afmformats Documentation

Release 0.18.0

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CONTENTS

Afmformats is a Python library for reading atomic force microscopy (AFM) data file formats. This is the documentation of afmformats version 0.18.0.

CHAPTER

ONE

GETTING STARTED

1.1 Installation

To install afmformats, use one of the following methods (the package dependencies will be installed automatically):

- **from PyPI**: `pip install afmformats`
- **from sources**: `pip install -e .`

1.2 Basic Usage

```
In [1]: import afmformats

In [2]: dslist = afmformats.load_data("data/force-save-example.jpk-force")

# dslist is a list of force-distance curves
In [3]: dslist
Out[3]: [<AFMForceDistance 'data/force-save-example.jpk-force'[0] at 0x7ff482798ac0>]

# available data columns of the first curve
In [4]: dslist[0].columns
Out[4]: ['force', 'height (measured)', 'height (piezo)', 'segment', 'time']

In [5]: dslist[0]["force"]
Out[5]:
array([-6.56678981e-10, -6.64172230e-10, -6.79510911e-10, ...,
       -7.61449435e-10, -7.68909858e-10, -7.58163174e-10])
```

1.3 Supported file formats

All supported file formats are listed in the table below. If you are interested in other file formats, please create a new issue.

Format introduced by	Description	Extension	Loader
AFM workshop	comma-separated values	.csv	*formats.fmt_workshop.ws_single.load_csv*
afmformats	HDF5-based	.h5	*formats.fmt_hdf5.load_hdf5*
Asylum Research	binary-wave	.ibw	*formats.fmt_igor.load_igor*
JPK Instruments	binary FD data	.jpk-force	*formats.fmt_jpk.load_jpk*
JPK Instruments	binary QMap data	.jpk-force-map	*formats.fmt_jpk.load_jpk*
JPK Instruments	binary QMap data	.jpk-qi-data	*formats.fmt_jpk.load_jpk*
JPK Instruments	binary QMap data	.jpk-qi-series	*formats.fmt_jpk.load_jpk*
afmformats	tab-separated values	.tab	*formats.fmt_tab.load_tab*
NT-MDT Spectrum Instruments	exported by NT-MDT Nova	.txt	*formats.fmt_ntmdt_txt.load_txt*
AFM workshop	QMAP as zipped comma-separated values	.zip	*formats.fmt_workshop.ws_map.load_map*

1.4 Notes

Afmformats is a base module for loading experimental data. You might want to use nanite or PyJibe for higher-level functionalities.

CHAPTER

TWO

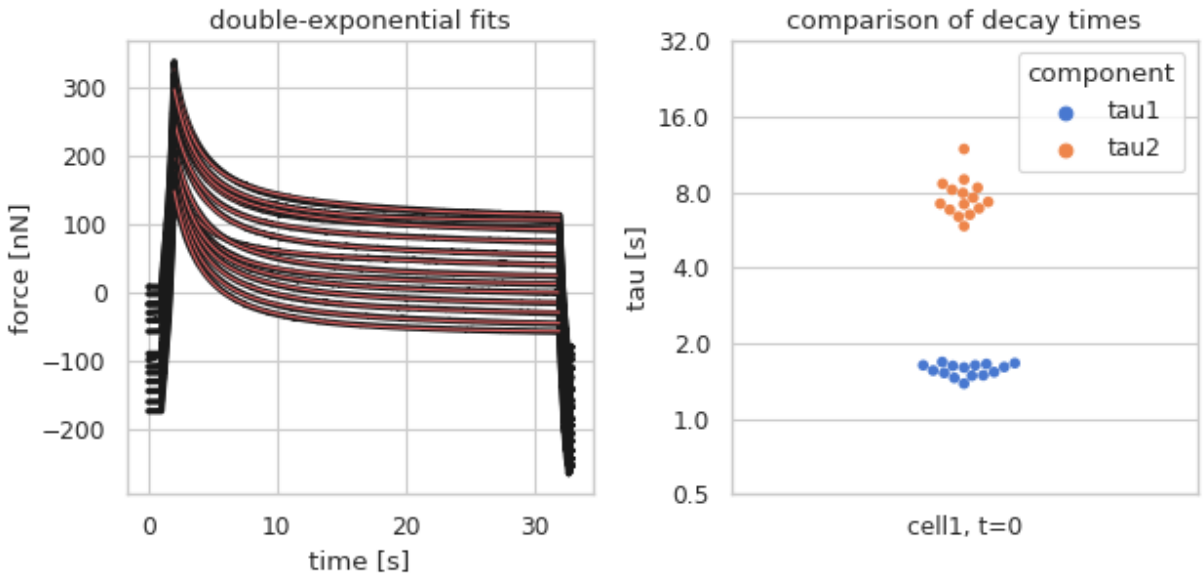
EXAMPLES

These are examples for the bare afmformats package. You might find other examples interesting to you in the nanite documentation.

2.1 Double-exponential fit to stress-relaxation data

This example reproduces the first entry in figure 5d (cell1) of [BAZ+22].

Please note that in the original manuscript, not all curves were used in the final figure. Some curves were excluded based on curve quality. The data were kindly provided by Alice Battistella.



stress_relaxation.py

```
import pathlib
import shutil
import tempfile

import afmformats

from lmfit.models import ConstantModel, ExponentialModel
```

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```
import matplotlib.pylab as plt
from matplotlib.ticker import ScalarFormatter
import numpy as np
import pandas
import seaborn as sns
sns.set_theme(style="whitegrid", palette="muted")


# extract the data to a temporary directory
data_path = pathlib.Path(__file__).parent / "data"
wd_path = pathlib.Path(tempfile.mkdtemp())
shutil.unpack_archive(data_path / "10.1002_btm2.10294_fig5d-cell1.zip",
                      wd_path)

# scale conversion constants
xsc = 1
ysc = 1e9
xl = "time [s]"
yl = "force [nN]"

# data extraction
data = []
for path in wd_path.glob("*.jpk-force"):
    data += afmformats.load_data(path)

# this is where the data for the swarm plot is stored
rdat = {
    "tau": [],
    "component": [],
    "cell": [],
}

data_fits = []

for di in data:
    # use intermediate `intr` segment data
    x = di.intr["time"] * xsc
    y = di.intr["force"] * ysc

    # fitting with double-exponential
    const = ConstantModel()
    exp_1 = ExponentialModel(prefix='exp1_')
    exp_2 = ExponentialModel(prefix='exp2_')

    pars = exp_1.guess(y, x=x)
    pars.update(exp_2.guess(y, x=x))
    pars["exp1_decay"].set(value=1, min=0.1)
    pars["exp2_decay"].set(value=8, min=2)
    pars.update(const.guess(y, x=x))
    pars["c"].set(value=np.min(y))

    mod = const + exp_1 + exp_2
```

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```
    init = mod.eval(pars, x=x)
    out = mod.fit(y, pars, x=x)
    data_fits.append([x, out.best_fit])

    rdat["tau"].append(out.params["exp1_decay"].value)
    rdat["component"].append("tau1")
    rdat["cell"].append("cell1, t=0")

    rdat["tau"].append(out.params["exp2_decay"].value)
    rdat["component"].append("tau2")
    rdat["cell"].append("cell1, t=0")


fig = plt.figure(figsize=(8, 4))

# plot all stress-relaxation curves
ax1 = plt.subplot(121, title="double-exponential fits")
for ii in range(len(data)):
    di = data[ii]
    ax1.plot(di["time"]*xsc, di["force"]*ysc, color="k", lw=3)
    xf, yf = data_fits[ii]
    ax1.plot(xf, yf, color="r", lw=1)
ax1.set_xlabel(xl)
ax1.set_ylabel(yl)

df = pandas.DataFrame(data=rdat)
# Draw a categorical scatterplot to show each observation
ax2 = plt.subplot(122, title="comparison of decay times")
ax2 = sns.swarmplot(data=df, x="cell", y="tau", hue="component")
ax2.set_yscale('log', base=2)
ax2.yaxis.set_major_formatter(ScalarFormatter())
ax2.set_yticks([0.5, 1, 2, 4, 8, 16, 32])
ax2.set(xlabel="", ylabel="tau [s]")

plt.tight_layout()

plt.show()
```

CHAPTER

THREE

ADVANCED USAGE

3.1 Grouping AFM data

AFM data can be organized in an *afmformats.AFMGroup* which comes with a few user-convenient functionalities:

```
In [1]: import afmformats

In [2]: group = afmformats.AFMGroup("data/force-map2x2-example.jpk-force-map")

# group contains all curves in the data file
In [3]: print(group)
AFMGroup: 'data/force-map2x2-example.jpk-force-map'
- AFMForceDistance 'data/force-map2x2-example.jpk-force-map'[0]
- AFMForceDistance 'data/force-map2x2-example.jpk-force-map'[1]
- AFMForceDistance 'data/force-map2x2-example.jpk-force-map'[2]
- AFMForceDistance 'data/force-map2x2-example.jpk-force-map'[3]

# you may add other data files to groups
In [4]: group += afmformats.load_data("data/force-save-example.jpk-force")

In [5]: print(group)
AFMGroup: 'None'
- AFMForceDistance 'data/force-map2x2-example.jpk-force-map'[0]
- AFMForceDistance 'data/force-map2x2-example.jpk-force-map'[1]
- AFMForceDistance 'data/force-map2x2-example.jpk-force-map'[2]
- AFMForceDistance 'data/force-map2x2-example.jpk-force-map'[3]
- AFMForceDistance 'data/force-save-example.jpk-force'[0]

# You can also extract a subgroup that matches a certin path
In [6]: subgroup = group.subgroup_with_path("data/force-map2x2-example.jpk-force-map")

In [7]: print(subgroup)
AFMGroup: 'data/force-map2x2-example.jpk-force-map'
- AFMForceDistance 'data/force-map2x2-example.jpk-force-map'[0]
- AFMForceDistance 'data/force-map2x2-example.jpk-force-map'[1]
- AFMForceDistance 'data/force-map2x2-example.jpk-force-map'[2]
- AFMForceDistance 'data/force-map2x2-example.jpk-force-map'[3]
```

CHAPTER

FOUR

IMPLEMENTING NEW FILE FORMATS

If you are interested in adding support for a new file format, please create a new issue to start a discussion. Please also attach a zip file with example data that can later on be used during testing.

