BASTet: Berkeley Analysis and Storage Toolkit

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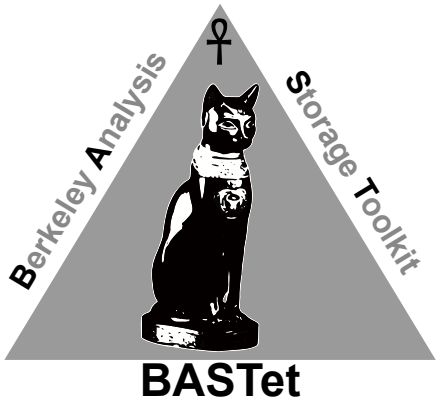

Berkeley Analysis
Storage Toolkit
BASTet

CHAPTER

ONE

INTRODUCTION

This documenation provides an introduction to the omsi HDF-based data format employed by the OpenMSI project as well as the omsi software stack including: i) the omsi file format API, ii) data analysis API, and iii) other tools and modules included in the omsi software stack

1.1 Mass Spectrometry Imaging

Metabolite and protein analysis is vital to understanding the phenotype of a biological sample. Specifically, metabolite levels dynamically vary in response to energy demands, diet, disease, and environment. Typical analysis of metabolite levels begins with homogenization of a sample and the spatial relationships of the biological material are lost. Mass spectrometry imaging of metabolite and protein levels overcomes this limitation by directly measuring the relative abundance of biomolecules and mapping their position. An "image" constitutes a relative abundance map for a given biomolecule and large-numbers of molecules can be imaged simultaneously. While this technique is certainly revolutionary, the in-depth analysis of these datasets often provides a barrier to many researchers. OpenMSI provides a gateway for the management and storage of these datafiles (where each file is the size of a typical hard drive), the visualization of the hyper-dimensional contents of the data, and the statistical analysis of the data.

Mass Spectrometry Imaging (MSI) plays a key role in the study of the metabolism and energetics of cells and cellular communities. Metabolite imaging and metabolomic analysis are used to map the connectivity, dynamics and spatial topography of complex cellular systems. In contrast to optical imaging, using MSI allows us to study large numbers of metabolic compounds in a single image. A mass spectrometry image provides for each pixel information about the entire mass spectrum, which is described by a high-resolution spectrum, currently consisting of up to 200,000 m/z bins. A single high-resolution 2D image slice requires on the order of 50GB and several TB's in 3D. Analysis of extremely large and complex MSI data is challenging from both a computational as well as visualization/analysis point of view. Users often require assistance by experts analysts to explore and analyze their MSI data.

1.2 OpenMSI: Science Gateway

The goal of OpenMSI is to provide a web-based gateway for management and storage of MSI data, the visualization of the hyper-dimensional contents of the data, and the statistical analysis of the data. Initially the gateway should support basic: i) data browsing capabilities and ii) data analysis and visualization capabilities. The visualization would provide easy-to-use selection capabilities allowing a user to: i) select regions of interest in a two-dimensional visualization of the imaging data and to retrieve and plot the spectra for the selected data portions and ii) to select peaks of interest in a spectrum and display an image showing which portions of the image contain similar features. Even such a simple exploratory tool would be extremely valuable in making the imaging data more accessible to end-users. In the longer term we envision to extend this simple browser step-by-step with more sophisticates analysis and interactions capabilities to support: i) interactive annotation of spectra, ii) execution of computationally intensive analysis tasks on remote parallel compute systems at NERSC, and iii) upload data and analysis results to OpenMSI to facilitate sharing of data/results with the MSI community. Similar to the CXIDB project at NERSC, we plan to us HDF5 to

enable efficient and flexible: i) data storage, ii) retrieval of data subsets, iii) storage of meta-data information, and iv) extension of the data to include additional derived data. As part of this project we also plan to investigate the use of HPC to speed-up a select set of compute intensive analysis tasks. Many of the analysis tasks currently performed in serial —such as peak detection and filtering— involve large numbers of independent computations (e.g., on a per spectrum basis) and could efficiently utilize parallel compute resources to speed-up the analysis.

1.3 OpenMSI: Software Infrastructure

The OpenMSI software infrastructure described in this document provides the foundations for interacting with and analyzing MSI data. In order to make MSI data accessible, the OpenMSI project has developed a HDF5 data layout scheme designed for MSI data. The data format enables storage of: i) raw MSI data, ii) metadata information about an experiment, sample and instrument, and iii) derived analysis results, in a single HDF5 file. Multiple experiments, each of which may included multiple MSI datasets and derived analysis results, may be stored in the same HDF5 file.

The OpenMSI software stack is based on Python using the h5py library for interacting with HDF5 files. omsi provides a custom API for reading/writing omsi HDF5 files. The file API employs a similar strucutre as the file format itself with each high-level HDF5 group being represented by a corresponding python class (see `omsi.dataformat.omsi_file`). The `omsi.analysis` package then provides an API for integrating new anlaysis functions with the HDF5 format and the OpenMSI software stack (as well as a series of analysis functions currently available within omis). Additional helpful tools are availabel via the `omsi.tools` and `omsi.examples` packages.

CHAPTER

TWO

CONVERTING AND FILES AND MAKING THEM ACCESSIBLE

2.1 Converting an MSI file at NERSC

To convert a mass spectrometry imaging file, e.g., in img or bruckerflex format, to HDF5 do the following:

```
ssh edison.nersc.gov
cd /project/projectdirs/openmsi/devel/convert
source setupEnvironment.csh
python convertToOMSI.py <infile1> <output HDF5File>
```

Note if you use the bash shell then use `setupEnvironment.bash` instead.

Note, if you want to use the output file from openmsi.nersc.gov then the output file path should be:

```
/project/projectdirs/openmsi/omsi_data_private/<username>/<filename>
```

where username is the name of the primary user that owns the file.

2.2 Making a converted file accessible to OpenMSI (Private)

The conversion script will by default automatically try to register new files with the OpenMSI site and assign them private to a single user if the output file is placed in the OpenMSI private data location:

```
python convertToOMSI.py <infile1> /project/projectdirs/openmsi/omsi_data_private/<username>/<filename
```

The username in the path will determine the user the file is assigned to. E.g: The filename will also be the name used in the listing on the site. In order to generate the HDF5 file without adding to the database, use the `--no-add-to-db` command line option, e.g,:

2.3 Changing file permissions:

Using the OpenMSI website the owner of the file can assign permissions to files online:

https://openmsi.nersc.gov/openmsi/resources/filemanager?file=<filename>

2.4 `convertToOMSI`: Usage and Options

NOTE: In order to view a current, complete list of conversions options use:

```
python convertToOMSI.py --help
```

```
python convertToOMSI.py --help
USAGE: Call "convertToOMSI [options] imgBaseFile1 imgBaseFile2 ... imgBaseFileN HDF5File"

This converter script takes the basename (i.e., path+basefilename) of a single
or multiple MSI files as input and converts them to HDF5. Each MSI file is
stored as a separate experiment in the output HDF5 file. If an input file
defines multiple regions, then those regions can either be stored as separate
datasets of the same experiment and/or merged to a single MSI dataset.
Using the various paramter settings described below, one can define how the
conversion should be performed, how the data should be stored in HDF5, and
indicate which analyses should be executed.

===HELPER OPTIONS===
--suggest-chunking : Iterate over all given input files and suggest a chunking strategy.
                     No data is converted when this option is given, i.e., no name for the
                     HDF5File should be given, but only input files should be listed.

===ERROR HANDLING OPTIONS===
--error-handling <options>: Define how errors should be handled. Options are:
                    i)   terminate-and-cleanup (default) : Terminate the conversion, delete the
                            the HDF5 file and do not add the file to the database.
                    ii)  terminate-only, : Leave the generated HDF5 output file in place but  do not
                             add the file to the database.
                    iii) continue-on-error: Ignore errors if possible and continue, even if this
                             means that some data may be missing from the output.
--email <email1 email2 ...>: Send notification in case of both error or success to the given email ad
--email-success <email1 email2 ...>>: Send notification in case of success to the given email address
--email-error <email1 email2 ...>>: Send notification in case of error to the given email address.

===INPUT DATA OPTIONS===

Default input data options: --format auto --regions split+merge
--format <option>: Define which file format is used as input. By default the program tries to
           automatically determine the input format. This option can be used to indicate
           the format explicitly to in case the auto option fails. Available options are:
          {'bruckerflex_file': <class 'omsi.dataformat.bruckerflex_file.bruckerflex_file'>, 'img_file
--regions <option>: Some file formats (e.g., brucker) allow multiple regions to be imaged and stored
           in a single file. This option allows one to specify how these regions should be
           treated during file conversion. E.g., one may want to store i) each region as a
           separate dataset in the output file (--regions split), ii) all regions combined
           in a single dataset (--regions merge), or both (--regions split+merge)
           Available options are:
          ['split', 'merge', 'split+merge']

===FILE WRITE OPTIONS===

---FILE WRITE OPTIONS: Chunking---

Default HDF5 Chunking options: Enabled by default using --auto-chunking :
--auto-chunking : Automatically decide which chunking should be used. This option
                automatically generates two copies of the data, one with a chunking
                optimized for selection of spectra and another one optimized for
                selection of ion image slices. All --chunking, --no-chunking, and
                --optimized-chunking options are ignored if this paramter is given
--chunking <x y z> : Use chunking when writing the HDF5 file. (DEFAULT, x=4,y=4,z=2048)
--no-chunking : Disable chunking when writing the HDF5 file. Use in combination with
```

```
                --no-compression since compression depends on chunking and will enable
                it if compression is used.
--optimized-chunking <x y z> : Use this option to generate additional copies of the data
                with different chunked data layouts. Generating multiple copies of the
                data with different chunked data layouts can be help accelerate selective
                data read opeations. (DEFAULT OFF). We recommend a spectra-aligned chunking
                for the raw data, e.g., '--chunking 1 1 32768' and an image-aligned chunked
                secondary copy of the data, e.g., '--optimzied-chunking 20 20 100'.

---FILE WRITE OPTIONS: Compression---
HDF5 Compression: Default ON using (gzip, 4):
--compression: Enable compression using (gzip,4). NOTE: Compression requires the use of chunking.
--no-compression: Disable the use of compression.

===I/O OPTIONS===
--io <option>: Available options are: ['chunk', 'spectrum', 'all']
             i) all : Read the full data in memory and write it at once
             ii) spectrum : Read one spectrum at a time and write it to the file.
             iii) chunk : Read one chunk at a time and write it to the file.

===DATABSE OPTIONS===

These options control whether the generated output file should be added to a server database
to manage web file access permissions
Default options are: --add-to-db --db-server http://openmsi.nersc.gov
--add-to-db : Add the output HDF5 file to the database.
--no-add-to-db : Disable adding the file to the database.
--db-server : Specify the online server where the file should be registers. Default is
              http://openmsi.nersc.gov
--owner : Name of the user that should be assigned as owner. By default the owner is
          determined automatically based on the file path.

===ANALYSIS OPTIONS===

NMF: Default ON: (nc=20, timeout=600, niter=2000, tolerance=0.0001, raw=False)
--nmf : Compute the nmf for all the input data files and store the results in the
        HDF5 file. NOTE: If global peak-finding (fpg) is performed, then
        nmf will be performed on the peak-cube, otherwise on the raw data
--no-nmf: Disable the execution of nmf
--nmf-nc <number>: Number of components to be computed by the NMF. (default nc=20)
--nmf-timeout <number>: Maximum time in seconds to be used for computing the NMF. (default timeout=6(
--nmf-niter <number>: Number of iterations (minimum is 2)(default niter=2000)
--nmf-tolerance <number>: Tolerance value for a relative stopping condition. (default tolerance=0.000
--nmf-raw <number>: Force execution of the NMF on the raw data. By default the results from
            the global peak finding (--fpg) are used to compute the NMF.

Global Peak Finding: Default ON:
--fpg : Compute the global peak finding for all input data files and save results
           in the HDF5 file (DEFAULT)
--no-fpg: Disable the global peak finding

Local Peak Finding: Default OFF:
--fpl : Compute the local peak finding for all input data files and save results
        in the HDF5 file
--no-fpl: Disable the local peak finding (DEFAULT)

---OTHER OPTIONS---
```

```
Generate Thumbnail image: Default OFF:
--thumbnail: Generate thumbnail image for the file based on, in order of availability:
             * The first three components of the NMF
             * The three most intense peaks from the global peak finding (fpg)
             * The three most intense peaks in the raw data that are at least 1 percent
               of the total m/z range apart.
--no-thumbnail: Do not generate a thumbnail image.

Generate XDMF header file for output file: Default OFF:
--xdmf: Write XDMF XML-based header-file for the output HDF5 file.
--no-xdmf: Do not generate a XDMF XML-based header for the HDF5 file.
```

