EXCOGITO

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Contents

Chapter 1

EXCOGITO

Chapter 2

python scripts

This folder contains a minimal conda environment that allows the user to:

- convert a GROMACS xtc file to an XYZ file (script `sample_convert_xtc_to_xyz.py`)
- generate a custom .ini parameter file (script `setup_parfile.py`)
- test the software (more info inside the *tests* folder)

Installation

In order to install the software you must have `conda` installed.

Then, it is sufficient to run the following command:

"‘ conda env create –file conda_env_excogito.yml "‘

to create the **excogito** environment. Once the packages are downloaded, **excogito** can be activated via:

"‘ conda activate excogito "‘

XTC to XYZ conversion

In order to convert a GROMACS XTC to XYZ you just need to run:

"‘ python3 sample_convert_xtc_to_xyz.py "‘

Once you provide GROMACS XTC and GRO files and a reasonable name for your output, the script will perform the conversion making use of the `MDTraj 1.9.5` software

Parameter file setup

Running

"‘ python3 setup_parfile.py "‘

will help you with the setup of the *ini* parameter file needed by EXCOGITO.

Contacts

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Chapter 3

README

EXCOGITO is the program to investigate the mapping problem in coarse-grained modelling of biomolecules.

If you use EXCOGITO in your research please cite:

EXCOGITO, an EXtensible COarse-GraIning TOol, M Giulini, R Fiorentini, L Tubiana, R Potestio, *in preparation*

An Information-Theory-Based Approach for Optimal Model Reduction of Biomolecules, M Giulini, R Menichetti, MS Shell, R Potestio, *Journal of chemical theory and computation 16 (11), 6795-6813*

A journey through mapping space: characterising the statistical and metric properties of reduced representations of macromolecules, R Menichetti, M Giulini, R Potestio, *The European Physical Journal B 94 (10), 1-26*

1. Installation

1.1 General requirements on Linux systems

The only requirement is to have `Openmp` installed on your machine.

1.2 Additional requirements on MAC OS

- Install `argp` by using homebrew. At the terminal, run this command: "' brew install argp-standalone "'
- Install `xcode` if your version is higher than MacOs 10.7. You are not required to install the Xcode App from AppStore. At the terminal, just run this command (about 15 Gb are required free on your disk even though, at the end of installation, only 2 Gb will be consumed) "' xcode-select –install "'

In order to have access to OpenMP libraries you can install `libomp` by using homebrew. At the terminal, run this command: "' brew install libomp "'

1.3 Compiling

The code can be compiled using `CMake`. A minimal installation is obtained following these steps:

1. create a directory in *excogito*, such as *build* "'bash mkdir build cd build "'
2. run cmake from *build*, calling the outer directory "'bash cmake .. "'
3. run make "'bash make "'

1.3.2 Compilation options

Cmake allows to specify several options, such as the C compiler, compilation links and compilation flags. For instance, if the optimized Intel C compiler (icc) is available, step 2 may be substitued by: "‘bash cmake .. -DCMAKE-_C_COMPILER=icc -DCMAKE_C_FLAGS="-Ofast -fopenmp -I./include -mkl -xSSE4.2 -parallel -ipo -mcpu=native" "‘

On MacOs, the C compiler identification should be AppleClang (check the first line printed on terminal after launching the command `cmake ..`).

2. Running

The typical usage of the program consists in a call to *excogito* with one of the following options:

- **optimize**: to optimize the coarse-grained mapping by minimising its mapping entropy;
- **random**: to randomly generate coarse-grained representations and measure the associated mapping entropies;
- **measure**: to measure the mapping entropy of a mapping provided by the user (in the form of a .txt file);
- **norm**: to calculate the norm of a mapping (provided by the user) throughout a trajectory;
- **cosine**: to calculate pairwise distance and cosine between a pair of mappings (provided by the user) throughout a trajectory;
- **distance**: to calculate the distance matrix between a data set of mappings (provided by the user) over a single conformation;
- **optimize_kl**: to optimize the coarse-grained mapping by minimising its mapping entropy, calculated using the original Kullback-Leibler divergence;
- **random_kl**: to randomly generate coarse-grained representations and measure the associated mapping entropies, calculated using the original Kullback-Leibler divergence;
- **measure_kl**: to measure the mapping entropy of a mapping provided by the user (in the form of a .txt file), calculated using the original Kullback-Leibler divergence.

Each task can require different input files, which are provided to the program in the form of command-line options.

For further information, please type on terminal `./excogito --help` or `./excogito -h`

Alternatively, for printing a short usage message, please type: `./excogito --usage` or `./excogito -u`

After selecting which task is suitable for your purposes, read carefully the documentation below according to your choice.

2.1. Optimize Task

The **optimize** task requires the *protein code* string and three input files: *parameter*, *trajectory*, and *energy*.

In order to launch the **optimize** task follow this syntax:

"‘bash ./excogito optimize -p $parameter_file.ini -t $trajectory_file.xyz -e $energy_file.txt -c $prot_code

or

./excogito optimize –p $parameter_file.ini –t $trajectory_file.xyz –e $energy_file.txt –code $prot_code "‘

For further information, please type on terminal `./excogito optimize`

2.2. Random Task

The **random** task requires the *protein code* string and three input files: *parameter*, *trajectory*, and *energy*.

In order to launch the **random** task follow this syntax:

"‘bash ./excogito random -p $parameter_file.ini -t $trajectory_file.xyz -e $energy_file.txt -c $prot_code

or

./excogito random –p $parameter_file.ini –t $trajectory_file.xyz –e $energy_file.txt –code $prot_code "‘

For further information, please type on terminal `./excogito random`

2.3. Measure Task

The **measure** task requires the *protein code* string and four input files: *parameter*, *trajectory*, *energy*, and *mapping*.

In order to launch the **measure** task follow this syntax:

"‘bash ./excogito measure -p $parameter_file.ini -t $trajectory_file.xyz -e $energy_file.txt -c $prot_code -m $mapping_file.txt

or

./excogito measure –p $parameter_file.ini –t $trajectory_file.xyz –e $energy_file.txt –prot_code $prot_code –m1 $mapping_file.txt "‘

For further information, please type on terminal `./excogito measure`

2.4. Norm Task

The **norm** task requires the *protein code* string and three input files: *parameter*, *trajectory*, and *mapping*.

In order to launch the **norm** task follow this syntax:

"‘bash ./excogito norm -p $parameter_file.ini -t $trajectory_file.xyz -c $prot_code -m $mapping_file.txt

or

./excogito norm –p $parameter_file.ini –t $trajectory_file.xyz –prot_code $prot_code –m1 $mapping_file.txt "‘

For further information, please type on terminal `./excogito norm`

2.5. Cosine Task

The **cosine** task requires the *protein code* string and four input files: *parameter*, *trajectory*, *1st mapping*, and *2nd mapping*.

In order to launch the **cosine** task follow this syntax:

"‘bash ./excogito cosine -p $parameter_file.ini -t $trajectory_file.xyz -c $prot_code -m $mapping_file.txt -n $mapping-_file2.txt

or

./excogito cosine –p $parameter_file.ini –t $trajectory_file.xyz –prot_code $prot_code –m1 $mapping_file.txt –m2 $mapping_file2.txt "‘

For further information, please type on terminal `./excogito cosine`

2.6. Distance Task

The **distance** task requires the *protein code* string and thre input files: *parameter*, *trajectory*, *mapping matrix*.

In order to launch the **distance** task follow this syntax:

"'bash ./excogito distance -p $parameter_file.ini -t $trajectory_file.xyz -c $prot_code -x $mapping_matrix_file.txt

or

./excogito distance –p $parameter_file.ini –t $trajectory_file.xyz –prot_code $prot_code –matrix $mapping_matrix-_file.txt

"'

For further information, please type on terminal `./excogito distance`

2.7. Optimize_kl Task

The **optimize_kl** task requires the *protein code* string and three input files: *parameter*, *trajectory*, and *probability*.

In order to launch the **optimize_kl** task follow this syntax:

"'bash ./excogito optimize -p $parameter_file.ini -t $trajectory_file.xyz -r $probability_file.txt -c $prot_code

or

./excogito optimize –p $parameter_file.ini –t $trajectory_file.xyz –probs $probability_file.txt –code $prot_code "'

For further information, please type on terminal `./excogito optimize_kl`

2.8. Random_kl Task

The **random_kl** task requires the *protein code* string and three input files: *parameter*, *trajectory*, and *probability*.

In order to launch the **random_kl** task follow this syntax:

"'bash ./excogito random_kl -p $parameter_file.ini -t $trajectory_file.xyz -r $probability_file.txt -c $prot_code

or

./excogito random_kl –p $parameter_file.ini –t $trajectory_file.xyz –probs $probability_file.txt –code $prot_code "'

For further information, please type on terminal `./excogito random_kl`

2.9. Measure_kl Task

The **measure_kl** task requires the *protein code* string and four input files: *parameter*, *trajectory*, *probability*, and *mapping*.

In order to launch the **measure_kl** task follow this syntax:

"'bash ./excogito measure_kl -p $parameter_file.ini -t $trajectory_file.xyz -r $probability_file.txt -c $prot_code -m $mapping_file.txt

or

./excogito measure_kl –p $parameter_file.ini –t $trajectory_file.xyz –probs $probability_file.txt –prot_code $prot_-code –m1 $mapping_file.txt "'

For further information, please type on terminal `./excogito measure_kl`

3. Which arguments are mandatory? A short explanation

As shown in **Section 2.x**, the *protein code* string and two files are always mandatory, namely the *parameter file* and the *xyz trajectory file.* The other files can be mandatory, depending on the chosen task.

What are these files?

- $**$$parameter_file.ini$**$ $\rightarrow$ Set of parameters in *ini* format for the algorithm (see 3.1). Examples are present in $*$/examples/parameters$*$;

- ∗∗$trajectory_file.xyz∗∗ → Trajectory in *xyz* format (see the Section 3.2). An example is present in ∗/examples/trajectories∗;
- ∗∗$energy_file.txt∗∗ → File with the energies corresponding to each configuration in the trajectory (see the Section 3.3). An example is present in ∗/examples/energies∗;
- ∗∗$prot_code∗∗ → Unique string that identifies the structure (see 3.4). It will be used to generate the output files;
- ∗∗$mapping_file.txt∗∗ → Mapping file, containing the indices of the retained atoms (see 3.5). An example is present in ∗/examples/mappings∗;
- ∗∗$mapping_file2.txt∗∗ → 2nd Mapping file, containing the indices of the retained atoms (see 3.5). An example is present in ∗/examples/mappings∗;
- ∗∗$mapping_matrix_file.txt∗∗ → Matrix with *n_mappings* CG mappings (see 3.6).
- ∗∗$probability_file.txt∗∗ → File with the probabilities corresponding to each configuration in the trajectory (see 3.7). They must sum to 1.0. An example is present in ∗/examples/probabilities∗;

3.1. Parameter FILE

The core element of EXCOGITO is the parameter file, which is employed to define the constants used in the different tasks.

A sample parameter file for each task can be found in /examples/parameters.

There exist 16 parameters, but only few of them are mandatory for the selected task. They are illustrated in the following table:

Parameter	Description	Type	Mandatory	Suggested value
atomnum	number of atoms in the system	int	all	
frames	number of frames in the trajectory	int	all	`$< 5000 \ \text{(on laptops),} \ < 15000 \ \text{if criterion} \ != 3$`
cgnum	number of CG sites	int	all	`$\in [\frac{\text{atomnum}}{20} , \frac{\text{atomnum}}{2}]$`
criterion	criterion for clustering	int	O-R-M	`$\in {0, 1, 2, 3, 4}$`
nclust	number of CG macrostates	int	C0 - C3	`$\in [\frac{\text{frames}}{500} \frac{\text{frames}}{100}]`
n_mappings	number of mappings in tasks **random** and **distance**	int	R-D	

MC_steps	number of MC step in task **optimize**	int	O	> 5000
rotmats_period	MC steps between two full alignments in task **optimize**	int	O	
t_zero	starting temperature in task **optimize**	double	O	
distance	cophenetic distance threshold	double	C1	
max_nclust	upper number of clusters	int	C2	$\in [\frac{\text{frames}}{100} \frac{\text{frames}}{50}]$
min_nclust	lower number of clusters	int	C2	$\in [\frac{\text{frames}}{1000 \ \text{and} \ << \text{\ max\_nclust}$
Ncores	number of cores	int	no	
decay_time	governs temperature decay in task **optimize**	double	O	
rsd	use rsd (if 1) instead of rmsd (if 0)	int	no	
stride	number of structures between two pivot configurations	int	C3	$\sim 10 \ \text{if frames} \in [10^4, 10^5]$

O-R-M-D refer to the tasks (optimize/optimize_kl, random/random_kl, measure/measure_kl, distance) in which the parameter is mandatory. C0 .. C3 indicates that the parameter is mandatory if the clustering criterion is equal to 0 .. 3, respectively.

Clustering

Four criteria for hierarchical clustering:

- **0** *Maxclust* clustering: configurations are lumped into *Nclust* macrostates;
- **1** *Maxdist* clustering: clustering with the cophenetic distance;
- **2** *Multiple maxclust*: as described in *Giulini et al.* (JCTC, 2020);
- **3** *Fast clustering*: as in criterion **0**, but applied to a set of pivot configurations. Labels of intermediate structures are assigned to the closer pivot;

3.2. Trajectory FILE

The trajectory should be provided in the xyz format. The first line of each frame indicates the number of atoms, while the second can contain an arbitrary string. As an example, a trajectory with 2 frames and 3 atoms should resemble the following string:

‘‘‘ 3

X 2.53 2.09 3.55 X 2.57 1.95 3.51 X 2.45 1.87 3.46 3

X 2.69 1.96 3.40 X 2.80 1.91 3.43 X 2.67 2.03 3.28 ‘‘‘

In the *python* subdirectory there is a script that helps with the conversion from GROMACS XTC to the XYZ format.

3.3. Energy FILE

Energy files, mandatory for tasks **optimize**, **random**, and **measure**, should contain one value for each frame in the trajectory.

3.4 Protein Code

The protein code is a string that is used to create output files. Don't insert spaces or special characters in this string

3.5 Mapping FILES

A mapping file, mandatory for tasks **measure**, **norm**, and **cosine** is a file with an integer per line. The value correspond to the index of the atom in the xyz trajectory. As an example, a mapping with 8 sites on a peptide of 50 sites should respect the following format:

"' 3 7 19 21 26 34 40 47 "'

3.6. Mapping Matrix FILES

A mapping matrix is mandatory for task **distance**. It is simply a series of transposed mappings. If we aim at computing the distance matrix between three mappings with 8 sites on a peptide of 50 sites, we must respect the following syntax:

"' 3 7 19 21 26 34 40 47 2 8 19 24 25 38 41 44 0 10 12 20 29 31 35 49 "'

3.7. Probability FILE

Probability files, mandatory for tasks **optimize_kl**, **random_kl**, and **measure_kl**, must contain one value for each frame in the trajectory and should be properly normalized to 1. For a trajectory of 5 frames, the following file is acceptable:

"' 0.1 0.15 0.6 0.05 0.1 "'

4. Examples

Inside the directory examples there are example files for the *6d93* protein, allowing the user to try all the different tasks:

- **optimize**: `./build/excogito optimize -p examples/parameters/parameters_-optimize_6d93_N31_small.ini -t examples/trajectories/6d93_100frames.xyz -e examples/energies/6d93_energies_100frames.txt -c 6d93`
- **random**: `./build/excogito random -p examples/parameters/parameters_random-_6d93_N31_small.ini -t examples/trajectories/6d93_100frames.xyz -e examples/energies _energies_100frames.txt -c 6d93`
- **measure**: `./build/excogito measure -p examples/parameters/parameters-_loadca_6d93_N31.ini -t examples/trajectories/6d93_1000frames.xyz -e examples/energies/6d93_energies_1000frames.txt -c 6d93 -m examples/mappings/tamapin-_ca_mapping.txt`
- **norm**: `./build/excogito norm -p examples/parameters/parameters_norm_6d93_-N31.ini -t examples/trajectories/6d93_1000frames.xyz -e examples/energies/6d93-_energies_1000frames.txt -c 6d93 -m examples/mappings/tamapin_ca_mapping.-txt`

- **cosine**: `./build/excogito cosine -p ./examples/parameters/parameters_-cosine_6d93_N31.ini -t ./examples/trajectories/6d93_1000frames.xyz -e ./examples/energies/6d93_energies_1000frames.txt -c 6d93 -m ./examples/mappings/tama _ca_mapping.txt --m2 ./examples/mappings/tamapin_nextca_mapping.txt`
- **distance**: `./build/excogito distance -p examples/parameters/parameters-_distance_6d93_N31.ini -t ./examples/trajectories/6d93_1frame.xyz -x examples/mappings/6d93_mapping_matrix.txt -c 6d93`
- **optimize**: `./build/excogito optimize_kl -p examples/parameters/parameters_-optimizekl_6d93_N31_notemp.ini -t examples/trajectories/6d93_100frames.-xyz -r examples/probabilities/6d93_probs_100frames.txt -c 6d93`
- **random_kl**: `./build/excogito random_kl -p examples/parameters/parameters-_randomkl_6d93_N31.ini -t examples/trajectories/6d93_100frames.xyz -r examples/probabilities/6d93_probs_100frames.txt -c 6d93`
- **measure_kl**: `./build/excogito measure_kl -p examples/parameters/parameters-_measurekl_6d93_N31.ini -t examples/trajectories/6d93_100frames.xyz -r examples/probabilities/6d93_probs_100frames.txt -c 6d93 -m examples/mappings/tamapir _ca_mapping.txt`

5. Scaling values

The approximated mapping entropy is calculated (tasks **optimize**, **random** and **measure**) without the scaling factor $\frac{k_B \beta^2}{2}$ (see. Giulini et al.). This factor should be computed by the user according to the temperature employed to simulate the system.

6. Documentation

File `refman.pdf` in the `docs` directory contains detailed documentation authomatically generated with doxygen version 1.8.5.

A custom documentation can be generated in `html` and `tex` format by running `doxygen excogito_-doxygen.conf`.

7. Contacts

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Chapter 4

How to test the software?

We employ python `Unittest` class to test our code. The file *test_suite.py* contains some Unittest Test Cases that should be run in order to be sure that the compilation went succesfully.