If you are familiar with GitHub, please create a pull request and make sure that

- the file format reader is located in `afmformats.formats.fmt_NAME` (it may be a directory or a file, depending on the complexity)
- the file format displays correctly in the docs and the docs compile without errors:

```
cd docs
pip install -r requirements.txt
sphinx-build . _build
# and open _build/index.html in a browser
```

- you updated the CHANGELOG
- your code is fully tested (create test functions in `tests/test_fmt_NAME.py`) and all other tests pass (There are a few general tests that all file format readers must pass):

```
pip install pytest
pytest tests
```

- the data files for examples are named according to `fmt-NAME-MOD_filename.suffix` where `MOD` can be e.g. `fd` for force-distance data.

If you cannot or will not work with GitHub, you may paste your code in the corresponding issue. If the file format is not too complicated, let's just hope that things don't get messy.

4.1 Basic file format reader structure

The best way to understand how file formats work in afmformats is to take a look at the file formats implemented already. For the sake of clarity, here is a `file format reader template`:

```
import pathlib

import numpy as np


__all__ = ["load_my_format"]
```

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```
def load_my_format(path, callback=None, meta_override=None):
    """Loads AFM data from my format

    This is the main function for loading your file format. Please
    add a description here.

    Parameters
    ----------
    path: str or pathlib.Path or io.TextIOBase
        path to a .tab file
    callback: callable
        function for progress tracking; must accept a float in
        [0, 1] as an argument.
    meta_override: dict
        if specified, contains key-value pairs of metadata that
        are used when loading the files
        (see :data:`afmformats.meta.META_FIELDS`)
    """
    if meta_override is None:
        meta_override = {}

    path = pathlib.Path(path)
    # Here you would start parsing your data and metadata from `path`
    # You should specify as many metadata keys as possible. See
    # afmformats.meta.DEF_ALL for a list of valid keys.
    metadata = {"path": path}
    # Valid column names are defined in afmformats.afm_data.known_columns.
    data = {"force": np.linspace(1e-9, 5e-9, 100),
            "height (measured)": np.linspace(2e-6, -1e-6, 100)}

    metadata.update(meta_override)
    dd = {"data": data,
          "metadata": metadata}

    if callback is not None:
        callback(1)

    # You may also return a list with more items in case the file format
    # contains more than one curve.
    return [dd]


recipe_myf = {
    "descr": "A short description",
    "loader": load_my_format,
    "suffix": ".myf",
    "modality": "force-distance",
    "maker": "designer of file format",
}
```

A few notes:

- The `recipe_myf` contains the recipe for loading the file format into afmformats. It must be registered in

`afmformats/formats/__init__.py`.

- You may call the `callback` function with a floating point value between 0 and 1 (progress tracking) in-between of your loading steps if you expect that your file format reader is slow (e.g. several curves have to be loaded). This will give users of e.g. PyJibe visual feedback on how long they will have to wait.
- The `meta_override` dictionary is useful if you file format does not contain essential metadata such as spring constant or sensitivity. In such cases, you can raise an *afmformats.errors.MissingMetaDataError* to signal PyJibe that it should ask the user for the missing metadata. For an example, please see the AFM workshop file format.

4.2 Optimizing data import

In most cases, it is not neccessary to actually load the data from disk in the *load_my_format* method, especially if you have to parse large binary blobs or text files. In such cases, you can make use of the lazy loaders implemented in afmformats. For metadata, you can use *afmformats.meta.LazyMetaValue* and for data columns, you can use *afmformats.lazy_loader.LazyData*. The JPK file reader makes heavy usage of those classes.

CHAPTER

FIVE

AFMFORMATS

5.1 Submodules

5.1.1 afmformats._version

Determine package version from git repository tag

Each time this file is imported it checks whether the package version can be determined using *git describe*. If this fails (because either this file is not located at the 1st level down the repository root or it is not under version control), the version is read from the script "_version_save.py" which is not versioned by git, but always included in the final distribution archive (e.g. via PyPI). If the git version does not match the saved version, then "_version_save.py" is updated.

Usage

1. Put this file in your main module directory:

   REPO_ROOT/package_name/_version.py

2. Add this line to REPO_ROOT/package_name/__init__.py

   from ._version import version as __version__ # noqa: F401

3. (Optional) Add this line to REPO_ROOT/.gitignore

   _version_save.py

Features

- supports Python 2 and 3
- supports frozen applications (e.g. PyInstaller)
- supports installing into a virtual environment that is located in a git repository
- saved version is located in a python file and therefore no other files (e.g. MANIFEST.in) need be edited
- fallback version is the creation date
- excluded from code coverage via "pragma: no cover"

Changelog

2019-11-06.2

- use os.path.split instead of counting os.path.sep (Windows)

2019-11-06

- remove deprecated imp dependency (replace with parser)
- check whether this file is versioned and its location is correct
- code cleanup and docs update

5.1.2 afmformats._version_save

5.1.3 afmformats.afm_data

Classes

- *AFMData*: General base class for AFM data

class afmformats.afm_data.**AFMData**(*data*, *metadata*, *diskcache=False*)

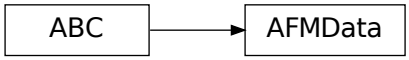
General base class for AFM data

Initialization

Parameters

- **data** (*dict-like*) – Experimental data
- **metadata** (*dict*) – Metadata
- **diskcache** (*bool*) – TODO

Inheritance



export_data(*out*, *metadata=True*, *fmt='tab'*)

Export all data columns to a file

Parameters

- **out** (*str, pathlib.Path, writable io.IOBase, or h5py.Group*) – Output path, open file, or h5py object
- **metadata** (*bool or list*) – If True, all available metadata are stored. If False, no metadata are stored. If a list, only the given metadata keys are stored.
- **fmt** (*str*) – "tab" for the tab separated values format and "hdf5" / "h5" for the HDF5 file format

Notes

- If you wish to append HDF5 data to an existing file, please open the file first and call this function with the h5py.File object, i.e.

```
with h5py.File(path, "a") as h5:
    fdist.export(out=h5, fmt="hdf5")
```

  Otherwise the file will be overridden.
- The column "index" is not exported in the HDF5 file format

reset_data()
Resets all data to the state they were after loading

Internally, only *self._data* is *clear`ed, which means that all calls to `__getitem__* fall-back to *self._raw_data*.

property columns
Available data columns

property columns_innate
Data columns available only in the original data file

property enum
Unique index of *self* in *self.path*

Indexing starts at "0"

property metadata
Unique index of *self* in *self.path*

abstract property modality
Imaging modality (e.g. force-distance)

property path
Path to the measurement file

Variables

- *column_dtypes*
- *column_units*
- *known_columns*

afmformats.afm_data.**column_dtypes**
Data types of all known columns (all other columns are assumed to be float)

```
{'force': <class 'float'>,
 'height (measured)': <class 'float'>,
 'height (piezo)': <class 'float'>,
 'index': <class 'int'>,
 'segment': <class 'numpy.uint8'>,
 'time': <class 'float'>,
 'tip position': <class 'float'>}
```

afmformats.afm_data.**column_units**
Units of all known columns

```
{'force': 'N',
 'height (measured)': 'm',
 'height (piezo)': 'm',
 'index': '',
 'segment': '',
 'time': 's',
 'tip position': 'm'}
```

afmformats.afm_data.**known_columns**
Known data columns