CHAPTER

THREE

INTEGRATING NEW FILE FORMATS

3.1 Developing a file reader

In order to develop a new file reader we need to implement a corresponding class for the file format that inherits form `file_reader_base` (for formats that always contain a single region) or `file_reader_base_with_regions` (for formats that support multiple imaging regions in a single file). Both base classes are availble in the `omsi.dataformat.file_reader_base` module. The developer then needs to implement the following functions:

```
from omsi.dataformat.file_reader_base import file_reader_base

class formatname_file(file_reader_base):

    # 1. Implement the init function which must accept basename and requires_slicing as inputs
    def __init__(self, basename=None, requires_slicing=True):
        """
        basename : Name of the file/folder to be opened
        requires_slicing: Boolean indicating whether the user requires array slicing via
            the __getitem__ function to work or not. This is an optimization, because many MSI
            data formats do not easily support arbitrary slicing of data but rather only
            iteration over spectra.
        """
        super(formatname_file, self).__init__(basename, requires_slicing)  # 1.1 Call super __init__
        self.data_type = 'uint16'    # 1.2 Define the data type used
        self.shape = [0, 0, 0]       # 1.3 Define the shape of the dataset
        self.mz = 0                  # 1.4 Define the m/z axis

    # 2. Implement __getitem__
    def __getitem__(self, key):
        # Implement array-based slicing for the format so that the data can be read
        # via [x,y,z]

    # 3. Implement close_file
    def close_file(self):
        # Function called to close any open files when deleting the object

    # 4. Implement is_valid_dataset
    @classmethod
    def is_valid_dataset(cls, name):
        # Given the name of a file or directory, determine whether the given
        # data defines a valid dataset for the current format
```

For file formats that support multiple regions the implementation is aside from a few additions he same. The main difference are:

1. Inherit from `file_reader_base_with_regions` instead of `file_reader_base`
2. Set the `self.region_dicts` and `self.select_region` attributes in the `__init__` function
3. Implement the `set_region_selection` function

```
from omsi.dataformat.file_reader_base import file_reader_base_with_regions

class formatname_file(file_reader_base):

    # 1. Implement the init function which must accept basename and requires_slicing as inputs
    def __init__(self, basename=None, requires_slicing=True):
        super(formatname_file, self).__init__(basename, requires_slicing)  # 1.1 Call super __init__
        self.data_type = 'uint16'     # 1.2 Define the data type used
        self.shape = [0, 0, 0]        # 1.3 Define the shape of the dataset
        self.mz = 0                   # 1.4 Define the m/z axis
        self.region_dicts = []        # 1.5 Define a list of dicts where each dict describes
                                      #     the parameters of a region. In the simplest case
                                      #     of rectangular regions, a dict would specify the
                                      #     `origin` and `extends` of a region.
        self.select_region = None     # 1.6 Define the index of the selected region.
                                      #     Set to None to treat dataset as a whole (i.e.,
                                      #     merge all regions). If set to a region index,
                                      #     then the __getitem__ function is expected to
                                      #     behave as if the file consisted of just the
                                      #     selected region and the self.shape parameter
                                      #     must be set accordingly

    # 2-4: Implement the other functions of file_reader_base as described above.
    #      Note, __getitem__ must consider the value of self.select_region and
    #      treat any data requests as if they referred to the selected region
    #      only. Depending on the data format this may require transformation
    #      of the selection keys to locate the appropriate data

    # 5. Implement the set_region_selection function to allow a user to select a region
    def set_region_selection(self, region_index=None):
    """Define which region should be selected for local data reads.

       :param region_index: The index of the region that should be read. The shape of the
                data will be adjusted accordingly. Set to None to select all regions and
                treat the data as a single full 3D image.
    """
    # 5.1 Select all data
    if region_index is None:
        self.select_region = None           # 5.1.1 Set the region selection to None
        self.shape = self.full_shape        # 5.1.2 Define shape of the complete data
    # 5.2 Select a particular region
    elif region_index < self.get_number_of_regions():
        self.select_region = region_index   # 5.2.1 Set region index
        self.shape = ...                    # 5.2.2 Define the 3D shape of the region
```

3.2 Integrating the file reader with OpenMSI

Integrating a new file reader with OpenMSI is simple:

1. Add the file reader module to the `omsi.dataformat` format module and
2. Add the name of your module to the `__all__` variable in `omis.dataformat.__init__.py`

Once these steps are complete, the `omsi.dataformat.file_reader_base` module will automatically detect the new format and make it available as part of the file conversion script `omsi.tools.convertToOMSI`. To check which formats are registered, simply do:

```
>>> from omsi.dataformat import *
>>> formats = file_reader_base.file_reader_base.available_formats()
>>> print formats
{'bruckerflex_file': <class 'omsi.dataformat.bruckerflex_file.bruckerflex_file'>,
 'img_file': <class 'omsi.dataformat.img_file.img_file'>}
```

Using this basic feature makes it possible to easily iterate over all available formats and the consistent interface described by the `file_format_base` module allows us to use all the formats in a consistent manner (avoiding special cases). E.g., if we want to read a file of an unknown format we can simply:

```
from omsi.dataformat import *
formats = file_reader_base.file_reader_base.available_formats()
filename = 'my_unknown_file'
filereader = None
formatname = None
for fname, fclass in formats.items():
    if fclass.is_valid_dataset(filename):
        filereader = fclass
        formatname = fname
if filereader is not None:
    print "Using "+str(formatname)+" to read the file"
    openfile = filereader(basename=filename, requires_slicing=True)
```

CHAPTER

FOUR

DEVELOPING A NEW ANALYSIS FOR BASTET

4.1 Overview:

The OpenMSI Toolkit includes a basic template for implementing new analyses as part of OpenMSI. The template is located in `omsi.templates.omsi_analysis_template.py`. The template provides step-by-step instructions on how to implement a new analysis. Simply search top-to-bottom for EDIT_ME markers to find locations that need to be edited and what changes need to be made.

The implementation of a new analysis is divided into three main steps. We here provide a brief overview of these steps. A detailed walk-through the required implementation is provided in the following sections.

Step 1) Basic integration of your analysis with OpenMSI (Required)

The basic integration is simple and should requires only minimal additional effort. The basic integration with the OpenMSI provides:

- full integration of the analysis with the OpenMSI file format and API
- full support for OpenMSI's data provenance capabilities
- full integration with analysis drivers (e.g, the command line driver) enabling direct execution of the analysis with automatic handling of user input specification, help, etc.
- basic integration of the analysis with the website, in that a user will be able to browse the analysis in the online file browser. The basic integration automatically provides full support for the `qmetadata` and `qcube` URL data access patterns. The basic integration provides limited support for the `qslice`, `qspectrum`, and `qmz` patterns, in that it automatically exposes all dependencies of the analysis that support these patterns but it does not expose the data of the analysis itself. This is part of step 2.

Step 2) Integrating your analysis with the OpenMSI web-based viewer (Recommended)

Once the basic integration is complete, you may want integrate your analysis fully with the OpenMSI online viewer, in order to make your analysis easily accesible to the OpenMSI user community. This step requires the implementation of the `qslice`, `qspectrum`, and `qmz` URL patterns for the analysis. This step completes the integration with the OpenMSI framework itself.

Step 3) Making your analysis self-sufficient (Recommended)

This step makes your analysis "self-sufficient" in that it allows you to execute your analysis from the command-line.

4.1.1 Some important features of `analysis_base`

`omsi.analysis.analysis_base` is the base class for all omsi analysis functionality. The class provides a large set of functionality designed to facilitate i) storage of analysis data in the omsi HDF5 file format and ii) integration of new analysis capabilities with the OpenMSI web API and the OpenMSI web-based viewer (see Viewer functions

below for details), iii) support for data provenance, and iv) in combination with the *omsi_analysis_driver* module enable the direct execution of analysis, e.g, from the command line

Slicing

`analysis_base` implements basic slicing to access data stored in the main member variables. By default the data is retrieved from __data_list by the __getitem__(key) function, which implements the [..] operator, i.e., the functions returns __data_list[key]['data']. The key is a string indicating the name of the paramter to be retrieved. If the key is not found in the __data_list then the function will try to retrieve the data from __parameter_list instead. By adding "parameter/key" or "dependency/key" one may also explicitly retrieve values from the __parameter_list and __dependency_list.

Important Member Variables

- `analysis_identifier` defines the name for the analysis used as key in search operations.
- `__data_list` defines a list of `omsi.analysis.analysis_data.analysis_data` objects to be written to the HDF5 file. Derived classes need to add all data that should be saved for the analysis in the omsi HDF5 file to this dictionary. See `omsi.analysis.analysis_data` for details.
- `parameters` List of `parameter_data` to be written to the HDF5 file. Derived classes need to add all parameter data that should be saved for the analysis in the omsi HDF5 file to this dictionary using the provided `add_parameter(...)` function. See `omsi.analysis.analysis_data` and `add_parameter(..)` function of `analysis_base` for details.
- `data_names` is a list of strings of all names of analysis output datasets. These are the target names for __data_list. **NOTE** Names of parameters specified in `parameters` and `data_names` should be distinct.

I/O functions

These functions can be optionally overwritten to control how the analysis data should be written/read from the omsi HDF5 file. Default implementations are provided here, which should be sufficient for most cases.

- `write_analysis_data` By default all data is written by `omsi.dataformat.omsi_file.analysis.omsi_file_a`
  By implementing this function we can implement the write for the main data (i.e., what is stored in self.__data_list) ourselves. In practice (at least in the serial case) this should not be needed. However, overwriting the function can be useful when implementing an analysis using MPI and we want to avoid gathering the data on rank the root rank (usually rank 0).
- `add_custom_data_to_omsi_file`: The default implementation is empty as the default data write is managed by the omsi_file_experiment.create_analysis() function. Overwrite this function, in case that the analysis needs to write data to the HDF5 omsi file beyond what the defualt omsi data API does.
- `read_from_omsi_file`: The default implementation tries to reconstruct the original data as far as possible, however, in particular in case that a custom add_custom_data_to_omsi_file funtion has been implemented, the default implementation may not be sufficien. The default implementation reconstructs: i) analysis_identifier and reads all custom data into ii)__data_list. Note, an error will be raised in case that the analysis type specified in the HDF5 file does not match the analysis type specified by get_analysis_type(). This function can be optionally overwritten to implement a custom data read.

Web API Functions

Several convenient functions are used to allow the OpenMSI online viewer to interact with the analysis and to visualize it. The default implementations provided here simply indicate that the analysis does not support the data access

operations required by the online viewer. Overwrite these functions in the derived analysis classes in order to interface them with the viewer. All viewer-related functions start with `v\_...` .

NOTE: the default implementation of the viewer functions defined in `analysis_base` are designed to take care of the common requirement for providing viewer access to data from all depencies of an analysis. In many cases, the default implementation is often sill called at the end of custom viewer functions.

NOTE: The viewer functions typically support a viewerOption parameter. viewerOption=0 is expected to refer to the analysis itself.

- `v_qslice`: Retrieve/compute data slices as requested via qslice URL requests. The corrsponding view of the DJANGO data access server already translates all input parameters and takes care of generating images/plots if needed. This function is only responsible for retrieving the data.
- `v_qspectrum`: Retrieve/compute spectra as requested via qspectrum URL requests. The corrsponding view of the DJANGO data access server already translates all input parameters and takes care of generating images/plots if needed. This function is only responsible for retrieving the data.
- `v_qmz`: Define the m/z axes for image slices and spectra as requested by qspectrum URL requests.
- `v_qspectrum_viewer_options`: Define a list of strings, describing the different viewer options available for the analysis for qspectrum requests (i.e., `v_qspectrum`). This feature allows the analysis developer to define multiple different visualization modes for the analysis. For example, when performing a data rediction (e.g., PCA or NMF) one may want to show the raw spectra or the loadings vector of the projection in the spectrum view (v_qspectrum). By providing different viewer options we allow the user to decide which option they are most interested in.
- `v_qslice_viewer_options`: Define a list of strings, describing the different viewer options available for the analysis for qslice requests (i.e., `v_qslice`). This feature allows the analysis developer to define multiple different visualization modes for the analysis. For example, when performing a data rediction (e.g., PCA or NMF) one may want to show the raw spectra or the loadings vector of the projection in the spectrum view (v_qspectrum). By providing different viewer options we allow the user to decide which option they are most interested in.

