwich), 61
resize_leaf_0() (Inlets method), 54
rev() (SmartRange method), 69
rev() (SmartRangeDecrement method), 69
rev() (SmartRangeEqual method), 69
rev() (SmartRangeFunction method), 68
rev() (SmartRangeIncrement method), 69
right() (in module aquaduct.traj.paths), 55
robust_and() (in module aquaduct.traj.paths), 65
robust_or() (in module aquaduct.traj.paths), 65
roman_emulation (class in aquaduct.traj.sandwich), 61
roots (ValveDataAccessRoots attribute), 38
rotate (SimpleProgressBar attribute), 63

**S**

sandwich() (MasterReader method), 59
sandwich_mode (MasterReader attribute), 58
save_config() (ValveConfig method), 39
save_config_stream() (ValveConfig method), 39
save_cric() (ValveConfig method), 39
save_file2tar() (SimpleTarWriteHelper method), 71
save_object2tar() (SimpleTarWriteHelper method), 71
SavgolSmooth (class in aquaduct.geom.smooth), 46
scatter() (MPLTracePlotter method), 73
scatter() (SinglePathPlotter method), 72
scope_name (GenericPathTypeCodes attribute), 55
Selection (class in aquaduct.traj.sandwich), 60
set_frame() (ReaderTraj method), 59
set_real_frame() (ReaderTraj method), 59
set_real_frame() (ReaderTrajViaMDA method), 60
set_savgol_function() (SavgolSmooth method), 47
set_variable() (ValveDataAccess_pickle method), 38
show() (SimpleProgressBar method), 64
showit() (in module aquaduct.visual.quickplot), 72
simple_types_distribution() (CTypePathsCollection static method), 42
SimplePathPlotter (class in aquaduct.visual.quickplot), 72
SimpleProgressbar (class in aquaduct.visual.html), 63
SimpleProteinPlotter (class in aquaduct.visual.pymol.connector), 71
SinglePath (class in aquaduct.traj.sandwich), 56
SinglePathID (class in aquaduct.traj.paths), 57
SinglePathPlotter (in module aquaduct.visual.pymol.connector), 72
SingleResidueSelection (class in aquaduct.traj.sandwich), 61
size (Inlets attribute), 54
size (MacroMolPath attribute), 57
sizes (MacroMolPath attribute), 57
sizes (PassingPath attribute), 58
small_clusters_to_outliers() (Inlets method), 54
smart_time_string() (in module aquaduct.utils.clui), 62
SmartRange (class in aquaduct.utils.helpers), 69
SmartRangeDecrement (class in aquaduct.utils.helpers), 69
SmartRangeEqual (class in aquaduct.utils.helpers), 68
SmartRangeFunction (class in aquaduct.utils.helpers), 68
SmartRangeIncrement (class in aquaduct.utils.helpers), 69
Smooth (class in aquaduct.geom.smooth), 44
smooth() (ActiveWindowOverMaxStepSmooth method), 47
smooth() (ActiveWindowSmooth method), 46
smooth() (DistanceWindowOverMaxStepSmooth method), 47
smooth() (DistanceWindowSmooth method), 46
smooth() (MaxStepSmooth method), 46
smooth() (SavgolSmooth method), 47
smooth() (Smooth method), 44
smooth() (WindowOverMaxStepSmooth method), 47
smooth() (WindowSmooth method), 46
smooth_coords_ranges() (in module aquaduct.traj.sandwich), 61
smooth_name() (ValveConfig static method), 38
sort_clusters() (Inlets method), 54
sortify() (in module aquaduct.utils.helpers), 66