```
['force',
 'height (measured)',
 'height (piezo)',
 'index',
 'segment',
 'time',
 'tip position']
```

5.1.4 afmformats.afm_group

Classes

- *AFMGroup*: Container for *afmformats.afm_data.AFMData*

class afmformats.afm_group.**AFMGroup**(*path=None*, *meta_override=None*, *callback=None*, *modality=None*, *data_classes_by_modality=None*)
Container for *afmformats.afm_data.AFMData*

Parameters

- **path** (*str or pathlib.Path or None*) – If this option is specified, then an AFMGroup is generated directly from a datafile.
- **meta_override** (*dict*) – Dictionary with metadata that is used when loading the data in *path*.
- **callback** (*callable or None*) – A method that accepts a float between 0 and 1 to externally track the process of loading the data.

- **data_classes_by_modality** (*dict*) – Override the default AFMData class to use for managing the data (see `default_data_classes_by_modality`): This is e.g. used by index to pass *Indentation* (which is a subclass of the default *AFMForceDistance*) for handling "force-indentation" data.

Inheritance

append(*afmdata*)
Append an AFMData instance

Parameters **afmdata** (afmformats.afm_data.AFMData) – AFM data

get_enum(*enum*)
Return the AFMData curve with this enum value

Raises

- **ValueError if multiple curves with the same enum value exist.** –
- **KeyError if the enum value is not found** –

subgroup_with_path(*path*)
Return a subgroup with AFMData matching *path*

5.1.5 afmformats.afm_qmap

- *Functions*
- *Classes*
- *Variables*

Functions

- *qmap_feature()*: Decorator for labeling AFMQMap features

afmformats.afm_qmap.**qmap_feature**(*name*, *unit*, *cache=False*)
Decorator for labeling AFMQMap features

The name and unit are stored as properties of the wrapped function. In addition, the return value of the function can be cached (see *cache* argument).

Parameters

- **name** (*str*) – Name of the feature
- **unit** (*str*) – Unit of the returned feature

- **cache** (*bool or callable*) – If boolean, determines whether the feature data should be cached or not. If callable, the callable gets an instance of AFMData as an argument and should return an identifier (str) for the current value. If that identifier is the same as in the cache, then the cached value is used.

Classes

- *AFMQMap*: Management of quantitative AFM data on a grid

class afmformats.afm_qmap.**AFMQMap**(*path_or_group*, *meta_override=None*, *callback=None*, *modality=None*, *data_classes_by_modality=None*)

Management of quantitative AFM data on a grid

Parameters

- **path_or_group** (*str or pathlib.Path or* afmformats.afm_group.AFMGroup) – The path to the data file or an instance of *AFMGroup*
- **meta_override** (*dict*) – Dictionary with metadata that is used when loading the data in *path*.
- **callback** (*callable or None*) – A method that accepts a float between 0 and 1 to externally track the process of loading the data.
- **data_classes_by_modality** (*dict*) – Override the default AFMData class to use for managing the data (see `default_data_classes_by_modality`): This is e.g. used by index to pass *Indentation* (which is a subclass of the default *AFMForceDistance*) for handling "force-indentation" data.

Inheritance

static feat_core_data_height_base_point_um(*afmdata*)

Compute the lowest height (measured)

static feat_core_data_piezo_range_um(*afmdata*)

Compute peak-to-peak piezo range

static feat_core_data_scan_order(*afmdata*)

Return the enumeration of the dataset

get_coords(*which='px'*)

Get the qmap coordinates for each curve in *AFMQMap.group*

Parameters **which** (*str*) – "px" for pixels or "um" for microns.

get_qmap(*feature*, *qmap_only=False*)

Return the quantitative map for a feature

Parameters

- **feature** (*str*) – Feature to compute map for (see `QMap.features`)
- **qmap_only** – Only return the quantitative map data, not the coordinates

Returns

- **x, y** (*1d ndarray*) – Only returned if *qmap_only* is False; Pixel grid coordinates along x and y
- **qmap** (*2d ndarray*) – Quantitative map

property extent
extent (x1, x2, y1, y2) [µm]

features
Available features

group
AFM data (instance of *afmformats.afm_group.AFMGroup*)

property shape
shape of the map [px]

Variables

- *unit_scales*

afmformats.afm_qmap.**unit_scales**
Scale conversion helper