“‘bash python3 test_suite.py -v “‘

If everything went smoothly the output should look like the following:

“‘bash ... Ran 20 tests in 0.140s

OK “‘

test_suite.py makes use of the following packages:

- unittest
- pathlib
- os
- subprocess

Chapter 5

Namespace Index

5.1 Namespace List

Here is a list of all namespaces with brief descriptions:

Chapter 6

Hierarchical Index

6.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

Chapter 7

Class Index

7.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

Chapter 8

File Index

8.1 File List

Here is a list of all files with brief descriptions:

Chapter 9

Namespace Documentation

9.1 sample_convert_xtc_to_xyz Namespace Reference

Variables

- tuple xtc_path = input("insert path to XTC file\n")
- tuple gro_path = input("insert path to GRO file\n")
- tuple xyz_filename = input("insert path to output XYZ file\n")
- tuple full_traj = mdtraj.load_xtc(xtc_path.strip(),top=gro_path.strip())
- full_traj_topology = full_traj.topology
- tuple no_h = full_traj_topology.select('type != H')
- tuple n_heavy_traj = len(no_h)
- tuple mdt_tr_heavy = mdtraj.load_xtc(xtc_path, top=gro_path, atom_indices = list(no_h))

9.1.1 Variable Documentation

9.1.1.1 tuple sample_convert_xtc_to_xyz.xtc_path = input("insert path to XTC file\n")

9.1.1.2 tuple sample_convert_xtc_to_xyz.gro_path = input("insert path to GRO file\n")

9.1.1.3 tuple sample_convert_xtc_to_xyz.xyz_filename = input("insert path to output XYZ file\n")

9.1.1.4 tuple sample_convert_xtc_to_xyz.full_traj = mdtraj.load_xtc(xtc_path.strip(),top=gro_path.strip())

9.1.1.5 sample_convert_xtc_to_xyz.full_traj_topology = full_traj.topology

9.1.1.6 tuple sample_convert_xtc_to_xyz.no_h = full_traj_topology.select('type != H')

9.1.1.7 tuple sample_convert_xtc_to_xyz.n_heavy_traj = len(no_h)

9.1.1.8 tuple sample_convert_xtc_to_xyz.mdt_tr_heavy = mdtraj.load_xtc(xtc_path, top=gro_path, atom_indices = list(no_h))

9.2 setup_parfile Namespace Reference

Functions

- def retrieve_parameter
- def get_mandatory_parameters

- def get_optional_parameters
- def write_parameters

Variables

- list tasks = ["optimize", "random", "measure", "norm", "cosine", "distance", "optimize_kl", "measure_kl"]
- dictionary mandatory_pars
- dictionary optional_pars
- dictionary pars_description
- dictionary pars_type
- dictionary clustering_pars
- tuple task = input("Insert the task you would like to perform among the following: " + str(tasks) + "\n")
- dictionary my_pars = {}
- tuple opt = input("Insert optional parameters? (y/n)")

9.2.1 Function Documentation

9.2.1.1 def setup_parfile.retrieve_parameter (*par_name*, *par_type*, *par_desc*)

9.2.1.2 def setup_parfile.get_mandatory_parameters (*task*)

9.2.1.3 def setup_parfile.get_optional_parameters (*task*)

9.2.1.4 def setup_parfile.write_parameters (*task*, *pars_dict*)

9.2.2 Variable Documentation

9.2.2.1 list setup_parfile.tasks = ["optimize", "random", "measure", "norm", "cosine", "distance", "optimize_kl", "measure_kl"]

9.2.2.2 dictionary setup_parfile.mandatory_pars

Initial value:

```
= {
    "optimize" : [ "atomnum", "frames", "cgnum", "MC_steps", "rotmats_period", "Ncores" ],
    "random" : [ "atomnum", "frames", "cgnum", "n_mappings" ],
    "measure" : [ "atomnum", "frames", "cgnum" ],
    "norm": [ "atomnum", "frames", "cgnum" ],
    "cosine" : [ "atomnum", "frames", "cgnum" ],
    "distance" : [ "atomnum", "frames", "cgnum", "n_mappings" ],
    "optimize_kl" : ["atomnum", "frames", "cgnum", "MC_steps", "Ncores"],
    "measure_kl" : [ "atomnum", "frames", "cgnum" ]
}
```

9.2.2.3 dictionary setup_parfile.optional_pars

Initial value:

```
= {
    "optimize" : [ "criterion", "t_zero", "decay_time"],
    "random" : [ "criterion"],
    "measure" : [ "criterion"],
    "norm": [],
    "cosine" : [],
    "distance" : [],
    "optimize_kl" : ["criterion", "t_zero", "decay_time"],
    "measure_kl" : [ "criterion"]
}
```

9.2.2.4 dictionary setup_parfile.pars_description

Initial value:

```
= {
    "atomnum" : "number of atoms in your structure",
    "frames" : "number of frames in your trajectory",
    "cgnum" : "number of coarse-grained sites",
    "n_mappings": "number of coarse-grained mappings",
    "MC_steps" : "number of Monte Carlo steps",
    "rotmats_period" : "steps between two calculations of rotation matrices ",
    "criterion" : "criterion for hierarchical clustering:\n0 : fixed number of clusters\n1 : cophenetic
     distance\n2 : multiple numbers of clusters\n3 : fast clustering on a subset of configurations (only for
     continuous trajectories)",
    "Ncores" : "number of cores to use",
     "t_zero" : "starting temperature for Simulated Annealing",
     "nclust" : "number of clusters",
     "distance" : "cophenetic distance",
     "max_nclust" : "upper limit to the number of clusters",
     "min_nclust" : "lower limit to the number of clusters",
     "decay_time" : "temperature decay for Simulated Annealing",
     "rsd" : "use RSD instead of RMSD",
     "stride" : "number of structures between two pivot configurations"
}
```

9.2.2.5 dictionary setup_parfile.pars_type

Initial value:

```
= {
    "atomnum" : int,
    "frames" : int,
    "cgnum" : int,
    "n_mappings": int,
    "MC_steps" : int,
    "rotmats_period" : int,
    "criterion" : int,
    "Ncores" : int,
     "t_zero" : float,
     "criterion" : int,
     "nclust" : int,
     "distance" : float,
     "max_nclust" : int,
     "min_nclust" : int,
     "Ncores" : int,
     "decay_time" : float,
     "rsd" : int,
     "stride" : int
}
```

9.2.2.6 dictionary setup_parfile.clustering_pars

Initial value:

```
= {
    0: [ "nclust" ],
    1: [ "distance" ],
    2: [ "min_nclust", "max_nclust" ],
    3: [ "stride", "nclust"]
}
```

9.2.2.7 tuple setup_parfile.task = input("Insert the task you would like to perform among the following: " + str(tasks) + "\n")

9.2.2.8 dictionary setup_parfile.my_pars = {}

9.2.2.9 tuple setup_parfile.opt = input("Insert optional parameters? (y/n)")

9.3 test_suite Namespace Reference

Classes

- class test0
- class test1
- class test2
- class test3
- class test4
- class test5
- class test6
- class test7
- class test8
- class test9
- class test10
- class test11
- class test12
- class test13
- class test14
- class test15
- class test16
- class test17
- class test18
- class test19
- class test20
- class test21
- class test22
- class test23
- class test24
- class test25
- class test26

Variables

- tuple t_start = dt.datetime.now()
- tuple bash_script = subprocess.Popen("./test_suite.sh", shell=True, stdout=subprocess.PIPE)

9.3.1 Detailed Description

```
\class test_suite

The file contains several python tests to check the correct installation of METool package.
```

9.3.2 Variable Documentation

9.3.2.1 tuple test_suite.t_start = dt.datetime.now()

9.3.2.2 tuple test_suite.bash_script = subprocess.Popen("./test_suite.sh", shell=True, stdout=subprocess.PIPE)

Chapter 10

Class Documentation

10.1 alignment Class Reference

library of functions that perform alignments of pairs of structures

10.1.1 Detailed Description

library of functions that perform alignments of pairs of structures

The documentation for this class was generated from the following file:

- lib/alignment.c

10.2 alignments Class Reference

structure that defines the current alignments stored in memory

`#include <alignment.h>`

Public Attributes

- double * rmsd_mat
- double ** rotation_matrices
- double ** coms
- int rsd
- double * rmsd_vector
- double ** rotation_matrices_vector

10.2.1 Detailed Description

structure that defines the current alignments stored in memory

10.2.2 Member Data Documentation

10.2.2.1 double* alignments::rmsd_mat

condensed pairwise RMSD matrix

10.2.2.2 double∗∗ alignments::rotation_matrices

condensed matrix of pairwise rotation matrices

10.2.2.3 double∗∗ alignments::coms

array of centers of mass

10.2.2.4 int alignments::rsd

RSD parameter. {0: use the RMSD, 1: use the RSD}

10.2.2.5 double∗ alignments::rmsd_vector

RMSD vector for fast, 1D, clustering

10.2.2.6 double∗∗ alignments::rotation_matrices_vector

vector of pairwise rotation matrices

The documentation for this class was generated from the following file:

- include/alignment.h

10.3 arguments Struct Reference

```
#include <io.h>
```

Public Attributes

- int silent
- int verbose
- char ∗ parameter_file
- char ∗ energy_file
- char ∗ mapping_file
- char ∗ mapping_file2
- char ∗ trajectory_file
- char ∗ prot_code
- char ∗ task
- char ∗ mapping_matrix
- char ∗ probability_file

10.3.1 Member Data Documentation

10.3.1.1 int arguments::silent

10.3.1.2 int arguments::verbose

10.3.1.3 char∗ arguments::parameter_file

input parameter file

10.3.1.4 char∗ arguments::energy_file

input energy file

10.3.1.5 char∗ arguments::mapping_file

input first mapping file

10.3.1.6 char∗ arguments::mapping_file2

input second mapping file

10.3.1.7 char∗ arguments::trajectory_file

input trajectory file

10.3.1.8 char∗ arguments::prot_code

protein code

10.3.1.9 char∗ arguments::task

task: (optimize, random, measure, norm, cosine, distance)

10.3.1.10 char∗ arguments::mapping_matrix

input mapping matrix

10.3.1.11 char∗ arguments::probability_file

input probability file

The documentation for this struct was generated from the following file:

- include/io.h

10.4 cg_mapping Class Reference

structure that defines a cg mapping

```
#include <mapping.h>
```

Public Attributes

- int n_at
- int n_cg
- int ∗ mapping
- double smap
- int ∗ clusters
- int ∗ size
- double ∗ norms

10.4.1 Detailed Description

structure that defines a cg mapping

10.4.2 Member Data Documentation

10.4.2.1 int cg_mapping::n_at

number of atoms in the atomistic structure

10.4.2.2 int cg_mapping::n_cg

number of CG sites

10.4.2.3 int* cg_mapping::mapping

binary array defining the CG mapping

10.4.2.4 double cg_mapping::smap

value of mapping entropy

10.4.2.5 int* cg_mapping::clusters

array CG macrostates

10.4.2.6 int* cg_mapping::size

sizes of CG macrostates

10.4.2.7 double* cg_mapping::norms

moduli of CG mapping over the trajectory

The documentation for this class was generated from the following file:

- include/mapping.h

10.5 cg_mapping_lib Class Reference

library of functions that perform simple operations on CG mappings

10.5.1 Detailed Description

library of functions that perform simple operations on CG mappings

The documentation for this class was generated from the following file:

- lib/mapping.c

10.6 clust_params Class Reference

structure that defines the parameters for hierarchical clustering

```
#include <hierarchical_clustering.h>
```

Public Attributes

- int crit
- int ncl
- int max_ncl
- int min_ncl
- double c_distance

10.6.1 Detailed Description

structure that defines the parameters for hierarchical clustering

10.6.2 Member Data Documentation

10.6.2.1 int clust_params::crit

criterion for clustering structures. {0: single nclust, 1: distance-based, 2: multiple nclust, 3: fast clustering}

10.6.2.2 int clust_params::ncl

number of clusters (if crit is 0)

10.6.2.3 int clust_params::max_ncl

maximum number of clusters (if crit is 2)

10.6.2.4 int clust_params::min_ncl

minimum number of clusters (if crit is 2)

10.6.2.5 double clust_params::c_distance

maximum cophenetic distance (if crit is 1)

The documentation for this class was generated from the following file:

- include/hierarchical_clustering.h

10.7 geometry Class Reference

library of functions that perform simple geometrical calculations

10.7.1 Detailed Description

library of functions that perform simple geometrical calculations

The documentation for this class was generated from the following file:

- lib/geometry.c

10.8 hierarchical_clustering Class Reference

library of functions that perform hierarchical clustering

10.8.1 Detailed Description

library of functions that perform hierarchical clustering

Credits to scipy authors:

Copyright (C) Damian Eads, 2007-2008. New BSD License.

hierarchy.py (derived from cluster.py, `http://scipy-cluster.googlecode.com`)

Author: Damian Eads Date: September 22, 2007

The documentation for this class was generated from the following file:

- lib/hierarchical_clustering.c

10.9 ini_parse_string_ctx Struct Reference

Public Attributes

- const char ∗ ptr
- size_t num_left

10.9.1 Member Data Documentation

10.9.1.1 const char∗ ini_parse_string_ctx::ptr

10.9.1.2 size_t ini_parse_string_ctx::num_left

The documentation for this struct was generated from the following file:

- lib/ini.c

10.10 io Class Reference

library of functions for all input-output operations

10.10.1 Detailed Description

library of functions for all input-output operations

The documentation for this class was generated from the following file:

- lib/io.c

10.11 MC_params Class Reference

structure that defines a the parameters of Monte Carlo sampling

```
#include <sampling.h>
```

Public Attributes

- double t_zero
- double decay_time
- int rotmats_period
- int MC_steps

10.11.1 Detailed Description

structure that defines a the parameters of Monte Carlo sampling

10.11.2 Member Data Documentation

10.11.2.1 double MC_params::t_zero

starting effective temperature

10.11.2.2 double MC_params::decay_time

decay parameter

10.11.2.3 int MC_params::rotmats_period

Simulated Annealing steps between two updates of the alignments

10.11.2.4 int MC_params::MC_steps

number of MC steps

The documentation for this class was generated from the following file:

- include/sampling.h

10.12 observables Class Reference

library of functions for the calculation of several observables

10.12.1 Detailed Description

library of functions for the calculation of several observables

The documentation for this class was generated from the following file:

- lib/observables.c

10.13 parameters Struct Reference

```
#include <io.h>
```

Public Attributes

- int atomnum
- int frames
- int cgnum
- int nclust
- int n_mappings
- int MC_steps
- int rotmats_period
- float t_zero
- float distance
- int criterion
- int max_nclust
- int min_nclust
- int Ncores
- float decay_time
- int rsd
- int stride
- int Flag_atomnum
- int Flag_frames
- int Flag_cgnum
- int Flag_nclust
- int Flag_n_mappings
- int Flag_MC_steps

- int Flag_rotmats_period
- int Flag_t_zero
- int Flag_distance
- int Flag_criterion
- int Flag_max_nclust
- int Flag_min_nclust
- int Flag_Ncores
- int Flag_decay_time
- int Flag_rsd
- int Flag_stride

10.13.1 Member Data Documentation

10.13.1.1 int parameters::atomnum

10.13.1.2 int parameters::frames

10.13.1.3 int parameters::cgnum

10.13.1.4 int parameters::nclust

10.13.1.5 int parameters::n_mappings

10.13.1.6 int parameters::MC_steps

10.13.1.7 int parameters::rotmats_period

10.13.1.8 float parameters::t_zero

10.13.1.9 float parameters::distance

10.13.1.10 int parameters::criterion

10.13.1.11 int parameters::max_nclust

10.13.1.12 int parameters::min_nclust

10.13.1.13 int parameters::Ncores

10.13.1.14 float parameters::decay_time

10.13.1.15 int parameters::rsd

10.13.1.16 int parameters::stride

10.13.1.17 int parameters::Flag_atomnum

10.13.1.18 int parameters::Flag_frames

10.13.1.19 int parameters::Flag_cgnum

10.13.1.20 int parameters::Flag_nclust

10.13.1.21 int parameters::Flag_n_mappings

10.13.1.22 int parameters::Flag_MC_steps

10.13.1.23 int parameters::Flag_rotmats_period

10.13.1.24 int parameters::Flag_t_zero

10.13.1.25 int parameters::Flag_distance

10.13.1.26 int parameters::Flag_criterion

10.13.1.27 int parameters::Flag_max_nclust

10.13.1.28 int parameters::Flag_min_nclust

10.13.1.29 int parameters::Flag_Ncores

10.13.1.30 int parameters::Flag_decay_time

10.13.1.31 int parameters::Flag_rsd

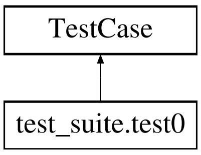
10.13.1.32 int parameters::Flag_stride

The documentation for this struct was generated from the following file:

- include/io.h

10.14 test_suite.test0 Class Reference

Inheritance diagram for test_suite.test0:



Public Member Functions

- def test0_exist
- def test0_SA
- def test0_log_exist
- def test0_head_tail

10.14.1 Detailed Description

```
class that checks a three-cores Simulated Annealing run
```

10.14.2 Member Function Documentation

10.14.2.1 def test_suite.test0.test0_exist (*self*)

```
check existence of .dat files
```

10.14.2.2 def test_suite.test0.test0_SA (*self*)

```
open files and check that the optimizations correctly finished
```

10.14.2.3 def test_suite.test0.test0_log_exist (*self*)

```
check existence of log file
```

10.14.2.4 def test_suite.test0.test0_head_tail (*self*)

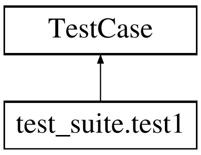
```
check first and last line of log
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.15 test_suite.test1 Class Reference

Inheritance diagram for test_suite.test1:



Public Member Functions

- def test1_exist
- def test1_exist_dat
- def test1_count_mapping
- def test1_head_tail

10.15.1 Detailed Description

```
class that checks the correct generation of random mappings and the measurement of their mapping entropy
```

10.15.2 Member Function Documentation

10.15.2.1 def test_suite.test1.test1_exist (*self*)

```
check existence of log file
```

10.15.2.2 def test_suite.test1.test1_exist_dat (*self*)

```
check existence of output file
```

10.15.2.3 def test_suite.test1.test1_count_mapping (*self*)

```
check for consistency between the declared and effective number of random mappings (and the number of calculat
```

10.15.2.4 def test_suite.test1.test1_head_tail (*self*)

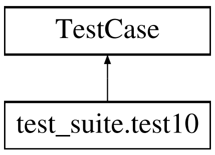
```
check log's head and tail
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.16 test_suite.test10 Class Reference

Inheritance diagram for test_suite.test10:



Public Member Functions

- def test10_log_exist
- def test10_err_exist
- def test10_err_correct

10.16.1 Detailed Description

```
class that checks the error output if the mapping file is not complete (longer than n_cg beads)
```

10.16.2 Member Function Documentation

10.16.2.1 def test_suite.test10.test10_log_exist (*self*)

```
check existence of log file
```

10.16.2.2 def test_suite.test10.test10_err_exist (*self*)

```
check existence of error file
```

10.16.2.3 def test_suite.test10.test10_err_correct (*self*)

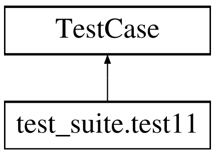
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.17 test_suite.test11 Class Reference

Inheritance diagram for test_suite.test11:



Public Member Functions

- def test11_log_exist
- def test11_err_exist
- def test11_err_correct

10.17.1 Detailed Description

```
class that checks the error output if the mapping file is not complete (value not between [0 ;n_at) )
```

10.17.2 Member Function Documentation

10.17.2.1 def test_suite.test11.test11_log_exist (*self*)

```
check existence of log file
```

10.17.2.2 def test_suite.test11.test11_err_exist (*self*)

```
check existence of error file
```

10.17.2.3 def test_suite.test11.test11_err_correct (*self*)

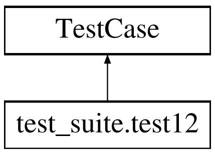
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.18 test_suite.test12 Class Reference

Inheritance diagram for test_suite.test12:



Public Member Functions

- def test12_log_exist
- def test12_err_exist
- def test12_err_correct

10.18.1 Detailed Description

```
class that checks the error output if the mapping file is not complete (each value must be INT)
```