Executing, saving, and restoring an analysis object

Using the command-line driver we can directly execute analysis as follows:

```
python omsi/analysis/omsi_analysis_driver <analysis_module_class> <analysis_parameters>
```

E.g. to execute a non-negative matrix factorization (NMF) using the *omsi.analysis.multivariate_stats.omsi_nmf* module we can simply:

```
python omsi/analysis/omsi_analysis_driver.py multivariate_stats/omsi_nmf.py
    --msidata "test_brain_convert.h5:/entry_0/data_0"
    --save "test_ana_save.h5"
```

Any analysis based on the infrastructure provided by `analysis_base` is fully integrated with OpenMSI file API provided by‘‘omsi.dataformat.omsi_file‘‘. This means the analysis can be directly saved to an OMSI HDF5 file and the saved analysis can be restored from file. In OMSI files, analyses are generally associated with experiments, so that we use the `omsi.dataformat.omsi_file.omsi_file_experiment` API here.

```
# Open the MSI file and get the desired experiment
from omsi.dataformat.omsi_file import *
f = omsi_file( filename, 'a' )
e = f.get_experiment(0)

# Execute the analysis
d = e.get_msidata(0)
```

```
a = omsi_myanalysis()
a.execute(msidata=d, integration_width=10, msidata_dependency=d)

# Save the analysis object.
analysis_object , analysis_index = exp.create_analysis( a )

# This single line is sufficient to store the complete analysis to the omsi file.
# By default the call will block until the write is complete. Setting the
# parameter flushIO=False enables buffered write, so that the call will
# return once all data write operations have been scheduled. Here we get
# an omsi.dataformat.omsi_file.omsi_file_analysis
# object for management of the data stored in HDF5 and the integer index of the analysis.

# To restore an analysis from file, i.e., read all the analysis data from file
# and store it in a corresponding analysis object we can do the following.
# Similar to the read_from_omsi_file(...) function of analysis_base
# mentioned below, we can decide via parameter settings of the function,
# which portions of the analysis should be loaded into memory
a2 = analysis_object.restore_analysis()

# If we want to now re-execute the same analysis we can simply call
a2.execute()

# If we want to rerun the analysis but change one or more parameter settings,
# then we can simply change those parameters when calling the execute function
d2 = e.get_msidata(1)    # Get another MSI dataset
a2.execute(msidata=d2)  # Execute the analysis on the new MSI dataset

# The omsi_file_analysis class also provides a convenient function that allows us
# to recreate, i.e., restore and run the analysis, in a single function call
a3 = analysis_object.recreate_analysis()

# The recreate_analysis(...) function supports additional keyword arguments
# which will be passed to the execute(...) call of the analysis, so that we
# can change parameter settings for the analysis also when using the
# recreate analysis call.

# If we know the type of analysis object (which we can also get from file), then we
# naturally also restore the analysis from file ourselves via
a4 = omsi_myanalysis().read_from_omsi_file(analysisGroup=analysis_object, \
                                           load_data=True, \
                                           load_parameters=True,\
                                           load_runtime_data=True, \
                                           dependencies_omsi_format=True )
# By setting load_data and/or load_parameters to False, we create h5py instead of
# numpy objects, avoiding the actual load of the data. CAUTION: To avoid the accidental
# overwrite of data we recommend to use load_data and load_parameters as False only
# when the file has been opened in read-only mode 'r'.

# Rerunning the same analysis again
a4.execute()
```

4.2 Integrating a new Analysis using the OpenMSI Analysis Template

4.2.1 Step 1) Basic integration

The simple steps outlined below provide you now with full integration of your analysis with the OpenMSI file format and API and full support for OpenMSI's data provenance capabilities. It also provides basic integration of your analysis with the OpenMSI website, in that a user will be able to browse your analysis in the online file browser. The basic integration also automatically provides full support for the `qmetadata` and `qcube` URL data access patterns, so that you can start to program against your analysis remotely. The basic integration provides limited support for the `qslice`, `qspectrum`, and `qmz` patterns, in that it automatically exposes all dependencies of the analysis that support these patterns but it does not expose the data of your analysis itself. This is part of step 2. Once you have completed the basic integation yout final analysis code should look something like this:

```
class omsi_mypeakfinder(analysis_base) :

    def __init__(self, name_key="undefined"):
        """Initalize the basic data members"""

        super(omsi_mypeakfinder,self).__init__()

        self.analysis_identifier = name_key
        # Define the names of the outputs generated by the analysis
        self.data_names = [ 'peak_cube' , 'peak_mz' ]

        # Define the input parameters of the analysis
        dtypes = self.get_default_dtypes()
        groups = self.get_default_parameter_groups()
        self.add_parameter(name='msidata',
                           help='The MSI dataset to be analyzed',
                           dtype=dtypes['ndarray'],
                           group=groups['input'],
                           required=True)
        self.add_parameter(name='mzdata',
                           help='The m/z values for the spectra of the MSI dataset',
                           dtype=dtypes['ndarray'],
                           group=groups['input'],
                           required=True)
        self.add_parameter(name='integration_width',
                           help='The window over which peaks should be integrated',
                           dtype=float,
                           default=0.1,
                           group=groups['settings'],
                           required=True)
        self.add_parameter(name='peakheight',
                           help='Peak height parameter',
                           dtype=int,
                           default=2,
                           group=groups['settings'],
                           required=True)


    def execute_analysis(self) :
        """..."""
        # Copy parameters to local variables. This is purely for convenience and is not mandatory.
        # NOTE: Input parameters are automatically record (i.e., we don't need to to anything specia
        msidata = self['msidata']
        mzdata = self['mzdata']
```

```
        integration_width = self['integration_width']
        peakheight = self['peakheight']

        # Implementation of my peakfinding algorithm

        ...

        # Return the result.
        # NOTE: We need to return the output in the order we specified them in self.data_names
        # NOTE: The outputs will be automatically recorded (i.e., we don't need to anything special)
        return peakCube, peakMZ
        self['peak_cube'] = peakCube

    ...

# Defining a main function is optional. However, allowing a user to directly execute your analysis
# from the command line is simple, as we can easily reuse the command-line driver module
if __name__ == "__main__":
    from omsi.analysis.omsi_analysis_driver import cl_analysis_driver
    cl_analysis_driver(analysis_class=omsi_mypeakfinder).main()
```

1.1 Creating a new analysis skeleton

- Copy the analysis template to the appropriate location where your analysis should live (NOTE: The analysis template may have been updated since this documentation was written). Any new analysis should be located in a submodule of the `omsi.analysis.` module. E.g., if you implement a new peak finding algorithm, it should be placed in omsi/analysis/findpeaks. For example:

```
cp omsi/templates/omsi_analysis_template.py openmsi-tk/omsi/analysis/findpeaks/omsi_mypeakfinder.py
```

- Replace all occurrences of `omsi_analysis_template` in the file with the name of your analysis class, e.g, omsi_mypeakfinder. You can do this easily using "Replace All" feature of most text editors. or on most Unix systems (e.g, Linux or MacOS) on the commandline via:

```
cd openmsi-tk/omsi/analysis/findpeaks
sed -i.bak 's/omsi_analysis_template/omsi_mypeakfinder/' omsi_mypeakfinder.py
rm omsi_mypeakfinder.py.bak
```

- Add your analysis to the `__init__.py` file of the python module where your analysis lives. In the `__init__.py` file you need to add the name of your analysis class to the `all__` list and add a an import of your class, e.g, `from omsi_mypeakfinder import *`. For example:

```
all__ = [ "omsi_mypeakfinder",  "omsi_findpeaks_global" , ...]
from omsi_findpeaks_global import *
from omsi_findpeaks_local import *
...
```

- The analysis template contains documentation on how to implement a new analysis. Simply search for *EDIT_ME* to locate where you should add code and descriptions of what code to add.

1.2 Specifying analysis inputs and outputs

In the `__init__` function specify the names of the input parameters of your analysis as well as the names of the output data generated by your analysis. Note, the `__init__` function should have a signature that allows us to instantiate the analysis without having to provide any inputs. E.g.,

```
def __init__(self, name_key="undefined"):
    """Initalize the basic data members"""

    super(omsi_mypeakfinder,self).__init__()
    self.analysis_identifier = name_key

    # Define the names of the outputs
    self.data_names = ['peak_cube', 'peak_mz']

    # Define the input parameters
    dtypes = self.get_default_dtypes()  # List of default data types. Build-in types are
                                        # available as well but can be safely used directly as well
    groups = self.get_default_parameter_groups() # List of default groups to organize parameters. We
                                                 # to use the 'input' group for all input data to be
                                                 # as this will make the integration with OpenMSI eas
    self.add_parameter(name='msidata',
                       help='The MSI dataset to be analyzed',
                       dtype=dtypes['ndarray'],
                       group=groups['input'],
                       required=True)
    self.add_parameter(name='mzdata',
                       help='The m/z values for the spectra of the MSI dataset',
                       dtype=dtypes['ndarray'],
                       group=groups['input'],
                       required=True)
    self.add_parameter(name='integration_width',
                       help='The window over which peaks should be integrated',
                       dtype=float,
                       default=0.1,
                       group=groups['settings'],
                       required=True)
    self.add_parameter(name='peakheight',
                       help='Peak height parameter',
                       dtype=int,
                       default=2,
                       group=groups['settings'],
                       required=True)
```

1.3: Implementing the `execute_analysis` function

1.3.1 Document your execute_analysis function. OpenMSI typically uses Sphynx notation in the doc-string. The doc-string of the execute_analysis(..) function and the class are used by the analysis driver modules to provide a description of your analysis as part of the help and will also be included in the help string generated by the *get_help_string()* inherited via *analysis_base* function.

```
def execute_analysis(self) :
    """This analysis computes global peaks in MSI data...
    """
```

1.3.2 Implement your analysis. For convenience it is often useful to assign the your parameters to local variables, although, this is by no means required. Note, all values are stored as 1D+ numpy arrays, however, are automatically converted for you, so that we can just do:

```
integration_width = self['integration_width']
```

1.3.4 Return the outputs of your analysis in the same order as specified in the *self.data_names* you specified in your *__init__* function (here *['peak_cube', 'peak_mz']*):

```
return peakCube, peakMZ
```

Results returned by your analysis will be automatically saved to the respective output variables. This allows users to conveniently access your results and it enables the OpenMSI file API to save your results to file. We here automatically convert single scalars to 1D numpy arrays to ensure consistency. Although, the data write function can handle a large range of python built_in types by automatically converting them to numpy for storage in HDF5, we generally recommend to convert use numpy directly here to save your data.

With this you have now completed the basic integration of your analysis with the OpenMSI framework.

4.2.2 Step 2) Integrating the Analysis with the OpenMSI Web API:

Once the analysis is stored in the OMSI file format, integration with `qmetadata` and `qcube` calls of the web API is automatic. The `qmetadata` and `qcube` functions provide general purpose access to the data so that we can immediatly start to program against our analysis.

Some applications—such as the OpenMSI web-based viewer—utilize the simplified, special data access patterns `qslice`, `qspectrum`, and `qmz` in order to interact with the data. The default implementation of these function available in `omsi.analysis.analysis_base` exposes the data from all depencdencies of the analysis that support these patterns. For full integration with the web API, however, we need to implement this functionality in our analysis class. The `qmz` pattern in particular is relevant to both the `qslice` and `qspectrum` pattern and should be always implemented as soon as one of the two patterns is defined.

2.1 Implementing the `qslice` pattern

```
class omsi_myanalysis(analysis_base) :
    ...

    @classmethod
    def v_qslice(cls , anaObj , z , viewer_option=0) :
        """Implement support for qslice URL requests for the viewer

           anaObj: The omsi_file_analysis object for which slicing should be performed.
           z: Selection string indicting which z values should be selected.
           viewer_option: An analysis can provide different default viewer behaviors
                          for how slice operation should be performed on the data.
                          This is a simple integer indicating which option is used.

           :returns: numpy array with the data to be displayed in the image slice
                     viewer. Slicing will be performed typically like [:,:,zmin:zmax].

        """
        from omsi.shared.omsi_data_selection import *
        #Implement custom analysis viewer options
        if viewer_option == 0 :
            dataset =  anaObj[ 'labels' ] #We assume labels was a 3D image cube of labels
            zselect = selection_string_to_object(z)
            return dataset[ : , :, zselect ]

        #Expose recursively the slice options for any data dependencies. This is useful
        #to allow one to trace back data and generate comlex visualizations involving
        #multiple different data sources that have some from of dependency in that they
        #led to the generation of this anlaysis. This behavior is already provided by
        #the default implementation of this function ins analysis_base.
        elif viewer_option >= 0 :
```

```
            #Note, the base class does not know out out viewer_options so we need to adjust
            #the vieweOption accordingly by substracting the number of our custom options.
            return super(omsi_myanalysis,cls).v_qslice( anaObj , z, viewer_option-1)
        #Invalid viewer_option
        else :
            return None

    @classmethod
        def v_qslice_viewer_options(cls , anaObj ) :
            """Define which viewer_options are supported for qspectrum URL's"""
            #Get the options for all data dependencies
            dependent_options = super(omsi_findpeaks_global,cls).v_qslice_viewer_options(anaObj)
            #Define our custom viewer options
            re = ["Labels"] + dependent_options
            return re
```

NOTE: We here convert the selection string to a python selection (i.e., a list, slice, or integer) object using the `omsi.shared.omsi_data_selection.check_selection_string(...)` . This has the advantage that we can use the given selection directly in our code and avoids the use of a potentially dangerous `eval` , e.g., `return eval("dataset[:,:, %s]" %(z,))` . While we can also check the validity of the seletion string using `omsi.shared.omsi_data_selection.check_selection_string(...)` , it is recommened to convert the string to a valid python selection to avoid possible attacks.