```
{'': 1, 'k': 1000.0, 'm': 0.001, 'n': 1e-09, 'p': 1e-12, 'µ': 1e-06}
```

5.1.6 afmformats.afm_segment

- *Classes*

Classes

- *AFMSegment*: Simple wrapper around dict-like *data* to expose a single segment

class afmformats.afm_segment.**AFMSegment**(*raw_data*, *data*, *segment*)
Simple wrapper around dict-like *data* to expose a single segment

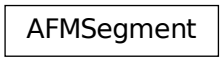
This class also caches the segment indices.

New Segment data

Parameters

- **raw_data** (*dict*) – dictionary containing valid column names as keys and 1d ndarrays as values; this is raw data (e.g. from the measurement file) that may be lazily-loaded
- **data** (*dict*) – same as raw_data, but in this case the data are already in memory; we distinguish between raw_data and data so that we know where the data came from (e.g. there might be "tip poisition" in both dictionaries, but we only always use (and override) the "tip position" in *data*. We never touch *raw_data*.

Inheritance



clear_cache()
Invalidates the segment indices corresponding to *self.data*

segment
The segment type (approach, intermediate, or retract)

property segment_indices
boolean array of segment indices

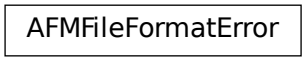
5.1.7 afmformats.errors

Classes

- *AFMFileFormatError*: Common base class for all exceptions
- *DataFileBrokenError*: Common base class for all exceptions
- *FileFormatMetaDataError*: Common base class for all exceptions
- *FileFormatNotSupportedError*: Common base class for all exceptions
- *InvalidFileFormatError*: Common base class for all exceptions
- *MissingMetaDataError*: Common base class for all exceptions

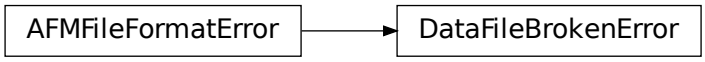
class afmformats.errors.**AFMFileFormatError**

Inheritance



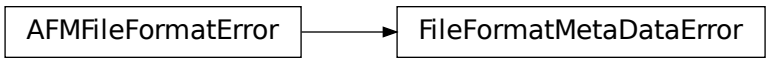
class afmformats.errors.**DataFileBrokenError**

Inheritance



class afmformats.errors.**FileFormatMetaDataError**

Inheritance

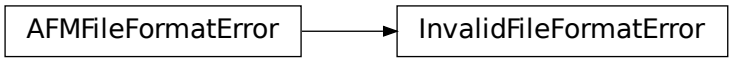


class afmformats.errors.**FileFormatNotSupportedError**

Inheritance

class afmformats.errors.**InvalidFileFormatError**

Inheritance



class afmformats.errors.**MissingMetaDataError**(*meta_keys*, **args*, ***kwargs*)
Special error class for missing metadata

The missing metadata keys are stored in the `meta_keys` property.

Inheritance

meta_keys
List of missing metadata keys

5.1.8 afmformats.formats

Submodules

afmformats.formats.fmt_hdf5

Functions

- *load_hdf5()*: Loads HDF5 files as exported by afmformats

afmformats.formats.fmt_hdf5.**load_hdf5**(*path_or_h5*, *callback=None*, *meta_override=None*)
Loads HDF5 files as exported by afmformats

The HDF5 format is self explanatory. The root attributes contain the version of afmformats used to create it. For each curve, one group is created, named according to "0", "1", … "9", "10", "11", etc. The attributes of each group are key-value pairs defined in *afmformats.meta.KEYS_VALID*. The group contains datasets named according to *afmformats.afm_data.known_columns* and have the attribute "unit" with the corresponding value in *afmformats.afm_data.column_units*.

Parameters

- **path_or_h5** (*str or pathlib.Path or h5py.Group*) – path to HDF5 file or an HDF5 group
- **callback** (*callable*) – function for progress tracking; must accept a float in [0, 1] as an argument.
- **meta_override** (*dict*) – if specified, contains key-value pairs of metadata that are used when loading the files (see *afmformats.meta.META_FIELDS*)

Notes

In case *path_or_h5* is a h5py.Group object, the "path" metadata variable will always be set to the path of the original HDF5 file. Keep this in mind if you think about storing multiple datasets (each containing multiple curves) in one HDF5 file (bad idea).

Classes

- *H5DictReader*: Undocumented.

class afmformats.formats.fmt_hdf5.**H5DictReader**(*path_or_h5*, *enum_key*)
Read-only HDF5-based dictionary for arrays

Parameters

- **path_or_h5** (*str or pathlib.Path or h5py.Group*) – Path to HDF5 file or an HDF5 group
- **enum_key** (*str*) – Name of the subgroup in *path_or_h5* that contains the data of the dictionary

Inheritance

afmformats.formats.fmt_igor

- *Functions*

Functions

- *load_igor()*: Load Asylum Research (Igor) binarywave .ibw files

afmformats.formats.fmt_igor.**load_igor**(*path*, *callback=None*, *meta_override=None*)
Load Asylum Research (Igor) binarywave .ibw files

The raw data are loaded with the Python module "igor" (http://blog.tremily.us/posts/igor/). The way column labels are assigend to the data is kind of hacky. The metadata assignment is largely guessed.

Test data were provided by Nicolas Hauck [HSC+18].

Parameters

- **path** (*str or pathlib.Path*) – path to in .ibw data file
- **callback** (*callable*) – function for progress tracking; must accept a float in [0, 1] as an argument.
- **meta_override** (*dict*) – if specified, contains key-value pairs of metadata that are used when loading the files (see *afmformats.meta.META_FIELDS*)

afmformats.formats.fmt_jpk

Submodules

afmformats.formats.fmt_jpk.jpk_data

Functions

- *find_column_dat()*: Find a column in a list of strings
- *load_dat_raw()*: Load data from binary JPK .dat files
- *load_dat_unit()*: Load data from a JPK .dat file with a specific calibration slot

afmformats.formats.fmt_jpk.jpk_data.**find_column_dat**(*loc_list*, *column*)
Find a column in a list of strings

Parameters

- **loc_list** (*list of str*) – The segment's data location list (within the archive), e.g.

  ['segments/0/channels/height.dat', 'segments/0/channels/vDeflection.dat', 'segments/0/channels/strainGaugeHeight.dat']

- **column** (*str*) – afmformats column name *afmformats.afm_data.known_columns*

Returns

- **name** (*str*) – Matched column name from *JPK_COLUMNS*, e.g. "strainGaugeHeight"
- **slot** (*str*) – Default slot location from *JPK_SLOTS*
- **loc** (*str*) – Matched data location in zip file, e.g. "segments/0/channels/strainGaugeHeight.dat"

afmformats.formats.fmt_jpk.jpk_data.**load_dat_raw**(*fd*, *name*, *properties*)

Load data from binary JPK .dat files

Parameters

- **fd** (*file*) – Open .dat file
- **name** (*str*) – Name of the data to read (required for scale conversions) (valid options are values in *JPK_COLUMNS*)
- **properties** (*dict*) – Property dictionary metadata (see also `JPKReader._get_index_segment_properties()`)

Returns **data** – A numpy array with the raw data.

Return type 1d ndarray

Notes

This method tries to correctly determine the data type of the binary data and scales it with the *data.encoder.scaling* values given in the header files.

See also:

load_dat_unit Includes conversion to useful units

afmformats.formats.fmt_jpk.jpk_data.**load_dat_unit**(*fd*, *name*, *properties*, *slot='default'*)

Load data from a JPK .dat file with a specific calibration slot

Parameters

- **fd** (*file*) – Open .dat file
- **name** (*str*) – Name of the data to read (required for scale conversions) (valid options are values in *JPK_COLUMNS*)
- **properties** (*dict*) – Property dictionary metadata (see also `JPKReader._get_index_segment_properties()`)
- **slot** (*str*) – The .dat files in the JPK measurement zip files come with different calibration slots. Valid values are
  - For the height of the piezo crystal during measurement (the piezo height is not as accurate as the measured height from the height sensor; the piezo movement is not linear): "height.dat": "volts", "nominal", "calibrated"
  - For the measured height of the cantilever: "strainGaugeHeight.dat": "volts", "nominal", "absolute" "measuredHeight.dat": "volts", "nominal", "absolute" "capacitiveSensorHeight": "volts", "nominal", "absolute" (they are all the same)
  - For the recorded cantilever deflection: "vDeflection.dat": "volts", "distance", "force"

Returns

- **data** (*1d ndarray*) – A numpy array containing the scaled data.
- **unit** (*str*) – A string representing the metric unit of the data.
- **name** (*str*) – The name of the data column.

Notes

The raw data (see *load_dat_raw*) is usually stored in "volts" and needs to be converted to e.g. "force" for "vDeflection" or "nominal" for "strainGaugeHeight". The conversion parameters (offset, multiplier) are stored in the header files and they are not stored separately for each slot, but the conversion parameters are stored relative to the slots. For instance, to compute the "force" slot from the raw "volts" data, one first needs to compute the "distance" slot. This conversion is taken care of by this method.

This is an example header:

channel.vDeflection.data.file.name=channels/vDeflection.dat channel.vDeflection.data.file.format=raw channel.vDeflection.data.type=short channel.vDeflection.data.encoder.type=signedshort channel.vDeflection.data.encoder.scaling.type=linear channel.vDeflection.data.encoder.scaling.style=offsetmultiplier channel.vDeflection.data.encoder.scaling.offset=-0.00728873489143207 channel.vDeflection.data.encoder.scaling.multiplier=3.0921021713588157E-4 channel.vDeflection.data.encoder.scaling.unit.type=metric-unit channel.vDeflection.data.encoder.scaling.unit.unit=V channel.vDeflection.channel.name=vDeflection channel.vDeflection.conversion-set.conversions.list=distance force channel.vDeflection.conversion-set.conversions.default=force channel.vDeflection.conversion-set.conversions.base=volts channel.vDeflection.conversion-set.conversion.volts.name=Volts channel.vDeflection.conversion-set.conversion.volts.defined=false channel.vDeflection.conversion-set.conversion.distance.name=Distance channel.vDeflection.conversion-set.conversion.distance.defined=true channel.vDeflection.conversion-set.conversion.distance.type=simple channel.vDeflection.conversion-set.conversion.distance.comment=Distance channel.vDeflection.conversion-set.conversion.distance.base-calibration-slot=volts channel.vDeflection.conversion-set.conversion.distance.calibration-slot=distance channel.vDeflection.conversion-set.conversion.distance.scaling.type=linear channel.vDeflection.conversion-set.conversion.distance.scaling.style=offsetmultiplier channel.vDeflection.conversion-set.conversion.distance.scaling.offset=0.0 channel.vDeflection.conversion-set.conversion.distance.scaling.multiplier=7.000143623002982E-8 channel.vDeflection.conversion-set.conversion.distance.scaling.unit.type=metric-unit channel.vDeflection.conversion-set.conversion.distance.scaling.unit.unit=m channel.vDeflection.conversion-set.conversion.force.name=Force channel.vDeflection.conversion-set.conversion.force.defined=true channel.vDeflection.conversion-set.conversion.force.type=simple channel.vDeflection.conversion-set.conversion.force.comment=Force channel.vDeflection.conversion-set.conversion.force.base-calibration-slot=distance channel.vDeflection.conversion-set.conversion.force.calibration-slot=force channel.vDeflection.conversion-set.conversion.force.scaling.type=linear channel.vDeflection.conversion-set.conversion.force.scaling.style=offsetmultiplier channel.vDeflection.conversion-set.conversion.force.scaling.offset=0.0 channel.vDeflection.conversion-set.conversion.force.scaling.multiplier=0.043493666407368466 channel.vDeflection.conversion-set.conversion.force.scaling.unit.type=metric-unit channel.vDeflection.conversion-set.conversion.force.scaling.unit.unit=N

To convert from the raw "volts" data to force data, these steps are performed:

- Convert from "volts" to "distance" first, because the "base-calibration-slot" for force is "distance".

  distance = volts*7.000143623002982E-8 + 0.0

- Convert from "distance" to "force":

force = distance*0.043493666407368466 + 0.0

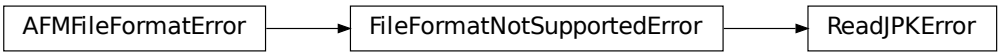
The multipliers shown above are the values for sensitivity and spring constant: sensitivity = 7.000143623002982E-8 m/V spring_constant = 0.043493666407368466 N/m

Classes

- *ReadJPKError*: Common base class for all exceptions

class afmformats.formats.fmt_jpk.jpk_data.**ReadJPKError**

Inheritance



Variables

- *JPK_COLUMNS*
- *JPK_SLOTS*
- *JPK_UNITS*

afmformats.formats.fmt_jpk.jpk_data.**JPK_COLUMNS**

Maps afmformats column names to JPK column names

```
{'force': ['vDeflection'],
 'height (measured)': ['strainGaugeHeight',
                       'capacitiveSensorHeight',
                       'measuredHeight'],
 'height (piezo)': ['height', 'head-height']}
```

afmformats.formats.fmt_jpk.jpk_data.**JPK_SLOTS**

Maps afmformats column names to default JPK normalization slots

```
{'force': 'force',
 'height (measured)': 'nominal',
 'height (piezo)': 'calibrated'}
```

afmformats.formats.fmt_jpk.jpk_data.**JPK_UNITS**

Maps afmformats column names to default JPK units

```
{'force': 'N', 'height (measured)': 'm', 'height (piezo)': 'm'}
```

afmformats.formats.fmt_jpk.jpk_meta

Variables

afmformats.formats.fmt_jpk.jpk_meta.**get_primary_meta_recipe**

```
<functools._lru_cache_wrapper object at 0x7ff491e5f0d0>
```

afmformats.formats.fmt_jpk.jpk_meta.**get_secondary_meta_recipe**