10.18.2 Member Function Documentation

10.18.2.1 def test_suite.test12.test12_log_exist (*self*)

```
check existence of log file
```

10.18.2.2 def test_suite.test12.test12_err_exist (*self*)

```
check existence of error file
```

10.18.2.3 def test_suite.test12.test12_err_correct (*self*)

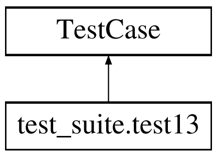
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.19 test_suite.test13 Class Reference

Inheritance diagram for test_suite.test13:



Public Member Functions

- def test13_log_exist
- def test13_err_exist
- def test13_err_correct

10.19.1 Detailed Description

```
class that checks the error output if the mapping file is not complete (it contains duplicates)
```

10.19.2 Member Function Documentation

10.19.2.1 def test_suite.test13.test13_log_exist (*self*)

```
check existence of log file
```

10.19.2.2 def test_suite.test13.test13_err_exist (*self*)

```
check existence of error file
```

10.19.2.3 def test_suite.test13.test13_err_correct (*self*)

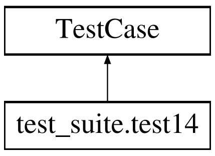
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.20 test_suite.test14 Class Reference

Inheritance diagram for test_suite.test14:



Public Member Functions

- def test14_log_exist
- def test14_err_exist
- def test14_err_correct

10.20.1 Detailed Description

```
class that checks the error output if the parameter file contains, at least, a string VALUE instead of integer
```

10.20.2 Member Function Documentation

10.20.2.1 def test_suite.test14.test14_log_exist (*self*)

```
check existence of log file
```

10.20.2.2 def test_suite.test14.test14_err_exist (*self*)

```
check existence of error file
```

10.20.2.3 def test_suite.test14.test14_err_correct (*self*)

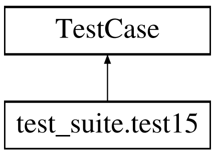
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.21 test_suite.test15 Class Reference

Inheritance diagram for test_suite.test15:



Public Member Functions

- def test15_log_exist
- def test15_err_exist
- def test15_err_correct

10.21.1 Detailed Description

```
class that checks the error output if the energy file contains, at least, an integer value instead of float
```

10.21.2 Member Function Documentation

10.21.2.1 def test_suite.test15.test15_log_exist (*self*)

```
check existence of log file
```

10.21.2.2 def test_suite.test15.test15_err_exist (*self*)

```
check existence of error file
```

10.21.2.3 def test_suite.test15.test15_err_correct (*self*)

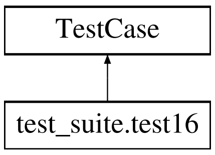
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.22 test_suite.test16 Class Reference

Inheritance diagram for test_suite.test16:



Public Member Functions

- def test16_log_exist
- def test16_err_exist
- def test16_err_correct

10.22.1 Detailed Description

```
class that checks the error output if the energy file contains, at least, one row containing more than one col
```

10.22.2 Member Function Documentation

10.22.2.1 def test_suite.test16.test16_log_exist (*self*)

```
check existence of log file
```

10.22.2.2 def test_suite.test16.test16_err_exist (*self*)

```
check existence of error file
```

10.22.2.3 def test_suite.test16.test16_err_correct (*self*)

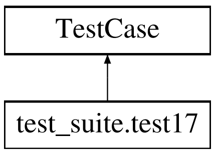
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.23 test_suite.test17 Class Reference

Inheritance diagram for test_suite.test17:



Public Member Functions

- def test17_log_exist
- def test17_err_exist
- def test17_err_correct

10.23.1 Detailed Description

```
class that checks the error output if the trajectory file contains an integer number != n_atoms when n_column
```

10.23.2 Member Function Documentation

10.23.2.1 def test_suite.test17.test17_log_exist (*self*)

```
check existence of log file
```

10.23.2.2 def test_suite.test17.test17_err_exist (*self*)

```
check existence of error file
```

10.23.2.3 def test_suite.test17.test17_err_correct (*self*)

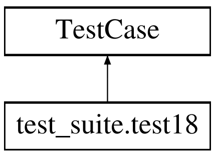
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.24 test_suite.test18 Class Reference

Inheritance diagram for test_suite.test18:



Public Member Functions

- def test18_log_exist
- def test18_err_exist
- def test18_err_correct

10.24.1 Detailed Description

```
class that checks the error output if the trajectory file contains, at least, one letter, instead of float at
```

10.24.2 Member Function Documentation

10.24.2.1 def test_suite.test18.test18_log_exist (*self*)

```
check existence of log file
```

10.24.2.2 def test_suite.test18.test18_err_exist (*self*)

```
check existence of error file
```

10.24.2.3 def test_suite.test18.test18_err_correct (*self*)

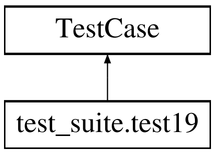
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.25 test_suite.test19 Class Reference

Inheritance diagram for test_suite.test19:



Public Member Functions

- def test19_output_exist
- def test19_correct_coord_number

10.25.1 Detailed Description

```
class that checks the correct calculation of the norm of the mapping for 4AKE
```

10.25.2 Member Function Documentation

10.25.2.1 def test_suite.test19.test19_output_exist (*self*)

```
check existence of output file
```

10.25.2.2 def test_suite.test19.test19_correct_coord_number (*self*)

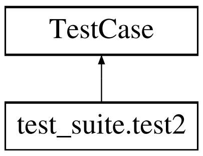
```
check correct atomistic coordination number
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.26 test_suite.test2 Class Reference

Inheritance diagram for test_suite.test2:



Public Member Functions

- def test2_log_exist
- def test2_output_exist
- def test2_head_tail
- def test2_correct_smap

10.26.1 Detailed Description

```
class that checks loading mapping task
```

10.26.2 Member Function Documentation

10.26.2.1 def test_suite.test2.test2_log_exist (*self*)

```
check existence of log file
```

10.26.2.2 def test_suite.test2.test2_output_exist (*self*)

```
check existence of output file
```

10.26.2.3 def test_suite.test2.test2_head_tail (*self*)

```
check parameter file is correct and that clusters are written
```

10.26.2.4 def test_suite.test2.test2_correct_smap (*self*)

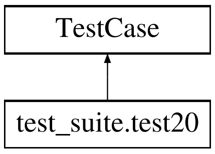
```
check that the mapping entropy is correct
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.27 test_suite.test20 Class Reference

Inheritance diagram for test_suite.test20:



Public Member Functions

- def test20_output_exist
- def test20_cosines
- def test20_distances

10.27.1 Detailed Description

```
class that checks calculation of cosines and distances between two identical mappings
```

10.27.2 Member Function Documentation

10.27.2.1 def test_suite.test20.test20_output_exist (*self*)

```
check existence of output file
```

10.27.2.2 def test_suite.test20.test20_cosines (*self*)

```
check that all cosines are calculated and equal to one
```

10.27.2.3 def test_suite.test20.test20_distances (*self*)

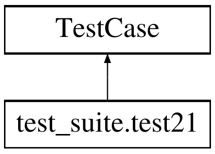
```
check that all distances are calculated and equal to zero
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.28 test_suite.test21 Class Reference

Inheritance diagram for test_suite.test21:



Public Member Functions

- def test21_output_exist
- def test21_consistent_norms

10.28.1 Detailed Description

```
class that checks the correct calculation of the norm of the Calpha mapping for 6D93
```

10.28.2 Member Function Documentation

10.28.2.1 def test_suite.test21.test21_output_exist (*self*)

```
check existence of output file
```

10.28.2.2 def test_suite.test21.test21_consistent_norms (*self*)

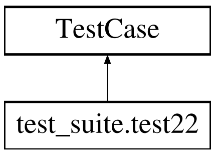
```
check consistency with calculated norms
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.29 test_suite.test22 Class Reference

Inheritance diagram for test_suite.test22:



Public Member Functions

- def test22_log_exist
- def test22_output_exist
- def test22_distmat_exist
- def test22_distmat_shape

10.29.1 Detailed Description

```
class that checks the correct calculation of distance matrix between mappings
```

10.29.2 Member Function Documentation

10.29.2.1 def test_suite.test22.test22_log_exist (*self*)

```
check existence of log file
```

10.29.2.2 def test_suite.test22.test22_output_exist (*self*)

```
check existence of output file
```

10.29.2.3 def test_suite.test22.test22_distmat_exist (*self*)

```
check existence of distance matrix file
```

10.29.2.4 def test_suite.test22.test22_distmat_shape (*self*)

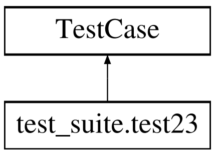
```
check shape of distance matrix
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.30 test_suite.test23 Class Reference

Inheritance diagram for test_suite.test23:



Public Member Functions

- def test23_output_exist
- def test23_correct_smap
- def test23_check_pairs

10.30.1 Detailed Description

```
class that checks the correct functioning of criterion 3 (fast clustering)
```

10.30.2 Member Function Documentation

10.30.2.1 def test_suite.test23.test23_output_exist (*self*)

```
check existence of output file
```

10.30.2.2 def test_suite.test23.test23_correct_smap (*self*)

```
check that the mapping entropy is correct
```

10.30.2.3 def test_suite.test23.test23_check_pairs (*self*)

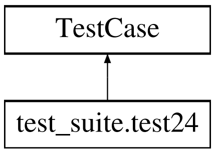
```
check existence of log file and that the number of pairs matches its expected value
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.31 test_suite.test24 Class Reference

Inheritance diagram for test_suite.test24:



Public Member Functions

- def test24_output_exist
- def test24_check_probabilities
- def test24_use_probabilities

10.31.1 Detailed Description

```
class that checks the correct functioning of task optimize_kl
```

10.31.2 Member Function Documentation

10.31.2.1 def test_suite.test24.test24_output_exist (*self*)

```
check existence of output file
```

10.31.2.2 def test_suite.test24.test24_check_probabilities (*self*)

```
check that the program is checking probabilities
```

10.31.2.3 def test_suite.test24.test24_use_probabilities (*self*)

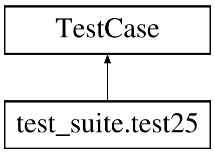
```
check that the program is using probabilities
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.32 test_suite.test25 Class Reference

Inheritance diagram for test_suite.test25:



Public Member Functions

- def test25_output_exist
- def test25_check_probabilities
- def test25_use_probabilities_correct_smap

10.32.1 Detailed Description

```
class that checks the correct functioning of task measure_kl
```

10.32.2 Member Function Documentation

10.32.2.1 def test_suite.test25.test25_output_exist (*self*)

```
check existence of output file
```

10.32.2.2 def test_suite.test25.test25_check_probabilities (*self*)

```
check that the program is checking probabilities
```

10.32.2.3 def test_suite.test25.test25_use_probabilities_correct_smap (*self*)

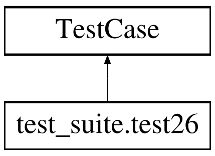
```
check that the program is using probabilities and that the mapping entropy is correct
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.33 test_suite.test26 Class Reference

Inheritance diagram for test_suite.test26:



Public Member Functions

- def test26_output_exist
- def test26_use_probabilities

10.33.1 Detailed Description

```
class that checks the correct functioning of task random_kl
```

10.33.2 Member Function Documentation

10.33.2.1 def test_suite.test26.test26_output_exist (*self*)

```
check existence of output file
```

10.33.2.2 def test_suite.test26.test26_use_probabilities (*self*)

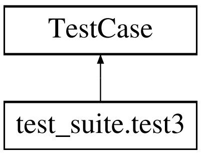
```
check that the program is using probabilities
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.34 test_suite.test3 Class Reference

Inheritance diagram for test_suite.test3:



Public Member Functions

- def test3_log_exist
- def test3_head_tail
- def test3_deltas

10.34.1 Detailed Description

```
class that checks the estimation of T_start inside optimisation
```

10.34.2 Member Function Documentation

10.34.2.1 def test_suite.test3.test3_log_exist (*self*)

```
check existence of log file
```

10.34.2.2 def test_suite.test3.test3_head_tail (*self*)

```
check log’s head and tail
```

10.34.2.3 def test_suite.test3.test3_deltas (*self*)

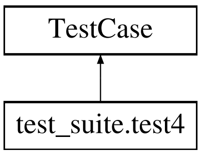
```
check delta dat files
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.35 test_suite.test4 Class Reference

Inheritance diagram for test_suite.test4:



Public Member Functions

- def test4_log_exist
- def test4_err_exist
- def test4_err_correct

10.35.1 Detailed Description

```
class that checks an invalid task ID (ex. optimizer)
```

10.35.2 Member Function Documentation

10.35.2.1 def test_suite.test4.test4_log_exist (*self*)

```
check existence of log file
```

10.35.2.2 def test_suite.test4.test4_err_exist (*self*)

```
check existence of error.dat
```

10.35.2.3 def test_suite.test4.test4_err_correct (*self*)

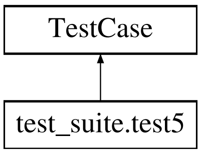
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.36 test_suite.test5 Class Reference

Inheritance diagram for test_suite.test5:



Public Member Functions

- def test5_log_exist
- def test5_count_alignments

10.36.1 Detailed Description

```
class that checks the expected number of alignments
```

10.36.2 Member Function Documentation

10.36.2.1 def test_suite.test5.test5_log_exist (*self*)

```
check existence of log file
```

10.36.2.2 def test_suite.test5.test5_count_alignments (*self*)

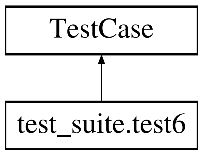
```
count the effective (from dat file) and expected (from log/parameter file) number of alignments. See if they m
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.37 test_suite.test6 Class Reference

Inheritance diagram for test_suite.test6:



Public Member Functions

- def test6_log_exist
- def test6_err_exist
- def test6_err_correct

10.37.1 Detailed Description

```
class that checks the error output if the trajectory does not respect the declared number of frames
```

10.37.2 Member Function Documentation

10.37.2.1 def test_suite.test6.test6_log_exist (*self*)

```
check existence of log file
```

10.37.2.2 def test_suite.test6.test6_err_exist (*self*)

```
check existence of error.dat
```

10.37.2.3 def test_suite.test6.test6_err_correct (*self*)

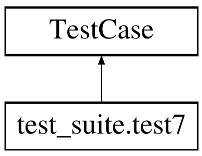
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.38 test_suite.test7 Class Reference

Inheritance diagram for test_suite.test7:



Public Member Functions

- def test7_log_exist
- def test7_err_exist
- def test7_err_correct

10.38.1 Detailed Description

```
class that checks the error output if the trajectory is cut at the last frame
```

10.38.2 Member Function Documentation

10.38.2.1 def test_suite.test7.test7_log_exist (*self*)

```
check existence of log file
```

10.38.2.2 def test_suite.test7.test7_err_exist (*self*)

```
check existence of error.dat
```

10.38.2.3 def test_suite.test7.test7_err_correct (*self*)

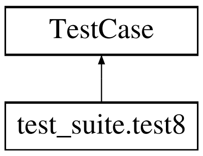
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.39 test_suite.test8 Class Reference

Inheritance diagram for test_suite.test8:



Public Member Functions

- def test8_log_exist
- def test8_err_exist
- def test8_err_correct

10.39.1 Detailed Description

```
class that checks the error output if the energy file is not complete
```

10.39.2 Member Function Documentation

10.39.2.1 def test_suite.test8.test8_log_exist (*self*)

```
check existence of log file
```

10.39.2.2 def test_suite.test8.test8_err_exist (*self*)

```
check existence of error.dat
```

10.39.2.3 def test_suite.test8.test8_err_correct (*self*)

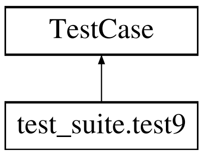
```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.40 test_suite.test9 Class Reference

Inheritance diagram for test_suite.test9:



Public Member Functions

- def test9_log_exist
- def test9_err_exist
- def test9_err_correct

10.40.1 Detailed Description

```
class that checks the error output if the mapping file is not complete (shorter than n_cg beads)
```

10.40.2 Member Function Documentation

10.40.2.1 def test_suite.test9.test9_log_exist (*self*)

```
check existence of log file
```

10.40.2.2 def test_suite.test9.test9_err_exist (*self*)

```
check existence of error file
```

10.40.2.3 def test_suite.test9.test9_err_correct (*self*)

```
check error file
```

The documentation for this class was generated from the following file:

- tests/test_suite.py

10.41 traj Class Reference

structure that defines a MD trajectory

```
#include <traj.h>
```

Public Attributes

- int frames
- double ** traj_coords
- double * energies
- int n_at
- int pairs
- int * strides
- int stride
- int eff_frames

10.41.1 Detailed Description

structure that defines a MD trajectory

10.41.2 Member Data Documentation

10.41.2.1 int traj::frames

number of frames in the trajectory

10.41.2.2 double∗∗ traj::traj_coords

2D array of xyz coordinates

10.41.2.3 double∗ traj::energies

1D array of energies. One value per frame.