2.2 Implementing the `qspectrum` pattern

```
class omsi_myanalysis(analysis_base) :
    ...
    @classmethod
    def v_qspectrum( cls, anaObj , x, y , viewer_option=0) :
        """Implement support for qspectrum URL requests for the viewer.

            anaObj: The omsi_file_analysis object for which slicing should be performed
            x: x selection string
            y: y selection string
            viewer_option: If multiple default viewer behaviors are available for a given
                           analysis then this option is used to switch between them.

            :returns: The following two elemnts are expected to be returned by this function :

                1) 1D, 2D or 3D numpy array of the requested spectra. NOTE: The spectrum axis,
                e.g., mass (m/z), must be the last axis. For index selection x=1,y=1 a 1D array
                is usually expected. For indexList selections x=[0]&y=[1] usually a 2D array
                is expected. For range selections x=0:1&y=1:2 we one usually expect a 3D array.
                This behavior is consistent with numpy and h5py.

                2) None in case that the spectra axis returned by v_qmz are valid for the
                returned spectrum. Otherwise, return a 1D numpy array with the m/z values
                for the spectrum (i.e., if custom m/z values are needed for interpretation
                of the returned spectrum).This may be needed, e.g., in cases where a
                per-spectrum peak analysis is performed and the peaks for each spectrum
                appear at different m/z values.

            Developer Note: h5py currently supports only a single index list. If the user provides
            an index-list for both x and y, then we need to construct the proper merged list and
            load the data manually, or, if the data is small enough, one can load the full data
            into a numpy array which supports mulitple lists in the selection. This, however, is
            only recommended for small datasets.
```

```
        """

        data = None
        customMZ = None
        if viewer_option == 0 :
            from omsi.shared.omsi_data_selection import *
            dataset =  anaObj[ 'labels' ]
            if (check_selection_string(x) == selection_type['indexlist']) and  \
               (check_selection_string(y) == selection_type['indexlist']) :
                #Assuming that the data is small enough, we can handle the multiple list
                #selection case here just by loading the full data use numpy to do the
                #subselection. Note, this version would work for all selection types but
                #we would like to avoid loading the full data if we don't have to.
                xselect = selection_string_to_object(x)
                yselect = selection_string_to_object(y)
                data = dataset[:][xselect,yselect,:]
                #Since we alredy confirmed that both selection strings are index lists we could
                #also just do an eval as follows.
                #data = eval("dataset[:][%s,%s, :]" %(x,y))
            else :
                xselect = selection_string_to_object(x)
                yselect = selection_string_to_object(y)
                data = dataset[xselect,yselect,:]
            #Return the spectra and indicate that no customMZ data values (i.e. None) are needed
            return data, None
        #Expose recursively the slice options for any data dependencies. This is useful
        #to allow one to trace back data and generate comlex visualizations involving
        #multiple different data sources that have some from of dependency in that they
        #led to the generation of this anlaysis. This behavior is already provided by
        #the default implementation of this function ins analysis_base.
        elif viewer_option >= 0 :
            #Note, the base class does not know out out viewer_options so we need to adjust
            #the vieweOption accordingly by substracting the number of our custom options.
            return super(omsi_findpeaks_global,cls).v_qspectrum( anaObj , x , y, viewer_option-1)

        return data , customMZ

    @classmethod
    def v_qspectrum_viewer_options(cls , anaObj ) :
        """Define which viewer_options are supported for qspectrum URL's"""
        #Get the options for all data dependencies
        dependent_options = super(omsi_findpeaks_global,cls).v_qspectrum_viewer_options(anaObj)
        #Define our custom viewer options
        re = ["Labels"] + dependent_options
        return re
```

2.3 Implementing the `qmz` pattern

```
class omsi_myanalysis(analysis_base) :
    ...

    @classmethod
        def v_qmz(cls, anaObj, qslice_viewer_option=0, qspectrum_viewer_option=0) :
            """Implement support for qmz URL requests for the viewer.

                Get the mz axes for the analysis
```

```
            anaObj: The omsi_file_analysis object for which slicing should be performed.
            qslice_viewer_option: If multiple default viewer behaviors are available for
                        a given analysis then this option is used to switch between them
                        for the qslice URL pattern.
            qspectrum_viewer_option: If multiple default viewer behaviors are available
                        for a given analysis then this option is used to switch between
                        them for the qspectrum URL pattern.

            :returns: The following four arrays are returned by the analysis:

              - mzSpectra : 1D numpy array with the static mz values for the spectra.
              - labelSpectra : String with lable for the spectral mz axis
              - mzSlice : 1D numpy array of the static mz values for the slices or
                          None if identical to the mzSpectra array.
              - labelSlice : String with label for the slice mz axis or None if
                             identical to labelSpectra.
              - valuesX: The values for the x axis of the image (or None)
              - labelX: Label for the x axis of the image
              - valuesY: The values for the y axis of the image (or None)
              - labelY: Label for the y axis of the image
              - valuesZ: The values for the z axis of the image (or None)
              - labelZ: Label for the z axis of the image

             Developer Note: Here we need to handle the different possible combinations
             for the differnent viewer_option patterns. It is in general safe to populate
             mzSlice and lableSlice also if they are identical with the spectrum settings,
             however, this potentially has a significant overhead when the data is transfered
             via a slow network connection, this is why we allow those values to be None
             in case that they are identical.

        """
        #The four values to be returned
        mzSpectra =  None
        labelSpectra = None
        mzSlice = None
        labelSlice = None
        peak_cube_shape = anaObj[ 'labels' ].shape #We assume labels was a 3D image cube of labe
        valuesX = range(0, peak_cube_shape[0])
        labelX = 'pixel index X'
        valuesY = range(0, peak_cube_shape[1])
        labelY = 'pixel index Y'
        valuesZ = range(0, peak_cube_shape[2]) if len(peak_cube_shape) > 3 else None
        labelZ = 'pixel index Z' if len(peak_cube_shape) > 3 else None

        #Both qslice and qspectrum here point to our custom analysis
        if qspectrum_viewer_option == 0 and qslice_viewer_option==0: #Loadings
            mzSpectra =  anaObj[ 'labels' ][:]
            labelSpectra = "Labels"
        #Both viewer_options point to a data dependency
        elif qspectrum_viewer_option > 0 and qslice_viewer_option>0 :
            mzSpectra, labelSpectra, mzSlice, labelSlice = \
                   super(omsi_findpeaks_global,cls).v_qmz( anaObj, \
                         qslice_viewer_option-1 , qspectrum_viewer_option-1)
        #Only the a qlice options point to a data dependency
        elif qspectrum_viewer_option == 0 and qslice_viewer_option>0 :
            mzSpectra =  anaObj[ 'peak_mz' ][:]
            labelSpectra = "m/z"
```

```
                tempA, tempB, mzSlice, labelSlice, valuesX, labelX, valuesY, labelY, valuesZ, labelZ
                        super(omsi_findpeaks_global,cls).v_qmz( anaObj, \
                                qslice_viewer_option-1 , 0)
            #Only the qspectrum option points to a data dependency
            elif qspectrum_viewer_option > 0 and qslice_viewer_option==0 :
                mzSlice =  anaObj[ 'peak_mz' ][:]
                labelSlice = "m/z"
                # Ignore the spatial axes and slize axis as we use our own
                mzSpectra, labelSpectra, tempA, tempB, vX, lX, vY, lY, vZ, lZ = \
                        super(omsi_findpeaks_global,cls).v_qmz( anaObj, \
                                0 , qspectrum_viewer_option-1)

            return mzSpectra, labelSpectra, mzSlice, labelSlice, valuesX, labelX, valuesY, labelY, va
```

4.2.3 Step 3) Making your analysis self-sufficient

Making your analysis self sufficient is trivial. If you used the analysis template provided by the toolkit, then you have already completed this step for free. In order to allow a user to run our analysis from the command line we need a main function. We here can simply reuse the command line driver provided by the toolkit. Using the command line driver we can run the analysis via:

```
python omsi/analysis/omsi_analysis_driver.py findpeaks.omsi_mypeakfinder
    --msidata "test_brain_convert.h5:/entry_0/data_0"
    --mzdata "test_brain_convert.h5:/entry_0/data_0/mz"
    --save "test_ana_save.h5"
```

To now enable us to execute our analysis module itself we simply need to add the following code (which is already part of the template)

```
if __name__ == "__main__":
    from omsi.analysis.omsi_analysis_driver import cl_analysis_driver
    cl_analysis_driver(analysis_class=omsi_mypeakfinder).main()
```

With this we can now directly execute our analysis from the command line, get a command-line help, specify all our input parameters on the command line, and save our analysis to file. To run the analysis we can now do:

```
python omsi/analysis/findpeaks/omsi_findpeaks_global.py
    --msidata "test_brain_convert.h5:/entry_0/data_0"
    --mzdata "test_brain_convert.h5:/entry_0/data_0/mz"
    --save "test_ana_save.h5"
```

This will run our peak finder on the given input data and save the result to the first experiment in the test_ana_save.h5 (the output file will be automatically created if it does not exist).

The command line driver also provides us a well-formated help based on the our parameter specification and the doc-string of the analysis class and its execute_analysis(...) function. E.g:

```
>>> python omsi/analysis/findpeaks/omsi_findpeaks_global.py --help

usage: omsi_findpeaks_global.py [-h] [--save SAVE] --msidata MSIDATA --mzdata
                                MZDATA [--integration_width INTEGRATION_WIDTH]
                                [--peakheight PEAKHEIGHT]
                                [--slwindow SLWINDOW]
                                [--smoothwidth SMOOTHWIDTH]

class description:

```

```
    Basic global peak detection analysis. The default implementation
    computes the peaks on the average spectrum and then computes the peak-cube data,
    i.e., the values for the detected peaks at each pixel.

    TODO: The current version assumes 2D data


execution description:

        Execute the global peak finding for the given msidata and mzdata.


optional arguments:
  -h, --help            show this help message and exit
  --save SAVE           Define the file and experiment where the analysis
                        should be stored. A new file will be created if the
                        given file does not exists but the directory does. The
                        filename is expected to be of the from:
                        <filename>:<entry_#> . If no experiment index is
                        given, then experiment index 0 (i.e, entry_0) will be
                        assumed by default. A validpath may, e.g, be
                        "test.h5:/entry_0" or jus "test.h5" (default: None)

analysis settings:
  Analysis settings

  --integration_width INTEGRATION_WIDTH
                        The window over which peaks should be integrated
                        (default: 0.1)
  --peakheight PEAKHEIGHT
                        Peak height parameter (default: 2)
  --slwindow SLWINDOW   Sliding window parameter (default: 100)
  --smoothwidth SMOOTHWIDTH
                        Smooth width parameter (default: 3)

input data:
  Input data to be analyzed

  --msidata MSIDATA     The MSI dataset to be analyzed (default: None)
  --mzdata MZDATA       The m/z values for the spectra of the MSI dataset
                        (default: None)

how to specify ndarray data?
----------------------------
n-dimensional arrays stored in OpenMSI data files may be specified as
input parameters via the following syntax:
      -- MSI data: <filename>.h5:/entry_#/data_#
      -- Analysis data: <filename>.h5:/entry_#/analysis_#/<dataname>
      -- Arbitrary dataset: <filename>.h5:<object_path>
E.g. a valid definition may look like: 'test_brain_convert.h5:/entry_0/data_0'
In rear cases we may need to manually define an array (e.g., a mask)
Here we can use standard python syntax, e.g, '[1,2,3,4]' or '[[1, 3], [4, 5]]'

This command-line tool has been auto-generated using the OpenMSI Toolkit
```

4.3 Advanced: Customizing core features

4.3.1 Custom data save

In most cases the default data save and restore functions should be sufficient. However, the `analysis_base` API also supports implementation of custom HDF5 write. To extend the existing data write code, simple implement the following function provided by `analysis_base` .

```
def add_custom_data_to_omsi_file(self , analysisGroup) :
    """This function can be optionally overwritten to implement a custom data write
       function for the analysis to be used by the omsi_file API.

       Note, this function should be used only to add additional data to the analysis
       group. The data that is written by default is typically still written by the
       omsi_file_experiment.create_analysis() function, i.e., the following data is
       wirtten by default: i) analysis_identifier ,ii) get_analysis_type,
       iii)__data_list, iv) __parameter_list , v) __dependency_list. Since the
       omsi_file.experiment.create_analysis() functions takes care of setting up the
       basic structure of the analysis storage (included the subgroubs for storing
       parameters and data dependencies) this setup can generally be assumed to exist
       before this function is called. This function is called automatically at the
       end omsi_file.experiment.create_analysis() (i.e, actually
       omsi_file_analysis.__populate_analysis__(..)) so that this function does not need
       to be called explicitly.

       Keyword Arguments:

       :param analysisGroup: The omsi_file_analysis object of the group for the
                             analysis that can be used for writing.

       """
    pass
```

4.3.2 Custom analysis restore

Similarly in order implement custom data restore behavior we can overwrite the default implementation of `omsi.analysis.analysis_base.analysis_base.read_from_omsi_file()` . In this case one will usually call the default implementation via `super(omsi_myanalysis,self).read_from_omsi_file(...)` first and then add any additional behavior.

4.3.3 Custom analysis execution

Analysis are typically executed using the `omsi.analysis.analysis_base.analysis_base.execute()` function we inherit from py:class:*omsi.analysis.analysis_base.analysis_base*. The `execute()` function controls many pieces, from recording and defining input parameters and outputs to executing the actual analysis. We, therefore, for NOT recommend to overwrite the `exceute(..)` function, but rather to customize specific portions of the execution. To do this, *execute()* is broken into a number of functions which are called in a specific order. In this way we can easily overwrite select functions to customize a particular feature without having to overwrite the complete `execute(..)` function.

Customizing setting of parameters

First, the execute function uses `omsi.analysis.analysis_base.analysis_base.update_analysis_parameters()` to set all parameters that have been passed to execute accordingly. The default implementation of `update_analysis_parameters(..)`, hence, simply calls `self.set_parameter_values(...)` to set all parameter values. We can customize this behavior simply by overwriting the `update_analysis_parameters(...)` function.

Customizing setting of default settings

Second, the execute function uses the `omsi.analysis.analysis_base.analysis_base.define_missing_parameter` function to set any required parameters that have not been set by the user to their respective values. Overwrite this function to customize how default parameter values are determined/set.

Customizing the recording of runtime information

The recording of runtime information is performed using the `omsi.shared.run_info_data.run_info_dict()` data structure. This data structure provides a series of functions that are called in order, in particular:

- `omsi.shared.run_info_data.run_info_dict.clear()` : This function is called first to clear the runtime dictionary. This is the same as the standard dict.clear.
- `omsi.shared.run_info_data.run_info_dict.record_preexecute()` : This function is called before the `execute_analysis` function is called and records basic system information,
- `omsi.shared.run_info_data.run_info_dict.record_postexecute()` : This function is called after the `execute_analysis` function has completed to record additional information, e.g, the time and duration of the analysis,
- `omsi.shared.run_info_data.run_info_dict..runinfo_clean_up()` : This function is called at the end to clean up the recorded runtime information. By default, `runinfo_clean_up()` removes any empty entries, i.e., key/value pairs where the value is either None or an empty string.