```
<functools._lru_cache_wrapper object at 0x7ff491e5f1f0>
```

afmformats.formats.fmt_jpk.jpk_reader

Classes

- *ArchiveCache*: Archive cache for fast access to zip data
- *JPKReader*: Undocumented.

class afmformats.formats.fmt_jpk.jpk_reader.**ArchiveCache**

Archive cache for fast access to zip data

If every *JPKReader* has its own instance of *ZipFile*, then on macOS (and possibly other OSes), we might run into an OSError; [Errno 24] Too many open files (https://github.com/AFM-analysis/afmformats/issues/10). The problem is, that if we don't leave the *ZipFile*, we have to re-open it every time we want to access some data. This is a huge overhead.

The solution is *ArchiveCache*, which keeps a reference to the last *max_archives=32* archives and closes the ones that were used least.

Inheritance

static get(*zip_path*)
Return the (possibly cached) *ZipFile* object for *zip_path*

class afmformats.formats.fmt_jpk.jpk_reader.**JPKReader**(*path*)

Inheritance

get_data(*column*, *index*, *segment=None*)
Return data for a given column, index, or segment

Parameters

- **column** (*str*) – Valid column from *afmformats.afm_data.known_columns*
- **index** (*int*) – Curve index in the current archive
- **segment** (*int or None*) – Segment index for chosen curve index

Returns **data** – Column data

Return type 1d ndarray

get_index_numbers()
Return int array with available index numbers

The numbers is what we refer to as "enum" in afmformats. Sometimes individual curves are missing from JPK files. These have to be correctly indexed.

get_index_path(*index*)
Return the path in the zip file for a specific curve index

get_index_segment_numbers(*index*)
Return available segment numbers for an index

get_index_segment_path(*index*, *segment*)
Return the path in the zip file for a specific index and segment

get_metadata(*index*, *segment=None*)
Return the metadata for a specific index and segment

Parameters

- **index** (*int*) – Curve index; For "single" hierarchy files, this should be 0.
- **segment** (*int or None*) – If None, then all segment-specific properties (e.g. approach and retract) are returned.

set_metadata(*metadata*)
Override internal metadata

This has a direct effect on `get_metadata()`.

property files
List of files and folders in the archive

property hierarchy
Format hierarchy ("single" or "indexed")

Functions

- *load_jpk()*: Loads JPK Instruments data files

afmformats.formats.fmt_jpk.**load_jpk**(*path*, *callback=None*, *meta_override=None*)
Loads JPK Instruments data files

These files are zip files containing java property files and integer-encoded binary data. The property files include recipes on how to convert the raw integer data to SI units.

Parameters

- **path** (*str or pathlib.Path*) – path to JPK data file
- **callback** (*callable*) – function for progress tracking; must accept a float in [0, 1] as an argument.
- **meta_override** (*dict*) – if specified, contains key-value pairs of metadata that are used when loading the files (see *afmformats.meta.META_FIELDS*)

afmformats.formats.fmt_ntmdt_txt

Functions

- *load_txt()*: Load text files exported by the NT-MDT Nova software

afmformats.formats.fmt_ntmdt_txt.**load_txt**(*path*, *callback=None*, *meta_override=None*)
Load text files exported by the NT-MDT Nova software

The columns are assumed to be: height (piezo) [nm], Deflection during approach (nA), Deflection during retraction (nA). The sensitivity in meta_override should be given in [m/A] (even though it is displayed as [m/V]).

This loader removes constant-value padding at the beginning of the data columns, an artifact that is sometimes introduced during data export. There are no metadata in this file format.

Test data were provided by Yuri Efremov [Efr20] [EBKS15].

Note that support for the original .mdt files is currently (2020) not possible. There exist binary readers for nt-mdt files (https://github.com/kaitai-io/kaitai_struct/), but this does not work for exemplary data. If the NT-MDT Nova software is not available, it should still be possible to load the data with Ggyddion and export it to something afmformats understands.

Parameters

- **path** (*str or pathlib.Path or io.TextIOBase*) – path to an ntmdt-exported .txt file
- **callback** (*callable*) – function for progress tracking; must accept a float in [0, 1] as an argument.
- **meta_override** (*dict*) – if specified, contains key-value pairs of metadata that are used when loading the files (see *afmformats.meta.META_FIELDS*)

afmformats.formats.fmt_tab

Functions

- *load_tab()*: Loads tab-separated-value files as exported by afmformats

afmformats.formats.fmt_tab.**load_tab**(*path*, *callback=None*, *meta_override=None*)
Loads tab-separated-value files as exported by afmformats

This is a simple tab-separated values files. The metadata may be present at the beginning of the file, commented out, as a json dump in a "BEGIN METADATA" - "END METADATA" block. The column data is listed below as a simple table.

Parameters

- **path** (*str or pathlib.Path or io.TextIOBase*) – path to a .tab file
- **callback** (*callable*) – function for progress tracking; must accept a float in [0, 1] as an argument.
- **meta_override** (*dict*) – if specified, contains key-value pairs of metadata that are used when loading the files (see *afmformats.meta.META_FIELDS*)

afmformats.formats.fmt_workshop

Submodules

afmformats.formats.fmt_workshop.ws_map

Functions

- *load_map()*: Load a set of zipped csv AFM workshop data

afmformats.formats.fmt_workshop.ws_map.**load_map**(*path*, *callback=None*, *meta_override=None*)

Load a set of zipped csv AFM workshop data

If you are recording quantitative force-maps (i.e. multiple curves on an x-y-grid) with AFM workshop setups, then you might have realized that you get *multiple* .csv files (one file per indentation) instead of *one* file that contains all the data (as you might be accustomed to from other manufacturers). Since afmformats expects one file per measurement, it would not be straight forward to obtain a properly enumerated quantitative imaging group.

This function offers a workaround - it loads a zip archive created from the the .csv files.

The files are structured like this:

```
Force-Distance Curve
File Format:    3

Date:    Wednesday, August 1, 2018
Time:    1:07:47 PM
Mode:    Mapping
Point:    16
X, um:    27.250000
Y, um:    27.250000

Extend Z-Sense(nm),Extend T-B(V),Retract Z-Sense(nm),Retract T-B(V)
13777.9288,0.6875,14167.9288,1.0917
13778.9288,0.6874,14166.9288,1.0722
13779.9288,0.6876,14165.9288,1.0693
13780.9288,0.6877,14164.9288,1.0824
13781.9288,0.6875,14163.9288,1.0989
...
```

Please make sure that the `Point` is enumerated from 1 onwards (and matches the alphanumerical order of the files in the archive) and that `Mode` is `Mapping`. The `X` and `Y` coordinates can be used by e.g. PyJibe to display QMap data on a grid.

Parameters

- **path** (*str or pathlib.Path*) – path to zip file containing AFM workshop .csv files
- **callback** (*callable*) – function for progress tracking; must accept a float in [0, 1] as an argument.
- **meta_override** (*dict*) – if specified, contains key-value pairs of metadata that are used when loading the files (see *afmformats.meta.META_FIELDS*)

afmformats.formats.fmt_workshop.ws_single

Functions

- *load_csv()*: Load csv data from AFM workshop

afmformats.formats.fmt_workshop.ws_single.**load_csv**(*path*, *callback=None*, *meta_override=None*, *mode='single'*)

Load csv data from AFM workshop

The files are structured like this:

```
Force-Distance Curve
File Format:    3

Date:    Wednesday, August 1, 2018
Time:    1:07:47 PM
Mode:    Single
Point:    1
X, um:    27.250000
Y, um:    27.250000

Extend Z-Sense(nm),Extend T-B(V),Retract Z-Sense(nm),Retract T-B(V)
13777.9288,0.6875,14167.9288,1.0917
13778.9288,0.6874,14166.9288,1.0722
13779.9288,0.6876,14165.9288,1.0693
13780.9288,0.6877,14164.9288,1.0824
13781.9288,0.6875,14163.9288,1.0989
...
```

The data for testing was kindly provided by Peter Eaton (afmhelp.com).

Parameters

- **path** (*str or pathlib.Path or io.TextIOBase*) – data file or an open file in text (not bytes) mode
- **callback** (*callable*) – function for progress tracking; must accept a float in [0, 1] as an argument.
- **meta_override** (*dict*) – if specified, contains key-value pairs of metadata that are used when loading the files (see *afmformats.meta.META_FIELDS*)
- **mode** (*str*) – curve mode to expect (either “single” or “mapping”); if an unexpected mode is found, AFMWorkshopFormatWarning is issued

Functions

- *find_data()*: Recursively find valid AFM data files
- *get_recipe()*: Return the file format recipe for a given path
- *load_data()*: Load AFM data

afmformats.formats.**find_data**(*path*, *modality=None*)
Recursively find valid AFM data files

Parameters

- **path** (*str or pathlib.Path*) – file or directory
- **modality** (*str*) – modality of the measurement ("force-distance")

Returns **file_list** – list of valid AFM data files

Return type list of pathlib.Path

afmformats.formats.**get_recipe**(*path*, *modality=None*)
Return the file format recipe for a given path

Parameters

- **path** (*str or pathlib.Path*) – file or directory
- **modality** (*str*) – modality of the measurement (see `IMAGING_MODALITIES`)

Returns **recipe** – file format recipe

Return type *AFMFormatRecipe*

afmformats.formats.**load_data**(*path*, *meta_override=None*, *modality=None*, *data_classes_by_modality=None*, *diskcache=False*, *callback=None*)
Load AFM data

Parameters

- **path** (*str or pathlib.Path*) – Path to AFM data file
- **meta_override** (*dict*) – Metadata dictionary that overrides experimental metadata
- **modality** (*str*) – Which acquisition modality to use (e.g. "force-distance")
- **data_classes_by_modality** (*dict*) – Override the default AFMData class to use for managing the data (see *default_data_classes_by_modality*): This is e.g. used by index to pass *Indentation* (which is a subclass of the default *AFMForceDistance*) for handling "force-indentation" data.
- **diskcache** (*bool*) – Whether to use caching (not implemented)
- **callback** (*callable*) – A method that accepts a float between 0 and 1 to externally track the process of loading the data

Returns **afm_list** – List where each element is on AFMData curve

Return type list of afmformats.afm_data.AFMData

Classes

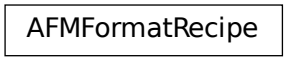
- *AFMFormatRecipe*: Undocumented.

class afmformats.formats.**AFMFormatRecipe**(*recipe*)

A wrapper class for file format recipes

Parameters **recipe** (*dict*) – file format recipe

Inheritance



detect(*path*)

Determine whether *path* can be opened with this recipe

Returns **valid** – True if *path* is openable, False otherwise.

Return type bool

Notes

If the underlying recipe does not implement a "detect" function, then only the file extension is checked.

get_modality(*path*)

Determine modality of a path

If a recipe provides several modalities, load the dataset and get the modality from the metadata.

property descr

description of file format

property loader

method for loading the data

property maker

who introduced the file format

property modalities

list of supported AFM imaging modalities

property suffix

file format suffix

Variables

- *default_data_classes_by_modality*
- *formats_available*
- *formats_by_suffix*
- *formats_by_modality*
- *supported_extensions*

afmformats.formats.**default_data_classes_by_modality**
dictionary with default data classes for each modality

