
Python-Relion Documentation

Release 0.9.7

Diamond Light Source - Scientific Software

Feb 03, 2022

CONTENTS:

1	Usage	3
2	API	5
2.1	Project object	5
2.2	Stage-specific information	5
3	Credits	9
	Index	11

Documentation: <https://python-relion.readthedocs.io>.

This package provides a python interface to the information contained in a Relion project folder. It does not run Relion itself.

Currently it caters for specific fields from the Motion Correction, CTF Find, 2D Classification and 3D Classification stages of the Relion pipeline, but this could readily be expanded to more stages and fields.

USAGE

To access a Relion project folder you first need to create a `relion.Project` object (c.f. [API](#) for more information):

```
import relion
proj = relion.Project("/path/to/relion/project/directory")
proj = relion.Project(pathlib.Path("/project/directory")) # path objects are supported
```

The directory structure inside a Relion directory is built up of stages and jobs. Each stage folder will contain one or more job folders. The job folder(s) contain files related to the stage, including the `*.star` files from which values can be read:

```
project_root
├── MotionCorr
│   ├── job002
│   │   ├── corrected_micrographs.star
│   │   └── ...
│   └── CTFFind
│       ├── job003
│       │   ├── micrographs_ctf.star
│       │   └── ...
│       └── Class2D
│           ├── job008
│           │   ├── run_it025_data.star
│           │   ├── run_it025_model.star
│           │   └── ...
│           ├── job013
│           │   ├── run_it_025_data.star
│           │   ├── run_it_025_model.star
│           │   └── ...
│           └── Class3D
│               ├── job016
│               │   ├── run_it_025_data.star
│               │   ├── run_it_025_model.star
│               │   └── ...
```

The desired EM values are extracted from `*.star` files. For example, a snippet from `MotionCorr/job002/corrected_micrographs.star` is shown below:

```
...
loop_
_rlnCtfPowerSpectrum #1
```

(continues on next page)

(continued from previous page)

```

_rlnMicrographName #2
_rlnMicrographMetadata #3
_rlnOpticsGroup #4
_rlnAccumMotionTotal #5
_rlnAccumMotionEarly #6
_rlnAccumMotionLate #7
MotionCorr/job002/Movies/20170629_00021_frameImage_PS.mrc MotionCorr/job002/Movies/
↪ 20170629_00021_frameImage.mrc MotionCorr/job002/Movies/20170629_00021_frameImage.star ↪
↪      1      16.420495      2.506308      13.914187
MotionCorr/job002/Movies/20170629_00022_frameImage_PS.mrc MotionCorr/job002/Movies/
↪ 20170629_00022_frameImage.mrc MotionCorr/job002/Movies/20170629_00022_frameImage.star ↪
↪      1      19.551677      2.478968      17.072709
MotionCorr/job002/Movies/20170629_00023_frameImage_PS.mrc MotionCorr/job002/Movies/
↪ 20170629_00023_frameImage.mrc MotionCorr/job002/Movies/20170629_00023_frameImage.star ↪
↪      1      17.547827      1.941103      15.606724
MotionCorr/job002/Movies/20170629_00024_frameImage_PS.mrc MotionCorr/job002/Movies/
↪ 20170629_00024_frameImage.mrc MotionCorr/job002/Movies/20170629_00024_frameImage.star ↪
↪      1      18.100817      1.722567      16.378250
...

```

To access the `_rlnAccumMotionTotal` column in this file you can use:

```

>>> [micrograph.total_motion for micrograph in proj.motioncorrection["job002"]]
['16.420495', '19.551677', '17.547827', '18.100817', ...]

```

Stages are dictionary-like objects, so can discover the list of all known jobs by:

```

>>> list(proj.class2D)
['job008', 'job013']

```

and use the other standard dictionary accessors (`.values()`, `.keys()`, `.items()`), too. You can also convert the stages into normal dictionaries:

```

>>> dict(p.ctffind)
{'job003': [CTFMicrograph(...), ...]}

```

For a list of supported stages and a list of supported values per stage please have a look at the [API](#) page.