We can customize any of these function by implementing a derived class of `omsi.shared.run_info_data.run_info_dict()` where we can overwrite the functions. In order to use our derived class we can then assign our object to `omsi.analysis.analysis_base.analysis_base.run_info()`. This design allows us to modularly use the runtime information tracking also for other tasks, not just with our analysis base infrastructure.

Customizing the analysis execution

The analysis is completely implemented in the `omsi.analysis.analysis_base.analysis_base.execute_analysis()` function, which we have to implement in our derived class, i.e, running the analysis is fully custom anyways.

Customizing the recording of analysis outputs

Finally (i.e., right before returning analysis results), `execute(..)` uses the `omsi.analysis.analysis_base.analysis_base.record_execute_analysis_outputs()` function to save all analysis outputs. Analysis outputs are stored in the self.__data_list variable. We can save analysis outputs simply by slicing and assignment, e.g., *self[output_name] = my_output*. By overwriting *record_execute_analysis_outputs(...)* we can customize the recording of data outputs.

4.4 Wrapping a function: The quick-and-dirty way

Sometimes developers just want to debug some analysis function or experiment with different variants of a code. At the same time, we want to be able to track the results of these kind of experiments in a simple fashion. The *omsi.analysis.generic()* provides us with such a quick-and-dirty solution. We say quick-and-dirty because it sacrifices some generality and features in favor for a very simple process.

Using the *omsi.analysis.generic.analysis_generic.from_function()* or *omsi.analysis.generic.bastet_analysis()* decorator, we can easily construct a generic *omsi.analysis.base.analysis_base* instance container object for a given function. We can then use this container object to execute our function, while tracking its provenance as well as save the results to file as we would with any other analysis object. This approach allows us to easily track, record, safe, share and reproduce code experiments with only minimal extra effort needed. Here we briefly outline the two main options to do this:

4.4.1 Option 1: Explicitly track specific excutions of a function

Instead of calling our analysis function `f()` directly, we create an instance of *omsi.analysis.generic.analysis_generic()* via `g = analysis_generic.from_function(f)` which we then use instead of our function. To execute our function we can now either call `g.execute(...)` as usual or treat `g` as a function and call it directly `g(...)`

```
import numpy as np
from omsi.analysis.generic import analysis_generic

# Define some example function we want to wrap to track results
def mysum(a):
    return np.sum(a)

# Create an analysis object for our function
g = analysis_generic.from_function(mysum)
g.execute(np.arange(10))  # This is the same as:  g(np.arange(10))
```

4.4.2 Option 2: Implicitly track the last execution of a function

If we are only interested in recording the last execution of our function, then we can alternatively wrap our function directly using the `@bastet_analysis` decorator. The main difference between the two approaches is that using the decorator we only record the last execution of our function, while using the explicit approach of option 1, we can create as many wrapped instances of our functions as we want and track the execution of each independently.

```
import numpy as np
from omsi.shared.log import log_helper
log_helper.set_log_level('DEBUG')
from omsi.analysis.generic import bastet_analysis
from omsi.dataformat.omsi_file.main_file import omsi_file

# Define some example function and wrap it
@bastet_analysis
def mysum(a):
    """Our own sum function"""
    return np.sum(a)

# Execute the analysis
res = mysum(a=np.arange(10))
```

4.4.3 Example 1: Defining and using wrapped functions

The code example shown below illustrates the "wrapping" of a simple example function `mysum(a)`, which simply uses `numpy.sum` to compute the sum of objects in an array. (NOTE: We could naturally also use `numpy.sum` directly, we use `mysum(a)` mainly to illustrate that this approach also works wit functions defined in the interpreter.)

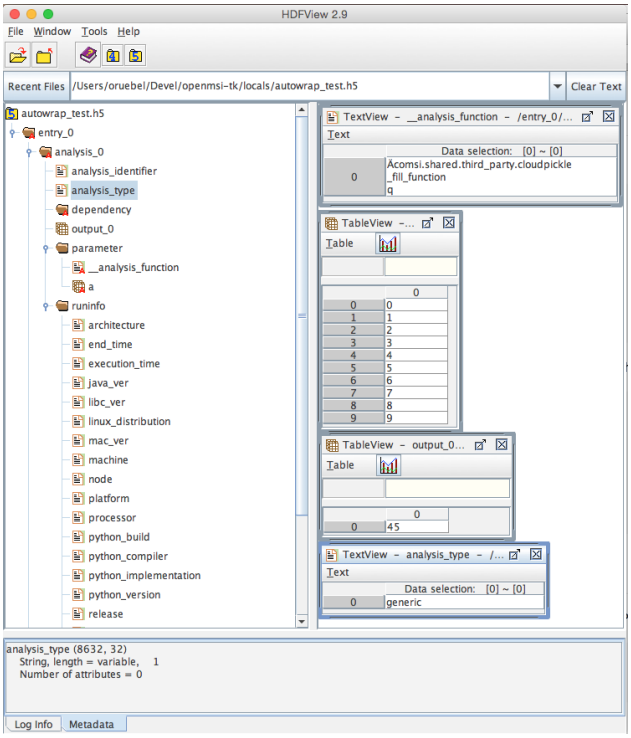
```
import numpy as np
from omsi.shared.log import log_helper
log_helper.set_log_level('INFO')
from omsi.analysis.generic import analysis_generic
from omsi.dataformat.omsi_file.main_file import omsi_file

# Define some example function we want to wrap to track results
def mysum(a):
    return np.sum(a)

# Create an analysis object for our function
g = analysis_generic.from_function(mysum)

# Execute the analysis
res = g.execute(a=np.arange(10))
log_helper.log_var(__name__, res=res)  # Logging the result

# Save the analysis to file
f = omsi_file('autowrap_test.h5', 'a')
e = f.create_experiment()
exp_index = e.get_experiment_index()
ana_obj, ana_index = e.create_analysis(g)
# Close the file
f.flush()
del f

# Restore the analysis from file
f = omsi_file('autowrap_test.h5', 'a')
e = f.get_experiment(exp_index)
a = e.get_analysis(ana_index)
g2 = a.restore_analysis()
res2 = g2.execute()
log_helper.log_var(__name__, res2=res2)  # Logging the result
if res == res2:
    log_helper.info(__name__, "CONGRATULATIONS---The results matched")
else:
    log_helper.error(__name__, "SORRY---The results did not match")
```

When we run our script, we can see that we were able to successfully capture the execution of our function and recreate the analysis from file.

```
machine:dir username$ python autowrap_function.py
2015-09-29 15:21:32,729 - __main__ - INFO - res = 45
2015-09-29 15:21:32,778 - __main__ - INFO - res2 = 45
2015-09-29 15:21:32,778 - __main__ - INFO - CONGRATULATIONS---The results matched
```

The figure below shows a view of the file generated by our wrapped function execution example shown above.

Note, we can use the wrapped function objects as usual in an analysis workflow to combine our functions with other analyses. For example, the simple example shown below shows how we can quickly define a simple filter to set all intensities that are less than 10 to a value of 0 before executing an analysis. We here first execute global peak finding to reduce the data, than apply a simple wrapped filter function to filter the data values, and then compute NMF on the filtered data.




```
from omsi.dataformat.omsi_file import *
from omsi.analysis.findpeaks.omsi_findpeaks_global import omsi_findpeaks_global
from omsi.analysis.multivariate_stats.omsi_nmf import omsi_nmf
from omsi.analysis.generic import analysis_generic
import numpy as np

f = omsi_file('/Users/oruebel/Devel/openmsi-data/msidata/20120711_Brain.h5' , 'r')
d = f.get_experiment(0).get_msidata(0)

# Specify the analysis workflow
a1 = omsi_findpeaks_global()
a1['msidata'] = d
a1['mzdata'] = d.mz

# Wrap a simple function to filter all peaks with less than 10 counts
def f(a):
    a[a<10] = 0
    return a
a2 = analysis_generic.from_function(f)
a2['a'] = a1['peak_cube']    # Use the peak_cube from a1 as input for the filter

# Create an NMF for the filtered data
a3 = omsi_nmf()
a3['msidata'] = a2['output_0']  # Make the output of our analysis the input of the NMF
a3['numIter'] = 2

# Run our simple workflow, i.e.,: peak_finder --> our_filter --> nmf
a3.execute_recursive()
```

By default, the outputs are named and numbered using the schema `output_#`, i.e., in the above example we used `a2['output_0']` to access the output our wrapped function. To define user-defined names for the out-

puts of a wrapped function we can simply provide a list of strings to the input parameter `output_names` of the `analysis_generic.from_function(...)`.

NOTE: Wrapping functions directly is not recommended for production workflows but is intended for development and debugging purposes only. This mechanism relies on that the library does the right thing in automatically determining input parameters, outputs, and their types and that we can handle all those types in the end-to-end process, from definition to storage. We do our best to make this mechanism work with a broad set of cases but we do not guarantee that the simple wrapping always work.

CHAPTER

FIVE

DEFINING AND EXECUTING ANALYSIS WORKFLOWS

Figure *Illustration of an example workflow for image normalization*, illustrates the basic steps of using analysis workflows, i.e,.:

1. Create the analysis tasks
2. Define the analysis inputs
3. Execute

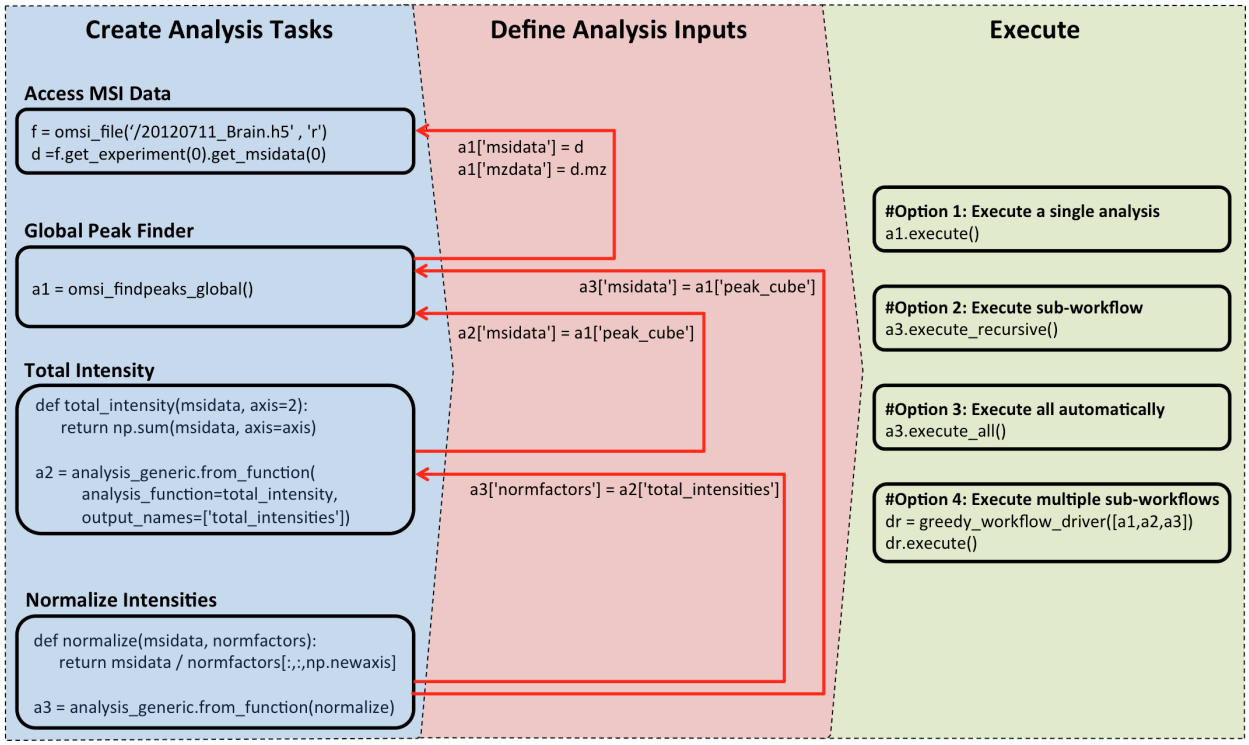


Fig. 5.1: Illustration of an example workflow for image normalization

In the following we will use a simple analysis—workflow in which we compute a peak-cube from a raw MSI dataset and then compute an NMF from the peak cube—to illustrate the main steps involved for performing complex analysis workflows.

