pyIMD Documentation

Release 0.0.8

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Contents:

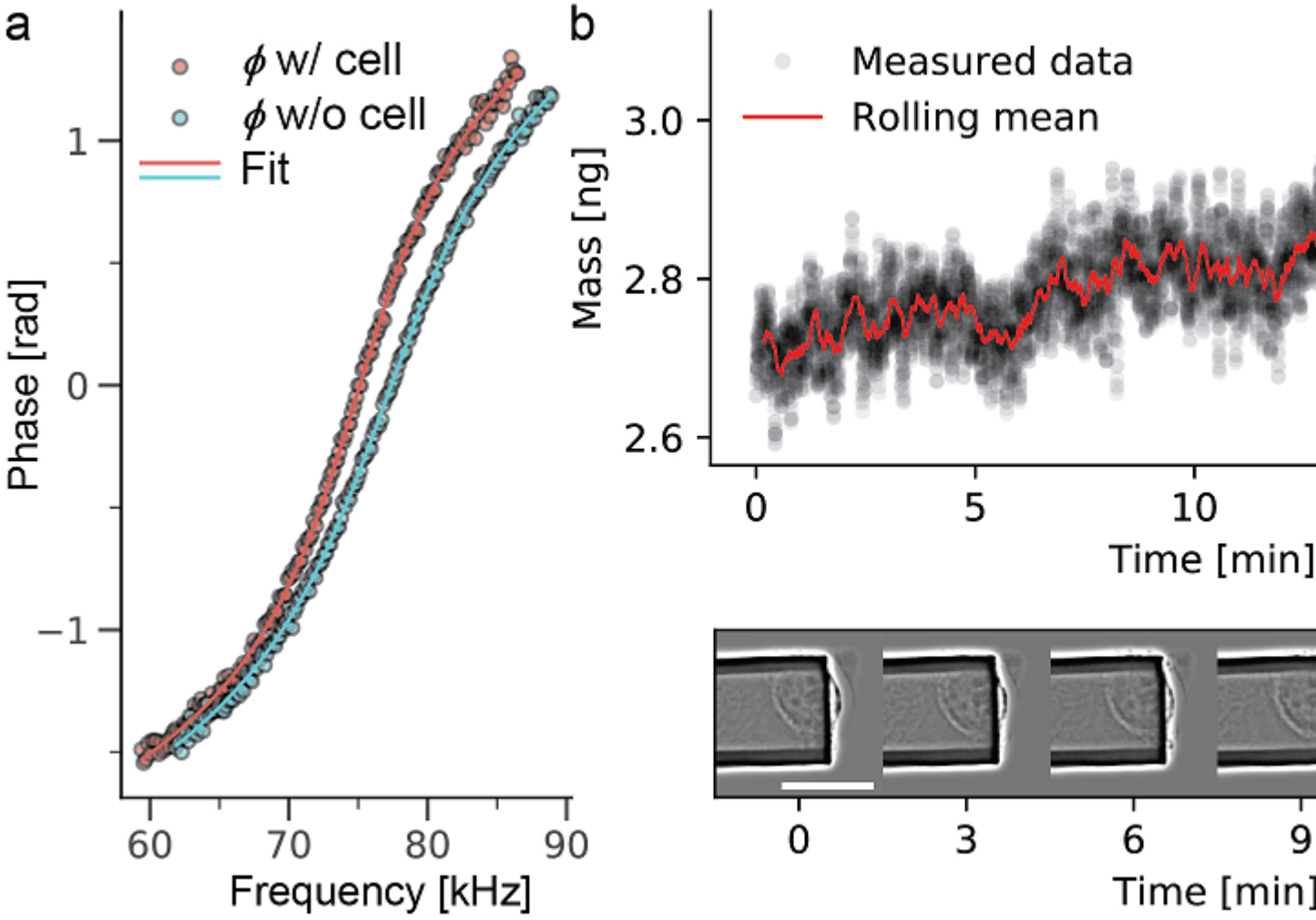

Fig. 1: Evolution of mass over time and the corresponding microscopy images are shown for a time span of 20min. The mass data was acquired every 10 ms (data shown in black), overlaid in red is the rolling mean with a window of 1000. Images taken every 3 min over the observed times span. The mammalian cell increases mass steadily..

The total mass of single cells can be accurately monitored in real time under physiological conditions with our recently developed picobalance. It is a powerful tool to investigate crucial processes in biophysics, cell biology or medicine, such as cell mass regulation. However, processing of the raw data can be challenging, as computation is needed to

extract the mass and long-term measurements can generate large amounts of data. Here, we introduce the software package **pyIMD** that automates raw data processing, particularly when investigating non-migrating cells. **pyIMD** stands for Python inertial mass determination and is implemented using Python 3.6 and can be used as a command line tool or as a stand-alone version including a graphical user interface.

This documentation of **pyIMD** describes the API and provides sample data sets as well as sample scripts to run **pyIMD** from Jupyter or the Python console. It also contains a tutorial about how **pyIMD** is used with the user interface.

CHAPTER 1

Installation

1.1 Stable release

1.1.1 As module

To install pyIMD, just run this command in your terminal:

```
$ pip install pyIMD
```

Installing pyIMD this way ensures that you get always the latest release.

If you don't have pip installed, this Python installation guide can guide you through the process.

1.1.2 As stand alone executable

If you want to install pyIMD on your system without installing Python yourself just download the pre-compiled executable matching your operating system:

pyIMD can then be used trough its graphical user interface (GUI) directly.

1.2 From sources

The latest sources for pyIMD can be downloaded from the Github repo.

You can clone the public repository:

```
$ git clone git://git.gitlab.com/csb.ethz/pyIMD.git
```

Once you have a copy of the source, navigate into the directory and run:

```
$ python setup.py install .
```

CHAPTER 2

Use and Examples

The examples show the basic usage of **pyIMD** to calculate the mass

2.1 pyIMD example script

This example script demonstrates the simplest interaction with **pyIMD**:

```
# /*****************************************************************************
# * Copyright © 2018-2019, ETH Zurich, D-BSSE, Andreas P. Cuny & Gotthold Fläschner
# * All rights reserved. This program and the accompanying materials
# * are made available under the terms of the GNU Public License v3.0
# * which accompanies this distribution, and is available at
# * http://www.gnu.org/licenses/gpl
# *
# * Contributors:
# *     Andreas P. Cuny - initial API and implementation
# *****************************************************************************/

from pyIMD.imd import InertialMassDetermination

# Create the inertial mass determination object
imd = InertialMassDetermination()

# Create a config file for the project / experiment to analyze using default values.␣
↪Note non default parameters can be
# added as optional arguments for e.g. spring_constant = 5.
file_path1 = "/pyIMD/examples/data/show_case/20170712_RSN_3_B"
file_path2 = "/pyIMD/examples/data/show_case/20170712_RSN_3_A"
file_path3 = "/pyIMD/examples/data/show_case/20170712_RSN_3_A_long_term.tdms"
imd.create_pyimd_project(file_path1, file_path2, file_path3, '\t', 23, 'PLL', figure_
↪width=5.4, figure_height=9.35,
                         initial_parameter_guess=[73.0, 5.2, 0.0, 0.0], upper_
↪parameter_bounds=[100.0, 7.0, 3.0, 3.0],
```

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```
                          spring_constant=8.0, cell_position=9.5, cantilever_
↪length=100.0, figure_format='pdf')

# Print the config file to the console to check if all parameters are set correctly␣
↪before starting the calculation.
imd.print_pyimd_project()

# If one needs to change a parameter on the fly just type: imd.settings.<parameter_
↪key> = value as eg.
# imd.settings.figure_resolution_dpi = 300. Note: Just hit imd.settings. + TAB to get␣
↪automatically a list of all
# available <parameter_keys>

# To enter all the parameters one can also start the settings user interface and␣
↪enter all the parameter values there.
# imd.show_settings_dialog()

# Run the inertial mass determination
imd.run_intertial_mass_determination()

# Save the config file for the project / experiment for documentation purpose or to␣
↪re-run with different /
# same parameter later
imd.save_pyimd_project("/pyIMD/examples/data/show_case/pyIMDProjectName.xml")

# To load an existing project type
imd.load_pyimd_project("/pyIMD/examples/data/show_case/pyIMDProjectName.xml")
# change a parameter i.e
imd.settings.figure_format = 'png'
# and run again
imd.run_intertial_mass_determination()
```

2.2 pyIMD example IPython/Jupyter notebook

[11]:
```
from pyIMD.imd import InertialMassDetermination
```

[12]:
```
imd = InertialMassDetermination()
```