```
{'creep-compliance': <class 'afmformats.mod_creep_compliance.AFMCreepCompliance'>,
 'force-distance': <class 'afmformats.mod_force_distance.AFMForceDistance'>,
 'stress-relaxation': <class 'afmformats.mod_stress_relaxation.AFMStressRelaxation'>
↪}
```

afmformats.formats.**formats_available**
available/supported file formats

```
[<AFMFormatRecipe from 'afmformats.formats.fmt_hdf5' at 0x7ff491e9fb50>,
 <AFMFormatRecipe from 'afmformats.formats.fmt_igor' at 0x7ff491e9fc70>,
 <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at 0x7ff491e6c580>,
 <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at 0x7ff491e6c6d0>,
 <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at 0x7ff491e6c730>,
 <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at 0x7ff491e6c790>,
 <AFMFormatRecipe from 'afmformats.formats.fmt_ntmdt_txt' at 0x7ff491e6c7f0>,
 <AFMFormatRecipe from 'afmformats.formats.fmt_tab' at 0x7ff491e6c850>,
 <AFMFormatRecipe from 'afmformats.formats.fmt_workshop.ws_map' at 0x7ff491e6c8b0>,
 <AFMFormatRecipe from 'afmformats.formats.fmt_workshop.ws_single' at␣
↪0x7ff491e6c910>]
```

afmformats.formats.**formats_by_suffix**
available file formats in a dictionary with suffix keys

```
{'.csv': [<AFMFormatRecipe from 'afmformats.formats.fmt_workshop.ws_single' at␣
↪0x7ff491e6c910>],
 '.h5': [<AFMFormatRecipe from 'afmformats.formats.fmt_hdf5' at 0x7ff491e9fb50>],
 '.ibw': [<AFMFormatRecipe from 'afmformats.formats.fmt_igor' at 0x7ff491e9fc70>],
 '.jpk-force': [<AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c580>],
 '.jpk-force-map': [<AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c6d0>],
 '.jpk-qi-data': [<AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c730>],
 '.jpk-qi-series': [<AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c790>],
 '.tab': [<AFMFormatRecipe from 'afmformats.formats.fmt_tab' at 0x7ff491e6c850>],
 '.txt': [<AFMFormatRecipe from 'afmformats.formats.fmt_ntmdt_txt' at␣
↪0x7ff491e6c7f0>],
 '.zip': [<AFMFormatRecipe from 'afmformats.formats.fmt_workshop.ws_map' at␣
↪0x7ff491e6c8b0>]}
```

afmformats.formats.**formats_by_modality**
available file formats in a dictionary for each modality

```
{'creep-compliance': [<AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c580>,
                      <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c6d0>,
                      <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c730>,
                      <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c790>],
 'force-distance': [<AFMFormatRecipe from 'afmformats.formats.fmt_hdf5' at␣
↪0x7ff491e9fb50>,
                    <AFMFormatRecipe from 'afmformats.formats.fmt_igor' at␣
↪0x7ff491e9fc70>,
                    <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c580>,
                    <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c6d0>,
                    <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c730>,
                    <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c790>,
                    <AFMFormatRecipe from 'afmformats.formats.fmt_ntmdt_txt' at␣
↪0x7ff491e6c7f0>,
                    <AFMFormatRecipe from 'afmformats.formats.fmt_tab' at␣
↪0x7ff491e6c850>,
                    <AFMFormatRecipe from 'afmformats.formats.fmt_workshop.ws_map'␣
↪at 0x7ff491e6c8b0>,
                    <AFMFormatRecipe from 'afmformats.formats.fmt_workshop.ws_single
↪' at 0x7ff491e6c910>],
 'stress-relaxation': [<AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c580>,
                       <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c6d0>,
                       <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c730>,
                       <AFMFormatRecipe from 'afmformats.formats.fmt_jpk' at␣
↪0x7ff491e6c790>]}
```

afmformats.formats.**supported_extensions**
list of supported extensions

```
['.csv',
 '.h5',
 '.ibw',
 '.jpk-force',
 '.jpk-force-map',
 '.jpk-qi-data',
 '.jpk-qi-series',
 '.tab',
 '.txt',
 '.zip']
```

5.1.9 afmformats.lazy_loader

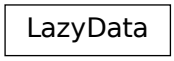
Classes

- *LazyData*: Lazily load data from function and kwargs

class afmformats.lazy_loader.**LazyData**
Lazily load data from function and kwargs

The idea is that the experimental data does not have to be loaded before the user requests it. Furthermore, this reduces the memory footprint (not all data are loaded).

Inheritance



set_lazy_loader(*column*, *func*, *kwargs*)
Add a lazy loader

Parameters

- **column** (*str*) – Column for which to register the loader
- **func** (*callable*) – Function to call to get the data
- **kwargs** – Keyword arguments to func

5.1.10 afmformats.meta

Functions

- *parse_time()*: Convert a time string to "HH:MM:SS.S"

afmformats.meta.**parse_time**(*value*)
Convert a time string to "HH:MM:SS.S"

- leading zeros are added where necessary
- trailing zeros after "." are stripped
- trailing "." is stripped

e.g.

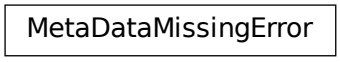
- "6:15:22 PM" -> "18:15:22"
- "6:15:22.00 AM" -> "06:15:22"
- "6:02:22.010 AM" -> "06:02:22.01"

Classes

- *MetaDataMissingError*: Raised when meta data is missing
- *LazyMetaValue*: A metadata value that is evaluated lazily in *MetaData*
- *MetaData*: Management of meta data variables

class afmformats.meta.**MetaDataMissingError**
Raised when meta data is missing

Inheritance



class afmformats.meta.**LazyMetaValue**(*func*, **args*, ***kwargs*)
A metadata value that is evaluated lazily in *MetaData*

Example usage:

```
meta = afmformats.meta.MetaData
meta["z range"] = afmformats.meta.LazyMetaValue(
     np.ptp,
     np.arange(10))
```

Parameters

- **func** (*callable*) – Function to call to get the metadata value
- **args** – arguments to func
- **kwargs** – Keyword arguments to func

Inheritance

class afmformats.meta.**MetaData**(**args*, ***kwargs*)

Management of meta data variables

Valid key names are defined in *afmformats.meta.KEYS_VALID*.

Inheritance

as_dict()

Convert to real dictionary

This is needed e.g. for *self.items* such that *json.dump* works in combination with *LazyMetaValue* (which is not JSON serializable)

copy()

Create a copy of the metadata

Returns **mdc** – Copy of the MetaData class (LazyMetaValue not copied)

Return type *MetaData*

get(*key*, *default=None*)

Return the value for key if key is in the dictionary, else default.

get_summary()

Convenience function returning the meta data summary

Returns a dict of dicts with keys matching the DEF_* dicts. Unset values are returned as *np.nan*.

items() → a set-like object providing a view on D's items

update([*E*], ***F*) → None. Update D from dict/iterable E and F.
If E is present and has a .keys() method, then does: for k in E: D[k] = E[k] If E is present and lacks a .keys() method, then does: for k, v in E: D[k] = v In either case, this is followed by: for k in F: D[k] = F[k]

values() → an object providing a view on D's values

Variables

- *IMAGING_MODALITIES*
- *META_FIELDS*
- *DEF_ALL*
- *KEYS_VALID*

afmformats.meta.**IMAGING_MODALITIES**
supported imaging modalities

```
['creep-compliance', 'force-distance', 'stress-relaxation']
```

afmformats.meta.**META_FIELDS**
Compendium of all allowed meta data keys, sorted by topic, and including units and validation methods