5.1 Step 1: Create the analysis tasks:

First we need to create our main analysis objects.

```
from omsi.dataformat.omsi_file import *
from omsi.analysis.findpeaks.omsi_findpeaks_global import omsi_findpeaks_global
from omsi.analysis.multivariate_stats.omsi_nmf import omsi_nmf

# Open a file to get some MSI data
f = omsi_file('/Users/oruebel/Devel/openmsi-data/msidata/20120711_Brain.h5' , 'r')
d = f.get_experiment(0).get_msidata(0)

# Specify the analysis workflow
# Create a global peak finding analysis
a1 = omsi_findpeaks_global()       # Create the analysis
# Create an NMF that processes our peak cube
a2['numIter'] = 2                  # Set input to perform 2 iterations only
```

5.2 Step 2: Define analysis inputs:

We can define the input parameters of analysis simply using standard dict-like assignment. Any dependencies between analysis tasks or OpenMSI files are created automatically for us.

```
# Define the inputs of the global peak finder
a1['msidata'] = d                  # Set the input msidata
a1['mzdata'] = d.mz                # Set the input mz data
# Define the inputs of the NMF
a2['msidata'] = a1['peak_cube']    # Set the input data to the peak cube
a2['numIter'] = 2                  # Set input to perform 2 iterations only
```

NOTE: So far we have only specified our workflow. We have not executed any analysis yet, nor have we loaded any actual data yet.

5.3 Step 3: Execute

Finally we need to execute our analyses. For this we have various options, depending on which parts of our workflow we want to execute.

5.3.1 Executing a single analysis

To execute a single analysis, we can simply call the `execute()` function of our analysis. Note, the execute may raise and `AnalysisReadyError` in case that the inputs of the analsis are not ready. E.g.:

```
a2.execute()    # Will fail with ``AnalysisReadyError``
```

```
a1.execute()    # Will successfully execute a1
```

5.3.2 Executing a single sub-workflow

To execute a single analysis including any missing dependencies, we can simply call the `execute_recursive()` function. E.g.:

```
a2.execute_recursive()    # Will successfully execute a1
```

The above will execute `a1` as well as `a2` since `a2` depends on `a1`.

NOTE: Recursive execution will only execute other analyses that are actually needed to complete our analysis and analysis results of dependent analyses that have been executed before will be reused. E.g., if we would call `a2.execute_recursive()` again, then only `a2` would be executed again.

NOTE: When executing multiple dependent analyses, then the execution is typically controlled by a workflow executor py:meth:*omsi.workflow.executor*. By default, `execute_recursive(..)` will automatically create a default driver. If we want to customize the driver to be used then we can simply assign a driver to the analysis before-hand by setting the py:var:*omsi.analysis.base.analysis_base.driver*‘ instance variable.

5.3.3 Executing all analyses

To run all analyses that have been created—independent of whether they depend on each other or not—we can simply call *omsi.analysis.base.analysis_base.execute_all()*.

```
a1.execute_all()    # Execute all analyses
```

The above will execute any analysis that have not up-to-date. NOTE: In contrast to py:meth:*omsi.analysis.base.analysis_base.execute* and py:meth:*omsi.analysis.base.analysis_base.execute_recursive*, this is a class-level method and not an object-method. Again, the function uses a workflow driver, which we can customize by providing as driver as input to the function.

5.3.4 Executing multiple sub-workflows

To explicitly execute a subset of analyses (and all their dependencies) we can explicitly define a driver for the workflow we want to execute:

```
from omsi.workflow.driver.greedy_executor import greedy_executor
driver = greedy_executor()  # Create a driver
driver.add_analysis(a1)             # Add one ore more analyses
driver.add_analysis(a2)
driver.execute()                    # Execute the workflow and its dependencies
```

```
driver2 = greedy_executor()
driver2.add_analysis_all()  # Add all analyses
driver2.execute()  # Execute all analyses
```

5.4 Example: Normalizing an image

The goal of this example is to 1) illustrate the general concepts of how we can define analysis workflows and 2) illustrate the use of simple wrapped functions in combination with integrated analytics to create complex analysis workflows. The example shown below defines a basic image normalization workflow in which we:

1. Compute a reduced peak cube from an MSI image using the global peak finding analysis provided by BASTet
2. Use a simple wrapped function to compute the total intensity image for the peak cube dataset computed in step 1
3. use a simple wrapped function to normalize the peak cube computed in step 1 using the total intensity image computed in step 2

This is the same workflow as shown in Figure *Illustration of an example workflow for image normalization*.

```
# Illustration of the basic image normalization workflow defined below:
#
# +-----------a1------------+       +-------------a2----------------+       +-----------a3-----------
# +---global-peak-finder----+       +------total_intensities--------+       +---normalize_intensitie
# |                         |       |                                |       |
# | msidata       peak_cube +---+---> msidata      total_intensities+-------> norm_factors     outpu
# |                         |   |   |                                |       |
# | mzdata                  |   |   | axis=2                         |   +---> msidata
# +-------------------------+   |   +--------------------------------+   |   +-------------------------
#                               |                                        |
#                               |                                        |
#                               +----------------------------------------+
```

```
import numpy as np
from omsi.shared.log import log_helper
log_helper.set_log_level('DEBUG')
from omsi.analysis.findpeaks.omsi_findpeaks_global import omsi_findpeaks_global
from omsi.dataformat.omsi_file.main_file import omsi_file
from omsi.analysis.generic import analysis_generic

# Define a simple function to compute the total intensity image
def total_intensity(msidata, axis=2):
    import numpy as np
    return np.sum(msidata, axis=axis)

# Define a simple function to normalize an MSI data cube by per-spectrum normalization factors
def normalize_intensities(msidata, normfactors):
    import numpy as np
    return msidata / normfactors[:,:,np.newaxis]

# Get an ezample MSI image
f = omsi_file('/Users/oruebel/Devel/openmsi-data/msidata/20120711_Brain.h5' , 'r')
d = f.get_experiment(0).get_msidata(0)

# Define the global peak finder
a1 = omsi_findpeaks_global()
a1['msidata'] = d
a1['mzdata'] = d.mz

# Define compute of total intensity image
a2 = analysis_generic.from_function(analysis_function=total_intensity,
                                    output_names=['total_intensities'])
a2['msidata'] = a1['peak_cube']

# Define the normalization of the peak cube
a3 = analysis_generic.from_function(normalize_intensities)
a3['msidata'] = a1['peak_cube']
a3['normfactors'] = a2['total_intensities']

# To run the workflow we now have several basic options
#
# 1) a3.execute_recursive()  : Recursively execute the last analysis and all its dependencies (i.e.,
# 2) a1.execute_all() : Tell any analysis to execute all available analyses (i.e., a1,a2,a3)
# 3) Create our own workflow driver to control the execution of the analyses
# 4) Manually call execute on a1, a2, and a3 in order of their dependencies

# Execute the workflow
```

```
45 a3.execute_recursive()
```

CHAPTER

SIX

WORKFLOW TOOLS

Similar to the *omsi.workflow.driver.cl_analysis_driver* (and the corresponding tool *omsi.tools.run_analysis*) for running single analysis tasks, BASTet provides basic tools for executing complete workflows via the concept of workflow dirvers. Users may implement their own drivers using the approbriate base classes *omsi.workflow.driver.base*.

Some basic drivers and tools are already available with BASTet, e.g., the *omsi.workflow.driver.cl_workflow_driver* module (and the corresponding tool `omsi.tools.run_workflow`) defines a driver for driving and executing one or multiple workflows defined via workflow scripts, directly from the command-line.

6.1 Workflow Scripts

Workflow scripts are regular python scripts that include the i) creation of the analusis objects, and ii) full or partial definition of analysis parameters but usually **NOT** the actual execution of any of the analyses. Following our example from earlier, we may simply save the following code in python source file, e.g, *normalize_image.py*.

```
import numpy as np
from omsi.analysis.findpeaks.omsi_findpeaks_global import omsi_findpeaks_global
from omsi.dataformat.omsi_file.main_file import omsi_file
from omsi.analysis.generic import analysis_generic

# Define a simple function to compute the total intensity image
def total_intensity(msidata, axis=2):
    import numpy as np
    return np.sum(msidata, axis=axis)

# Define a simple function to normalize an MSI data cube by per-spectrum normalization factors
def normalize_intensities(msidata, normfactors):
    import numpy as np
    return msidata / normfactors[:,:,np.newaxis]

# Define the global peak finder
a1 = omsi_findpeaks_global()

# Define compute of total intensity image
a2 = analysis_generic.from_function(analysis_function=total_intensity,
                                    output_names=['total_intensities'])
a2['msidata'] = a1['peak_cube']

# Define the normalization of the peak cube
a3 = analysis_generic.from_function(normalize_intensities)
```

```
a3['msidata'] = a1['peak_cube']
a3['normfactors'] = a2['total_intensities']
```

When using our command-line tool, all parameters that are not defined for any of the analyses are automatically exposed via command-line options. In contrast to our previous example, we here, e.g., do not set the input msidata and mzdata parameters for our global peak finder (a1). In this way, we can now easily set the input file we want to process directly via the command line. In cases where we want to expose a parameter via the command line but still want to provide a good default setting for the user, we can set the default value of a parameter via, e.g, `a1.get_parameter_data_by_name('peakheight')['default'] = 3`.

To execute our above example from the command line we can now simply do the following:

```
python run_workflow.py --script normalize_image.py
                       --ana_0:msidata $HOME/20120711_Brain.h5:/entry_0/data_0
                       --ana_0:mzdata  $HOME/20120711_Brain.h5:/entry_0/data_0/mz
```

In order to avoid collisions between parameters with the same name for different analyses, the tool prepends the unique `analysis_identifier` to each parameter. Since we did not set any explicit `analysis_identifier` (e.g, via ``a1.analysis_identifier='a1'`), the tool automatically generated unique identifiers (i.e, `ana_0`, `ana_1`, and `ana_3` for our 3 analyses). To view all available command line option we can simply call the script with `--help`. If one or more workflow scipts are given (here via seperate `--script` parameters), then all unfilled options of those workflows and the corresponding analyses will be listed as. E.g.

```
newlappy:tools oruebel$ python run_workflow.py --script normalize_image.py --help
usage: run_workflow.py --script SCRIPT [--save SAVE] [--profile]
                       [--memprofile]
                       [--loglevel {INFO,WARNING,CRITICAL,ERROR,DEBUG,NOTSET}]
                       --ana_0:msidata ANA_0:MSIDATA --ana_0:mzdata
                       ANA_0:MZDATA
                       [--ana_0:integration_width ANA_0:INTEGRATION_WIDTH]
                       [--ana_0:peakheight ANA_0:PEAKHEIGHT]
                       [--ana_0:slwindow ANA_0:SLWINDOW]
                       [--ana_0:smoothwidth ANA_0:SMOOTHWIDTH]
                       [--ana_1:axis ANA_1:AXIS]
                       [--reduce_memory_usage REDUCE_MEMORY_USAGE]
                       [--synchronize SYNCHRONIZE] [-h]

Execute analysis workflow(s) based on a given set of scripts

required arguments:
  --script SCRIPT       The workflow script to be executed. Multiple scripts
                        may be added via separate --script arguments (default:
                        None)

optional arguments:
  --save SAVE           Define the file and experiment where all analysis
                        results should be stored. A new file will be created
                        if the given file does not exists but the directory
                        does. The filename is expected to be of the from:
                        <filename>:<entry_#> . If no experiment index is
                        given, then experiment index 0 (i.e, entry_0) will be
                        assumed by default. A validpath may, e.g, be
                        "test.h5:/entry_0" or jus "test.h5" (default: None)
  --profile             Enable runtime profiling of the analysis. NOTE: This
                        is intended for debugging and investigation of the
                        runtime behavior of an analysis.Enabling profiling
                        entails certain overheads in performance (default:
                        False)
```

```
  --memprofile          Enable runtime profiling of the memory usage of
                        analysis. NOTE: This is intended for debugging and
                        investigation of the runtime behavior of an analysis.
                        Enabling profiling entails certain overheads in
                        performance. (default: False)
  --loglevel {INFO,WARNING,CRITICAL,ERROR,DEBUG,NOTSET}
                        Specify the level of logging to be used. (default:
                        INFO)
  -h, --help            show this help message and exit

ana_0:omsi.analysis.findpeaks.omsi_findpeaks_global:analysis settings:
  Analysis settings

  --ana_0:integration_width ANA_0:INTEGRATION_WIDTH
                        The window over which peaks should be integrated
                        (default: 0.1)
  --ana_0:peakheight ANA_0:PEAKHEIGHT
                        Peak height parameter (default: 2)
  --ana_0:slwindow ANA_0:SLWINDOW
                        Sliding window parameter (default: 100)
  --ana_0:smoothwidth ANA_0:SMOOTHWIDTH
                        Smooth width parameter (default: 3)

ana_0:omsi.analysis.findpeaks.omsi_findpeaks_global:input data:
  Input data to be analyzed

  --ana_0:msidata ANA_0:MSIDATA
                        The MSI dataset to be analyzed (default: None)
  --ana_0:mzdata ANA_0:MZDATA
                        The m/z values for the spectra of the MSI dataset
                        (default: None)

ana_1 : generic:
  --ana_1:axis ANA_1:AXIS

optional workflow executor options:
  Additional, optional settings for the workflow execution controls

  --reduce_memory_usage REDUCE_MEMORY_USAGE
                        Reduce memory usage by pushing analyses to file each
                        time they complete, processing dependencies out-of-
                        core. (default: False)
  --synchronize SYNCHRONIZE
                        Place an MPI-barrier at the beginning of the exection
                        of the workflow. This can be useful when we require
                        that all MPI ranks are fully initalized. (default:
                        False)

how to specify ndarray data?
----------------------------
n-dimensional arrays stored in OpenMSI data files may be specified as
input parameters via the following syntax:
      -- MSI data: <filename>.h5:/entry_#/data_#
      -- Analysis data: <filename>.h5:/entry_#/analysis_#/<dataname>
      -- Arbitrary dataset: <filename>.h5:<object_path>
E.g. a valid definition may look like: 'test_brain_convert.h5:/entry_0/data_0'
In rear cases we may need to manually define an array (e.g., a mask)
Here we can use standard python syntax, e.g, '[1,2,3,4]' or '[[1, 3], [4, 5]]'
```

```
94
95 This command-line tool has been auto-generated by BASTet (Berkeley Analysis & Storage Toolkit)
```

CHAPTER

SEVEN

OMSI DATA FORMAT

The following discusses the specification and use of OMSI mass spectrometry imaging data files.