10.41.2.4 int traj::n_at

number of atoms in the atomistic structure

10.41.2.5 int traj::pairs

number of possible pairs of structures

10.41.2.6 int∗ traj::strides

vector of configurations to consider (criterion 3)

10.41.2.7 int traj::stride

number of configurations between each pivot for clustering (criterion 3)

10.41.2.8 int traj::eff_frames

number of effective frames in the trajectory (criterion 3)

The documentation for this class was generated from the following file:

- include/traj.h

Chapter 11

File Documentation

11.1 excogito.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <math.h>
#include <my_malloc.h>
#include <time.h>
#include <omp.h>
#include <sys/types.h>
#include <unistd.h>
#include <limits.h>
#include <stdbool.h>
#include <sampling.h>
#include <io.h>
#include <geometry.h>
#include <mapping.h>
#include <observables.h>
#include <alignment.h>
#include <ini.h>
#include <traj.h>
#include <optimize.h>
#include <random_mapping.h>
#include <measure.h>
#include <norm.h>
#include <cosine.h>
#include <distance.h>
#include <argp.h>
#include <measure_kl.h>
#include <optimize_kl.h>
#include <random_mapping_kl.h>
```

Functions

- int main (int argc, char ∗argv[])

11.1.1 Function Documentation

11.1.1.1 int main (int *argc,* char ∗ *argv[]*)

main file of the program

11.2 include/alignment.h File Reference

```
#include <mapping.h>
#include <traj.h>
```

Classes

- class alignments

  structure that defines the current alignments stored in memory

Typedefs

- typedef struct alignments alignments

Functions

- void free_new_alignment (alignments ∗new_align)
- void free_alignment (alignments ∗align)
- void align_two_frames (double ∗frame_ref, double ∗frame_middle, int ref_id, int middle_id, cg_mapping ∗mapping, alignments ∗align)
- double optimal_alignment (double ∗∗x, double ∗∗y, int mapping_length, double u[][3])
- void correct_rmsd (alignments ∗new_align, traj ∗Trajectory, alignments ∗prev_align, int cgnum, int removed, int added)
- void cycle_alignment (traj ∗Trajectory, alignments ∗align, cg_mapping ∗mapping)
- void cycle_alignment_fastclust (traj ∗Trajectory, alignments ∗align, cg_mapping ∗mapping)
- void correct_rmsd_fastclust (alignments ∗new_align, traj ∗Trajectory, alignments ∗prev_align, int cgnum, int removed, int added)
- void cycle_alignment_stride (traj ∗Trajectory, alignments ∗align, cg_mapping ∗mapping)
- void align_traj_to_reference (traj ∗Trajectory, int ref_id)

11.2.1 Typedef Documentation

11.2.1.1 typedef struct **alignments alignments**

11.2.2 Function Documentation

11.2.2.1 void free_new_alignment (**alignments** ∗ *new_align*)

routine that frees an alignments object used in criterion 3

Parameters

`new_align`: alignments object

11.2.2.2 void free_alignment (**alignments** ∗ *align*)

routine that frees an alignments object

Parameters

`align`: alignments object

11.2.2.3 void align_two_frames (double ∗ *frame_ref,* double ∗ *frame_middle,* int *ref_id,* int *middle_id,* **cg_mapping** ∗ *mapping,* **alignments** ∗ *align*)

routine that aligns a pair of frames in a trajectory, calling `optimal_alignment`

Parameters

`frame_ref` : reference frame

`frame_middle` : frame in between two pivot clusters

`ref_id` : id (index) of frame_ref in the trajectory

`middle_id` : id (index) of frame_middle in the trajectory

`mapping` : cg_mapping object

`align` : alignments object

11.2.2.4 double optimal_alignment (double ∗∗ *x,* double ∗∗ *y,* int *mapping_length,* double *u[ ][3]*)

routine that computes the Kabsch alignment and the rmsd between two configurations

Parameters

`x`, `y` : CG structures

`cgnum` : length of CG mapping

`u` : rotation matrix

11.2.2.5 void correct_rmsd (**alignments** ∗ *new_align,* **traj** ∗ *Trajectory,* **alignments** ∗ *prev_align,* int *cgnum,* int *removed,* int *added*)

routine that computes the rmsd matrix without aligning frames over frames

Parameters

`new_align` : trial alignments object

`Trajectory` : traj object

`align` : alignments object

`cgnum` : number of CG sites (useful to normalize)

`removed` : index of removed atom

`added` : index of added atom

11.2.2.6 void cycle_alignment (**traj** ∗ *Trajectory,* **alignments** ∗ *align,* **cg_mapping** ∗ *mapping*)

routine that cycles over all pairs of frames in a trajectory, calling `optimal_alignment`

Parameters

`Trajectory` : traj object

`align` : alignments object

`mapping` : cg_mapping object

11.2.2.7 void cycle_alignment_fastclust (**traj** ∗ *Trajectory,* **alignments** ∗ *align,* **cg_mapping** ∗ *mapping*)

routine that computes the alignments if clustering must be fast

Parameters

`Trajectory` : traj object

`align` : alignments object

`mapping` : cg_mapping object

11.2.2.8 void correct_rmsd_fastclust (**alignments** ∗ *new_align,* **traj** ∗ *Trajectory,* **alignments** ∗ *prev_align,* int *cgnum,* int *removed,* int *added*)

routine that computes the rmsd matrix without aligning frames over frames

Parameters

`new_rmsd_mat` : new condensed pairwise RMSD matrix

`Trajectory` : traj object

`align` : alignments object

`cgnum` : number of CG sites (useful to normalize)

`removed` : index of removed atom

`added` : index of added atom

11.2.2.9 void cycle_alignment_stride (**traj** ∗ *Trajectory,* **alignments** ∗ *align,* **cg_mapping** ∗ *mapping*)

routine that cycles over all pairs of frames in a trajectory, calling `optimal_alignment`

Parameters

`Trajectory` : traj object

`align` : alignments object

`mapping` : cg_mapping object

11.2.2.10 void align_traj_to_reference (**traj** ∗ *Trajectory,* int *ref_id*)

routine that aligns the trajectory to a reference frame

Parameters

`Trajectory` : traj object

`ref_id` : reference frame

11.3 include/cosine.h File Reference

```
#include <stdio.h>
#include <io.h>
```

Functions

- void cosine (arguments ∗arguments, parameters ∗cc)

11.3.1 Function Documentation

11.3.1.1 void cosine (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to calculate pairwise distance and cosine between a pair of mappings (provided by the user) throughout a trajectory

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.4 include/distance.h File Reference

```
#include <stdio.h>
#include <io.h>
```

Functions

- void distance (arguments ∗arguments, parameters ∗cc)

11.4.1 Function Documentation

11.4.1.1 void distance (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to calculate the distance matrix between a data set of mappings (provided by the user) over a single conformation

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.5 include/geometry.h File Reference

Functions

- void vecprod_d (double ∗a, double ∗b, double ∗c)
- double scal_d (double ∗a, double ∗b, int dim)
- double coseno (double ∗vec1, double ∗vec2, int dim)
- double norm_d (double ∗a, int dim)
- void normalize_d (double ∗a, int dim)
- double dist_d (double ∗a, double ∗b, int dim)
- double det (double a1, double a2, double a3, double b1, double b2, double b3, double c1, double c2, double c3)
- void vec_sum_d (double ∗a, double ∗b, double ∗c, double d, int dim)
- void print_vec_d (double ∗a, int dim)
- void zero_vec_d (double ∗a, int dim)
- void zero_vec_i (int ∗a, int dim)
- void zero_matrix_d (double ∗∗a, int dim1, int dim2)
- void myjacobi (double a[ ][3], int n, double ∗d, double v[ ][3], int ∗nrot)

11.5.1 Function Documentation

11.5.1.1 void vecprod_d (double ∗ *a*, double ∗ *b*, double ∗ *c*)

11.5.1.2 double scal_d (double ∗ *a*, double ∗ *b*, int *dim*)

11.5.1.3 double coseno (double ∗ *vec1*, double ∗ *vec2*, int *dim*)

11.5.1.4 double norm_d (double ∗ *a*, int *dim*)

11.5.1.5 void normalize_d (double ∗ *a*, int *dim*)

11.5.1.6 double dist_d (double ∗ *a*, double ∗ *b*, int *dim*)

11.5.1.7 double det (double *a1*, double *a2*, double *a3*, double *b1*, double *b2*, double *b3*, double *c1*, double *c2*, double *c3*)

11.5.1.8 void vec_sum_d (double ∗ *a*, double ∗ *b*, double ∗ *c*, double *d*, int *dim*)

11.5.1.9 void print_vec_d (double ∗ *a*, int *dim*)

11.5.1.10 void zero_vec_d (double ∗ *a*, int *dim*)

11.5.1.11 void zero_vec_i (int ∗ *a*, int *dim*)

11.5.1.12 void zero_matrix_d (double ∗∗ *a*, int *dim1*, int *dim2*)

11.5.1.13 void myjacobi (double *a[ ][3]*, int *n*, double ∗ *d*, double *v[ ][3]*, int ∗ *nrot*)

11.6 include/hierarchical_clustering.h File Reference

Classes

- class clust_params

  structure that defines the parameters for hierarchical clustering

Typedefs

- typedef struct clust_params clust_params

Functions

- void mergesort_merge (double ∗∗arr, int l, int m, int r, int dim, int dims)
- void my_mergesort (double ∗∗arr, int l, int r, int dim, int dims)
- int condensed_index (int frames, int i, int j)
- double new_dist (double d_xi, double d_yi, double d_xy, int size_x, int size_y, int size_i)
- int is_visited (unsigned char ∗bitset, int i)
- void set_visited (unsigned char ∗bitset, int i)
- void get_max_dist_for_each_cluster (double ∗∗Z, double ∗MD, int frames)
- void cluster_monocrit (double ∗∗Z, double ∗MC, int ∗T, double cutoff, int frames)
- void cluster_maxclust_monocrit (double ∗∗Z, double ∗MC, int ∗T, int n, int max_nc)
- void cluster_maxclust_dist (double ∗∗Z, int ∗T, int frames, int Nclust)
- void cluster_dist (double ∗∗Z, int ∗T, double cutoff, int frames)
- int find (int x, int ∗self_parent)
- int merge (int ∗self_parent, int ∗self_size, int next_label, int x, int y)
- void label (double ∗∗Z, int frames)
- void hierarchical_clustering (double ∗rmsd_mat, int n, int couples, int ∗size, double ∗∗Z)
- void compute_clusters_list (int ∗clusters, int ∗cluster_list, int ∗cluster_list_idx, int frames, int Nclust)

11.6.1 Typedef Documentation

11.6.1.1 typedef struct **clust_params clust_params**

11.6.2 Function Documentation

11.6.2.1 void mergesort_merge (double ∗∗ *arr,* int *l,* int *m,* int *r,* int *dim,* int *dims*)

11.6.2.2 void my_mergesort (double ∗∗ *arr,* int *l,* int *r,* int *dim,* int *dims*)

11.6.2.3 int condensed_index (int *frames,* int *i,* int *j*)

`frames` : number of observations

`i` : node

`j` : node

11.6.2.4 double new_dist (double *d_xi,* double *d_yi,* double *d_xy,* int *size_x,* int *size_y,* int *size_i*)

11.6.2.5 int is_visited (unsigned char ∗ *bitset,* int *i*)

routine that checks if node i was visited.

Parameters

`bitset` : char defining visits

`i` : node

11.6.2.6 void set_visited (unsigned char ∗ *bitset,* int *i*)

routine that marks node i as visited.

Parameters

`bitset` : char defining visits

`i` : node

11.6.2.7 void get_max_dist_for_each_cluster (double ∗∗ *Z,* double ∗ *MD,* int *frames*)

Get the maximum inconsistency coefficient for each non-singleton cluster.

Parameters

`Z` : linkage matrix.

`MD` : array to store the result.

`frames` : number of observations.

11.6.2.8 void cluster_monocrit (double ∗∗ *Z,* double ∗ *MC,* int ∗ *T,* double *cutoff,* int *frames*)

Form flat clusters by monocrit criterion.

Parameters

`Z` : linkage matrix.

`MC` : monotonic criterion array.

`T` : array to store the cluster numbers. The i'th observation belongs to cluster `T[i]`.

`cutoff` : Clusters are formed when the MC values are less than or equal to `cutoff`.

`frames` : number of observations

11.6.2.9 void cluster_maxclust_monocrit (double ∗∗ *Z,* double ∗ *MC,* int ∗ *T,* int *n,* int *max_nc*)

Form flat clusters by maxclust_monocrit criterion.

Parameters

`Z` : linkage matrix

`MC` : monotonic criterion array

`T` : array to store the cluster numbers. The i'th observation belongs to cluster `T[i]`

`frames` : number of observations

`max_nc` : The maximum number of clusters

11.6.2.10 void cluster_maxclust_dist (double ∗∗ *Z,* int ∗ *T,* int *frames,* int *Nclust*)

routine that converts the dendrogram into nclust clusters

Parameters

`Z` : linkage matrix.

`T` : array to store the cluster numbers. The i'th observation belongs to cluster `T[i]`.

`frames` : number of observations.

`nclust` : number of desired clusters.

11.6.2.11 void cluster_dist (double ∗∗ *Z,* int ∗ *T,* double *cutoff,* int *frames*)

11.6.2.12 int find (int *x,* int ∗ *self_parent*)

11.6.2.13 int merge (int ∗ *self_parent,* int ∗ *self_size,* int *next_label,* int *x,* int *y*)

11.6.2.14 void label (double ∗∗ *Z,* int *frames*)

routine that correctly labels clusters in the unsorted dendrogram

Parameters

`Z` : linkage matrix

`frames` : number of observations

11.6.2.15 void hierarchical_clustering (double ∗ *rmsd_mat,* int *n,* int *couples,* int ∗ *size,* double ∗∗ *Z*)

overall routine for hierarchical clustering

Parameters

`rmsd_mat` : condensed pairwise RMSD matrix

`frames` : number of observations

`pairs` : possible pairs of structures

`size` : size of the clusters (it is nclust long)

`Z` : linkage matrix

11.6.2.16 void compute_clusters_list (int ∗ *clusters,* int ∗ *cluster_list,* int ∗ *cluster_list_idx,* int *frames,* int *Nclust*)

routine that computes the list of cluster IDs

Parameters

`clusters` : list of labels (one for each frame)

`cluster_list` : ordered list of labels

`cluster_list_idx` : is an index vector that stores the sum of populations up to each index

`frames` : number of observations

`nclust` : number of clusters

$<$ array that stores the population of each clusters

11.7 include/ini.h File Reference

```
#include <stdio.h>
```

Macros

- #define INI_HANDLER_LINENO 0
- #define INI_ALLOW_MULTILINE 1
- #define INI_ALLOW_BOM 1
- #define INI_START_COMMENT_PREFIXES ";#"
- #define INI_ALLOW_INLINE_COMMENTS 1
- #define INI_INLINE_COMMENT_PREFIXES ";"
- #define INI_USE_STACK 1
- #define INI_MAX_LINE 200
- #define INI_ALLOW_REALLOC 0
- #define INI_INITIAL_ALLOC 200
- #define INI_STOP_ON_FIRST_ERROR 0
- #define INI_CALL_HANDLER_ON_NEW_SECTION 0
- #define INI_ALLOW_NO_VALUE 0
- #define INI_CUSTOM_ALLOCATOR 0

Typedefs

- typedef int(∗ ini_handler)(void ∗user, const char ∗section, const char ∗name, const char ∗value)
- typedef char ∗(∗ ini_reader)(char ∗str, int num, void ∗stream)

Functions

- int ini_parse (const char ∗filename, ini_handler handler, void ∗user)
- int ini_parse_file (FILE ∗file, ini_handler handler, void ∗user)
- int ini_parse_stream (ini_reader reader, void ∗stream, ini_handler handler, void ∗user)
- int ini_parse_string (const char ∗string, ini_handler handler, void ∗user)

11.7.1 Macro Definition Documentation

11.7.1.1 #define INI_HANDLER_LINENO 0

11.7.1.2 #define INI_ALLOW_MULTILINE 1

11.7.1.3 #define INI_ALLOW_BOM 1

11.7.1.4 #define INI_START_COMMENT_PREFIXES ";#"

11.7.1.5 #define INI_ALLOW_INLINE_COMMENTS 1

11.7.1.6 #define INI_INLINE_COMMENT_PREFIXES ";"

11.7.1.7 #define INI_USE_STACK 1

11.7.1.8 #define INI_MAX_LINE 200

11.7.1.9 #define INI_ALLOW_REALLOC 0

11.7.1.10 #define INI_INITIAL_ALLOC 200

11.7.1.11 #define INI_STOP_ON_FIRST_ERROR 0

11.7.1.12 #define INI_CALL_HANDLER_ON_NEW_SECTION 0

11.7.1.13 #define INI_ALLOW_NO_VALUE 0

11.7.1.14 #define INI_CUSTOM_ALLOCATOR 0

11.7.2 Typedef Documentation

11.7.2.1 typedef int(∗ ini_handler)(void ∗user, const char ∗section, const char ∗name, const char ∗value)

11.7.2.2 typedef char∗(∗ ini_reader)(char ∗str, int num, void ∗stream)

11.7.3 Function Documentation

11.7.3.1 int ini_parse (const char ∗ *filename*, ini_handler *handler*, void ∗ *user*)

11.7.3.2 int ini_parse_file (FILE ∗ *file*, ini_handler *handler*, void ∗ *user*)

11.7.3.3 int ini_parse_stream (ini_reader *reader*, void ∗ *stream*, ini_handler *handler*, void ∗ *user*)

11.7.3.4 int ini_parse_string (const char ∗ *string*, ini_handler *handler*, void ∗ *user*)

11.8 include/io.h File Reference

```
#include <stdio.h>
#include <string.h>
#include <argp.h>
#include <ini.h>
#include <stdlib.h>
```

Classes

- struct arguments
- struct parameters

Functions

- FILE ∗ open_file_w (char ∗filename)
- FILE ∗ open_file_r (char ∗filename)
- FILE ∗ open_file_a (char ∗filename)
- void close_file (FILE ∗fp)
- void print_help_main (char ∗argv[ ])
- void print_help (char ∗argv[ ])
- static error_t parse_opt (int key, char ∗arg, struct argp_state ∗state)
- int handler (void ∗config, const char ∗section, const char ∗name, const char ∗value)
- parameters pp_config (parameters config)
- void print_usage_main (char ∗argv[ ])

- void check_files (char ∗∗pars, char ∗∗pars_names, int n_pars, char ∗argv[ ])
- void check_empty_file (FILE ∗f, char ∗filename)
- int n_rows (FILE ∗f)
- void check_empty_rows (char ∗str)
- void check_int_string (const char ∗str, int row, char ∗fname)
- void check_int_string_iniFile (const char ∗str, char ∗fname, char ∗name)
- void check_argv_errors (char ∗argv[ ], int argc)
- void check_float_string (char ∗str, int row, char ∗fname)
- void check_float_string_iniFile (const char ∗str, char ∗fname, char ∗name)
- int columns (char ∗string)
- void mandatory_files_present (arguments ∗arguments, char ∗argv[ ])
- void read_ParameterFile (arguments ∗arguments, parameters ∗cc)
- void check_optional_parameters (parameters ∗cc)
- void check_parameters (int ∗pars, char ∗∗pars_names, int n_pars)
- void read_mapping_matrix (char ∗mappings_filename, FILE ∗f_out_l, struct cg_mapping ∗mapping_matrix[ ], int nmaps)

Variables

- static char doc_main [ ]
- static char args_doc_main [ ] = "random\noptimize\nmeasure\nnorm\ncosine\ndistance"
- static struct argp_option options_main [ ]
- static struct argp argp = { options_main, parse_opt, args_doc_main, doc_main }

11.8.1 Function Documentation

11.8.1.1 FILE∗ open_file_w (char ∗ *filename*)

routine that opens a file in write mode

11.8.1.2 FILE∗ open_file_r (char ∗ *filename*)

routine that opens a file in read mode

11.8.1.3 FILE∗ open_file_a (char ∗ *filename*)

routine that opens a file in append mode

11.8.1.4 void close_file (FILE ∗ *fp*)

routine that closes a file

11.8.1.5 void print_help_main (char ∗ *argv[ ]*)

routine that prints detailed information about the program

Parameter

`argv[]` : array of command line arguments

11.8.1.6 void print_help (char ∗ *argv[]*)

routine that prints some help

Parameter

`argv[]` : array of command line arguments

11.8.1.7 static error_t parse_opt (int *key,* char ∗ *arg,* struct argp_state ∗ *state*) [static]

11.8.1.8 int handler (void ∗ *config,* const char ∗ *section,* const char ∗ *name,* const char ∗ *value*)

11.8.1.9 parameters pp_config (parameters *config*)

11.8.1.10 void print_usage_main (char ∗ *argv[]*)

routine that prints the usage of the program

Parameter

`argv[]` : array of command line arguments

11.8.1.11 void check_files (char ∗∗ *pars,* char ∗∗ *pars_names,* int *n_pars,* char ∗ *argv[]*)

routine that checks if all command line arguments are correctly provided

Parameter

`pars` : parameters

`pars_names` : names of parameters

`n_pars` : number of parameters

`argv[]` : array of command line arguments

11.8.1.12 void check_empty_file (FILE ∗ *f,* char ∗ *filename*)

routine that checks if the file required exists. If it is the case, check if it is empty or not.

Parameters

`f` : FILE structure that represents the file opened.

`filename` : filename read

11.8.1.13 int n_rows (FILE ∗ *f*)

routine that returns the number of rows in a file. It counts correctly this number even if the last row does not present

Parameter

`f` : FILE structure that represents the file opened.

11.8.1.14 void check_empty_rows (char ∗ *str*)

routine that checks if a generic line is empty or not

Parameter

`str` : string token in account

11.8.1.15 void check_int_string (const char ∗ *str,* int *row,* char ∗ *fname*)

routine that checks if the string token in account reading a generic FILE is an INTEGER number

Parameters

`str` : string token in account

`row` : number of row where the string is found.

`fname` : filename read

11.8.1.16 void check_int_string_iniFile (const char ∗ *str,* char ∗ *fname,* char ∗ *name*)

routine that checks if the string token in account is an INTEGER number. It works only for ini Files

Parameters

`str` : string token in account

`fname` : parameter filename

`name` : name of each parameter in the file

11.8.1.17 void check_argv_errors (char ∗ *argv[ ],* int *argc*)

routine that checks the correctness of command line arguments

Parameter

`argv[]` : array of command line arguments

`argc` : number of command line arguments

11.8.1.18 void check_float_string (char ∗ *str,* int *row,* char ∗ *fname*)

routine that checks if the string token in account reading a generic FILE is an Float number

Parameters

`str` : string token in account

`row` : number of row where the string is found.

`fname` : filename read

11.8.1.19 void check_float_string_iniFile (const char ∗ *str,* char ∗ *fname,* char ∗ *name*)

routine that checks if the string token in account is an Float number. It works only for ini Files

Parameters

`str` : string token in account

`fname` : parameter filename

`name` : name of each parameter in the file

11.8.1.20 int columns (char ∗ *string*)

routine that returns the number of columns for each row inside the file chosen.

Parameter

`string` : string token in account

11.8.1.21 void mandatory_files_present (arguments ∗ *arguments,* char ∗ *argv[]*)

routine that checks if the mandatory files are present

Parameters

`arguments` : command line arguments

`argv[]` : array of command line arguments

11.8.1.22 void read_ParameterFile (arguments ∗ *arguments,* parameters ∗ *cc*)

routine that reads the input parameter file

Parameter

`ParameterFileName` : parameter filename

11.8.1.23 void check_optional_parameters (parameters ∗ *cc*)

routine that checks optional parameters for the tasks that need them

Parameters

`cc` : parameters

11.8.1.24 void check_parameters (int ∗ *pars,* char ∗∗ *pars_names,* int *n_pars*)

routine that checks if all mandatory parameters are correctly provided

Parameter

`pars` : parameters

`pars_names` : names of parameters

`n_pars` : number of parameters

11.8.1.25 void read_mapping_matrix (char ∗ *mappings_filename,* FILE ∗ *f_out_l,* cg_mapping ∗ *mapping_matrix[ ],* int *nmaps*)

routine that reads the input mapping matrix

Parameters

filename : mapping filename

f_out_l : output filename

cg_mapping : cg_mapping object routine that reads the input mapping matrix

Parameters

`filename` : mapping filename

`f_out_l` : output filename

`cg_mapping` : cg_mapping object

`nmaps` : number of mappings defined in parameter file

11.8.2 Variable Documentation

11.8.2.1 char doc_main[ ] [static]

Initial value:

```
=
"\n---------------------------------------------------------------------------\n\
Please, choose one of the following tasks:\n\n\
   *random*          To randomly generate coarse-grained representations\n\
                             and measure the associated mapping entropies;\n\n\
   *optmize*             To optimize the coarse-grained mapping by minimising\n\
                             its mapping entropy\n\n\
   *measure*             To measure the mapping entropy of a mapping\n\
                             provided by the user (in the form of a .txt file)\n\n\
   *norm*            To calculate the norm of a mapping (provided by the user)\n\
                             throughout a trajectory\n\n\
   *cosine*          To calculate pairwise distance and cosine between a pair\n\
                 of mappings (provided by the user) throughout a trajectory\n\n\
   *distance*            To calculate the distance matrix between a data set\n\
                 of mappings (provided by the user) over a single conformation\n\
-------------------------------------------------------------------------\n\n\
Hereafter the list of OPTIONS:"
```

11.8.2.2 char args_doc_main[ ] = "random\noptimize\nmeasure\nnorm\ncosine\ndistance" [static]

11.8.2.3 struct argp_option options_main[ ] [static]

Initial value:

```
= {
   {"verbose",      'v',          0,  0,  "Produce verbose output" },
   {"quiet",        'q',         0,  OPTION_HIDDEN,  "Don't produce any output" },
   {"help",         'h',         0,  0,  "Give this help list"},
   {"p",            'p',      "FILE", OPTION_HIDDEN,  "Parameter file in ini.format (mandatory)"},
   {"e",            'e',      "FILE", OPTION_HIDDEN,  "Energy file (mandatory for tasks 0, 1, 2, 3)"},
   {"m1",           'm',      "FILE", OPTION_HIDDEN,  "Mapping file1 (mandatory for tasks 2, 4, 5)" },
   {"m2",           'n',      "FILE", OPTION_HIDDEN,  "Mapping file2 (mandatory for task 5)" },
   {"t",        't',      "FILE", OPTION_HIDDEN,  "Trajectory file in .xyz format (mandatory)"},
   {"code",         'c',      "STR",  OPTION_HIDDEN,  "String that identifies your structure (mandatory)"},
   {"matrix",       'x',      "STR",  OPTION_HIDDEN,  "mapping_matrix"},
   {"prob",         'r',      "FILE", OPTION_HIDDEN,  "Probability file"},
   { 0 }
}
```

11.8.2.4 struct argp argp = { options_main, parse_opt, args_doc_main, doc_main } [static]

11.9 include/mapping.h File Reference

```
#include <stdio.h>
```

Classes

- class cg_mapping

  structure that defines a cg mapping

Typedefs

- typedef struct cg_mapping cg_mapping

Functions

- void free_mapping (cg_mapping *mapping)
- void convert_mapping (cg_mapping *mapping, FILE *f_out)
- void generate_random_mapping (cg_mapping *mapping, FILE *f_out)
- void update_mapping (cg_mapping *curr_mapping, cg_mapping *old_mapping, int frames)
- void read_MappingFile (char *MappingFileName, FILE *f_out_l, cg_mapping *mapping)
- void read_mapping_matrix (char *mappings_filename, FILE *f_out_l, cg_mapping *mapping_matrix[], int nmaps)

11.9.1 Typedef Documentation

11.9.1.1 typedef struct cg_mapping cg_mapping

11.9.2 Function Documentation

11.9.2.1 void free_mapping (cg_mapping * *mapping*)

routine that frees the mapping

Parameters

`mapping` : cg_mapping object

11.9.2.2 void convert_mapping (cg_mapping ∗ *mapping,* FILE ∗ *f_out*)

routine that prints out the mapping

Parameters

`mapping` : cg_mapping object

`f_out` : file to write on

11.9.2.3 void generate_random_mapping (cg_mapping ∗ *mapping,* FILE ∗ *f_out*)

routine that generates a random mapping

Parameters

`mapping` : cg_mapping object

`f_out` : file to write on

11.9.2.4 void update_mapping (cg_mapping ∗ *curr_mapping,* cg_mapping ∗ *old_mapping,* int *frames*)

routine that updates old_mapping with the data contained in curr_mapping

Parameters

`curr_mapping` : current cg_mapping object

`old_mapping` : cg_mapping object to be updated

`frames` : length of the MD trajectory

11.9.2.5 void read_MappingFile (char ∗ *MappingFileName,* FILE ∗ *f_out_l,* cg_mapping ∗ *mapping*)

routine that reads the input mapping file

Parameters

`MappingFileName` : mapping filename

`f_out_l` : output filename

`cg_mapping` : cg_mapping object

11.9.2.6 void read_mapping_matrix (char ∗ *mappings_filename,* FILE ∗ *f_out_l,* cg_mapping ∗ *mapping_matrix[ ],* int *nmaps*)

routine that reads the input mapping matrix

Parameters

filename : mapping filename

f_out_l : output filename

cg_mapping : cg_mapping object routine that reads the input mapping matrix

Parameters

`filename` : mapping filename

`f_out_l` : output filename

`cg_mapping` : cg_mapping object

`nmaps` : number of mappings defined in parameter file

11.10 include/measure.h File Reference

```
#include <stdio.h>
#include <io.h>
```

Functions

- void measure (arguments ∗arguments, parameters ∗cc)

11.10.1 Function Documentation

11.10.1.1 void measure (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to measure the mapping entropy of a mapping provided by the user

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.11 include/measure_kl.h File Reference

```
#include <stdio.h>
#include <io.h>
```

Functions

- void measure_kl (arguments ∗arguments, parameters ∗cc)

11.11.1 Function Documentation

11.11.1.1 void measure_kl (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to measure the KL divergence version of the mapping entropy for a mapping provided by the user

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.12 include/my_malloc.h File Reference

```
#include "stdio.h"
```

Functions

- void readeol (FILE ∗fp)
- FILE ∗∗ F2t (int n1)
- FILE ∗∗∗ F3t (int n1, int n2)
- char ∗ c1t (int n1)
- char ∗∗ c2t (int n1, int n2)
- char ∗∗∗ c3t (int n1, int n2, int n3)
- char ∗∗∗∗ c4t (int n1, int n2, int n3, int n4)
- void free_c4t (char ∗∗∗∗p)
- void free_c3t (char ∗∗∗p)
- void free_c2t (char ∗∗p)
- void free_c1t (char ∗p)
- short ∗ s1t (int n1)
- short ∗∗ s2t (int n1, int n2)
- short ∗∗∗ s3t (int n1, int n2, int n3)
- short ∗∗∗∗ s4t (int n1, int n2, int n3, int n4)
- void free_s4t (short ∗∗∗∗p)
- void free_s3t (short ∗∗∗p)
- void free_s2t (short ∗∗p)
- void free_s1t (short ∗p)
- int ∗ i1t (int n1)
- int ∗∗ i2t (int n1, int n2)
- int ∗∗∗ i3t (int n1, int n2, int n3)
- int ∗∗∗∗ i4t (int n1, int n2, int n3, int n4)
- void free_i4t (int ∗∗∗∗p)
- void free_i3t (int ∗∗∗p)
- void free_i2t (int ∗∗p)
- void free_i1t (int ∗p)
- float ∗ f1t (int n1)
- float ∗∗ f2t (int n1, int n2)
- float ∗∗∗ f3t (int n1, int n2, int n3)
- float ∗∗∗∗ f4t (int n1, int n2, int n3, int n4)
- float ∗∗∗∗∗ f5t (int n1, int n2, int n3, int n4, int n5)
- void free_f5t (float ∗∗∗∗∗p)
- void free_f4t (float ∗∗∗∗p)
- void free_f3t (float ∗∗∗p)
- void free_f2t (float ∗∗p)
- void free_f1t (float ∗p)
- double ∗ d1t (int n1)
- double ∗∗ d2t (int n1, int n2)
- double ∗∗∗ d3t (int n1, int n2, int n3)
- double ∗∗∗∗ d4t (int n1, int n2, int n3, int n4)
- void free_d4t (double ∗∗∗∗p)
- void free_d3t (double ∗∗∗p)
- void free_d2t (double ∗∗p)
- void free_d1t (double ∗p)
- void pdarray (int n, int m, double ∗∗a)
- void pdvector (int n, double ∗a)

- void pfarray (int n, int m, float **a)
- void pfvector (int n, float *a)
- void piarray (int n, int m, int **a)
- void pivector (int n, int *a)
- void zdarray (int n, int m, double **a)
- void zdvector (int n, double *a)
- void zfarray (int n, int m, float **a)
- void zfvector (int n, float *a)
- void ziarray (int n, int m, int **a)
- void zivector (int n, int *a)
- void failed (char msg[])

11.12.1 Function Documentation

11.12.1.1 void readeol (FILE * *fp*)

11.12.1.2 FILE** F2t (int *n1*)

11.12.1.3 FILE*** F3t (int *n1,* int *n2*)

11.12.1.4 char* c1t (int *n1*)

11.12.1.5 char** c2t (int *n1,* int *n2*)

11.12.1.6 char*** c3t (int *n1,* int *n2,* int *n3*)

11.12.1.7 char**** c4t (int *n1,* int *n2,* int *n3,* int *n4*)

11.12.1.8 void free_c4t (char **** *p*)

11.12.1.9 void free_c3t (char *** *p*)

11.12.1.10 void free_c2t (char ** *p*)

11.12.1.11 void free_c1t (char * *p*)

11.12.1.12 short* s1t (int *n1*)

11.12.1.13 short** s2t (int *n1,* int *n2*)

11.12.1.14 short*** s3t (int *n1,* int *n2,* int *n3*)

11.12.1.15 short**** s4t (int *n1,* int *n2,* int *n3,* int *n4*)

11.12.1.16 void free_s4t (short **** *p*)

11.12.1.17 void free_s3t (short *** *p*)

11.12.1.18 void free_s2t (short ** *p*)

11.12.1.19 void free_s1t (short * *p*)

11.12.1.20 int* i1t (int *n1*)

11.12.1.21 int** i2t (int *n1,* int *n2*)

11.12.1.22 int∗∗∗ i3t (int *n1*, int *n2*, int *n3*)

11.12.1.23 int∗∗∗∗ i4t (int *n1*, int *n2*, int *n3*, int *n4*)

11.12.1.24 void free_i4t (int ∗∗∗∗ *p*)

11.12.1.25 void free_i3t (int ∗∗∗ *p*)

11.12.1.26 void free_i2t (int ∗∗ *p*)

11.12.1.27 void free_i1t (int ∗ *p*)

11.12.1.28 float∗ f1t (int *n1*)

11.12.1.29 float∗∗ f2t (int *n1*, int *n2*)

11.12.1.30 float∗∗∗ f3t (int *n1*, int *n2*, int *n3*)

11.12.1.31 float∗∗∗∗ f4t (int *n1*, int *n2*, int *n3*, int *n4*)

11.12.1.32 float∗∗∗∗∗ f5t (int *n1*, int *n2*, int *n3*, int *n4*, int *n5*)

11.12.1.33 void free_f5t (float ∗∗∗∗∗ *p*)

11.12.1.34 void free_f4t (float ∗∗∗∗ *p*)

11.12.1.35 void free_f3t (float ∗∗∗ *p*)

11.12.1.36 void free_f2t (float ∗∗ *p*)

11.12.1.37 void free_f1t (float ∗ *p*)

11.12.1.38 double∗ d1t (int *n1*)

11.12.1.39 double∗∗ d2t (int *n1*, int *n2*)

11.12.1.40 double∗∗∗ d3t (int *n1*, int *n2*, int *n3*)

11.12.1.41 double∗∗∗∗ d4t (int *n1*, int *n2*, int *n3*, int *n4*)

11.12.1.42 void free_d4t (double ∗∗∗∗ *p*)

11.12.1.43 void free_d3t (double ∗∗∗ *p*)

11.12.1.44 void free_d2t (double ∗∗ *p*)

11.12.1.45 void free_d1t (double ∗ *p*)

11.12.1.46 void pdarray (int *n*, int *m*, double ∗∗ *a*)

11.12.1.47 void pdvector (int *n*, double ∗ *a*)

11.12.1.48 void pfarray (int *n*, int *m*, float ∗∗ *a*)

11.12.1.49 void pfvector (int *n*, float ∗ *a*)

11.12.1.50 void piarray (int *n*, int *m*, int ∗∗ *a*)

11.12.1.51 void pivector (int *n*, int ∗ *a*)

11.12.1.52 void zdarray (int *n*, int *m*, double ∗∗ *a*)

11.12.1.53 void zdvector (int *n*, double ∗ *a*)

11.12.1.54 void zfarray (int *n*, int *m*, float ∗∗ *a*)

11.12.1.55 void zfvector (int *n*, float ∗ *a*)

11.12.1.56 void ziarray (int *n*, int *m*, int ∗∗ *a*)

11.12.1.57 void zivector (int *n*, int ∗ *a*)

11.12.1.58 void failed (char *msg[]*)

11.13 include/norm.h File Reference

```
#include <stdio.h>
#include <io.h>
```

Functions

- void norm (arguments ∗arguments, parameters ∗cc)

11.13.1 Function Documentation

11.13.1.1 void norm (**arguments** ∗ *arguments*, **parameters** ∗ *cc*)

subprogram to To calculate the norm of a mapping (provided by the user) throughout a trajectory

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.14 include/observables.h File Reference

```
#include <stdio.h>
#include <mapping.h>
#include <hierarchical_clustering.h>
#include <traj.h>
#include <alignment.h>
```

Functions

- void compute_coupling_matrix (double ∗coupling_mat, traj ∗Trajectory, int fr_id, float sigma)

- double compute_atomistic_coord_number (double ∗coupling_mat, traj ∗Trajectory, FILE ∗f_out_l)
- void compute_norm (cg_mapping ∗mapping, double ∗coupling_mat, double n_coord_at, int fr_id, FILE ∗f_-out_l)
- double compute_distance (cg_mapping ∗mapping, cg_mapping ∗mapping_prime, double ∗coupling_mat, double n_coord_at, int fr_id, FILE ∗f_out_l)
- void compute_mapping_norms (traj ∗Trajectory, cg_mapping ∗mapping, FILE ∗f_out_l)
- void compute_mapping_distances (traj ∗Trajectory, cg_mapping ∗mapping, cg_mapping ∗mapping_prime, FILE ∗f_out_l)
- void compute_mapping_distmat (traj ∗Trajectory, cg_mapping ∗mapping_matrix[ ], int nmaps, FILE ∗f_out_l, char ∗distmat_filename)
- void compute_variances (int Nclust, double ∗variances, int ∗cluster_list, int ∗cluster_list_idx, double ∗energies)
- double get_smap (int frames, int curr_nclust, int ∗clusters, double ∗energies)
- void overall_compute_smap (alignments ∗align, clust_params ∗clustering, traj ∗Trajectory, cg_mapping ∗mapping, int verbose, int kl_flag)

11.14.1 Function Documentation

11.14.1.1 void compute_coupling_matrix (double ∗ *coupling_mat,* traj ∗ *Trajectory,* int *fr_id,* float *sigma*)

routine that computes the coupling matrix over a frame

`coupling_mat` : coupling matrix

`Trajectory` : traj object

`fr_id` : frame ID

`sigma` : sigma parameter

11.14.1.2 double compute_atomistic_coord_number (double ∗ *coupling_mat,* traj ∗ *Trajectory,* FILE ∗ *f_out_l*)

routine that computes the atomistic coordination number for a certain coupling matrix. Double counting is necessary to ensure proper normalisation to norm and scalar product

`coupling_mat` : coupling matrix

`Trajectory` : traj object

`f_out_l` : output filename

11.14.1.3 void compute_norm (cg_mapping ∗ *mapping,* double ∗ *coupling_mat,* double *n_coord_at,* int *fr_id,* FILE ∗ *f_out_l*)

routine that computes the norm of a mapping over a frame of a trajectory

Parameters

`mapping` : cg_mapping object

`coupling_mat` : coupling matrix

`n_coord_at` : atomistic coordination number

`fr_id` : frame index

`f_out_l` : output filename

11.14.1.4 double compute_distance (**cg_mapping** ∗ *mapping,* **cg_mapping** ∗ *mapping_prime,* double ∗ *coupling_mat,* double *n_coord_at,* int *fr_id,* FILE ∗ *f_out_l*)

routine that computes the distance and cosine between a pair of cg mappings

Parameters

`mapping`, `mapping_prime` : cg_mapping objects

`coupling_mat` : coupling matrix

`n_coord_at` : atomistic coordination number

`fr_id` : frame index

`f_out_l` : output filename

11.14.1.5 void compute_mapping_norms (**traj** ∗ *Trajectory,* **cg_mapping** ∗ *mapping,* FILE ∗ *f_out_l*)

routine that computes the norm of a mapping over a MD trajectory

Parameters

`Trajectory` : traj object

`mapping` : cg_mapping object

`f_out_l` : output filename

11.14.1.6 void compute_mapping_distances (**traj** ∗ *Trajectory,* **cg_mapping** ∗ *mapping,* **cg_mapping** ∗ *mapping_prime,* FILE ∗ *f_out_l*)

routine that computes the distances and cosines between two mappings provided by the user over a MD trajectory

Parameters

`Trajectory` : traj object

`mapping`, `mapping_prime` : cg_mapping objects

`f_out_l` : output filename

11.14.1.7 void compute_mapping_distmat (**traj** ∗ *Trajectory,* **cg_mapping** ∗ *mapping_matrix[],* int *nmaps,* FILE ∗ *f_out_l,* char ∗ *distmat_filename*)

routine that computes the distance matrix between a set of mappings over a single structure

Parameters

`Trajectory` : traj object

`mappings_filename` : filename with the chosen mappings

`namps` : number of mappings

`f_out_l` : output filename

11.14.1.8 void compute_variances (int *Nclust*, double ∗ *variances*, int ∗ *cluster_list*, int ∗ *cluster_list_idx*, double ∗ *energies*)

routine that computes the variance of the energies

Parameters

`nclust` : number of macrostates

`variances` : vector of variances

`cluster_list` : list of cluster IDs

`cluster_list_idx` : list of cluster indices

`energies` : array of energies

11.14.1.9 double get_smap (int *frames*, int *curr_nclust*, int ∗ *clusters*, double ∗ *energies*)

routine that computes the observable given the current `nclust` and the current `clusters`

Parameters

`frames` : number of frames

`curr_nclust` : current index of CG macrostate

`clusters` : list of cluster IDs

`energies` : array of energies

11.14.1.10 void overall_compute_smap (alignments ∗ *align*, clust_params ∗ *clustering*, traj ∗ *Trajectory*, cg_mapping ∗ *mapping*, int *verbose*, int *kl_flag*)

routine that calls `get_smap` with the correct parameters

Parameters

`rmsd_mat` : condensed matrix of pairwise RMSDs

`clustering` : clust_params object

`Trajectory` : traj object

`mapping` : cg_mapping object

`verbose` : tunes the level of verbosity

`f_out` : output filename

11.15 include/optimize.h File Reference