```
2019-03-24 22:05:11 - pyIMD.imd - Object constructed successfully
```

[13]:
```
file_path1 = "../data/pll/20170712_RSN_3_B"
file_path2 = "../data/pll/20170712_RSN_3_A"
file_path3 = "../data/pll/20170712_RSN_3_A_long_term.tdms"
```

[14]:
```
imd.create_pyimd_project(file_path1, file_path2, file_path3, '\t', 23, 'PLL', figure_
↪height=40,
                         figure_unit='cm',initial_parameter_guess=[70.0, 2, 0.0, 0.0],
                         upper_parameter_bounds=[100.0, 5, 3.0, 3.0], spring_
↪constant=1.05,
                         cell_position=3.23, cantilever_length=59.84, figure_format=
↪'png',
                         correct_for_frequency_offset=True, frequency_offset_n_
↪measurements_used=15)
```

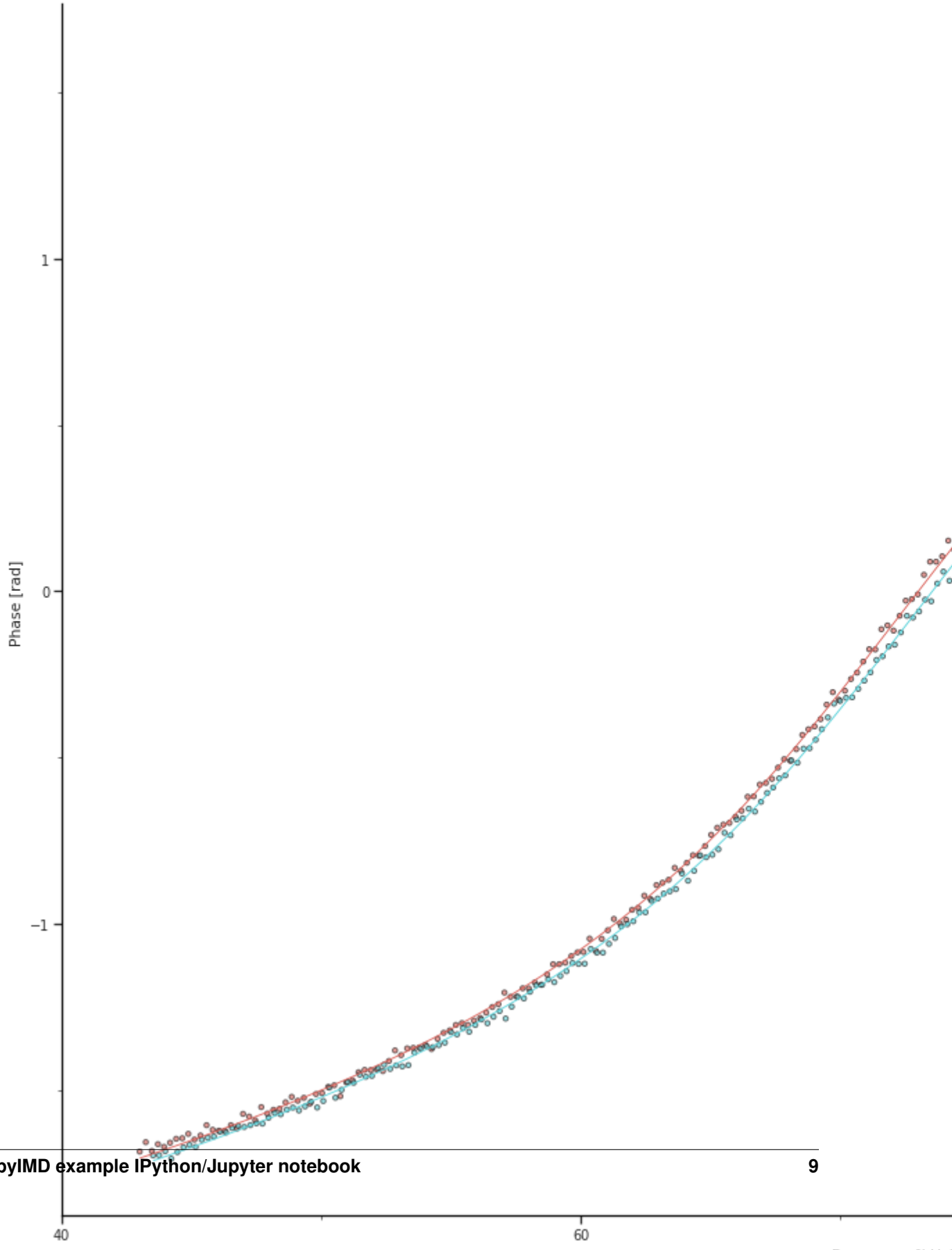
[15]:
```
imd.run_inertial_mass_determination()
```

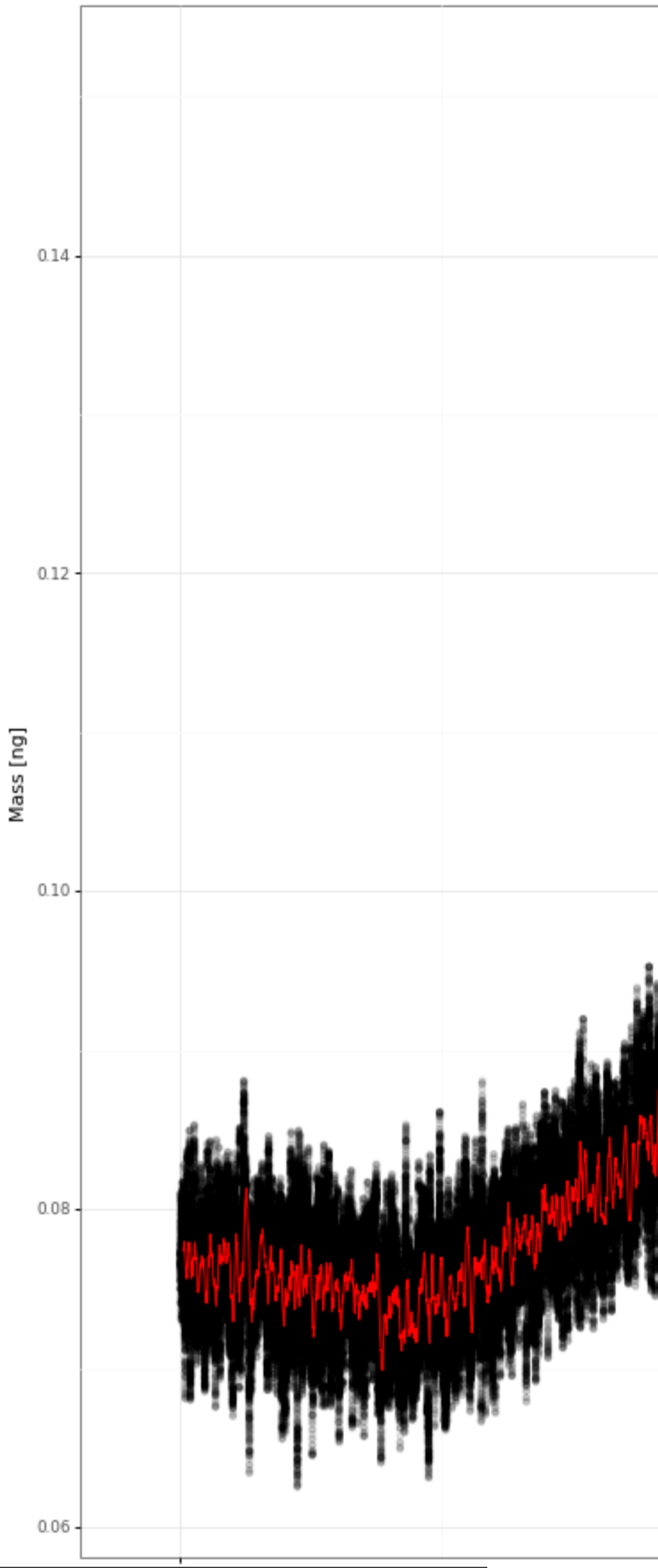
```
2019-03-24 22:05:12 - pyIMD.imd - Start reading all files
2019-03-24 22:06:32 - pyIMD.imd - Done reading all files
2019-03-24 22:06:32 - pyIMD.imd - Done converting units
2019-03-24 22:06:33 - pyIMD.imd - Done with pre start no cell resonance frequency␣
↪calculation
2019-03-24 22:06:34 - pyIMD.imd - Done with pre start with cell resonance frequency␣
↪calculation
2019-03-24 22:06:36 - pyIMD.imd - Done with pre start frequency shift figure␣
↪generation
2019-03-24 22:06:36 - pyIMD.imd - Offset calculation result: -0.10173519457150339
100%|| 692625/692625 [00:21<00:00, 32255.79it/s]
2019-03-24 22:06:57 - pyIMD.imd - Start writing figure to disk
2019-03-24 22:08:50 - pyIMD.imd - Done writing figure to disk
2019-03-24 22:08:50 - pyIMD.imd - Start writing data to disk
2019-03-24 22:08:54 - pyIMD.imd - Done writing data to disk
2019-03-24 22:08:54 - pyIMD.imd - Done with all calculations
```

The **run_intertial_mass_determination()** method generates automatically figures of the curve fitting for the per pre experiment data with and without a cell attached to the cantilever. A combined figure illustrating the shift in the phase response and the function fits and the resulting calculated cell mass of the long term measurement data.

2.2.1 Show resulting plots

- Shift in the phase response with and without cell attached to the cantilever and the corresponding function fit





- Final result of the mass calculation for the long term data set

[ ]:

2.3 pyIMD tutorial with user interface

Before starting, make sure pyIMD is *installed*

This tutorial provides a simple example with a test dataset, teaching step by step how to:

- create a pyIMD project
- calculate the mass form the measured data

The layout of the following windows and the paths are set for windows and might differ for Mac or Unix. First, lets have a look at the input data. The typical data set consists of 3 files: 1) a sweep file of the cantilever WITHOUT cell (text file with multi-line header) 2) a sweep file of the cantilever WITH cell (text file with multi-line header) and 3) the actual (long-term) measurement file, which is either a text file or TDMS file (lab-view specific file type). A typical time resolution is 10 ms for the data acquisition so these files can be quite large. **Fig. 1** visualizes the data input which can be found as example data set for download and testing.

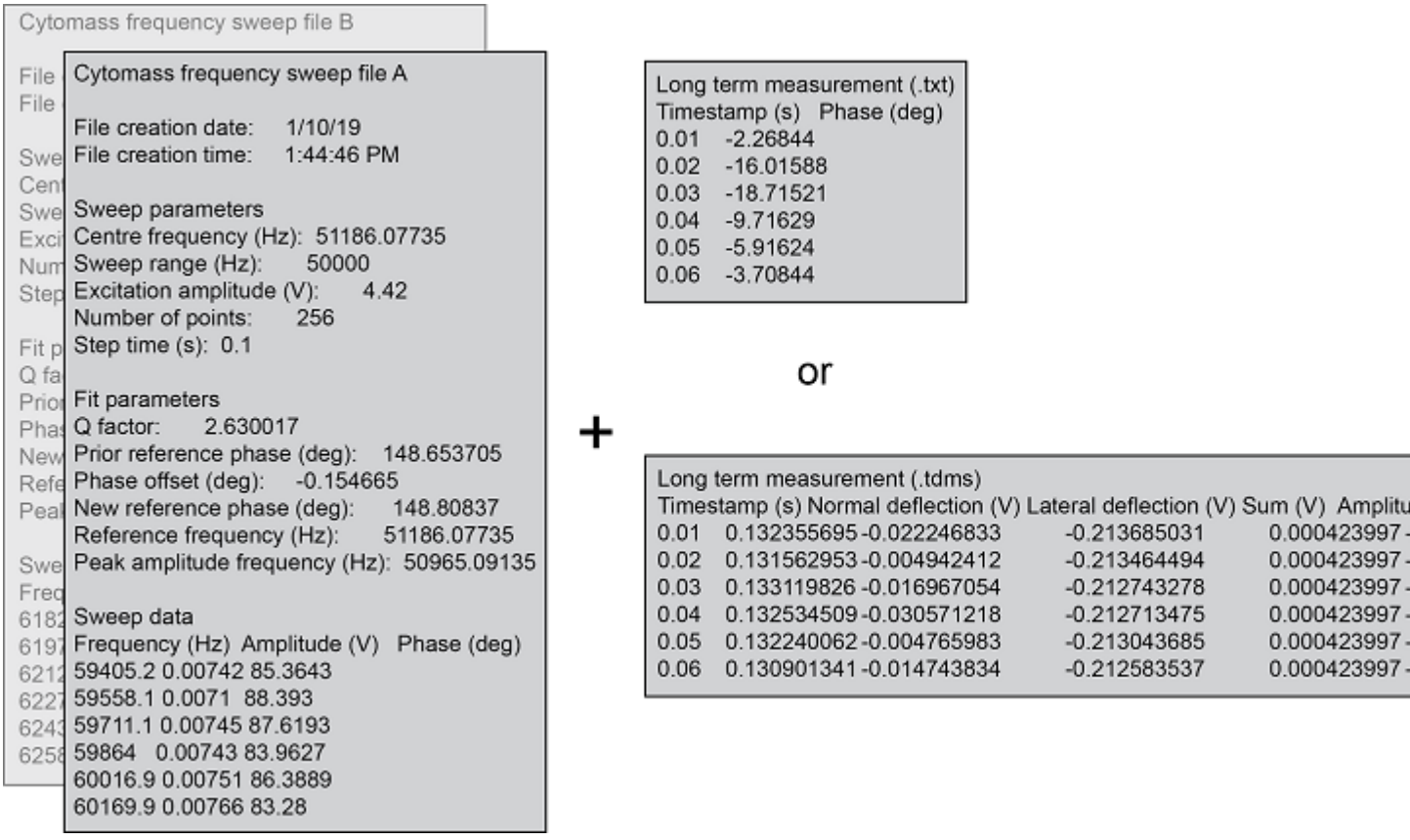


Fig. 1: **Figure 1**: Data format for pyIMD. pyIMD supports data from picobalance device controllers. (Cytomass and Nanonis)

The example pyIMD script section demonstrates how a pyIMD project is created on the console:

```
from pyIMD.imd import InertialMassDetermination

# Create the inertial mass determination object
imd = InertialMassDetermination()

# Create a config file for the project / experiment to analyze using default values.␣
↪Note non default parameters can be
# added as optional arguments for e.g. cell_position = 9.5.
file_path1 = "/pyIMD/examples/data/show_case/0190110_ShowCase_PLL_B.txt"
file_path2 = "/pyIMD/examples/data/show_case/20190110_ShowCase_PLL_A.txt"
file_path3 = "/pyIMD/examples/data/show_case/20190110_ShowCase_PLL_LongTerm.txt"
imd.create_pyimd_project(file_path1, file_path2, file_path3, '\t', 23, 'PLL', figure_
↪width=16.5, figure_height=20,
                         initial_parameter_guess=[60.0, 2.0, 0.0, 0.0], cell_
↪position=9.5, figure_format='pdf')
```

When using pyIMD through its user interface (UI) in the stand alone mode, the pyIMD project is created in exact the same way in the background. Yet, the user does not need to take care to type the paths or arguments correctly as all the input entered trough the UI will be validated automatically. **Fig. 2** shows the main window and the settings window of the pyIMD application. A new pyIMD project is created by selecting the three data files required for the calculation from a directory (3). Next, it needs to be declared which measurement each file contains and what the measurement mode is (5). Using the menu (1), opens the settings dialog and lets you determine all project related parameters such as the names of the output figures. After all settings are set, the mass calculation is started with (6).

The tools menu in **Fig. 2 (7)** allows for data concatenation from multiple files into a single one, in case the data was acquired with the Nanonis data logger. The resulting file can then be loaded as mentioned above along with the before and after cell attachment file.

```
# Run the inertial mass determination
imd.run_inertial_mass_determination()
```

The console (8) logs all actions performed with the UI and indicates when all calculations are done. The results can be viewed in the results tab (2), where as all the output figures are listed as well as the data can be inspected.

The first output created by pyIMD are control figures visualizing the fit of the cantilevers phase response is shown for the case with and without cell (**Fig. 3**). The shift towards lower frequencies can be clearly seen, when the cell is attached. Moreover, the Q-factor changes and therefore the slope of the response curve. If the fits are not fitting the raw data the parameter 'initial_parameter_guess', 'lower_parameter_bounds', 'upper_parameter_bounds' need to be adjusted in the settings dialog.

The analysis output by the software is shown in **Fig. 4**, the exemplary data for a mammalian cell is provided for download. The evolution of mass vs time is shown for a time span of 20 min. The mass data was acquired every 10 ms (data shown in black), overlaid in red is the rolling mean with a window of 1000 (adjustable parameter 'rolling_window_size'). Images taken every 3 min over the observed time span, we see on average a steady increase of the cell mass, the spring constant is 8 N/m (adjustable parameter 'sprint_constant'). The position of the cell projected along the long axis of the cantilever was 9.5 um (adjustable parameter, 'cell_position') and did not change, which is of importance for the current use of the software.

The project can either be re-run with different parameters, to i.e. improve the function fits or be saved using the menu (**Fig. 2**, (1)).