7.1 Data Layout

Experiment Information

- `/entry_#` *(HDF5 group)* : Each /entry# groups stores data for a single imaging experiment. Data from multiple related experiments may be stored in different /entry_# groups within the same file. To link data from related experiments that are stored in separate HDF5 files, one could create a master-file in which the /entry_# are softlinks to the corresponding groups in the external HDF5 files
  - `/entry_#/experiment_identifier` *(String dataset)* : For each experiment a user-defined identifier name —which should be unique— is stored. This can be used to search for a particular experiment based on its name.

  MSI Data

  - `/entry_#/data_#` *(HDF5 dataset)* : Multiple original images may be stored for each imaging experiment. The OMSI format manages the data associated with each dataset in a seperate group. For a standard MSI dataset this group contains the following datasets:
    - `/entry_#/data_#/data_#` *(3D dataset)* : Each data group may contain multiple copies of the same data. This is to allow for optimziations of the data layout for different selective read operations. This is important to enable fast data access to spectra and images via the web. By default the omsi format uses 3D arrays to store the spectral imaging data because:
      - This allows the use of chunking in HDF5 to optimize data access for slicing operations in all dimensions. 1D and 2D layout allow for optimization only for a limited set of selection operations.
      - When using, e.g., a 1D data array to store the data, one would also need to store the resolution and order of the different dimensions to make sure that one can interpreted and read the data correctly.
    - `/entry_#/data_#/format` *(String dataset)* : Simple string dataset describing the internal layout type of the dataset. While the most common data layout is to store the data in a single 3D array, other data layouts are supported as well, e.g., to enable more efficient storage for sparse MSI datasets.
    - `/entry_#/data_#/mz` *(1D dataset)* : The m/z values associated with the data.

  Instrument Information

  - `/entry_#/instrument` *(HDF5 group)* : For each experiment a group with additional data about the instrument is stored. The example shown above defines a name for the instrument but we could define a larger list of optional instrument information that we would like to store here. The CXIDB format allows multiple instruments for each experiment. To assign data uniquely to an instrument the data is stored in the corresponding instrument group. However, to ease access to the data, CXIDB defines soft-links to the data

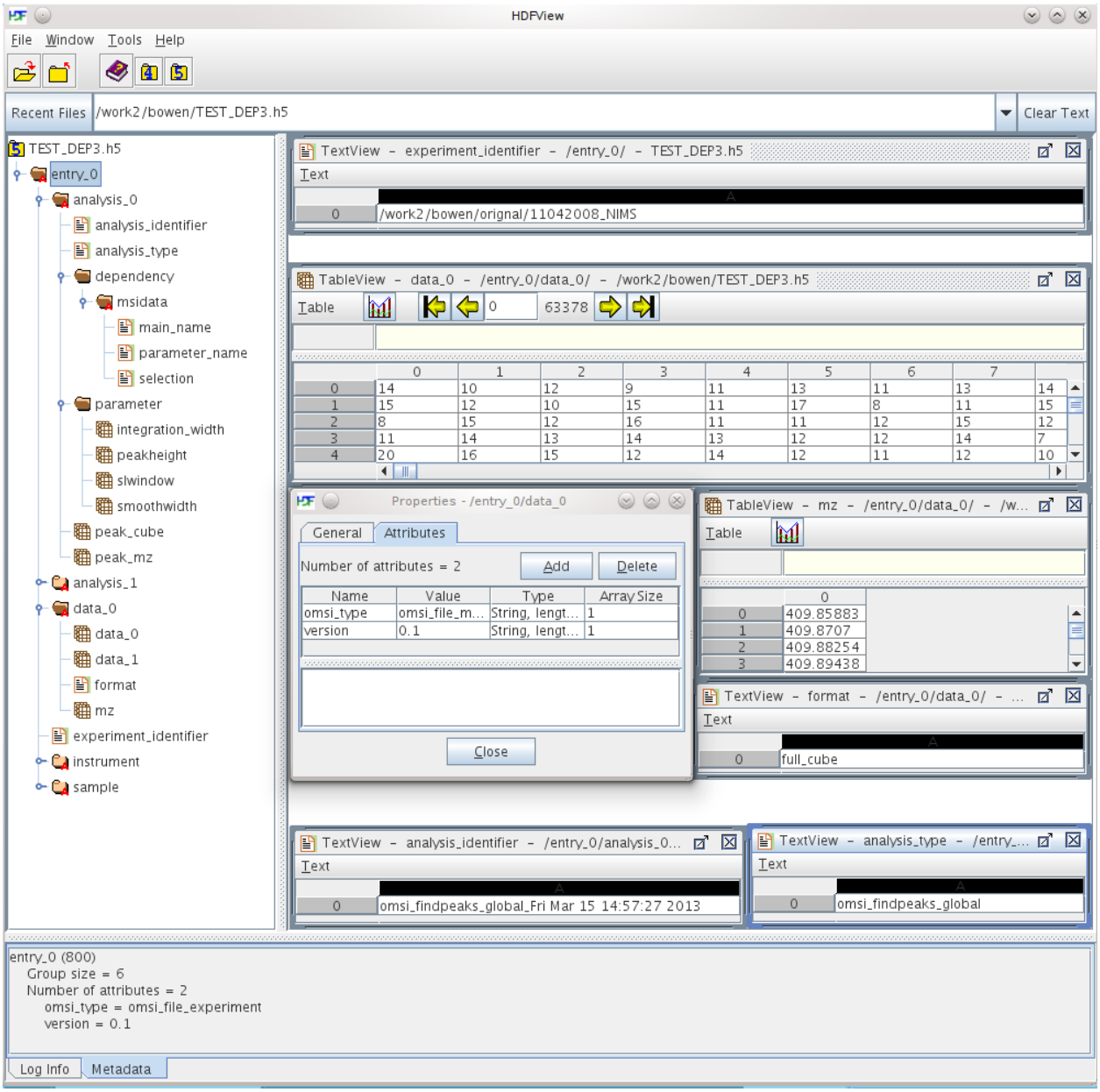


Fig. 7.1: Illustration of an example HDF5 file using the OpenMSI data format.

in the /entry_# group for the experiment as well. Allowing multiple instruments for a single experiment makes the format very complicated and is unnecceasry in most cases. In the OMSI format defined here, one can still store data from related experiments in a single file, simply by creating separate `entry_# group`.

* `/entry_#/instrument/name` *(String dataset)* : The name of instrument used
* `/entry_#/instrument/mz` *(1D dataset)* : The mz data of the instrument

Sample Information

- `/entry_#/sample` *(HDF5 group)* : For each experiment a group with additional data about the sample used in the experiment is stored. The example shown below only defines a name for the sample but we could define a larger list of optional instrument information that we would like to store here. The proposed format here makes a similar simplification compared to the CXIDB format as in the case of the instrument. For each experiment —represented by a `/entry_# group`— only a single sample may by used. Data from related samples may be stored in the proposed format in separate `/entry_#` groups representing different experiments.
  * `/entry_#/sample/name` *(String dataset)* : Name of the sample imaged.

Data Analysis Results

- `/entry_#/analysis_#` *(HDF5 group)* : Multiple derived analysis results may be stored in the proposed format in analysis_# groups associated with the experiment they were created from. Similar to the experiment a user-defined analysis-identifier string should be given to each analysis to allow searches for analysis results by name. Which data needs to be stored for an analysis will depend on the analysis. The omsi python API specifies some base classes to ease integration of analysis algorithms with the API and the HDF5 data format. Further formalizations may be specified to ease support of specific types of analysis results —e.g., clustering results— via the OpenMSI web-interface.
  * `/entry_#/analysis_#/analysis_identifier` *(String dataset)* : For each analysis a user-defined identifier name —which should be unique— is stored. This can be used to search for a particular experiment based on its name.
  * `/entry_#/analysis_#/analysis_type` *(String dataset)* : String describing the type of analysis. This should be high-level category, e.g., peak_finding_local, peak_finding_global, clustering etc. We will define a set of these categories that should be used. Having high-level categories for different algorithms that store their data in the same fashion will help later on with analyzing and visualizing the results from different algorithms that essentially produce the same output.
  * `/entry_#/analysis_#/...` *(Arbitrary HDF5 dataset)* : In the example shown in *Illustration of an example HDF5 file using the OpenMSI data format.* above, we have an example /entry_0/analysis_0/peakcube. The name for the output datasets from the analysis is currently not restricted. A set of name convention will however be defined by the omsi_analysis associated with the indicated analysis_type to ensure that the data can be handled gracefully. Otherwise, if an unkown analysis type is given then all datasets in the /entry_#/analysis_#/ group that are not part of the standard are assumed to be analysis datasets.
  * `/entry_#/analysis_#/parameter` *(HDF5 Group)* : Group containing addional datasets with input parameters of the analysis
    * `/entry_#/analysis_#/parameter/...` *(Arbitrary HDF5 datasets)* : Datasets defining input parameters of the analysis
  * `/entry_#/analysis_#/dependency` *(HDF5 Group)* : Group containing additional datasets specifying dependnecies of the analysis.

    `/entry_#/analysis_#/dependency/...` *(HDF5 Group)* : Each dependency is defined in a seperate group containting the following required datasets

- `/entry_#/analysis_#/dependency/.../main_name` *(String dataset)* : Path to the HDF5 object the analysis depends on.
- `/entry_#/analysis_#/dependency/.../parameter_name` *(String dataset)* : Name of the analysis parameter that has the dependency.
- `/entry_#/analysis_#/dependency/.../selection` *(String dataset)* : Optional Numpy selection string, indicating the subset of the data used.

Attributes

HDF5 attributes are used by the OMSI file format only to store format related information but not to store any data. Currently the following attributes are associated with the different high level groups:

- `omsi_type` *(String)* : Attribute indicating the omsi_file API object to be used to manage the given groupt. If the attribute is not present then the API decides which API object to use base on the name conventions described above.
- `version` *(String)* : Attribute indicating the version of the API class that should be used to represent this group.

7.2 Accessing OMSI data files

The `omsi.dataformat.omsi_file` module provides a convenient python-based API for reading and writing OMSI data files. The class also provides a convenient function for generating a XML-format XMDF header for the OMSI HDF5 file. Using the XDMF header file, the HDF5 data can be loaded in VisIt using VisIt's XDMF file reader. OMSI data files are valid HDF5 data files and can be accessed via the standard HDF5 libraries.

- **C/C++:**
  - More information about HDF5 can be found here: http://www.hdfgroup.org/HDF5/
- **Python:**
  - H5Py is a python interface to the HDF5 library. More detailed information can be found here: http://h5py.alfven.org/docs-2.0/
- **MATLAB:**
  - MATLAB provides both high-level and low-level access functions to HDF5. For more details see http://www.mathworks.com/help/techdoc/ref/hdf5.html
  - Simple example usin the high-level API:

```
file='~/Data/Imaging/DoubleV.hdf5'
h5disp(file)
mz=h5read(file,'/entry_0/instrument/mz');
[m mx]=min(abs(mz-746.22))
tic
y=h5read(file,'/entry_0/data_0',[mx 1 1],[1 250 160]);
toc
imagesc(squeeze(y))
axis equal
axis tight
```

  - Simple example using the low-level API:

```
file='~/Data/Imaging/DoubleV.hdf5'
plist = 'H5P_DEFAULT';
fid = H5F.open(file);
gid = H5G.open(fid,'/entry_0');
dset_id = H5D.open(fid,'/entry_0/data_0');
```

```
        dims = [160 250 1];
        offset = [0 0 mx]
        block = dims;
        mem_space_id = H5S.create_simple(3,dims,[]);
        file_space_id = H5D.get_space(dset_id);
        H5S.select_hyperslab(file_space_id,'H5S_SELECT_SET',offset,[],[],block);
        tic
        data = H5D.read(dset_id,'H5ML_DEFAULT',mem_space_id,file_space_id,plist);
        toc
        H5D.close(dset_id);
        H5F.close(fid);
        data=squeeze(data);
        imagesc(data)
        axis equal
        axis tight
```

- **Using HDF5 at NERSC**
  - Overview of python at NERSC: http://www.nersc.gov/users/software/development-tools/python-tools/
  - HDF5 modules are installed on most machines at NERSC:

```
        module load hdf5
        module load python
        python
        >>> import h5py
        >>> import numpy
```

7.3 Convert Mass Spectrometry Imaging Data to OMSI (HDF5) format

See section *Converting and Files and Making them Accessible* for details.

- `omsi.tools.convertToOMSI` : This python script, which is available via the OMSI software toolkit, provides functionality for converting img files to HDF5. The script takes a single or multiple img files as input and writes them to a single HDF5 file. The data of each img file is stored in a separate `/entry_#/data_#` object. The script also supports execution of a number of different analysis, such as, peak finding or nmf, directly during the data conversion. For up-to-date information about the usage of the script see `python imgToHDF5 --help`. A summary of the main command-line options of the tool are available below.
- `omsi.dataformat.omsi_file` : Module containing a set of python class for reading and writing HDF5 data files for the proposed OMSI HDF5 data layout.
- `omsi.dataformat.img_file` : Simple python class for reading img data files.
- `omsi.dataformat.bruckerflex_file` : Simple python class for reading bruckerflex files.