```
#include <stdio.h>
#include <io.h>
```

Functions

- void optimize (arguments ∗arguments, parameters ∗cc)

11.15.1 Function Documentation

11.15.1.1 void optimize (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to optimize the coarse-grained mapping by minimising its mapping entropy

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.16 include/optimize_kl.h File Reference

```
#include <stdio.h>
#include <io.h>
```

Functions

- void optimize_kl (arguments ∗arguments, parameters ∗cc)

11.16.1 Function Documentation

11.16.1.1 void optimize_kl (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to optimize the coarse-grained mapping by minimising the KL divergence version of its mapping entropy

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.17 include/random_mapping.h File Reference

```
#include <stdio.h>
#include <io.h>
```

Functions

- void random_mapping (arguments ∗arguments, parameters ∗cc)

11.17.1 Function Documentation

11.17.1.1 void random_mapping (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to randomly generate coarse-grained representations and measure the associated mapping entropies

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.18 include/random_mapping_kl.h File Reference

```
#include <stdio.h>
#include <io.h>
```

Functions

- void random_mapping_kl (arguments ∗arguments, parameters ∗cc)

11.18.1 Function Documentation

11.18.1.1 void random_mapping_kl (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to randomly generate coarse-grained representations and measure the KL divergence version of their mapping entropy

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.19 include/sampling.h File Reference

```
#include <mapping.h>
#include <alignment.h>
#include <hierarchical_clustering.h>
```

Classes

- class MC_params

  structure that defines a the parameters of Monte Carlo sampling

Typedefs

- typedef struct MC_params MC_params

Functions

- void my_make_a_move (cg_mapping ∗old_mapping, cg_mapping ∗new_mapping, int rem_add[2])
- void simulated_annealing (traj ∗Trajectory, clust_params ∗clustering, MC_params ∗SA_params, int cgnum, int rsd, int verbose, int kl_flag, FILE ∗f_out_l)

- double tzero_estimation (traj ∗Trajectory, clust_params ∗clustering, int cgnum, int rsd, int verbose, int kl_flag, FILE ∗f_out_l)

11.19.1 Typedef Documentation

11.19.1.1 typedef struct **MC_params MC_params**

11.19.2 Function Documentation

11.19.2.1 void my_make_a_move (**cg_mapping** ∗ *old_mapping,* **cg_mapping** ∗ *new_mapping,* int *rem_add[2]*)

function that swaps two atoms inside a CG mapping

Parameters

`old_mapping` : cg_mapping object

`new_mapping` : cg_mapping object

`rem_add` : vector of length 2 containing the removed and added atom index

11.19.2.2 void simulated_annealing (**traj** ∗ *Trajectory,* **clust_params** ∗ *clustering,* **MC_params** ∗ *SA_params,* int *cgnum,* int *rsd,* int *verbose,* int *kl_flag,* FILE ∗ *f_out_l*)

simulated annealing optimisation

Parameters

`Trajectory` : traj object

`alignments` : align object

`mapping` : cg_mapping object

`SA_params` : set of Monte Carlo parameters

`verbose` : tunes the level of verbosity

`f_out_l` : output filename

11.19.2.3 double tzero_estimation (**traj** ∗ *Trajectory,* **clust_params** ∗ *clustering,* int *cgnum,* int *rsd,* int *verbose,* int *kl_flag,* FILE ∗ *f_out_l*)

routine that makes *nrun* unbiased moves. It is used to estimate the starting temperature for Simulated Annealing.

Parameters

`Trajectory` : traj object

`alignments` : align object

`mapping` : cg_mapping object

`verbose` : tunes the level of verbosity

11.20 include/traj.h File Reference

```
#include <stdio.h>
#include <string.h>
#include <argp.h>
#include <ini.h>
#include <io.h>
```

Classes

- class traj

    structure that defines a MD trajectory

Typedefs

- typedef struct traj traj

Functions

- int check_probabilities (double ∗probabilities, int prob_length)
- void read_EnergyFile (char ∗EnergyFileName, traj ∗Trajectory)
- void read_TrajectoryFile (char ∗TrajFileName, traj ∗Trajectory)

11.20.1 Typedef Documentation

11.20.1.1 typedef struct **traj traj**

11.20.2 Function Documentation

11.20.2.1 int check_probabilities (double ∗ *probabilities,* int *prob_length*)

routine that checks that input probabilities sum to 1

Parameters

`probabilities` : array of probabilities

`prob_length` : array length

11.20.2.2 void read_EnergyFile (char ∗ *EnergyFileName,* traj ∗ *Trajectory*)

routine that reads the input energy file

Parameters

`EnergyFileName` : energies filename

`Trajectory` : traj object

11.20.2.3 void read_TrajectoryFile (char ∗ *TrajFileName,* traj ∗ *Trajectory*)

routine that reads the input xyz coordinate file

Parameters

`TrajFileName` : trajectory filename

`Trajectory` : traj object

11.21 lib/alignment.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <my_malloc.h>
#include <alignment.h>
#include <geometry.h>
```

Functions

- void free_new_alignment (alignments ∗new_align)
- void free_alignment (alignments ∗align)
- double optimal_alignment (double ∗∗x, double ∗∗y, int cgnum, double u[ ][3])
- void align_two_frames (double ∗frame_ref, double ∗frame_middle, int ref_id, int middle_id, cg_mapping ∗mapping, alignments ∗align)
- void cycle_alignment_stride (traj ∗Trajectory, alignments ∗align, cg_mapping ∗mapping)
- void cycle_alignment_fastclust (traj ∗Trajectory, alignments ∗align, cg_mapping ∗mapping)
- void cycle_alignment (traj ∗Trajectory, alignments ∗align, cg_mapping ∗mapping)
- void correct_rmsd (alignments ∗new_align, traj ∗Trajectory, alignments ∗align, int cgnum, int removed, int added)
- double correct_rmsd_two_frames (traj ∗Trajectory, double u[9], double com_ref[3], double com_other[3], int cgnum, int removed, int added, int ref_id, int other_id, double prev_rmsd)
- void correct_rmsd_fastclust (alignments ∗new_align, traj ∗Trajectory, alignments ∗prev_align, int cgnum, int removed, int added)
- void align_traj_to_reference (traj ∗Trajectory, int ref_id)

11.21.1 Function Documentation

11.21.1.1 void free_new_alignment (alignments ∗ *new_align*)

routine that frees an alignments object used in criterion 3

Parameters

`new_align`: alignments object

11.21.1.2 void free_alignment (alignments ∗ *align*)

routine that frees an alignments object

Parameters

`align`: alignments object

11.21.1.3 double optimal_alignment (double ∗∗ *x,* double ∗∗ *y,* int *cgnum,* double *u[ ][3]*)

routine that computes the Kabsch alignment and the rmsd between two configurations

Parameters

`x`, `y` : CG structures

`cgnum` : length of CG mapping

`u` : rotation matrix

11.21.1.4 void align_two_frames (double ∗ *frame_ref,* double ∗ *frame_middle,* int *ref_id,* int *middle_id,* cg_mapping ∗ *mapping,* alignments ∗ *align*)

routine that aligns a pair of frames in a trajectory, calling `optimal_alignment`

Parameters

`frame_ref` : reference frame

`frame_middle` : frame in between two pivot clusters

`ref_id` : id (index) of frame_ref in the trajectory

`middle_id` : id (index) of frame_middle in the trajectory

`mapping` : cg_mapping object

`align` : alignments object

11.21.1.5 void cycle_alignment_stride (traj ∗ *Trajectory,* alignments ∗ *align,* cg_mapping ∗ *mapping*)

routine that cycles over all pairs of frames in a trajectory, calling `optimal_alignment`

Parameters

`Trajectory` : traj object

`align` : alignments object

`mapping` : cg_mapping object

11.21.1.6 void cycle_alignment_fastclust (traj ∗ *Trajectory,* alignments ∗ *align,* cg_mapping ∗ *mapping*)

routine that computes the alignments if clustering must be fast

Parameters

`Trajectory` : traj object

`align` : alignments object

`mapping` : cg_mapping object

11.21.1.7 void cycle_alignment (**traj** ∗ *Trajectory,* **alignments** ∗ *align,* **cg_mapping** ∗ *mapping*)

routine that cycles over all pairs of frames in a trajectory, calling `optimal_alignment`

Parameters

`Trajectory` : traj object

`align` : alignments object

`mapping` : cg_mapping object

11.21.1.8 void correct_rmsd (**alignments** ∗ *new_align,* **traj** ∗ *Trajectory,* **alignments** ∗ *align,* int *cgnum,* int *removed,* int *added*)

routine that computes the rmsd matrix without aligning frames over frames

Parameters

`new_align` : trial alignments object

`Trajectory` : traj object

`align` : alignments object

`cgnum` : number of CG sites (useful to normalize)

`removed` : index of removed atom

`added` : index of added atom

11.21.1.9 double correct_rmsd_two_frames (**traj** ∗ *Trajectory,* double *u[9],* double *com_ref[3],* double *com_other[3],* int *cgnum,* int *removed,* int *added,* int *ref_id,* int *other_id,* double *prev_rmsd*)

routine that corrects the rmsd between two frames

Parameters

`Trajectory` : traj object

`u` : rotation matrix

`com_ref` : reference center of mass

`com_other` : other center of mass

`removed` : index of removed atom

`added` : index of added atom

`ref_id` : index of reference frame

`other_id` : index of other frame

`prev_rmsd` : previous rmsd

11.21.1.10 void correct_rmsd_fastclust (**alignments** ∗ *new_align,* **traj** ∗ *Trajectory,* **alignments** ∗ *prev_align,* int *cgnum,* int *removed,* int *added*)

routine that computes the rmsd matrix without aligning frames over frames

Parameters

`new_rmsd_mat` : new condensed pairwise RMSD matrix

`Trajectory` : traj object

`align` : alignments object

`cgnum` : number of CG sites (useful to normalize)

`removed` : index of removed atom

`added` : index of added atom

11.21.1.11 void align_traj_to_reference (**traj** ∗ ***Trajectory,*** int ***ref_id***)

routine that aligns the trajectory to a reference frame

Parameters

`Trajectory` : traj object

`ref_id` : reference frame

11.22 lib/cosine.c File Reference

```
#include <io.h>
#include <stdlib.h>
#include <my_malloc.h>
#include <traj.h>
#include <mapping.h>
#include <math.h>
#include <geometry.h>
#include <observables.h>
```

Functions

- void cosine (arguments ∗arguments, parameters ∗cc)

11.22.1 Function Documentation

11.22.1.1 void cosine (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to calculate pairwise distance and cosine between a pair of mappings (provided by the user) throughout a trajectory

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.23 lib/distance.c File Reference

```
#include <io.h>
#include <stdlib.h>
#include <my_malloc.h>
#include <traj.h>
#include <mapping.h>
#include <math.h>
#include <geometry.h>
#include <observables.h>
```

Functions

- void distance (arguments ∗arguments, parameters ∗cc)

11.23.1 Function Documentation

11.23.1.1 void distance (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to calculate the distance matrix between a data set of mappings (provided by the user) over a single conformation

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.24 lib/geometry.c File Reference

```
#include <stdio.h>
#include <math.h>
#include <geometry.h>
```

Macros

- #define ROTATE(a, i, j, k, l) g=a[i][j];h=a[k][l];a[i][j]=g-s∗(h+g∗tau);a[k][l]=h+s∗(g-h∗tau);

Functions

- void vecprod_d (double ∗a, double ∗b, double ∗c)
- double scal_d (double ∗a, double ∗b, int dim)
- double coseno (double ∗vec1, double ∗vec2, int dim)
- double norm_d (double ∗a, int dim)
- void normalize_d (double ∗a, int dim)
- double dist_d (double ∗a, double ∗b, int dim)
- double det (double a1, double a2, double a3, double b1, double b2, double b3, double c1, double c2, double c3)
- void vec_sum_d (double ∗a, double ∗b, double ∗c, double d, int dim)
- void print_vec_d (double ∗a, int dim)

- void zero_vec_d (double ∗a, int dim)
- void zero_vec_i (int ∗a, int dim)
- void myjacobi (double a[ ][3], int n, double ∗d, double v[ ][3], int ∗nrot)
- void zero_matrix_d (double ∗∗a, int dim1, int dim2)

11.24.1 Macro Definition Documentation

11.24.1.1 #define ROTATE(*a, i, j, k, l*) g=a[i][j];h=a[k][l];a[i][j]=g-s∗(h+g∗tau);a[k][l]=h+s∗(g-h∗tau);

11.24.2 Function Documentation

11.24.2.1 void vecprod_d (double ∗ *a,* double ∗ *b,* double ∗ *c*)

11.24.2.2 double scal_d (double ∗ *a,* double ∗ *b,* int *dim*)

11.24.2.3 double coseno (double ∗ *vec1,* double ∗ *vec2,* int *dim*)

11.24.2.4 double norm_d (double ∗ *a,* int *dim*)

11.24.2.5 void normalize_d (double ∗ *a,* int *dim*)

11.24.2.6 double dist_d (double ∗ *a,* double ∗ *b,* int *dim*)

11.24.2.7 double det (double *a1,* double *a2,* double *a3,* double *b1,* double *b2,* double *b3,* double *c1,* double *c2,* double *c3*)

11.24.2.8 void vec_sum_d (double ∗ *a,* double ∗ *b,* double ∗ *c,* double *d,* int *dim*)

11.24.2.9 void print_vec_d (double ∗ *a,* int *dim*)

11.24.2.10 void zero_vec_d (double ∗ *a,* int *dim*)

11.24.2.11 void zero_vec_i (int ∗ *a,* int *dim*)

11.24.2.12 void myjacobi (double *a[ ][3],* int *n,* double ∗ *d,* double *v[ ][3],* int ∗ *nrot*)

11.24.2.13 void zero_matrix_d (double ∗∗ *a,* int *dim1,* int *dim2*)

11.25 lib/hierarchical_clustering.c File Reference

```
#include <stdlib.h>
#include <math.h>
#include <my_malloc.h>
#include <string.h>
#include <hierarchical_clustering.h>
```

Functions

- void mergesort_merge (double ∗∗arr, int l, int m, int r, int dim, int dims)
- void my_mergesort (double ∗∗arr, int l, int r, int dim, int dims)
- int condensed_index (int frames, int i, int j)
- double new_dist (double d_xi, double d_yi, double d_xy, int size_x, int size_y, int size_i)
- int is_visited (unsigned char ∗bitset, int i)
- void set_visited (unsigned char ∗bitset, int i)

- void get_max_dist_for_each_cluster (double ∗∗Z, double ∗MD, int frames)
- void cluster_monocrit (double ∗∗Z, double ∗MC, int ∗T, double cutoff, int frames)
- void cluster_maxclust_monocrit (double ∗∗Z, double ∗MC, int ∗T, int frames, int max_nc)
- void cluster_maxclust_dist (double ∗∗Z, int ∗T, int frames, int nclust)
- void cluster_dist (double ∗∗Z, int ∗T, double cutoff, int frames)
- int find (int x, int ∗self_parent)
- int merge (int ∗self_parent, int ∗self_size, int next_label, int x, int y)
- void label (double ∗∗Z, int frames)
- void hierarchical_clustering (double ∗rmsd_mat, int frames, int pairs, int ∗size, double ∗∗Z)
- void compute_clusters_list (int ∗clusters, int ∗cluster_list, int ∗cluster_list_idx, int frames, int nclust)

11.25.1 Function Documentation

11.25.1.1 void mergesort_merge (double ∗∗ *arr,* int *l,* int *m,* int *r,* int *dim,* int *dims*)

11.25.1.2 void my_mergesort (double ∗∗ *arr,* int *l,* int *r,* int *dim,* int *dims*)

11.25.1.3 int condensed_index (int *frames,* int *i,* int *j*)

`frames` : number of observations

`i` : node

`j` : node

11.25.1.4 double new_dist (double *d_xi,* double *d_yi,* double *d_xy,* int *size_x,* int *size_y,* int *size_i*)

11.25.1.5 int is_visited (unsigned char ∗ *bitset,* int *i*)

routine that checks if node i was visited.

Parameters

`bitset` : char defining visits

`i` : node

11.25.1.6 void set_visited (unsigned char ∗ *bitset,* int *i*)

routine that marks node i as visited.

Parameters

`bitset` : char defining visits

`i` : node

11.25.1.7 void get_max_dist_for_each_cluster (double ∗∗ *Z,* double ∗ *MD,* int *frames*)

Get the maximum inconsistency coefficient for each non-singleton cluster.

Parameters

`Z` : linkage matrix.

`MD` : array to store the result.

`frames` : number of observations.

11.25.1.8 void cluster_monocrit (double ∗∗ *Z,* double ∗ *MC,* int ∗ *T,* double *cutoff,* int *frames*)

Form flat clusters by monocrit criterion.