```
# save a pyIMD project
imd.save_pyimd_project("/pyIMD/examples/data/show_case/pyIMDShowCaseProject.xml")
```

A previously saved project can be loaded again at a later time from the menu (**Fig. 2**, (1))or also from the command line without the user interface:

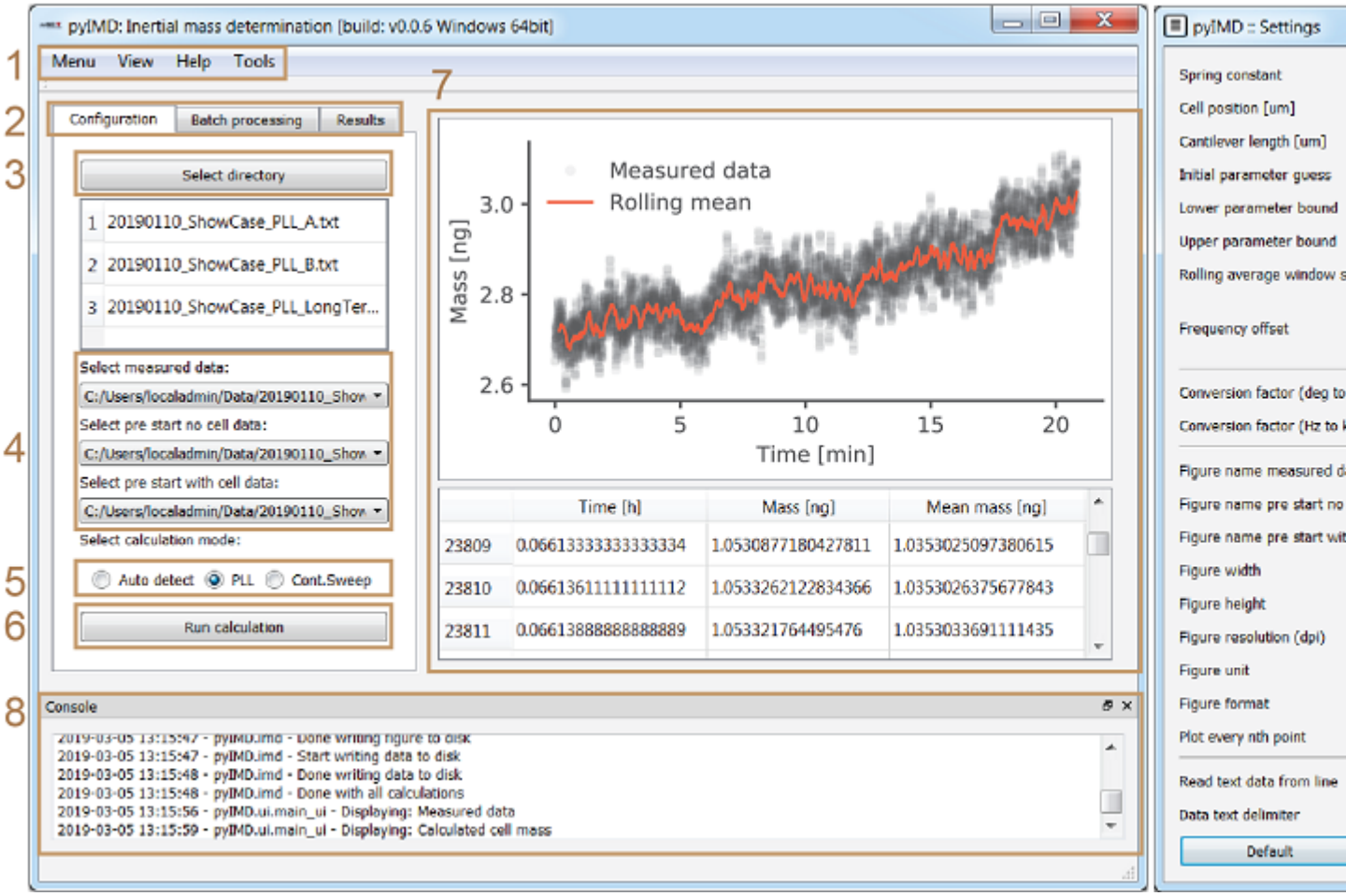


Fig. 2: **Figure 2**: . Through the menu bar (1) the pyIMD project can be loaded, saved, and the settings and parameter dialog opened (shown at the right-hand side). The help menu contains the software documentation, the quick help (also shown during startup), change log and information about the software dependencies and authors. The tabs (2) allow to switch between single calculation, batch calculation, and results. After all calculations are done the results tab is enabled and shows the latest result figures and data table in (7). (3) Creates a new pyIMD project while selecting at least three data files required for the calculation. After the files have been selected, it needs to be declared which type of data they contain, i.e. whether it is the single reference measurement of the cantilever without cell or the reference measurement with cell or the time resolved data (4). (5) Sets the acquisition mode that was used to collect the experimental long-term data. (6) Starts the mass calculation. If the batch processing is selected in (2) one or multiple pyIMD project files can be loaded, which will be run sequentially in different threads. With the settings dialog on the right, all the required parameters needed for the calculation as well as the output file formats or file names are set. The user input is validated live and if a parameter of a wrong type is entered, the input field turns yellow to notify the user of the mistake. When the user has inserted all necessary parameters correctly and started the calculation, a process is reported in the info window (8), and finally the result is shown in the main window.

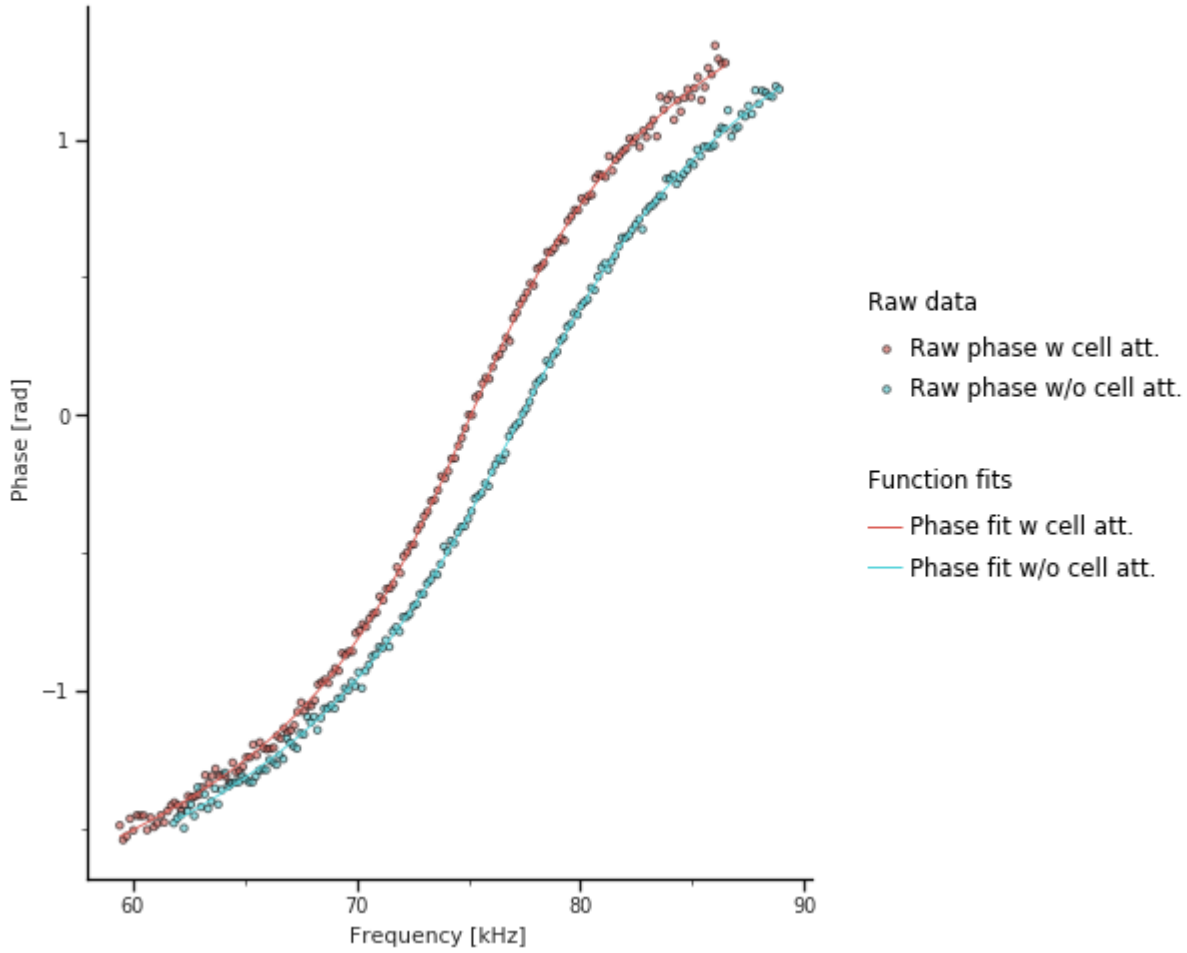


Fig. 3: **Figure 3**: Frequency vs cantilever phase response

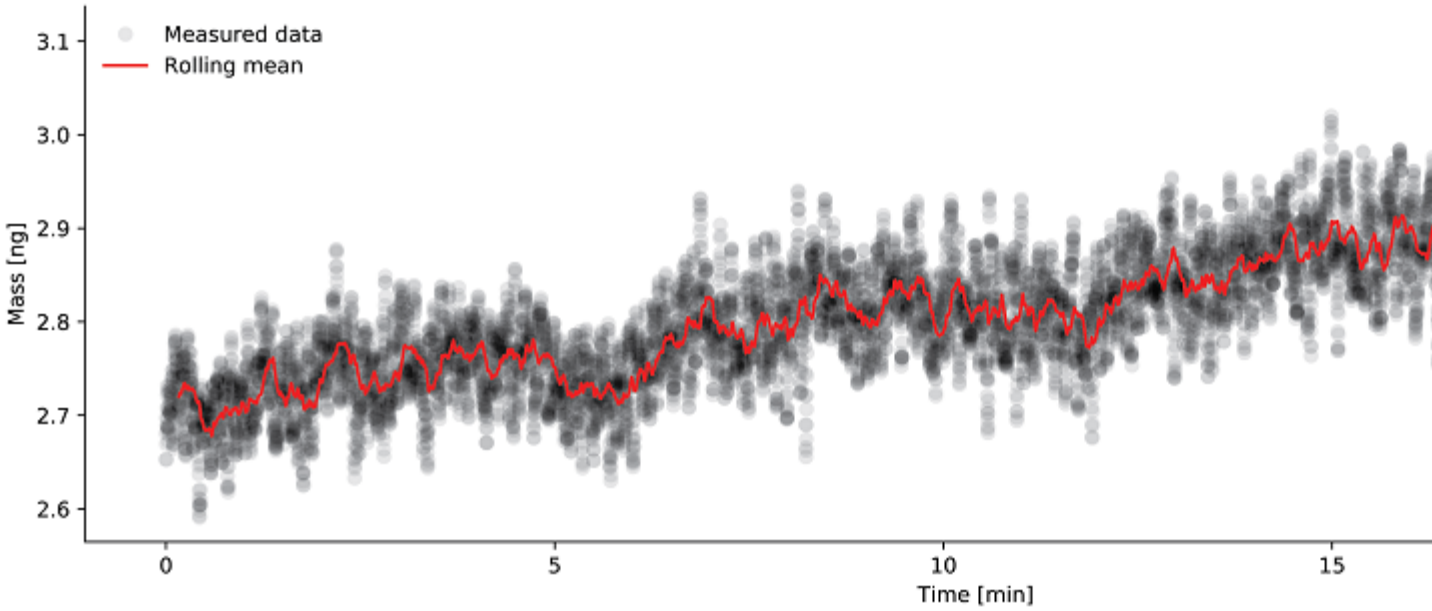


Fig. 4: **Figure 4**: Evolution of mass over time