```
{'acquisition': {'feedback mode': ['Feedback mode',
                                   '',
                                   <function vd_str_in.<locals>.str_in at␣
↪0x7ff4927b3940>],
                 'imaging mode': ['Imaging modality',
                                  '',
                                  <function vd_str_in.<locals>.str_in at␣
↪0x7ff4927b3e50>],
                 'sensitivity': ['Sensitivity', 'm/V', <class 'float'>],
                 'spring constant': ['Cantilever spring constant',
                                     'N/m',
                                     <class 'float'>]},
 'dataset': {'duration': ['Duration', 's', <class 'float'>],
             'duration approach': ['Duration of approach segment',
                                   's',
                                   <class 'float'>],
             'duration retract': ['Duration of retract segment',
                                  's',
                                  <class 'float'>],
             'enum': ['Dataset index within the experiment',
                      '',
                      <function fint at 0x7ff4927b3ca0>],
             'point count': ['Size of the dataset in points',
                             '',
                             <function fint at 0x7ff4927b3ca0>],
             'rate approach': ['Sampling rate of approach segment',
                               'Hz',
                               <class 'float'>],
             'rate retract': ['Sampling rate of retract segment',
                              'Hz',
                              <class 'float'>],
             'segment count': ['Number of segments',
                               '',
                               <function fint at 0x7ff4927b3ca0>],
             'setpoint': ['Target indentation force', 'N', <class 'float'>],
             'speed approach': ['Piezo speed of approach segment',
                                'm/s',
```

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```
                              <class 'float'>],
            'speed retract': ['Piezo speed of retract segment',
                              'm/s',
                              <class 'float'>],
            'z range': ['Axial piezo range', 'm', <class 'float'>]},
 'dataset-mod creep-compliance': {'duration intermediate': ['Duration of '
                                                            'intermediate '
                                                            'segment',
                                                            's',
                                                            <class 'float'>]},
 'qmap': {'grid center x': ['Horizontal center of grid', 'm', <class 'float'>],
          'grid center y': ['Vertical center of grid', 'm', <class 'float'>],
          'grid index x': ['Horizontal grid position index',
                           '',
                           <function fint at 0x7ff4927b3ca0>],
          'grid index y': ['Vertical grid position index',
                           '',
                           <function fint at 0x7ff4927b3ca0>],
          'grid shape x': ['Horizontal grid shape',
                           'px',
                           <function fint at 0x7ff4927b3ca0>],
          'grid shape y': ['Vertical grid shape',
                           'px',
                           <function fint at 0x7ff4927b3ca0>],
          'grid size x': ['Horizontal grid image size', 'm', <class 'float'>],
          'grid size y': ['Vertical grid image size', 'm', <class 'float'>],
          'position x': ['Horizontal position', 'm', <class 'float'>],
          'position y': ['Vertical position', 'm', <class 'float'>]},
 'setup': {'instrument': ['Instrument', '', <class 'str'>],
           'software': ['Acquisition software', '', <class 'str'>],
           'software version': ['Acquisition software version',
                                '',
                                <class 'str'>]},
 'storage': {'curve id': ['Curve identifier', '', <class 'str'>],
             'date': ['Recording date', '', <class 'str'>],
             'format': ['File format', '', <class 'str'>],
             'path': ['Path', '', <class 'pathlib.Path'>],
             'session id': ['Dataset identifier', '', <class 'str'>],
             'time': ['Recording time', '', <class 'str'>]}}
```

afmformats.meta.**DEF_ALL**

A dictionary for all metadata definitions

```
{'curve id': ['Curve identifier', '', <class 'str'>],
 'date': ['Recording date', '', <class 'str'>],
 'duration': ['Duration', 's', <class 'float'>],
 'duration approach': ['Duration of approach segment', 's', <class 'float'>],
 'duration intermediate': ['Duration of intermediate segment',
                           's',
                           <class 'float'>],
 'duration retract': ['Duration of retract segment', 's', <class 'float'>],
 'enum': ['Dataset index within the experiment',
```

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```
         '',
         <function fint at 0x7ff4927b3ca0>],
'feedback mode': ['Feedback mode',
                  '',
                  <function vd_str_in.<locals>.str_in at 0x7ff4927b3940>],
'format': ['File format', '', <class 'str'>],
'grid center x': ['Horizontal center of grid', 'm', <class 'float'>],
'grid center y': ['Vertical center of grid', 'm', <class 'float'>],
'grid index x': ['Horizontal grid position index',
                 '',
                 <function fint at 0x7ff4927b3ca0>],
'grid index y': ['Vertical grid position index',
                 '',
                 <function fint at 0x7ff4927b3ca0>],
'grid shape x': ['Horizontal grid shape',
                 'px',
                 <function fint at 0x7ff4927b3ca0>],
'grid shape y': ['Vertical grid shape',
                 'px',
                 <function fint at 0x7ff4927b3ca0>],
'grid size x': ['Horizontal grid image size', 'm', <class 'float'>],
'grid size y': ['Vertical grid image size', 'm', <class 'float'>],
'imaging mode': ['Imaging modality',
                 '',
                 <function vd_str_in.<locals>.str_in at 0x7ff4927b3e50>],
'instrument': ['Instrument', '', <class 'str'>],
'path': ['Path', '', <class 'pathlib.Path'>],
'point count': ['Size of the dataset in points',
                '',
                <function fint at 0x7ff4927b3ca0>],
'position x': ['Horizontal position', 'm', <class 'float'>],
'position y': ['Vertical position', 'm', <class 'float'>],
'rate approach': ['Sampling rate of approach segment', 'Hz', <class 'float'>],
'rate retract': ['Sampling rate of retract segment', 'Hz', <class 'float'>],
'segment count': ['Number of segments', '', <function fint at 0x7ff4927b3ca0>],
'sensitivity': ['Sensitivity', 'm/V', <class 'float'>],
'session id': ['Dataset identifier', '', <class 'str'>],
'setpoint': ['Target indentation force', 'N', <class 'float'>],
'software': ['Acquisition software', '', <class 'str'>],
'software version': ['Acquisition software version', '', <class 'str'>],
'speed approach': ['Piezo speed of approach segment', 'm/s', <class 'float'>],
'speed retract': ['Piezo speed of retract segment', 'm/s', <class 'float'>],
'spring constant': ['Cantilever spring constant', 'N/m', <class 'float'>],
'time': ['Recording time', '', <class 'str'>],
'z range': ['Axial piezo range', 'm', <class 'float'>]}
```

afmformats.meta.**KEYS_VALID**

List of all valid meta data keys

```
['curve id',
 'date',
 'duration',
```

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```
'duration approach',
'duration intermediate',
'duration retract',
'enum',
'feedback mode',
'format',
'grid center x',
'grid center y',
'grid index x',
'grid index y',
'grid shape x',
'grid shape y',
'grid size x',
'grid size y',
'imaging mode',
'instrument',
'path',
'point count',
'position x',
'position y',
'rate approach',
'rate retract',
'segment count',
'sensitivity',
'session id',
'setpoint',
'software',
'software version',
'speed approach',
'speed retract',
'spring constant',
'time',
'z range']
```

5.1.11 afmformats.mod_creep_compliance

Classes

- *AFMCreepCompliance*: Base class for AFM creep-compliance data

class afmformats.mod_creep_compliance.**AFMCreepCompliance**(**args*, ***kwargs*)

Base class for AFM creep-compliance data

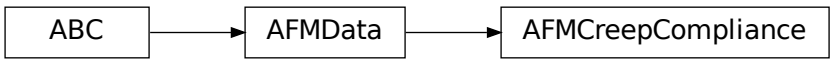
A creep-compliance dataset consists of an approach, an intermediate (with constant Force), and a retract curve.

Initialization

Parameters

- **data** (*dict-like*) – Experimental data
- **metadata** (*dict*) – Metadata
- **diskcache** (*bool*) – TODO

Inheritance



appr
Dictionary-like interface to the approach segment

intr
Dictionary-like interface to the intermediate segment

property modality
Imaging modality

retr
Dictionary-like interface to the retract segment

5.1.12 afmformats.mod_force_distance

Classes

- *AFMForceDistance*: Base class for AFM force-distance data

class afmformats.mod_force_distance.**AFMForceDistance**(**args*, ***kwargs*)
Base class for AFM force-distance data

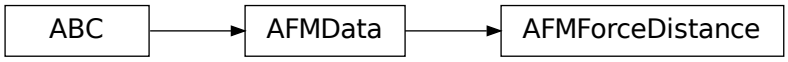
A force-distance dataset consists of an approach and a retract curve.

Initialization

Parameters

- **data** (*dict-like*) – Experimental data
- **metadata** (*dict*) – Metadata
- **diskcache** (*bool*) – TODO

Inheritance



appr
Dictionary-like interface to the approach segment

property modality
Imaging modality

retr
Dictionary-like interface to the retract segment

5.1.13 afmformats.mod_stress_relaxation

Classes

- *AFMStressRelaxation*: Base class for AFM stress-relaxation data

class afmformats.mod_stress_relaxation.**AFMStressRelaxation**(**args*, ***kwargs*)
Base class for AFM stress-relaxation data

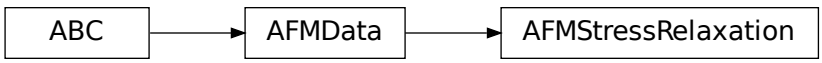
A stress-relaxation dataset consists of a pre-approach (with constant height), an approach (with a predefined indentation depth), an intermediate (with constant height), and a retract curve.