Parameters

`Z` : linkage matrix.

`MC` : monotonic criterion array.

`T` : array to store the cluster numbers. The i'th observation belongs to cluster `T[i]`.

`cutoff` : Clusters are formed when the MC values are less than or equal to `cutoff`.

`frames` : number of observations

11.25.1.9 void cluster_maxclust_monocrit (double ∗∗ *Z,* double ∗ *MC,* int ∗ *T,* int *frames,* int *max_nc*)

Form flat clusters by maxclust_monocrit criterion.

Parameters

`Z` : linkage matrix

`MC` : monotonic criterion array

`T` : array to store the cluster numbers. The i'th observation belongs to cluster `T[i]`

`frames` : number of observations

`max_nc` : The maximum number of clusters

11.25.1.10 void cluster_maxclust_dist (double ∗∗ *Z,* int ∗ *T,* int *frames,* int *nclust*)

routine that converts the dendrogram into nclust clusters

Parameters

`Z` : linkage matrix.

`T` : array to store the cluster numbers. The i'th observation belongs to cluster `T[i]`.

`frames` : number of observations.

`nclust` : number of desired clusters.

11.25.1.11 void cluster_dist (double ∗∗ *Z,* int ∗ *T,* double *cutoff,* int *frames*)

11.25.1.12 int find (int *x,* int ∗ *self_parent*)

11.25.1.13 int merge (int ∗ *self_parent,* int ∗ *self_size,* int *next_label,* int *x,* int *y*)

11.25.1.14 void label (double ∗∗ *Z*, int *frames*)

routine that correctly labels clusters in the unsorted dendrogram

Parameters

`Z` : linkage matrix

`frames` : number of observations

11.25.1.15 void hierarchical_clustering (double ∗ *rmsd_mat*, int *frames*, int *pairs*, int ∗ *size*, double ∗∗ *Z*)

overall routine for hierarchical clustering

Parameters

`rmsd_mat` : condensed pairwise RMSD matrix

`frames` : number of observations

`pairs` : possible pairs of structures

`size` : size of the clusters (it is nclust long)

`Z` : linkage matrix

11.25.1.16 void compute_clusters_list (int ∗ *clusters*, int ∗ *cluster_list*, int ∗ *cluster_list_idx*, int *frames*, int *nclust*)

routine that computes the list of cluster IDs

Parameters

`clusters` : list of labels (one for each frame)

`cluster_list` : ordered list of labels

`cluster_list_idx` : is an index vector that stores the sum of populations up to each index

`frames` : number of observations

`nclust` : number of clusters

< array that stores the population of each clusters

11.26 lib/ini.c File Reference

```
#include <stdio.h>
#include <ctype.h>
#include <string.h>
#include "ini.h"
#include <stdlib.h>
```

Classes

- struct ini_parse_string_ctx

Macros

- #define ini_malloc malloc
- #define ini_free free
- #define ini_realloc realloc
- #define MAX_SECTION 50
- #define MAX_NAME 50
- #define HANDLER(u, s, n, v) handler(u, s, n, v)

Functions

- static char ∗ rstrip (char ∗s)
- static char ∗ lskip (const char ∗s)
- static char ∗ find_chars_or_comment (const char ∗s, const char ∗chars)
- static char ∗ strncpy0 (char ∗dest, const char ∗src, size_t size)
- int ini_parse_stream (ini_reader reader, void ∗stream, ini_handler handler, void ∗user)
- int ini_parse_file (FILE ∗file, ini_handler handler, void ∗user)
- int ini_parse (const char ∗filename, ini_handler handler, void ∗user)
- static char ∗ ini_reader_string (char ∗str, int num, void ∗stream)
- int ini_parse_string (const char ∗string, ini_handler handler, void ∗user)

11.26.1 Macro Definition Documentation

11.26.1.1 #define ini_malloc malloc

11.26.1.2 #define ini_free free

11.26.1.3 #define ini_realloc realloc

11.26.1.4 #define MAX_SECTION 50

11.26.1.5 #define MAX_NAME 50

11.26.1.6 #define HANDLER(*u*, *s*, *n*, *v*) handler(u, s, n, v)

11.26.2 Function Documentation

11.26.2.1 static char∗ rstrip (char ∗ *s*) [static]

11.26.2.2 static char∗ lskip (const char ∗ *s*) [static]

11.26.2.3 static char∗ find_chars_or_comment (const char ∗ *s*, const char ∗ *chars*) [static]

11.26.2.4 static char∗ strncpy0 (char ∗ *dest*, const char ∗ *src*, size_t *size*) [static]

11.26.2.5 int ini_parse_stream (ini_reader *reader*, void ∗ *stream*, ini_handler *handler*, void ∗ *user*)

11.26.2.6 int ini_parse_file (FILE ∗ *file*, ini_handler *handler*, void ∗ *user*)

11.26.2.7 int ini_parse (const char ∗ *filename*, ini_handler *handler*, void ∗ *user*)

11.26.2.8 static char∗ ini_reader_string (char ∗ *str*, int *num*, void ∗ *stream*) [static]

11.26.2.9 int ini_parse_string (const char ∗ *string*, ini_handler *handler*, void ∗ *user*)

11.27 lib/io.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <io.h>
#include <argp.h>
#include <ini.h>
#include <traj.h>
#include <mapping.h>
```

Macros

- #define MATCH(s, n) strcmp(section, s) == 0 && strcmp(name, n) == 0

Functions

- void check_int_string (const char *str, int row, char *fname)
- void check_int_string_iniFile (const char *str, char *fname, char *name)
- int handler (void *config, const char *section, const char *name, const char *value)
- parameters pp_config (parameters config)
- void check_empty_file (FILE *f, char *filename)
- int n_rows (FILE *f)
- void check_empty_rows (char *str)
- void check_argv_errors (char *argv[], int argc)
- void check_float_string (char *str, int row, char *fname)
- void check_float_string_iniFile (const char *str, char *fname, char *name)
- int columns (char *string)
- void print_usage_main (char *argv[])
- void print_help_main (char *argv[])
- void print_help (char *argv[])
- void check_files (char **pars, char **pars_names, int n_pars, char *argv[])
- void check_parameters (int *pars, char **pars_names, int n_pars)
- void check_optional_parameters (parameters *cc)
- void mandatory_files_present (arguments *arguments, char *argv[])
- void init_parameters (parameters *cc)
- void read_ParameterFile (arguments *arguments, parameters *cc)
- FILE * open_file_w (char *filename)
- FILE * open_file_r (char *filename)
- FILE * open_file_a (char *filename)
- void close_file (FILE *fp)

Variables

- const char * argp_program_bug_address = "<raffaele.fiorentini@unitn.it>"

11.27.1 Macro Definition Documentation

11.27.1.1 #define MATCH(*s*, *n*) strcmp(section, s) == 0 && strcmp(name, n) == 0

11.27.2 Function Documentation

11.27.2.1 void check_int_string (const char ∗ *str*, int *row*, char ∗ *fname*)

routine that checks if the string token in account reading a generic FILE is an INTEGER number

Parameters

`str` : string token in account

`row` : number of row where the string is found.

`fname` : filename read

11.27.2.2 void check_int_string_iniFile (const char ∗ *str*, char ∗ *fname*, char ∗ *name*)

routine that checks if the string token in account is an INTEGER number. It works only for ini Files

Parameters

`str` : string token in account

`fname` : parameter filename

`name` : name of each parameter in the file

11.27.2.3 int handler (void ∗ *config*, const char ∗ *section*, const char ∗ *name*, const char ∗ *value*)

11.27.2.4 parameters pp_config (parameters *config*)

11.27.2.5 void check_empty_file (FILE ∗ *f*, char ∗ *filename*)

routine that checks if the file required exists. If it is the case, check if it is empty or not.

Parameters

`f` : FILE structure that represents the file opened.

`filename` : filename read

11.27.2.6 int n_rows (FILE ∗ *f*)

routine that returns the number of rows in a file. It counts correctly this number even if the last row does not present

Parameter

`f` : FILE structure that represents the file opened.

11.27.2.7 void check_empty_rows (char * *str*)

routine that checks if a generic line is empty or not

Parameter

`str` : string token in account

11.27.2.8 void check_argv_errors (char * *argv[ ],* int *argc*)

routine that checks the correctness of command line arguments

Parameter

`argv[]` : array of command line arguments

`argc` : number of command line arguments

11.27.2.9 void check_float_string (char * *str,* int *row,* char * *fname*)

routine that checks if the string token in account reading a generic FILE is an Float number

Parameters

`str` : string token in account

`row` : number of row where the string is found.

`fname` : filename read

11.27.2.10 void check_float_string_iniFile (const char * *str,* char * *fname,* char * *name*)

routine that checks if the string token in account is an Float number. It works only for ini Files

Parameters

`str` : string token in account

`fname` : parameter filename

`name` : name of each parameter in the file

11.27.2.11 int columns (char * *string*)

routine that returns the number of columns for each row inside the file chosen.

Parameter

`string` : string token in account

11.27.2.12 void print_usage_main (char * *argv[ ]*)

routine that prints the usage of the program

Parameter

`argv[]` : array of command line arguments

11.27.2.13 void print_help_main (char * *argv[]*)

routine that prints detailed information about the program

Parameter

`argv[]` : array of command line arguments

11.27.2.14 void print_help (char * *argv[]*)

routine that prints some help

Parameter

`argv[]` : array of command line arguments

11.27.2.15 void check_files (char ** *pars,* char ** *pars_names,* int *n_pars,* char * *argv[]*)

routine that checks if all command line arguments are correctly provided

Parameter

`pars` : parameters

`pars_names` : names of parameters

`n_pars` : number of parameters

`argv[]` : array of command line arguments

11.27.2.16 void check_parameters (int * *pars,* char ** *pars_names,* int *n_pars*)

routine that checks if all mandatory parameters are correctly provided

Parameter

`pars` : parameters

`pars_names` : names of parameters

`n_pars` : number of parameters

11.27.2.17 void check_optional_parameters (parameters * *cc*)

routine that checks optional parameters for the tasks that need them

Parameters

`cc` : parameters

11.27.2.18 void mandatory_files_present (arguments ∗ *arguments,* char ∗ *argv[]*)

routine that checks if the mandatory files are present

Parameters

`arguments` : command line arguments
`argv[]` : array of command line arguments

11.27.2.19 void init_parameters (parameters ∗ *cc*)

routine that initialises the parameters

Parameters

`cc` : parameters object

11.27.2.20 void read_ParameterFile (arguments ∗ *arguments,* parameters ∗ *cc*)

routine that reads the input parameter file

Parameter

`ParameterFileName` : parameter filename

11.27.2.21 FILE∗ open_file_w (char ∗ *filename*)

routine that opens a file in write mode

11.27.2.22 FILE∗ open_file_r (char ∗ *filename*)

routine that opens a file in read mode

11.27.2.23 FILE∗ open_file_a (char ∗ *filename*)

routine that opens a file in append mode

11.27.2.24 void close_file (FILE ∗ *fp*)

routine that closes a file

11.27.3 Variable Documentation

11.27.3.1 const char∗ argp_program_bug_address = "<raffaele.fiorentini@unitn.it>"

11.28 lib/mapping.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <mapping.h>
#include <io.h>
#include <my_malloc.h>
```

Functions

- void free_mapping (cg_mapping ∗mapping)
- void convert_mapping (cg_mapping ∗mapping, FILE ∗f_out)
- void generate_random_mapping (cg_mapping ∗mapping, FILE ∗f_out)
- void update_mapping (cg_mapping ∗curr_mapping, cg_mapping ∗old_mapping, int frames)
- void read_MappingFile (char ∗MappingFileName, FILE ∗f_out_l, cg_mapping ∗mapping)
- void read_mapping_matrix (char ∗mappings_filename, FILE ∗f_out_l, cg_mapping ∗mapping_matrix[], int nmaps)

11.28.1 Function Documentation

11.28.1.1 void free_mapping (**cg_mapping** ∗ *mapping*)

routine that frees the mapping

Parameters

`mapping` : cg_mapping object

11.28.1.2 void convert_mapping (**cg_mapping** ∗ *mapping,* FILE ∗ *f_out*)

routine that prints out the mapping

Parameters

`mapping` : cg_mapping object

`f_out` : file to write on

11.28.1.3 void generate_random_mapping (**cg_mapping** ∗ *mapping,* FILE ∗ *f_out*)

routine that generates a random mapping

Parameters

`mapping` : cg_mapping object

`f_out` : file to write on

11.28.1.4 void update_mapping (**cg_mapping** ∗ *curr_mapping,* **cg_mapping** ∗ *old_mapping,* int *frames*)

routine that updates old_mapping with the data contained in curr_mapping

Parameters

`curr_mapping` : current cg_mapping object

`old_mapping` : cg_mapping object to be updated

`frames` : length of the MD trajectory

11.28.1.5 void read_MappingFile (char ∗ *MappingFileName*, FILE ∗ *f_out_l*, cg_mapping ∗ *mapping*)

routine that reads the input mapping file

Parameters

`MappingFileName` : mapping filename

`f_out_l` : output filename

`cg_mapping` : cg_mapping object

11.28.1.6 void read_mapping_matrix (char ∗ *mappings_filename*, FILE ∗ *f_out_l*, cg_mapping ∗ *mapping_matrix[ ]*, int *nmaps*)

routine that reads the input mapping matrix

Parameters

filename : mapping filename

f_out_l : output filename

cg_mapping : cg_mapping object routine that reads the input mapping matrix

Parameters

`filename` : mapping filename

`f_out_l` : output filename

`cg_mapping` : cg_mapping object

`nmaps` : number of mappings defined in parameter file

11.29 lib/measure.c File Reference

```
#include <io.h>
#include <stdlib.h>
#include <my_malloc.h>
#include <traj.h>
#include <hierarchical_clustering.h>
#include <alignment.h>
#include <mapping.h>
#include <sampling.h>
#include <math.h>
#include <geometry.h>
#include <observables.h>
```

Functions

- void measure (arguments ∗arguments, parameters ∗cc)

11.29.1 Function Documentation

11.29.1.1 void measure (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to measure the mapping entropy of a mapping provided by the user

Parameters

`arguments`	: `arguments` object (command line arguments)
`parameters`	: `parameters` object

11.30 lib/measure_kl.c File Reference

```
#include <io.h>
#include <stdlib.h>
#include <my_malloc.h>
#include <traj.h>
#include <hierarchical_clustering.h>
#include <alignment.h>
#include <mapping.h>
#include <sampling.h>
#include <math.h>
#include <geometry.h>
#include <observables.h>
```

Functions

- void measure_kl (arguments ∗arguments, parameters ∗cc)

11.30.1 Function Documentation

11.30.1.1 void measure_kl (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to measure the KL divergence version of the mapping entropy for a mapping provided by the user

Parameters

`arguments`	: `arguments` object (command line arguments)
`parameters`	: `parameters` object

11.31 lib/my_malloc.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
```

Functions

- void failed (char message[])
- FILE ∗∗ F2t (int n1)
- FILE ∗∗∗ F3t (int n1, int n2)
- char ∗ c1t (int n1)
- char ∗∗ c2t (int n1, int n2)
- char ∗∗∗ c3t (int n1, int n2, int n3)
- char ∗∗∗∗ c4t (int n1, int n2, int n3, int n4)
- short ∗ s1t (int n1)
- short ∗∗ s2t (int n1, int n2)
- short ∗∗∗ s3t (int n1, int n2, int n3)
- short ∗∗∗∗ s4t (int n1, int n2, int n3, int n4)
- int ∗ i1t (int n1)
- int ∗∗ i2t (int n1, int n2)
- int ∗∗∗ i3t (int n1, int n2, int n3)
- int ∗∗∗∗ i4t (int n1, int n2, int n3, int n4)
- float ∗ f1t (int n1)
- float ∗∗ f2t (int n1, int n2)
- float ∗∗∗ f3t (int n1, int n2, int n3)
- float ∗∗∗∗ f4t (int n1, int n2, int n3, int n4)
- float ∗∗∗∗∗ f5t (int n1, int n2, int n3, int n4, int n5)
- double ∗ d1t (int n1)
- double ∗∗ d2t (int n1, int n2)
- double ∗∗∗ d3t (int n1, int n2, int n3)
- double ∗∗∗∗ d4t (int n1, int n2, int n3, int n4)
- void readeol (FILE ∗fp)
- void pdarray (int n, int m, double ∗∗a)
- void pdvector (int n, double ∗a)
- void pfarray (int n, int m, float ∗∗a)
- void pfvector (int n, float ∗a)
- void piarray (int n, int m, int ∗∗a)
- void pivector (int n, int ∗a)
- void zdarray (int n, int m, double ∗∗a)
- void zdvector (int n, double ∗a)
- void zfarray (int n, int m, float ∗∗a)
- void zfvector (int n, float ∗a)
- void ziarray (int n, int m, int ∗∗a)
- void zivector (int n, int ∗a)
- void free_c4t (char ∗∗∗∗p)
- void free_c3t (char ∗∗∗p)
- void free_c2t (char ∗∗p)
- void free_c1t (char ∗p)
- void free_s4t (short ∗∗∗∗p)
- void free_s3t (short ∗∗∗p)
- void free_s2t (short ∗∗p)
- void free_s1t (short ∗p)
- void free_i4t (int ∗∗∗∗p)
- void free_i3t (int ∗∗∗p)
- void free_i2t (int ∗∗p)
- void free_i1t (int ∗p)
- void free_f5t (float ∗∗∗∗∗p)
- void free_f4t (float ∗∗∗∗p)
- void free_f3t (float ∗∗∗p)
- void free_f2t (float ∗∗p)

- void free_f1t (float ∗p)
- void free_d4t (double ∗∗∗∗p)
- void free_d3t (double ∗∗∗p)
- void free_d2t (double ∗∗p)
- void free_d1t (double ∗p)

11.31.1 Function Documentation

11.31.1.1 void failed (char *message[ ]*)

11.31.1.2 FILE∗∗ F2t (int *n1*)

11.31.1.3 FILE∗∗∗ F3t (int *n1,* int *n2*)

11.31.1.4 char∗ c1t (int *n1*)

11.31.1.5 char∗∗ c2t (int *n1,* int *n2*)

11.31.1.6 char∗∗∗ c3t (int *n1,* int *n2,* int *n3*)

11.31.1.7 char∗∗∗∗ c4t (int *n1,* int *n2,* int *n3,* int *n4*)

11.31.1.8 short∗ s1t (int *n1*)

11.31.1.9 short∗∗ s2t (int *n1,* int *n2*)

11.31.1.10 short∗∗∗ s3t (int *n1,* int *n2,* int *n3*)

11.31.1.11 short∗∗∗∗ s4t (int *n1,* int *n2,* int *n3,* int *n4*)

11.31.1.12 int∗ i1t (int *n1*)

11.31.1.13 int∗∗ i2t (int *n1,* int *n2*)

11.31.1.14 int∗∗∗ i3t (int *n1,* int *n2,* int *n3*)

11.31.1.15 int∗∗∗∗ i4t (int *n1,* int *n2,* int *n3,* int *n4*)

11.31.1.16 float∗ f1t (int *n1*)

11.31.1.17 float∗∗ f2t (int *n1,* int *n2*)

11.31.1.18 float∗∗∗ f3t (int *n1,* int *n2,* int *n3*)

11.31.1.19 float∗∗∗∗ f4t (int *n1,* int *n2,* int *n3,* int *n4*)

11.31.1.20 float∗∗∗∗∗ f5t (int *n1,* int *n2,* int *n3,* int *n4,* int *n5*)

11.31.1.21 double∗ d1t (int *n1*)

11.31.1.22 double∗∗ d2t (int *n1,* int *n2*)

11.31.1.23 double∗∗∗ d3t (int *n1,* int *n2,* int *n3*)

11.31.1.24 double∗∗∗∗ d4t (int *n1,* int *n2,* int *n3,* int *n4*)

11.31.1.25 void readeol (FILE ∗ *fp*)

11.31.1.26 void pdarray (int *n*, int *m*, double ∗∗ *a*)

11.31.1.27 void pdvector (int *n*, double ∗ *a*)

11.31.1.28 void pfarray (int *n*, int *m*, float ∗∗ *a*)

11.31.1.29 void pfvector (int *n*, float ∗ *a*)

11.31.1.30 void piarray (int *n*, int *m*, int ∗∗ *a*)

11.31.1.31 void pivector (int *n*, int ∗ *a*)

11.31.1.32 void zdarray (int *n*, int *m*, double ∗∗ *a*)

11.31.1.33 void zdvector (int *n*, double ∗ *a*)

11.31.1.34 void zfarray (int *n*, int *m*, float ∗∗ *a*)

11.31.1.35 void zfvector (int *n*, float ∗ *a*)

11.31.1.36 void ziarray (int *n*, int *m*, int ∗∗ *a*)

11.31.1.37 void zivector (int *n*, int ∗ *a*)

11.31.1.38 void free_c4t (char ∗∗∗∗ *p*)

11.31.1.39 void free_c3t (char ∗∗∗ *p*)

11.31.1.40 void free_c2t (char ∗∗ *p*)

11.31.1.41 void free_c1t (char ∗ *p*)

11.31.1.42 void free_s4t (short ∗∗∗∗ *p*)

11.31.1.43 void free_s3t (short ∗∗∗ *p*)

11.31.1.44 void free_s2t (short ∗∗ *p*)

11.31.1.45 void free_s1t (short ∗ *p*)

11.31.1.46 void free_i4t (int ∗∗∗∗ *p*)

11.31.1.47 void free_i3t (int ∗∗∗ *p*)

11.31.1.48 void free_i2t (int ∗∗ *p*)

11.31.1.49 void free_i1t (int ∗ *p*)

11.31.1.50 void free_f5t (float ∗∗∗∗∗ *p*)

11.31.1.51 void free_f4t (float ∗∗∗∗ *p*)

11.31.1.52 void free_f3t (float ∗∗∗ *p*)

11.31.1.53 void free_f2t (float ∗∗ *p*)

11.31.1.54 void free_f1t (float ∗ *p*)

11.31.1.55 void free_d4t (double ∗∗∗∗ *p*)

11.31.1.56 void free_d3t (double ∗∗∗ *p*)

11.31.1.57 void free_d2t (double ∗∗ *p*)

11.31.1.58 void free_d1t (double ∗ *p*)

11.32 lib/norm.c File Reference