```
# load a pyIMD project
imd.load_pyimd_project("/pyIMD/examples/data/show_case/pyIMDShowCaseProject.xml")
```

2.4 pyIMD example script Nanonis long term

This example script demonstrates the command line interface use with **pyIMD** and Nanonis long term type of data:

```
# /*******************************************************************************
# * Copyright © 2018-2019, ETH Zurich, D-BSSE, Andreas P. Cuny & Gotthold Fläschner
# * All rights reserved. This program and the accompanying materials
# * are made available under the terms of the GNU Public License v3.0
# * which accompanies this distribution, and is available at
# * http://www.gnu.org/licenses/gpl
# *
# * Contributors:
# *     Andreas P. Cuny - initial API and implementation
# *******************************************************************************/

from pyIMD.imd import InertialMassDetermination

# Create the inertial mass determination object
imd = InertialMassDetermination()

# Create a config file for the project / experiment to analyze using default values.␣
↪Note non default parameters can be
# added as optional arguments for e.g. spring_constant = 5.
file_path1 = "/pyIMD/examples/data/nanonis_long_term/20190510_LC_05_B001.dat"
file_path2 = "/pyIMD/examples/data/nanonis_long_term/20190510_LC_05_A001.dat"
file_path3 = "/pyIMD/examples/data/nanonis_long_term/20190510_LC_05_Longterm001.dat"
imd.create_pyimd_project(file_path1, file_path2, file_path3, '\t', 23, 'PLL', figure_
↪width=5.4, figure_height=9.35,
```

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```
                        initial_parameter_guess=[73.0, 5.2, 0.0, 0.0], upper_
↪parameter_bounds=[100.0, 8.0, 3.0, 3.0],
                        spring_constant=8.0, cell_position=10, cantilever_length=100.
↪0)

# Print the config file to the console to check if all parameters are set correctly␣
↪before starting the calculation.
imd.print_pyimd_project()

# Save the config file for the project / experiment for documentation purpose or to␣
↪re-run with different /
# same parameter later
imd.save_pyimd_project("/pyIMD/examples/data/nanonis_long_term/pyIMDProjectName.xml")

# Run the inertial mass determination
imd.run_intertial_mass_determination()
```

CHAPTER 3

API Reference

3.1 analysis

pyIMD.analysis.curve_fit.**fit_function**(*x*, *fn*, *q*, *a*, *b*)

Defines the phase response of a damped harmonic oscillator (i.e. the cantilever with or without cell). It is called from calculate_resonance_frequencies, to be fitted to the data primarily to extract the natural resonance frequency.

Parameters

- **x** (*float*) – Frequency (the independent variable of that function)
- **fn** (*float*) – Natural resonance frequency
- **q** (*float*) – Q factor (losses)
- **a** (*float*) – Linear factor accounting for a linear background
- **b** (*float*) – Constant Phase-Offset

Returns Returns the phase.

Return type phase (*float*)

pyIMD.analysis.calculations.**calculate_mass**(*spring_constant*, *res_freq_after_cell_load*, *res_freq_before_cell_load*)

Calculates the mass given the spring constant of the cantilever and the resonance frequency without and with cell attached to the cantilever.

Args:

spring_constant (*float*): Stiffness of the cantilever [in N/m] res_freq_after_cell_load (*float*): Resonance frequency of the cantilever AFTER the cell is picked up, at time point t [in kHz] res_freq_before_cell_load (*float*): Resonance frequency of the cantilever BEFORE the cell is picked up [in kHz]

Returns: mass (*float*): Returns data as float, which is the mass at time point t.

pyIMD.analysis.calculations.**calculate_position_correction**(*cell_position*, *cantilever_length*)

Calculates the correction factor with which the measured mass needs to be multiplied to get all the mass present on the cantilever. This is needed as the cantilever is differently sensitive to mass, depending on the location where this mass is attached. The measurements are performed with the first mode of vibration, which is described by the factor kL = 1.875. For higher modes, different would be used (4.694 for the second , 7.855 for the third etc.)

Parameters

- **cell_position** (*float*) – Cell position from the free end of the cantilever [in micrometer]
- **cantilever_length** (*float*) – Cantilever length [in micrometer]

Returns Returns a double which is the correction factor.

Return type correction_factor (*float*)

pyIMD.analysis.calculations.**calculate_resonance_frequencies**(*frequency_array*, *phase_array*, *initial_param_guess*, *lower_param_bounds*, *upper_param_bounds*)

Calculate_resonance_frequencies calculates the resonance frequency from input frequency and phase array. It does so via fitting the phase response of a harmonic oscillator (defined in pyIMD.analysis.curve_fit). The first fit parameter of the fit parameter array is the resonance frequency.

Parameters

- **frequency_array** (*float array*) – Array of frequencies [in kHz]
- **phase_array** (*float array*) – Array of phase [in Rad]
- **initial_param_guess** (*float*) – Initial parameter guess (1x4 array)
- **lower_param_bounds** (*float*) – Lower bounds (1x4 array)
- **upper_param_bounds** (*float*) – Upper bounds (1x4 array)

Returns Resonance frequency [in kHz]

Return type resonance_frequency (*float*)

Returns

Curve fit parameters curve_fit_parameter[0] := Q factor (losses)

curve_fit_parameter[1] := Linear factor accounting for a linear background

curve_fit_parameter[2] := Offset of the background

Return type curve_fit_parameter (*float array*)

3.2 configuration

class pyIMD.configuration.config.**Settings**

Bases: object

Settings initialization with default parameter values stored in pyIMD.configuration.defaults

calculation_mode
Parameter defining the calculation mode.

Parameters **mode** (*str*) – The calculation mode. PLL, Cont.Sweep or Auto.

cantilever_length
Parameter defining the cantilever length.