2.1 Project object

class relion.**Project**(*path, database='ISPyB', run_options=None, message_constructors=None*)

Reads information from a Relion project directory and makes it available in a structured, object-oriented, and pythonic fashion.

property **class2D**

access the 2D classification stage of the project. Returns a dictionary-like object with job names as keys, and lists of Class2DParticleClass namedtuples as values.

property **class3D**

access the 3D classification stage of the project. Returns a dictionary-like object with job names as keys, and lists of Class3DParticleClass namedtuples as values.

property **ctffind**

access the CTFFind stage of the project. Returns a dictionary-like object with job names as keys, and lists of CTFFMicrograph namedtuples as values.

property **motioncorrection**

access the motion correction stage of the project. Returns a dictionary-like object with job names as keys, and lists of MCMicrograph namedtuples as values.

The individual stage accessors `.ctffind`, `.class2D`, etc. return a dictionary-like object that allows you to access individual Relion jobs within that particular stage. The dictionary key names are the relion job names (usually `jobXXX`), the dictionary value is a list of stage-specific named tuples, listed below.

2.2 Stage-specific information

class relion._parser.ctffind.**CTFFMicrograph**(*micrograph_name, astigmatism, defocus_u, defocus_v, defocus_angle, max_resolution, fig_of_merit, amp_contrast, diagnostic_plot_path*)

Contrast Transfer Function stage.

property **amp_contrast**

Amplitude contrast.

property **astigmatism**

Estimated astigmatism. Units angstrom (A).

property **defocus_angle**

Estimated angle of astigmatism.

property defocus_u

Averaged with Defocus V to give estimated defocus. Units angstrom (A).

property defocus_v

Averaged with Defocus U to give estimated defocus. Units angstrom (A).

property diagnostic_plot_path

Path to the CTF diagnostic (fit/data comparison) plot (jpeg).

property fig_of_merit

Figure of merit/CC/correlation value. Confidence of the defocus estimation.

property max_resolution

Maximum resolution that the software can detect. Units angstrom (A).

property micrograph_name

Micrograph name. Useful for reference.

```
class relion._parser.motioncorrection.MCMicrograph(micrograph_name,  
                                                    micrograph_snapshot_full_path,  
                                                    micrograph_number, total_motion, early_motion,  
                                                    late_motion, micrograph_timestamp, drift_data)
```

Motion Correction stage.

property drift_data

Alias for field number 7

property early_motion

Early motion.

property late_motion

Late motion.

property micrograph_name

Micrograph name. Useful for reference.

property micrograph_number

Micrograph number: sequential in time.

property micrograph_snapshot_full_path

Path to jpeg of the motion corrected micrograph.

property micrograph_timestamp

Time stamp at which the micrograph was created.

property total_motion

Total motion. The amount the sample moved during exposure. Units angstrom (A).

```
class relion._parser.class2D.Class2DParticleClass(particle_sum, reference_image, class_distribution,  
                                                  accuracy_rotations, accuracy_translations_angst,  
                                                  estimated_resolution,  
                                                  overall_fourier_completeness, job)
```

2D Classification stage.

property accuracy_rotations

Accuracy rotations.

property accuracy_translations_angst

Accuracy translations angst.

property class_distribution

Class Distribution. Proportional to the number of particles per class.

property estimated_resolution

Estimated resolution.

property job

Job number of the Class2D job.

property overall_fourier_completeness

Overall Fourier completeness.

property particle_sum

Sum of all particles in the class. Gives a tuple with the class number first, then the particle sum.

property reference_image

Reference image.

```
class relion._parser.class3D.Class3DParticleClass(particle_sum, reference_image, class_distribution,  
                                                  accuracy_rotations, accuracy_translations_angst,  
                                                  estimated_resolution,  
                                                  overall_fourier_completeness,  
                                                  initial_model_num_particles, job)
```

3D Classification stage.

property accuracy_rotations

Accuracy rotations.

property accuracy_translations_angst

Accuracy translations angst.

property class_distribution

Class Distribution. Proportional to the number of particles per class.

property estimated_resolution

Estimated resolution.

property initial_model_num_particles

The number of particles used to generate the initial model.

property job

Job number of the Class3D job.

property overall_fourier_completeness

Overall Fourier completeness.

property particle_sum

Sum of all particles in the class. Gives a tuple with the class number first, then the particle sum.

property reference_image

Reference image.

