# Python-Relion Documentation

*Release 0.9.9*

**Diamond Light Source - Scientific Software**

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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.

CHAPTER

ONE

# 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
```

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```
_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.

CHAPTER

TWO

# API

## 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 CTFMicrograph 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.**CTFMicrograph**(*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

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- Colin M. Palmer
- Daniel Hatton
- Donovan Webb
- Markus Gerstel
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- Takanori Nakane

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