Parameters **cantilever_length** (*float*) – Cantilever length in microns.

cell_position
Parameter defining the cell position offset.

Parameters **cell_position** (*float*) – Cell position offset in microns from the free end of the cantilever.

conversion_factor_deg_to_rad
Parameter defining the data conversion factor from degrees to radians.

Parameters **factor** (*float*) – Data conversion factor from degrees to radians.

conversion_factor_hz_to_khz
Parameter defining the data conversion factor from Hz to kHz.

Parameters **factor** (*float*) – Data conversion factor from hertz to kilo hertz.

correct_for_frequency_offset
Parameter defining if PLL measurement data should be corrected for a potential frequency offset between the frequency pre start measured after a cell is attached to the cantilever and the actual measurement.

Parameters **correction** (*boolean*) – Boolean. False by default. True runs in the PLL case a frequency offset correction.

figure_format
Parameter defining the result figure(s) format.

Parameters **unit** (*str*) – Pdf and png ar currently supported.

figure_height
Parameter defining the result figure(s) height.

Parameters **height** (*float*) – Figure height in the unit specified.

figure_name_measured_data
Parameter defining the figure name for resulting calculated mass of the measured data.

Parameters **name** (*str*) – Figure name for resulting calculated mass of the measured data.

figure_name_pre_start_no_cell
Parameter defining the figure name for the function fit pre start no cell.

Parameters **name** (*str*) – Figure name for the function fit pre start no cell.

figure_name_pre_start_with_cell
Parameter defining the figure name for the function fit pre start with cell.

Parameters **name** (*str*) – Figure name for the function fit pre start with cell.

figure_plot_every_nth_point
Parameter defining how many data points are used for visualization. For very large data sets a number > 1 could increase the readability of the figure and lower the file size.

Parameters **nth_point** (*int*) – Pdf and png ar currently supported.

figure_resolution_dpi
Parameter defining the result figure(s) resolution in dpi.

Parameters **resolution** (*int*) – Figure resolution. E.g. 72, 150, 300.

figure_units
Parameter defining the result figure(s) unit.

Parameters **unit** (*str*) – Figure unit. E.g. mm, cm, in.

figure_width
Parameter defining the result figure(s) width.

Parameters **width** (*float*) – Figure width in the unit specified.

frequency_offset
Parameter defining the frequency offset.

Parameters **freq_offset** (*int*) – Frequency offset with which the measurement data will be corrected with.

frequency_offset_mode
Parameter defining the mode to be used to calculate the frequency offset. This applies only to in PLL recorded data.

Parameters **mode** (*str*) – Mode for frequency offset calculation. Either Auto or Manual.

frequency_offset_n_measurements_used
Parameter defining how many data points of the measurement should be used to calculate the average frequency offset.

Parameters **n_measurements** (*int*) – Number of measurement data points to be used to calculate the average freq. offset.

initial_parameter_guess
Parameter defining the initial parameter guess.

Parameters **array** (*list*) – Initial parameter guess.

lower_parameter_bounds
Parameter defining the lower parameter bounds.

Parameters **array** (*list*) – Lower parameter bounds.

measurements_path
Parameter defining the path to the measurement file.

Parameters **path** (*str*) – Path to the measurement file. (.tdms or .txt file).

new_pyimd_project(*pre_start_no_cell_path*, *pre_start_with_cell_path*, *measurements_path*, *text_data_delimiter*, *read_text_data_from_line*, *calculation_mode*, ***kwargs*)
Create a new pyIMD project with the following arguments. Two modes enable the analysis of different experimental setups. PLL mode and Cont.Sweep mode. For more information please read the documentation.

Parameters

- **pre_start_no_cell_path** (*str*) – File path + file name of initial frequency shift measurement before cell attachment (txt file).
- **pre_start_with_cell_path** (*str*) – File path + file name of initial frequency shift measurement after cell attachment (txt file).
- **measurements_path** (*str*) – File path + file name of the actual measurement (tdms file (default) or txt file).
- **text_data_delimiter** (*str*) – Text file data delimiter i.e ‘ ‘ for tab delimited or ‘,’ for comma separated data.

- **read_text_data_from_line** (*int*) – Line number from which data of pre start measurements should be read. Typically the first few lines contain header information and no data.
- **calculation_mode** (*str*) – PLL := phase lock loops mode Cont.Sweep := sweep mode Auto := Auto detection of the mode (experimental)

Keyword Arguments

- **figure_width** (*float*) – Width of result figures
- **figure_height** (*float*) – Height of result figures
- **figure_units** (*str*) – Figure units i.e cm, inch
- **figure_format** (*str*) – Figure format i.e png or pdf
- **figure_resolution_dpi** (*int*) – Resolution of result figures in dpi
- **figure_name_pre_start_no_cell** (*str*) – Figure name of function fit for pre start with no cell loaded data
- **figure_name_pre_start_with_cell** (*str*) – Figure name of function fit for pre start with cell loaded data
- **figure_name_measured_data** (*str*) – Figure name of the resulting mass of the measured data
- **figure_plot_every_nth_point** (*'int'*) – Parameter defining how many data points will be plotted. For large data stets to increase readability and reducing file size.
- **conversion_factor_hz_to_khz** (*float*) – Conversion factor to convert from hertz to kilo hertz
- **conversion_factor_deg_to_rad** (*float*) – Conversion factor to convert from degrees to radian
- **spring_constant** (*float*) – Spring constant value of the cantilever
- **initial_parameter_guess** (*list*) – Initial parameter guess
- **lower_parameter_bounds** (*list*) – Lower parameter bounds
- **upper_parameter_bounds** (*list*) – Upper parameter bounds
- **rolling_window_size** (*'int'*) – Window size for calculating the rolling average.
- **correct_for_frequency_offset** (*'bool'*) – Correct for potential frequency offset during PLL mode.
- **frequency_offset_mode** (*'str'*) – Frequency offset correction mode (Auto or Manual)
- **frequency_offset_n_measurements_used** (*'int'*) – Number of measurement data points to be used for automatic frequency offset correction
- **frequency_offset** (*'float'*) – Frequency offset either set manually or calculated automatically
- **cantilever_length** (*float*) – Cantilever length in microns
- **cell_position** (*float*) – Cell position offset from cantilever tip in microns
- **project_folder_path** (*str*) – Path to project data files. Also used to store pyIMD results such as data and figures.

pre_start_no_cell_path
Parameter defining the path to the pre start no cell file.

Parameters **path** (*str*) – Path to the pre start no cell file (.txt).

pre_start_with_cell_path
Parameter defining the path to the pre start with cell file.

Parameters **path** (*str*) – Path to the pre start with cell file (.txt).

project_folder_path
Parameter defining the path to the files.

Parameters **path** (*str*) – The path to the files.

read_pyimd_project (*file_path*)
Read a pre defined pyIMD project form a XML file from disk.

Parameters **file_path** (*str*) –

Returns String reporting the success of failure of loading a pyIMD project.

Return type status (*str*)

read_text_data_from_line
Parameter defining the length of the header inside the initial sweep files. From this line number the data will be imported.

Parameters **line_number** (*int*) – Line number from where on to read the data from.

rolling_window_size
Parameter defining the window size of the rolling window applied to the data for visualizing the trend.

Parameters **window_size** (*int*) – Rolling window size.

selected_files
Parameter defining the selected files for calculation.

Parameters **files** (*list*) – Selected files for calculation.

spring_constant
Parameter defining the spring constant of the cantilever.

Parameters **spring_constant** (*float*) – Spring constant of the cantilever.

text_data_delimiter
Parameter defining the text file data delimiter.

Parameters **delimiter** (*str*) – Text file data delimiter i.e ‘ ‘ for tab delimited or ‘,’ for comma separated data.

upper_parameter_bounds
Parameter defining the upper parameter bounds.

Parameters **array** (*list*) – Upper parameter bounds.

write_pyimd_project (*file_path*)
Write the current pyIMD project as XML file to disk. :param file_path: :type file_path: *str*

Returns String reporting the success of failure of loading a pyIMD project.

Return type status (*str*)

3.3 io

pyIMD.io.read_from_disk.**read_from_dat**(*file*, *delimiter*)
Method to read data from dat files (i.e from Nanonis software).

Parameters

- **file** (*str*) – File path + file name.
- **delimiter** (*str*) – Delimiter used in the data file to separate columns

Returns Returns data structured in a pandas data frame.

Return type data (*pandas data frame*)

pyIMD.io.read_from_disk.**read_from_file**(*file*, *delimiter*)
Method to read data from a file.

Parameters

- **file** (*str*) – File path + file name to a .TDMS or .txt file.
- **delimiter** (*str*) – Delimiter used in the data file to separate columns

Returns Returns data structured in a pandas data frame.

Return type data (*pandas data frame*)

pyIMD.io.read_from_disk.**read_from_tdms**(*file*)
Method to read data from National Instruments technical data management streaming files (TDMS).