Index 85
spath2ctype() (Inlets method), 54
spath2spheres() (WhereToCut method), 52
spath_spectrum() (in module aquaduct.visual.quickplot), 72
spaths2ctypes() (Inlets method), 54
spaths_spectra() (in module aquaduct.visual.quickplot), 72
Sphere (class in aquaduct.traj.barber), 51
split_list() (in module aquaduct.utils.helpers), 68
stage_I_run() (in module aquaduct.apps.valvecore), 39
stage_II_run() (in module aquaduct.apps.valvecore), 39
stage_III_run() (in module aquaduct.apps.valvecore), 39
stage_IV_run() (in module aquaduct.apps.valvecore), 39
stage_V_run() (in module aquaduct.apps.valvecore), 39
stage_VI_run() (in module aquaduct.apps.valvecore), 39
Stageartize (class in aquaduct.geom.pca), 44
strech_zip() (in module aquaduct.utils.helpers), 68
surface (ProtoInletTypeCodes attribute), 53
surface_incoming (InletTypeCodes attribute), 53
surface_outgoing (InletTypeCodes attribute), 53
T
thead() (in module aquaduct.utils.cli), 63
thread_count (CpuThreadsCount attribute), 70
tictoc (class in aquaduct.utils.clui), 62
TmpDumpWriterOfMDA (class in module aquaduct.traj.dumps), 52
topology (MasterReader attribute), 58
toRoman() (roman_emulation method), 61
trajectory (MasterReader attribute), 58
triangle_angles() (in module aquaduct.geom.traces), 47
triangle_angles_last() (in module aquaduct.geom.traces), 48
triangle_height() (in module aquaduct.geom.traces), 48
TriangleLinearize (class in aquaduct.geom.traces), 50
tsep() (in module aquaduct.utils.cli), 63
ttime() (SimpleProgressBar method), 64
tupleify() (in module aquaduct.utils.helpers), 67
type (SmartRangeDecrement attribute), 69
type (SmartRangeEqual attribute), 68
type (SmartRangeIncrement attribute), 69
types (GenericPaths attribute), 55
types (Inlets attribute), 54
types (MacroMolPath attribute), 57
types (PassingPath attribute), 58
types_cont (MacroMolPath attribute), 57
types_distribution() (CTypeSpathsCollection method), 43
types_in (MacroMolPath attribute), 56
types_object (MacroMolPath attribute), 56
types_out (MacroMolPath attribute), 56
types_prob_to_types() (CTypeSpathsCollection method), 43
U
underline() (in module aquaduct.utils.clui), 63
undo() (Center method), 43
undo() (Normalize method), 44
undo() (PCA method), 44
undo() (Standartize method), 44
union() (in module aquaduct.traj.paths), 55
union_full() (in module aquaduct.traj.paths), 55
union_smartr() (in module aquaduct.traj.paths), 55
uniqify() (in module aquaduct.utils.helpers), 67
uniqify() (Selection method), 60
unknown_names (ValveDataAccess_pickle attribute), 38
update() (CTypeSpathsCollection method), 42
update() (SimpleProgressBar method), 64
V
valve_begin() (in module aquaduct.apps.valvecore), 39
valve_end() (in module aquaduct.apps.valvecore), 39
valve_exec_stage() (in module aquaduct.apps.valvecore), 39
valve_load_config() (in module aquaduct.apps.valvecore), 39
ValveConfig (class in aquaduct.apps.valvecore), 38
ValveDataAccess (in module aquaduct.apps.data), 38
ValveDataAccess_nc (class in aquaduct.apps.data), 38
ValveDataAccess_pickle (class in aquaduct.apps.data), 37
ValveDataAccessRoots (class in aquaduct.apps.data), 38
vdw() (AtomSelection method), 60
VdW_radii (in module aquaduct.traj.sandwich), 59
vector_norm() (in module aquaduct.geom.traces), 48
VectorLinearize (class in aquaduct.geom.traces), 50
vectors_angle() (in module aquaduct.geom.traces), 48
vectors_angle_alt() (in module aquaduct.geom.traces), 49
vectors_angle_alt_anorm() (in module aquaduct.geom.traces), 49
vectors_angle_anorm() (in module aquaduct.geom.traces), 49
version() (in module aquaduct), 73
version_nice() (in module aquaduct), 73
W
what2what() (in module aquaduct.utils.helpers), 68
WhereToCut (class in aquaduct.traj.barber), 52
Window (class in aquaduct.traj.sandwich), 58
window (MasterReader attribute), 58
WindowOverMaxStepSmooth (class in module aquaduct.geom.smooth), 47
WindowSmooth (class in aquaduct.geom.smooth), 45
X
xor() (in module aquaduct.traj.paths), 55
xor_full() (in module aquaduct.traj.paths), 55
xor_smartr() (in module aquaduct.traj.paths), 55
y

yield_generic_paths() (in module aquaduct.traj.paths), 56

yield_single_paths() (in module aquaduct.traj.paths), 56

yield_spath_len_and_smooth_diff_in_types_slices()
  (in module aquaduct.visual.quickplot), 72

z

zip_zip() (in module aquaduct.utils.helpers), 68