**CHAPTER
THREE**

CREDITS

- Anna Horstmann
- Colin M. Palmer
- Daniel Hatton
- Donovan Webb
- Markus Gerstel
- Sjors H.W. Scheres
- Takanori Nakane

INDEX

A

accuracy_rotations (re-
lion._parser.class2D.Class2DParticleClass
property), 6

accuracy_rotations (re-
lion._parser.class3D.Class3DParticleClass
property), 7

accuracy_translations_angst (re-
lion._parser.class2D.Class2DParticleClass
property), 6

accuracy_translations_angst (re-
lion._parser.class3D.Class3DParticleClass
property), 7

amp_contrast (reliion._parser.ctffind.CTFMicrograph
property), 5

astigmatism (reliion._parser.ctffind.CTFMicrograph
property), 5

C

class2D (reliion.Project property), 5

Class2DParticleClass (class in re-
lion._parser.class2D), 6

class3D (reliion.Project property), 5

Class3DParticleClass (class in re-
lion._parser.class3D), 7

class_distribution (re-
lion._parser.class2D.Class2DParticleClass
property), 6

class_distribution (re-
lion._parser.class3D.Class3DParticleClass
property), 7

ctffind (reliion.Project property), 5

CTFMicrograph (class in reliion._parser.ctffind), 5

D

defocus_angle (reliion._parser.ctffind.CTFMicrograph
property), 5

defocus_u (reliion._parser.ctffind.CTFMicrograph prop-
erty), 5

defocus_v (reliion._parser.ctffind.CTFMicrograph prop-
erty), 6

diagnostic_plot_path (re-
lion._parser.ctffind.CTFMicrograph property),
6

drift_data (reliion._parser.motioncorrection.MCMicrograph
property), 6

E

early_motion (reliion._parser.motioncorrection.MCMicrograph
property), 6

estimated_resolution (re-
lion._parser.class2D.Class2DParticleClass
property), 6

estimated_resolution (re-
lion._parser.class3D.Class3DParticleClass
property), 7

F

fig_of_merit (reliion._parser.ctffind.CTFMicrograph
property), 6

I

initial_model_num_particles (re-
lion._parser.class3D.Class3DParticleClass
property), 7

J

job (reliion._parser.class2D.Class2DParticleClass prop-
erty), 7

job (reliion._parser.class3D.Class3DParticleClass prop-
erty), 7

L

late_motion (reliion._parser.motioncorrection.MCMicrograph
property), 6

M

max_resolution (reliion._parser.ctffind.CTFMicrograph
property), 6

MCMicrograph (class in re-
lion._parser.motioncorrection), 6

micrograph_name (re-
 lion._parser.ctffind.CTFMicrograph property),
 6

micrograph_name (re-
 lion._parser.motioncorrection.MCMicrograph
 property), 6

micrograph_number (re-
 lion._parser.motioncorrection.MCMicrograph
 property), 6

micrograph_snapshot_full_path (re-
 lion._parser.motioncorrection.MCMicrograph
 property), 6

micrograph_timestamp (re-
 lion._parser.motioncorrection.MCMicrograph
 property), 6

motioncorrection (relion.Project property), 5

O

overall_fourier_completeness (re-
 lion._parser.class2D.Class2DParticleClass
 property), 7

overall_fourier_completeness (re-
 lion._parser.class3D.Class3DParticleClass
 property), 7

P

particle_sum (relion._parser.class2D.Class2DParticleClass
 property), 7

particle_sum (relion._parser.class3D.Class3DParticleClass
 property), 7

Project (class in relion), 5

R

reference_image (re-
 lion._parser.class2D.Class2DParticleClass
 property), 7

reference_image (re-
 lion._parser.class3D.Class3DParticleClass
 property), 7

T

total_motion (relion._parser.motioncorrection.MCMicrograph
 property), 6