Parameters **file** (*str*) – File path + file name string.

Returns Returns data structured in a pandas data frame.

Return type data (*pandas data frame*)

pyIMD.io.read_from_disk.**read_from_text**(*file*, *delimiter*, *read_from_row*)
Method to read data from text files.

Parameters

- **file** (*str*) – File path + file name.
- **delimiter** (*str*) – Delimiter used in the data file to separate columns
- **read_from_row** (*int*) – Row number from where to start reading data to be able to skip heading text rows. Make sure that you keep the Frequency, Amplitude and Phase headers.

Returns Returns data structured in a pandas data frame.

Return type data (*pandas data frame*)

pyIMD.io.write_to_disk.**write_concat_data**(*directory*, *delimiter*, *time_interval*)
Method to write concatenate data from single dat files (i.e data logger from Nanonis software).

Parameters

- **directory** (*str*) – Directory containing files to concatenate.
- **delimiter** (*str*) – Delimiter to be used in the data file to separate columns.
- **time_interval** (*int*) – Measurement time interval in milliseconds.

Returns Writes concatenated data to single .csv file.

Return type file (*void*)

pyIMD.io.write_to_disk.**write_to_disk_as**(*file_format*, *plot_object*, *file*, ***kwargs*)
Method to write figures in various file formats

Parameters

- **file_format** (*str*) – File format identifier i.e. png or pdf
- **plot_object** (*ggplot object*) – ggplot object
- **file** (*str*) – File path + file name of the figure to save

Keyword Arguments

- **width** (*int*) – Figure width (optional)
- **height** (*int*) – Figure height (optional)
- **units** (*'str`*) – Figure units (optional) 'in', 'mm' or 'cm'
- **resolution** (*int*) – Figure resolution in dots per inch [dpi] (optional)

Returns Writes figure to disk in the respective file format

Return type file (*void*)

pyIMD.io.write_to_disk.**write_to_pdf**(*plot_object*, *file*, ***kwargs*)
Method to write figures in pdf format to current directory

Parameters

- **plot_object** (*ggplot object*) – ggplot object
- **file** (*str*) – File path + file name of figure to save

Keyword Arguments

- **width** (*int*) – Figure width (optional)
- **height** (*int*) – Figure height (optional)
- **units** (*'str`*) – Figure units (optional) 'in', 'mm' or 'cm'
- **resolution** (*int*) – Figure resolution in dots per inch [dpi] (optional)

Returns Writes figure to disk as pdf

Return type pdf file (*void*)

pyIMD.io.write_to_disk.**write_to_png**(*plot_object*, *file*, ***kwargs*)
Method to write figures in png format to current directory

Parameters

- **plot_object** (*ggplot obj*) – ggplot object
- **file** (*str*) – File path + file name of the figure to save

Keyword Arguments

- **width** (*int*) – Figure width (optional)
- **height** (*int*) – Figure height (optional)
- **units** (*str*) – Figure units (optional) 'in', 'mm' or 'cm'
- **resolution** (*int*) – Figure resolution in dots per inch [dpi] (optional)

Returns Writes figure to disk as png

Return type png file (*void*)

3.4 plotting

pyIMD.plotting.figures.**create_montage_array**(*img_stack*, *size*)

Creates an image montage of a 3D numpy array with the shape [image frames, image row, image col] for the specified size.

Parameters

- **img_stack** (*3D numpy array*) – 3D numpy image array [image row, image col, image frames].
- **size** (*numpy array*) – Array specifying the amount of images displayed in the montage per row and column. If one argument is replaced with np.nan, the needed amount of rows or columns is calculated automatically. E. g. [5, np.nan]

Returns 2D numpy array with the image montage

Return type montage (*2D numpy array*)

pyIMD.plotting.figures.**get_montage_array_size**(*size*, *image_row_count*, *image_col_count*, *frame_count*)

Calculates the final size of a numpy array needed to hold a the number of specified image frames given the row and column count of the final array.

Parameters

- **size** (*numpy array*) – Array specifying the amount of images displayed in the montage per row and column. If one argument is replaced with np.nan, the needed amount of rows or columns is calculated automatically. E. g. [5, np.nan]
- **image_row_count** (*int*) – Number of rows per image
- **image_col_count** (*int*) – Number of columns per image
- **frame_count** (*int*) – Number of image frames in the stack

Returns Array with the number of rows and columns needed in the montage array for the images

Return type montage_size (*numpy array*)

pyIMD.plotting.figures.**plot_fitting**(*x*, *y*, *resonance_frequency*, *parameter*)

Plots the phase response and the corresponding fit of the harmonic damped oscillator.

Parameters

- **x** (*float array*) – X coordinates (frequency in kHz)
- **y** (*float array*) – Y coordinates (phase in radians)
- **resonance_frequency** (*float array*) – Resonance frequency given by the fit of x and y
- **parameter** (*float array*) – Others parameters of function fit (Q factor, offset, linear background)

Returns Returns a ggplot object

Return type p (*ggplot object*)

pyIMD.plotting.figures.**plot_mass**(*calculated_cell_mass*, *plot_every_nth_point*)

Plots the resulting mass

Parameters

- **calculated_cell_mass** (*pandas data frame*) – Pandas data frame [Nx3] with time and calculated cell mass and rolling mean averaged cell mass

- **plot_every_nth_point** (*int*) – If 1 all data points are plotted. Otherwise every nth data point is used for plotting.

Returns Returns a ggplot plot object

Return type p (*ggplot object*)

pyIMD.plotting.figures.**plot_response_shift**(*x*, *y*, *resonance_frequency_without*, *parameter_without*, *xx*, *yy*, *resonance_frequency_with*, *parameter*)

Plots the phase response of pre start data without and with cell attached to cantilever with the respective function fit.

Parameters

- **x** (*float array*) – X coordinates w/o cell (frequency in kHz)
- **y** (*float array*) – Y coordinates w/o cell (phase in radians)
- **xx** (*float array*) – X coordinates w/ cell(frequency in kHz)
- **yy** (*float array*) – Y coordinates w/ cell (phase in radians)
- **resonance_frequency_without** (*float array*) – Resonance frequency given by the fit of x and y w/o cell
- **resonance_frequency_with** (*float array*) – Resonance frequency given by the fit of x and y w/ cell
- **parameter** (*float array*) – Others parameters of function fit (Q factor, offset, linear background) w/o cell
- **parameter_without** (*float array*) – Others parameters of function fit (Q factor, offset, linear background) w/ cell

Returns Returns a ggplot object

Return type p (*ggplot object*)

3.5 ui

class pyIMD.ui.main_ui.**IMDWindow**

Bases: PyQt5.QtWidgets.QMainWindow

Implementation of the pyIMD main user interface window.

closeEvent(*event*)

Application close event override of QMainWindow closeEvent

Parameters **event** (*QCloseEvent*) – A QCloseEvent

Returns O when process finished correctly otherwise >0

Return type status_code (*int*)

close_application(*event*)

Opens a message box to handle program exit properly asking the user if the project should be saved first.

Parameters **event** (*QCloseEvent*) – A QCloseEvent

Returns 0 when process finished correctly, otherwise >0

Return type status_code (*int*)

static get_logger_object(*name*)
Gets a logger object to log messages of pyIMD status to the console in a standardized format.

Returns Returns a logger object with correct string formatting.

Return type logger (*object*)

handle_change_console_text(*text*)
Implementation of the handle_change_console_text slot.

Parameters **text** (*str*) – String received from Settings instance to print to the console.

on_about()
Displays the about window.

on_change_log()
Displays the change log window.

on_combo_box_changed(*index*)
Prints the selected item of the data drop down list to the console.

Parameters **index** (*int*) – Index of the selected item from the drop down list.

on_concatenation()
Opens concatenation dialog and starts file concatenation in new thread.

on_data_list_selection_changed()
Adds the selected data to the PandasDataFrameModel model to be displayed in the results table view.

on_quick_instructions()
Displays the quick instructions window.

static on_read_documentation()
Opens the documentation in the default web browser.

on_settings_changed(*changed_settings*)
Update settings from settings dialog to settings configuration as soon as user commits parameter changes.

Parameters **changed_settings** (*dict*) – Settings dictionary

Returns Updates the changed settings on the object directly

Return type Null (*void*)

on_task_finished(*task*)
Enable the Result tab after the inertial mass determination run is finished.

Args: task: ThreadPoolExecutor task

on_update_text(*text*)
Writes new text to the console at the last text cursor position

Parameters **text** (*str*) – Text to be shown on the console.

open_project()
Opens a pyIMD project file (.xml) using the IntertialMassDetermination.load_pyimd_project method

print_to_console(*text*)
Print text to console.