Initialization

Parameters

- **data** (*dict-like*) – Experimental data
- **metadata** (*dict*) – Metadata
- **diskcache** (*bool*) – TODO

Inheritance



appr
Dictionary-like interface to the approach segment

intr
Dictionary-like interface to the intermediate segment

property modality
Imaging modality

prep
Dictionary-like interface to the pre-measurement segment

retr
Dictionary-like interface to the retract segment

5.1.14 afmformats.parse_funcs

Functions

- *fbool()*: boolean
- *fint()*: integer
- *vd_str_in()*: Return a validator that tests whether a string is in a list

afmformats.parse_funcs.**fbool**(*value*)
boolean

afmformats.parse_funcs.**fint**(*value*)
integer

afmformats.parse_funcs.**vd_str_in**(*alist*)
Return a validator that tests whether a string is in a list

CHAPTER

SIX

CHANGELOG

List of changes in-between afmformats releases.

6.1 version 0.18.0

- ref: JPK calibration files are now not ignored anymore
- ref: allow to specify custom metadata for JPK files
- ref: replaced ReadJPKMetaKeyError with MissingMetaDataError
- ref: support *return_modality* in *detect* methods of recipes
- ref: cleanup of JPK reader class

6.2 version 0.17.1

- maintenance release

6.3 version 0.17.0

- feat: support loading stress-relaxation data from .jpk-force files (#9)
- docs: add example for stress-relaxation data analysis

6.4 version 0.16.7

- maintenance release

6.5 version 0.16.6

- setup: bump igor2 from 0.4.0 to 0.5.0

6.6 version 0.16.5

- setup: migrate from igor to igor2 (Python 3 support)
- tests: add test for files that contain force data but no spring constant

6.7 version 0.16.4

- enh: implement *AFMData.columns_innate* which is a list of columns present in the original data file
- enh: implement *AFMData.reset_data* to remove all user-defined column data (i.e. columns not in *AFMData.columns_innate* or columns that override those)

6.8 version 0.16.3

- fix: setting column data to *AFMSegment* did not work when column did only exist in raw data property

6.9 version 0.16.2

- enh: implement *__setitem__* for *AFMSegment*
- ref: make *data* and *raw_data* private properties of *AFMSegment*

6.10 version 0.16.1

- enh: support .jpk-qi-series files (by extension)
- enh: improve error handling when data exported from the JPK software does not contain encoder scaling offset and multiplier
- ref: use f-strings more often

6.11 version 0.16.0

- BREAKING CHANGE: "segment" column is no longer boolean, so it cannot be used directly for indexing (#15)
- fix: support modified AFM workshop file format (#17)
- fix: segment data via *AFMData.appr* and *AFMData.retr* did not use user-defined data to identify segments, but the "segment" column from the raw data (this does not affect PyJibe or nanite which fo not make excessive use of these properties)
- enh: add "segment count" key to meta data

- enh: optimize segment handling: new class AFMSegment that caches segment indices (#16)
- enh: properly test data types of metadata when setting them

6.12 version 0.15.0

- feat: generally support creep-compliance and stress-relaxation data via the new "modalities" (supercedes "modality") recipe key
- feat: support for JPK creep-compliance data
- enh: extract segment duration from JPK files
- fix: ignore NaN values in JPK property files
- ref: add separate meta data section for modality-related keys
- ref: improvements of JPK metadata reader
- tests: rename test data files to reflect format

6.13 version 0.14.4

- docs: add section for implementing new file formats (#13)
- fix: IndexError when trying to open .txt files that are no AFM files
- ref: separate submodule for formats

6.14 version 0.14.3

- enh: implement LazyMetaValue to speed-up loading JPK files
- enh: perform caching in LazyData (minor speed-up)

6.15 version 0.14.2

- fix: partially revert breaking change in 0.14.0 ("imaging mode" was previously used when exporting data in PyJibe and this metadata key should not change)
- fix: add detect function for HDF5 format (afmformats attempted to load nanite rating containers)
- enh: added height span for QMap data
- tests: add .tab and .h5 test files
- ref: renamed QMap feature "lowest height" to "height base point"
- ref: changed prefix to "data" for all QMap data

6.16 version 0.14.1

- fix: populate AFMQMap grid metadata for AFM workshop format (#12)
- enh: speed-up QMap computation by decorator-based caching
- ref: move QMap grid index computation to MetaData class

6.17 version 0.14.0

- BREAKING CHANGE: changed 'mode' to 'modality' throughout afmformats
- feat: introduced afmformats.AFMGroup, a container for AFMData (#11)
- feat: introduced afmformats.AFMQMap for managing quantitative AFMData (#11)
- feat: allow to use other derived classes of AFMData when loading experimental data via the *data_classes_by_modality* option
- ref: *AFMData.export* is deprecated in favor of *AFMData.export_data*
- ref: renamed submodule afm_fdist to mod_force_distance

6.18 version 0.13.3

- enh: improve speed when loading data by avoiding accessing data during initialization
- fix: JPK file format reader speed regression caused by #10 (implemented ArchiveCache)

6.19 version 0.13.2

- enh: make sure people don't think they can load a data file with a different spring constant or sensitivity

6.20 version 0.13.1

- fix: make sure callback functions are always used

6.21 version 0.13.0

- feat: support zipped AFM workshop map data (#5)
- feat: added *find_data* method
- enh: make MissingMetaDataError class special (missing metadata are stored as property)
- enh: add "detect" function for JPK file format
- docs: add missing objects to `__all__` (autoapi)
- ref: code cleanup

6.22 version 0.12.6

- ref: DeprecationWarning: np.float from numpy 1.20

6.23 version 0.12.5

- fix: JPK file format reader kept the zip files open indefinitely which resulted in OSError "Too many open files" (#10)
- ci: removed appveyor build

6.24 version 0.12.4

- fix: opening .h5 files failed with AttributeError
- ref: setup.py test is deprecated

6.25 version 0.12.3

- build: migrate to GitHub Actions

6.26 version 0.12.2

- fix: properly sort curves within JPK files

6.27 version 0.12.1

- maintenance release

6.28 version 0.12.0

- ref: rewrite JPK data file reader: new JPKReader class (#4)
- enh: add new LazyData class for loading data on demand (#4)

6.29 version 0.11.0

- feat: allow defining "detect" method to determine whether a recipe can open a file (#7)

6.30 version 0.10.2

- maintenance release

6.31 version 0.10.1

- fix: parsing issue when loading .ibw files without AM/PM in "Time" metadata (#8)
- enh: make sure "time" is always parsed as HH:MM:SS.S when adding it to *MetaData*
- enh: compute "curve id" and "session id" from "date", "time", and "enum" if not given in *MetaData*

6.32 version 0.10.0

- feat: allow to override metadata when loading data
- feat: support new file format from AFM workshop (.csv)
- feat: support new file format from JPK (.jpk-qi-data)
- feat: support new file format from NT-MDT (.txt exported by Nova)
- enh: implement *AFMFormatRecipe* class for handling and verifying recipe dictionaries
- enh: implement *register_format* function

6.33 version 0.9.0

- feat: support new file format from Asylum Research, Igor (.ibw)
- ref: always compute piezo range metadata instead of taking it from the set value in the acquisition settings (JKP format)

6.34 version 0.8.0

- enh: do not export "index" column to HDF5 files to save disk space
- enh: save column units when exporting to HDF5
- ref: moved class methods and constants from "afm_fdist" to "afm_data"
- docs: add code reference, basic usage, and list of file formats

6.35 version 0.7.1

- fix: exporting to HDF5 did not work when a h5py.Group was used
- fix: exporting to HDF5 did not reset the "enum" key
- enh: use gzip compression in HDF5 file format
- enh: allow "h5" and "hdf5" as HDF5 file format specifiers during export

6.36 version 0.7.0

- BREAKING CHANGE: piezo height is now loaded as "calibrated" and not as "nominal" (JPK file format)
- fix: metadata acquisition "duration" and "point count" only showed data of apporach part (JPK file format)
- enh: load metadata "speed" and "rate" separately for approach and retract part
- ref: restructured meta data organization

6.37 version 0.6.0

- feat: force-distance metadata can now be saved and loaded for the .tab file format (#3)
- feat: implement new HDF5-based file format (read/write)
- feat: support piezo height (JPK file format)
- enh: improve parsing of JPK files (#1)

6.38 version 0.5.2

- ref: drop pandas dependency (#2)

6.39 version 0.5.1

- fix: allow "force-modulation" feedback mode

6.40 version 0.5.0

- feat: meta data summary with *MetaData.get_summary*

6.41 version 0.4.1

- ref: group meta data by topic
- fix: identifier in JPK file format was actually session identifier

6.42 version 0.4.0

- BREAKING CHANGE: change metadata key names
- enh: add class for checking metadata

6.43 version 0.3.0

- feat: support tab-separated values file format (.tab)
- fix: file formats were not registered correctly
- ref: derive file format errors from own error classes

6.44 version 0.2.0

- compatibility changes towards nanite

6.45 version 0.1.0

- initial version

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