```
#include <io.h>
#include <stdlib.h>
#include <my_malloc.h>
#include <traj.h>
#include <mapping.h>
#include <math.h>
#include <geometry.h>
#include <observables.h>
```

Functions

- void norm (arguments ∗arguments, parameters ∗cc)

11.32.1 Function Documentation

11.32.1.1 void norm (arguments ∗ *arguments,* parameters ∗ *cc*)

subprogram to To calculate the norm of a mapping (provided by the user) throughout a trajectory

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.33 lib/observables.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <my_malloc.h>
#include <observables.h>
#include <io.h>
#include <time.h>
#include <geometry.h>
#include <alignment.h>
```

Functions

- void compute_coupling_matrix (double ∗coupling_mat, traj ∗Trajectory, int fr_id, float sigma)
- double compute_atomistic_coord_number (double ∗coupling_mat, traj ∗Trajectory, FILE ∗f_out_l)
- void compute_norm (cg_mapping ∗mapping, double ∗coupling_mat, double n_coord_at, int fr_id, FILE ∗f_-out_l)
- double compute_distance (cg_mapping ∗mapping, cg_mapping ∗mapping_prime, double ∗coupling_mat, double n_coord_at, int fr_id, FILE ∗f_out_l)
- void compute_mapping_norms (traj ∗Trajectory, cg_mapping ∗mapping, FILE ∗f_out_l)
- void compute_mapping_distances (traj ∗Trajectory, cg_mapping ∗mapping, cg_mapping ∗mapping_prime, FILE ∗f_out_l)
- void compute_mapping_distmat (traj ∗Trajectory, cg_mapping ∗mapping_matrix[ ], int nmaps, FILE ∗f_out_l, char ∗distmat_filename)
- void compute_variances (int nclust, double ∗variances, int ∗cluster_list, int ∗cluster_list_idx, double ∗energies)
- void compute_pR (int nclust, double ∗p_R, int ∗cluster_list, int ∗cluster_list_idx, double ∗energies)
- double get_smap (int frames, int curr_nclust, int ∗clusters, double ∗energies)
- double get_kl (int frames, int curr_nclust, int ∗clusters, double ∗energies)
- void overall_compute_smap (alignments ∗align, clust_params ∗clustering, traj ∗Trajectory, cg_mapping ∗mapping, int verbose, int kl_flag)

11.33.1 Function Documentation

11.33.1.1 void compute_coupling_matrix (double ∗ *coupling_mat,* traj ∗ *Trajectory,* int *fr_id,* float *sigma*)

routine that computes the coupling matrix over a frame

`coupling_mat` : coupling matrix

`Trajectory` : traj object

`fr_id` : frame ID

`sigma` : sigma parameter

11.33.1.2 double compute_atomistic_coord_number (double ∗ *coupling_mat,* traj ∗ *Trajectory,* FILE ∗ *f_out_l*)

routine that computes the atomistic coordination number for a certain coupling matrix. Double counting is necessary to ensure proper normalisation to norm and scalar product

`coupling_mat` : coupling matrix

`Trajectory` : traj object

`f_out_l` : output filename

11.33.1.3 void compute_norm (cg_mapping ∗ *mapping,* double ∗ *coupling_mat,* double *n_coord_at,* int *fr_id,* FILE ∗ *f_out_l*)

routine that computes the norm of a mapping over a frame of a trajectory

Parameters

`mapping` : cg_mapping object

`coupling_mat` : coupling matrix

`n_coord_at` : atomistic coordination number

`fr_id` : frame index

`f_out_l` : output filename

11.33.1.4 double compute_distance (**cg_mapping** ∗ *mapping,* **cg_mapping** ∗ *mapping_prime,* double ∗ *coupling_mat,* double *n_coord_at,* int *fr_id,* FILE ∗ *f_out_l*)

routine that computes the distance and cosine between a pair of cg mappings

Parameters

`mapping`, `mapping_prime` : cg_mapping objects

`coupling_mat` : coupling matrix

`n_coord_at` : atomistic coordination number

`fr_id` : frame index

`f_out_l` : output filename

11.33.1.5 void compute_mapping_norms (**traj** ∗ *Trajectory,* **cg_mapping** ∗ *mapping,* FILE ∗ *f_out_l*)

routine that computes the norm of a mapping over a MD trajectory

Parameters

`Trajectory` : traj object

`mapping` : cg_mapping object

`f_out_l` : output filename

11.33.1.6 void compute_mapping_distances (**traj** ∗ *Trajectory,* **cg_mapping** ∗ *mapping,* **cg_mapping** ∗ *mapping_prime,* FILE ∗ *f_out_l*)

routine that computes the distances and cosines between two mappings provided by the user over a MD trajectory

Parameters

`Trajectory` : traj object

`mapping`, `mapping_prime` : cg_mapping objects

`f_out_l` : output filename

11.33.1.7 void compute_mapping_distmat (**traj** ∗ *Trajectory,* **cg_mapping** ∗ *mapping_matrix[ ],* int *nmaps,* FILE ∗ *f_out_l,* char ∗ *distmat_filename*)

routine that computes the distance matrix between a set of mappings over a single structure

Parameters

`Trajectory` : traj object

`mappings_filename` : filename with the chosen mappings

`namps` : number of mappings

`f_out_l` : output filename

11.33.1.8 void compute_variances (int *nclust,* double ∗ *variances,* int ∗ *cluster_list,* int ∗ *cluster_list_idx,* double ∗ *energies*)

routine that computes the variance of the energies

Parameters

`nclust` : number of macrostates

`variances` : vector of variances

`cluster_list` : list of cluster IDs

`cluster_list_idx` : list of cluster indices

`energies` : array of energies

11.33.1.9 void compute_pR (int *nclust,* double ∗ *p_R,* int ∗ *cluster_list,* int ∗ *cluster_list_idx,* double ∗ *energies*)

routine that computes the variance of the energies

Parameters

`nclust` : number of macrostates

`variances` : vector of variances

`cluster_list` : list of cluster IDs

`cluster_list_idx` : list of cluster indices

`energies` : array of energies

11.33.1.10 double get_smap (int *frames,* int *curr_nclust,* int ∗ *clusters,* double ∗ *energies*)

routine that computes the observable given the current `nclust` and the current `clusters`

Parameters

`frames` : number of frames

`curr_nclust` : current index of CG macrostate

`clusters` : list of cluster IDs

`energies` : array of energies

11.33.1.11 double get_kl (int *frames,* int *curr_nclust,* int ∗ *clusters,* double ∗ *energies*)

routine that computes the observable given the current `nclust` and the current `clusters`

Parameters

`frames` : number of frames

`curr_nclust` : current index of CG macrostate

`clusters` : list of cluster IDs

`energies` : array of energies

11.33.1.12 void overall_compute_smap (alignments * *align*, clust_params * *clustering*, traj * *Trajectory*, cg_mapping * *mapping*, int *verbose*, int *kl_flag*)

routine that calls `get_smap` with the correct parameters

Parameters

`rmsd_mat` : condensed matrix of pairwise RMSDs

`clustering` : clust_params object

`Trajectory` : traj object

`mapping` : cg_mapping object

`verbose` : tunes the level of verbosity

`f_out` : output filename

11.34 lib/optimize.c File Reference

```
#include <io.h>
#include <stdlib.h>
#include <my_malloc.h>
#include <traj.h>
#include <hierarchical_clustering.h>
#include <alignment.h>
#include <mapping.h>
#include <sampling.h>
#include <math.h>
#include <omp.h>
```

Functions

- void optimize (arguments *arguments, parameters *cc)

11.34.1 Function Documentation

11.34.1.1 void optimize (arguments * *arguments*, parameters * *cc*)

subprogram to optimize the coarse-grained mapping by minimising its mapping entropy

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.35 lib/optimize_kl.c File Reference

```
#include <io.h>
#include <stdlib.h>
#include <my_malloc.h>
#include <traj.h>
#include <hierarchical_clustering.h>
#include <alignment.h>
#include <mapping.h>
#include <sampling.h>
#include <math.h>
#include <omp.h>
```

Functions

- void optimize_kl (arguments ∗arguments, parameters ∗cc)

11.35.1 Function Documentation

11.35.1.1 void optimize_kl (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to optimize the coarse-grained mapping by minimising the KL divergence version of its mapping entropy

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.36 lib/random_mapping.c File Reference

```
#include <io.h>
#include <stdlib.h>
#include <my_malloc.h>
#include <traj.h>
#include <hierarchical_clustering.h>
#include <alignment.h>
#include <mapping.h>
#include <sampling.h>
#include <math.h>
#include <geometry.h>
#include <observables.h>
```

Functions

- void random_mapping (arguments ∗arguments, parameters ∗cc)

11.36.1 Function Documentation

11.36.1.1 void random_mapping (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to randomly generate coarse-grained representations and measure the associated mapping entropies

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.37 lib/random_mapping_kl.c File Reference

```
#include <io.h>
#include <stdlib.h>
#include <my_malloc.h>
#include <traj.h>
#include <hierarchical_clustering.h>
#include <alignment.h>
#include <mapping.h>
#include <sampling.h>
#include <math.h>
#include <geometry.h>
#include <observables.h>
```

Functions

- void random_mapping_kl (arguments ∗arguments, parameters ∗cc)

11.37.1 Function Documentation

11.37.1.1 void random_mapping_kl (**arguments** ∗ ***arguments,*** **parameters** ∗ ***cc***)

subprogram to randomly generate coarse-grained representations and measure the KL divergence version of their mapping entropy

Parameters

`arguments` : `arguments` object (command line arguments)

`parameters` : `parameters` object

11.38 lib/sampling.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <my_malloc.h>
#include <math.h>
#include <sampling.h>
#include <alignment.h>
#include <mapping.h>
#include <observables.h>
```

Functions

- void my_make_a_move (cg_mapping ∗old_mapping, cg_mapping ∗new_mapping, int rem_add[2])
- void accept_move (int rem_add[2], cg_mapping ∗mapping, cg_mapping ∗new_mapping, alignments ∗align, alignments ∗new_align, traj ∗Trajectory, clust_params ∗clustering, double ∗∗new_coefficients_matrix)
- double tzero_estimation (traj ∗Trajectory, clust_params ∗clustering, int cgnum, int rsd, int verbose, int kl_flag, FILE ∗f_out_l)
- void simulated_annealing (traj ∗Trajectory, clust_params ∗clustering, MC_params ∗SA_params, int cgnum, int rsd, int verbose, int kl_flag, FILE ∗f_out_l)

11.38.1 Function Documentation

11.38.1.1 void my_make_a_move (**cg_mapping** ∗ *old_mapping,* **cg_mapping** ∗ *new_mapping,* int *rem_add[2]*)

function that swaps two atoms inside a CG mapping

Parameters

`old_mapping` : cg_mapping object

`new_mapping` : cg_mapping object

`rem_add` : vector of length 2 containing the removed and added atom index

11.38.1.2 void accept_move (int *rem_add[2],* **cg_mapping** ∗ *mapping,* **cg_mapping** ∗ *new_mapping,* **alignments** ∗ *align,* **alignments** ∗ *new_align,* **traj** ∗ *Trajectory,* **clust_params** ∗ *clustering,* double ∗∗ *new_coefficients_matrix*)

routine that accepts a Simulated Annealing move. It updates all the relevant observables.

Parameters

`rem_add` : vector of length 2 containing the removed and added atom index

`alignments` : align object

`mapping` : cg_mapping object

`verbose` : tunes the level of verbosity

11.38.1.3 double tzero_estimation (**traj** ∗ *Trajectory,* **clust_params** ∗ *clustering,* int *cgnum,* int *rsd,* int *verbose,* int *kl_flag,* FILE ∗ *f_out_l*)

routine that makes *nrun* unbiased moves. It is used to estimate the starting temperature for Simulated Annealing.

Parameters

`Trajectory` : traj object

`alignments` : align object

`mapping` : cg_mapping object

`verbose` : tunes the level of verbosity

11.38.1.4 void simulated_annealing (traj ∗ *Trajectory,* clust_params ∗ *clustering,* MC_params ∗ *SA_params,* int *cgnum,* int *rsd,* int *verbose,* int *kl_flag,* FILE ∗ *f_out_l*)

simulated annealing optimisation

Parameters

`Trajectory` : traj object

`alignments` : align object

`mapping` : cg_mapping object

`SA_params` : set of Monte Carlo parameters

`verbose` : tunes the level of verbosity

`f_out_l` : output filename

11.39 lib/traj.c File Reference

```
#include <traj.h>
#include <stdio.h>
#include <io.h>
#include <stdlib.h>
#include <ini.h>
```

Functions

- int check_probabilities (double ∗probabilities, int prob_length)
- void read_EnergyFile (char ∗EnergyFileName, traj ∗Trajectory)
- void read_TrajectoryFile (char ∗TrajFileName, traj ∗Trajectory)

11.39.1 Function Documentation

11.39.1.1 int check_probabilities (double ∗ *probabilities,* int *prob_length*)

routine that checks that input probabilities sum to 1

Parameters

`probabilities` : array of probabilities

`prob_length` : array length

11.39.1.2 void read_EnergyFile (char ∗ *EnergyFileName,* traj ∗ *Trajectory*)

routine that reads the input energy file

Parameters

`EnergyFileName` : energies filename

`Trajectory` : traj object

11.39.1.3 void read_TrajectoryFile (char ∗ *TrajFileName*, traj ∗ *Trajectory*)

routine that reads the input xyz coordinate file

Parameters

`TrajFileName` : trajectory filename

`Trajectory` : traj object

11.40 python/README.md File Reference

11.41 README.md File Reference

11.42 tests/README.md File Reference

11.43 python/sample_convert_xtc_to_xyz.py File Reference

Namespaces

- sample_convert_xtc_to_xyz

Variables

- tuple sample_convert_xtc_to_xyz.xtc_path = input("insert path to XTC file\n")
- tuple sample_convert_xtc_to_xyz.gro_path = input("insert path to GRO file\n")
- tuple sample_convert_xtc_to_xyz.xyz_filename = input("insert path to output XYZ file\n")
- tuple sample_convert_xtc_to_xyz.full_traj = mdtraj.load_xtc(xtc_path.strip(),top=gro_path.strip())
- sample_convert_xtc_to_xyz.full_traj_topology = full_traj.topology
- tuple sample_convert_xtc_to_xyz.no_h = full_traj_topology.select('type != H')
- tuple sample_convert_xtc_to_xyz.n_heavy_traj = len(no_h)
- tuple sample_convert_xtc_to_xyz.mdt_tr_heavy = mdtraj.load_xtc(xtc_path, top=gro_path, atom_indices = list(no_h))

11.44 python/setup_parfile.py File Reference

Namespaces

- setup_parfile

Functions

- def setup_parfile.retrieve_parameter
- def setup_parfile.get_mandatory_parameters
- def setup_parfile.get_optional_parameters
- def setup_parfile.write_parameters

Variables

- list setup_parfile.tasks = ["optimize", "random", "measure", "norm", "cosine", "distance", "optimize_kl", "measure_kl"]
- dictionary setup_parfile.mandatory_pars
- dictionary setup_parfile.optional_pars
- dictionary setup_parfile.pars_description
- dictionary setup_parfile.pars_type
- dictionary setup_parfile.clustering_pars
- tuple setup_parfile.task = input("Insert the task you would like to perform among the following: " + str(tasks) + "\n")
- dictionary setup_parfile.my_pars = {}
- tuple setup_parfile.opt = input("Insert optional parameters? (y/n)")

11.45 tests/test_suite.py File Reference

Classes

- class test_suite.test0
- class test_suite.test1
- class test_suite.test2
- class test_suite.test3
- class test_suite.test4
- class test_suite.test5
- class test_suite.test6
- class test_suite.test7
- class test_suite.test8
- class test_suite.test9
- class test_suite.test10
- class test_suite.test11
- class test_suite.test12
- class test_suite.test13
- class test_suite.test14
- class test_suite.test15
- class test_suite.test16
- class test_suite.test17
- class test_suite.test18
- class test_suite.test19
- class test_suite.test20
- class test_suite.test21
- class test_suite.test22
- class test_suite.test23
- class test_suite.test24
- class test_suite.test25
- class test_suite.test26

Namespaces

- test_suite

Variables

- tuple test_suite.t_start = dt.datetime.now()
- tuple test_suite.bash_script = subprocess.Popen("./test_suite.sh", shell=True, stdout=subprocess.PIPE)