Parameters **text** (*str*) –

run_batch_calculation()
Implementation of the pyIMD calculation batch mode based on pyIMD project files.

run_calculation()
Implementation of the pyIMD calculation start as new thread.

save_project()
Saves a pyIMD project file as .xml using the IntertialMassDetermination.save_pyimd_project method

Returns Saves pyIMD project as xml file to disk

Return type Null (*void*)

select_batch_files()
Selection of .xml pyIMD project files for batch calculation.

select_data_files()
Select data files to create a new pyIMD project

send_to_console_signal
pyqtSignal used to send a text to the console.

Parameters **message** (*str*) –

setup_console_connection()
Set up the console connection between the settings and the main window.

show_console()
Show and hide the console with the program log.

show_data()
Display the selected file names om the file viewer.

show_settings_dialog()
Show the settings dialog.

sync_settings()
Synchronizes the settings of the UI with the pyIMD object settings object.

class pyIMD.ui.main_ui.**Stream**
Bases: PyQt5.QtCore.QObject

Implementation of a stream to handle logging messages

stream_signal
pyqtsignal to redirect sterr

write(*text: object*) → object
Emits text formatted as string. :param text: :type text: *str*

class pyIMD.ui.settings.**SettingsDialog**(*settings_dictionary*)
Bases: PyQt5.QtWidgets.QDialog

Settings QDialog user interface implementation.

check_state()
Live validation if parameters entered by user are valid.

Returns Returns color formatter validator state.

Return type sender (*obj*)

close_settings_dialog()
Close the settings UI dialog without saving changes made on parameters

Returns None.

Return type Null (*void*)

commit_parameters()
Saves changes on parameters.

Returns Returns the changed parameters as dictionary.

Return type Parameters (*dict*)

find_checked_radiobutton()
Find the checked radiobutton

Returns Returns the name of the selected radio button.

Return type selected radio (*str*)

on_frequency_offset_mode_auto(*checked*)
Enables the auto offset mode fields

Parameters **checked** (*bool*) – Boolean enabling or disabling the frequency offset spin

Returns None

Return type Null (*void*)

on_frequency_offset_mode_manual(*checked*)
Enables the manual offset mode fields

Parameters **checked** (*bool*) – Boolean enabling or disabling the frequency offset field

Returns None

Return type Null (*void*)

on_toggle_frequency_offset(*state*)
Enables or disables the frequency offset optional parameters

Parameters **state** (*int*) – State enabling or disabling the frequency offset correction

Returns None

Return type Null (*void*)

print_to_console(*text*)
Print changes to console

Parameters **text** (*str*) – Text to print to the console

Returns Prints message to console.

Return type Message (*str*)

send_to_console_signal
pyqtSignal sends message to console

Returns Status message to be send to console.

Return type message (*str*)

set_defaults()
Set parameters default values to user interface.

Returns None

Return type Null (*void*)

set_values()
Set parameter values to user interface.

Returns None

Return type Null (*void*)

settings_has_changed_signal
pyqtSignal sends dictionary with all settings

Returns Dictionary with settings.

Return type settings (*dict*)

3.6 imd

class pyIMD.imd.**InertialMassDetermination**
Bases: PyQt5.QtCore.QObject

Constructs a IntertialMassDetermination object

concatenate_files(*directory*, *time_interval*, ***kwargs*)
Method to write concatenate data from single dat files (i.e data logger files from Nanonis software).

Parameters

- **directory** (*str*) – Directory containing files to concatenate.
- **time_interval** (*int*) – Measurement time interval in milliseconds.

Keyword Arguments **delimiter** (*str*) – Delimiter to be used in the data file to separate columns.(i.e. , s) If empty it uses default given by settings.

Returns Writes concatenated data to single .csv file.

Return type file (*void*)

convert_data()
Converts imported data to correct units needed for further calculation.

create_pyimd_project(*pre_start_no_cell_path*, *pre_start_with_cell_path*, *measurements_path*, *text_data_delimiter*, *read_text_data_from_line*, *calculation_mode*, ***kwargs*)
Create a pyIMD project with the following arguments. Two modes enable the analysis of different experimental setups. PLL mode and Cont.Sweep mode. For more information please read the documentation.

Parameters

- **pre_start_no_cell_path** (*str*) – File path + file name of initial frequency shift measurement before cell attachment (txt file).
- **pre_start_with_cell_path** (*str*) – File path + file name of initial frequency shift measurement after cell attachment (txt file).
- **measurements_path** (*str*) – File path + file name of the actual measurement (tdms file (default) or txt file).
- **text_data_delimiter** (*str*) – Text file data delimiter i.e ‘ ‘ for tab delimited or ‘,’ for comma separated data.
- **read_text_data_from_line** (*int*) – Line number from which data of pre start measurements should be read Typically the first few lines contain header information and no data.
- **calculation_mode** (*str*) – PLL := phase lock loops mode Cont.Sweep := sweep mode Auto := Auto detection of the mode (experimental)

Keyword Arguments

- **figure_width** (*float*) – Width of result figures
- **figure_height** (*float*) – Height of result figures
- **figure_units** (*str*) – Figure units i.e cm, inch
- **figure_format** (*str*) – Figure format i.e png or pdf
- **figure_resolution_dpi** (*int*) – Resolution of result figures in dpi
- **figure_name_pre_start_no_cell** (*str*) – Figure name of function fit for pre start with no cell loaded data
- **figure_name_pre_start_with_cell** (*str*) – Figure name of function fit for pre start with cell loaded data
- **figure_name_measured_data** (*str*) – Figure name of the resulting mass of the measured data
- **figure_plot_every_nth_point** (*'int'*) – Parameter defining how many data points will be plotted. For large data stets to increase readability and reducing file size.
- **conversion_factor_hz_to_khz** (*float*) – Conversion factor to convert from hertz to kilo hertz
- **conversion_factor_deg_to_rad** (*float*) – Conversion factor to convert from degrees to radian
- **spring_constant** (*float*) – Spring constant value of the cantilever
- **initial_parameter_guess** (*list*) – Initial parameter guess
- **lower_parameter_bounds** (*list*) – Lower parameter bounds
- **upper_parameter_bounds** (*list*) – Upper parameter bounds
- **rolling_window_size** (*'int'*) – Window size for calculating the rolling average.
- **correct_for_frequency_offset** (*'bool'*) – Correct for potential frequency offset during PLL mode.
- **frequency_offset_mode** (*'str'*) – Frequency offset correction mode (Auto or Manual)
- **frequency_offset_n_measurements_used** (*'int'*) – Number of measurement data points to be used for automatic frequency offset correction
- **frequency_offset** (*'float'*) – Frequency offset either set manually or calculated automatically
- **cantilever_length** (*float*) – Cantilever length in microns
- **cell_position** (*float*) – Cell position offset from cantilever tip in microns
- **project_folder_path** (*str*) – Path to project data files. Also used to store pyIMD results such as data and figures.

establish_console_connection()
Establish console connection between the imd object and the settings dialog.

static get_logger_object(*name*)
Gets a logger object to log messages of pyIMD status to the console in a standardized format.

Returns Returns a logger object with correct string formatting.

Return type logger (*object*)

handle_change_console_text(*string*)

Parameters **string** (*str*) – String received from Settings instance to print to the console.

load_pyimd_project(*file_path*)
Loads a pre defined pyIMD project form a XML file.

Parameters **file_path** (*str*) – Full path + file name to the pyIMD project file.

Returns String reporting the success of failure of loading a pyIMD project.

Return type status (*str*)

on_settings_changed(*changed_settings*)
Update settings

print_pyimd_project()
Prints the current pyIMD settings and parameters to the console.

Returns pyIMD settings and parameter summary as formatted string.

Return type pyIMD project summary (*str*)

run_batch_inertial_mass_determination(**args*)
Runs the inertial mass determination calculation in batch mode. Specify one or multiple pyIMD project files which will be run sequentially. NOTE: In a future release this will be parallelized using multiple threads to perform the calculations in parallel to gain speed. Currently the focus is not on speed but the idea is to analyze many experiments conveniently over night for example.

Parameters **args** (*list*) – List of one or many file paths + file names to valid pyIMD project files.

Returns Returns result structured in a pandas data frame and saves function fit plots as pdf files.

Return type void

run_inertial_mass_determination()
Runs the inertial mass determination calculation

Returns Returns result structured in a pandas data frame and saves function fit plots as pdf or png files directly to the disk.

Return type void

save_pyimd_project(*file_path*)
Saves the current pyIMD project as XML file.

Parameters **file_path** (*str*) – Full path + file name to the pyIMD project file.

Returns String reporting the success of failure of loading a pyIMD project.

Return type status (*str*)

show_settings_dialog()
Shows the settings dialog in a pop up window.

CHAPTER 4

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CHAPTER 5

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