CHAPTER

EIGHT

HDF5 I/O PERFORMANCE

Analysis and visualization of mass spectrometry imaging (MSI) data is often based on selected subsets of the data, e.g., single or multiple spectra or m/z data slices. It is, therefore, crucial that we are able to quickly access select subsets of the data. In the context of web-based applications —such as the OpenMSI Viewer— this is particularly crucial in order to enable interactive data analysis and to provide a satisfactory user experience. The tests described here focus on characterizing and optimizing the performance of data access operations performed in serial on OMSI HDF5 files. While we here focus on the performance of serial data accesses, the optimizations described here are fundamental to optimizing parallel data access as well.

In the following, we first identify a select set of target compute platforms (Section *Test Platforms*) and define a set of representative use cases in order to evaluate the performance of different data layouts (Section *Test Cases*). We then discuss the basic layout of the MSI data (Section *Dataset Layout*) and establish the baseline performance using the default contiguous data layout (Section *Baseline Performance*). Afterwards, we explore further optimization of the data layout using HDF5's data chunking (Section *Chunking: Part 1*) and data compression (Section *Compression*) capabilities. We conclude this study with a discussion of lessons-learned in Section *Discussion*.

8.1 Test Platforms

All tests were performed on two main compute systems: i) login node of `hopper.nersc.gov` (short `hopper`) and ii) `portal-auth.nersc.gov` (short `portal`). On `hopper` we utilized the LUSTRE-based `/scratch` file system, as well as the global GPFS-based `/project` file system. On `portal` we can only access the `/project` file system. We chose these systems because: i) `hopper` is our candidate system for performing large-scale parallel analysis of MSI data and ii) `portal` is our target system for providing web-based access to MSI data.

8.1.1 `hopper.nersc.gov`

The `hopper` system has 12 login nodes with 4 quad-core AMD 2.4 GHz Opteron 8378 processors (16 cores total) each on 8 of the login nodes and 4 8-core AMD 2.0 GHz Opteron 6128 processors (32 cores total) each on 4 of the login nodes. Each login node has 128 GB of memory. The login nodes are external to the main Cray XE6 system. All tests were performed using `hopper` login nodes.

Scratch: There are two Lustre file systems on `hopper` —mounted as `/scratch` and `/scratch2` (in the following we use `/scratch2`)— with the following setup:

- 13 LSI 7900 disk controllers (Each disk controller is served by 2 I/O Object Storage Servers (OSSs))
- Each OSS host 6 OSTs (Object Storage Target) (simplified speaking a software abstraction of a physical disk)
- Fiber Channel 8 connectivity from OSSs to the LSI disk controllers
- Infiniband connects the Lustre router nodes in the 3d torus through a QDR switch to the OSSs

- In total each `/scratch` file system has 156 OSTs which is the lowest layer with which users need to interact. When a file is created in `/scratch` it is by default "striped" or split across two different OSTs. Striping is a technique to increase I/O performance. Instead of writing to a single disk, striping to two disks allows the user to potentially double read and write bandwidth. In the following experiments we use the default stripping settings but depending on file size, larger stripe settings may be advantageous. Using the `/scratch` file system for temporary storage of MSI data files can be advantageous when performing complex I/O intensive analysis.

Global `/project` **:** This is a large (1606 TB), permanent, medium-performance GPFS-based file system. We utilized the `/project` file system in the context of the OpenMSI project for permanent storage of MSI data.

8.1.2 `portal-auth.nersc.gov`

The `portal` system is used at NERSC for any data services that require public access from the Internet (such as Science Gateways) and as such also hosts the OpenMSI webpage and science gateway. The system consists of 2 quad-core AMD Opteron 2378 processors (8 cores total) with 24GB of memory. This system has only access to the `/project` file system.

8.2 Test Cases

In order to evaluate the performance of different data layouts, we designed a set of test-cases modeling the most common data access patterns in the analysis of MSI data. One particular focus of this study is to optimize the performance of the file format for web-based access to the data required for OpenMSI's online data viewing, analysis and exploration functionality. In this context it is most important that we are able to quickly access select subsets of the data, in particular, image slices, spectra or subcubes of the data. These type of data access patterns, however, are very common also for a large range of data analyses, e.g., peak finding on individual spectra, data clustering and many others. In contrast to analysis performed with direct access to the compute system, the abilities for data caching are typically much more limited in a web-based setting due to the fact that: i) http accesses are stateless, i.e., a file is typically reopend for each incoming request and closed again afterwards and ii) access patterns to the data are much more irregular with multiple users working with different datasets and/or different subsets of the data at the same time. While the median performance for repeated data selection operations on the same open file is often very important for data analysis, in a web-based setting the maximum time for the first access to the data is often much more important. In the following we report for each selection test case the median time (indicating the sustained performance on an open file) and the maximum time (indicating the selection performance after the first opening of the file). We usually repeat each selection test case 50 times for each data layout using randomized selection parameters.

8.2.1 Case 1: m/z Slice Selection

This test case models the selection of a series of z-slices of the data (i.e., slices in a mass range), and extracts a set of consecutive, full images of the data. This type of operation is required in the OpenMSI viewer when updating channels in the image viewer itself. It is also a common operation in many other analyses, e.g, when analyzing the distribution for a particular peak across the image.

- **Randomized Selection Parameters:** `zmin`
- **Dependent Selection Parameters:** `zmax = zmin+25`
- **Extracted Dataset:** $100 \times 100 \times 25 = 250,000$ records $= 500,000$ bytes $= 0.5$MB

8.2.2 Case 2: Spectra Selection

This test case models the selection of a 5×5 set of full spectra. In the OpenMSI viewer, access to single and multiple neighboring spectra is required when updating the spectrum plot's. This is also a typical operation for many analyses

that operate on a per spectrum basis, e.g., peak finding for a single spectrum.

- **Randomized Selection Parameters:** `xmin` , `ymin`
- **Dependent Selection Parameters:** `xmax = xmin+5` , `ymax = ymin+5`
- **Extracted Dataset:** $5 \times 5 \times 100,000 = 200,000$ records $= 2,500,000$ bytes $= 5$MB

8.2.3 Case 3: 3D Subcube Selection

This selection models the general access to consecutive sub-pieces of the data, e.g., when accessing data from a particular spatial region of the data related to a particular set of m/z data values. This type of operation is required, e.g., when analyzing the data of a cluster of pixels with a particular set of peaks of interest.

- **Randomized Selection Parameters:** `xmin` , `ymin`, `zmin`
- **Dependent Selection Parameters:** `xmax = xmin+5` , `ymax = ymin+5`, `zmax = zmin+1000`
- **Extracted Dataset:** $5 \times 5 \times 1,000 = 25,000$ records $= 50,000$ bytes $= 0.05$ MB

8.2.4 Case 4: Data Write

As described above, the aim of this study is to optimize the performance of selective data read operations (termed hyperslap selections in HDF5). In contrast to the data read, data write is a one-time cost during the file conversion step and is, therefore, less critical to the operation of OpenMSI. A reduced write performance may, therefore, be acceptable in lieu of an increase in read performance as long as an acceptable write performance is maintained. During selection performance tests, the data write is repeated only 3 times for each data layout (i.e.,once for each of the three selection test cases). For selected cases (indicated in the plot titles) we ran dedicated data write tests with 10 repeats. We here typically report the average times for data write.

8.2.5 Case 5: File Size

The size of data files is important to this study as different file layouts may have different space requirements (e.g., due to padding and additional metadata). While reduction of the size of data files is not the main objective of this work, it is important to avoid unnecessary overheads in file size and, hence, storage cost. The size of files reported in this study have been determined using the Python command `os.stat( filename ).st_size`.

8.2.6 Test Data

For this study we use a $100 \times 100 \times 100,000$ test dataset. The dataset is stored as a 3D array of UInt (16bit) data values using the OMSI HDF5 format described in Chapter *OMSI Data Format* . Data write and hyperslap performance are independent of the data values being written/read, so to test the baseline write-performance, we simply assign to each data element the index of the corresponding data chunk. For test cases that utilize data compression, we use a donor MSI data file to fill the file with realistic data. We may replicate data from the donor file in case that the testfile is larger than the donor file. In case that a donor file is used, we read the donor data into memory prior to writing of the test dataset. For each test case (i.e., data layout + selection case) we generate a new test data file to reduce/eliminate effects of data caching. The newly generated file is then opened and the current selection (i.e., hyperslap selection) is repeated 50 times using randomized selection parameters.

Raw data files used in this study are:

- **Dataset A:** (default donor file)
  - **Name:** 11042008_NIMS.h5

  - **Dimensions:** $227 \times 108 \times 63,378$
  - **Raw Data Size:** 3.2GB
  - **File Size:** 3.3GB (including results from global peak finding and nmf)
- **Dataset B:**
  - **Name:** 2012_0403_KBL_platename.h5 (DoubleV)
  - **Dimensions:** $160 \times 250 \times 116,152$
  - **Raw Data Size:** 9.3GB
  - **File Size:** 9.5GB (including results from global peak finding and nmf)

8.3 Dataset Layout

A single (2D) MSI dataset defines a 3D data volume with the spatial coordinates x, y and the m/z (mass) as third dimension (z). In raw block-of-uint format (e.g, in the IMG format) the data is often stored in a 1D linearized fashion: $spectrum_{0,0}$, $spectrum_{0,1}$, ... , $spectrum_{l,m}$. While such a layout is well-suited for accessing single full spectra, access to single image z-slices requires $l * m$ seek operations and traversal of the complete dataset (with l, m being the number of pixel in x,y ,respectively). Selection of spectra and z-slices of the data are orthogonal selection operations, i.e., a 1D data layout can always just optimize one of the two access operations but not both. Similarly, a 2D data layout can be defined to enable easy access to full spectra as well as full z-slices, but does not easily support to optimize access to 3D subsets of the data. We, therefore, store MSI data as a 3D array in HDF5 to: i) be be able to optimize and find a good performance compromise for selection of spectra, z-slices as well as 3D subcubes of the data and ii) because the 3D array reflects the true dimensionally of the data.

HDF5 can represent array datasets with as many as 32 dimensions. However, in the file the data is linearized in order to store it as part of the 1-dimensional stream of data that is the low-level file. The data layout determines in which way the multidimensional dataset is mapped to the serial file. The simplest way to accomplish this is to flatten the dataset (similar to how arrays are stored in memory) and to store the entire dataset into a monolithic block on disk. We here use this, so-called, contiguous layout as baseline for our performance tests (see Section *Baseline Performance*).

Chunking provides an alternative to the contiguous layout. In contrast to storing the data in a single block in the HDF5 file, using chunking the data is split into multiple chunks. Each chunk of a dataset is allocated separately and stored at independent locations throughout the HDF5 file. The chunks of a dataset can then be read/written independently, enabling independent parallel I/O and potentially improving performance when operating on a subset of the dataset. Data chunks may be stored in arbitrary order and position within the HDF5 file. HDF5 uses a B-tree to map a chunks N-dimensional address to a physical file addresses. The size of the B-tree directly depends on the number of chunks allocated for a dataset. The more chunks are allocated for a dataset: i) the larger overhead for traversal of the B-tree, ii) the higher the potential contention for the metadata cache, and iii) the larger the number of I/O operations. An introduction to data chunking in HDF5 is provided at http://www.hdfgroup.org/HDF5/doc/Advanced/Chunking/ . The performance of different chunking strategies for storing MSI data is evaluated in Section *Chunking: Part 1*.

Use of chunking also enables the use of HDF5 I/O filters. We here investigate the use of compression filters. I/O filters are applied in HDF5 to each chunk individually, and entire chunks are processed at once. I/O filters enabled for a dataset are executed every time a chunk is loaded or flushed to disk. Choosing proper settings for the chunking (and chunk cache) are, therefore, critical for the performance of filtered datasets. The potential use of `gzip` compression for improving file size and hyperslap selection of MSI datasets is evaluated in Section *Compression*.

Chunking and HDF5 I/O filters (e.g., data compression) are implemented transparently in HDF5, i.e, the API functions for reading/writing chunked/compressed datasets are the same ones used to read/write datasets with a uncompressed, contiguous layout. The layout (i.e., chunking scheme and compression options) is defined via a single function call to set up the layout on a property list before the dataset is created.

8.3.1 Baseline Performance

The goal of this section is to establish a baseline for the performance of the basic HDF5 contiguous data layout (i.e., without chunking). The baseline performance for the three selection test cases are shown in Figures i) *Baseline performance for the slice selection test case*, ii) *Baseline performance for the spectra selection test case*, and iii) *Baseline performance for the subcube selection test*. The bar plots show the minimum (blue), median (blue+red), average (blue+red+green), and maximum (blue+red+green+lilac) times for retrieving the selected data. We observe that `hopper` using `/scratch` provides much better performance for selection of spectra and 3D subcubes of the data. For the z-slice selection we observe that `hopper` achieves good median and average selection performance, whereas the performance of the z-slice selection on `portal` is generally poor. In all cases, we observe poor worst-case (maximum) times for the z-slice selection case.

For serial data write performance we observe that `/project` provides better write performance. However, for parallel write operations, the LUSTRE-based `/scratch` file system is expected to outperform `/project`.

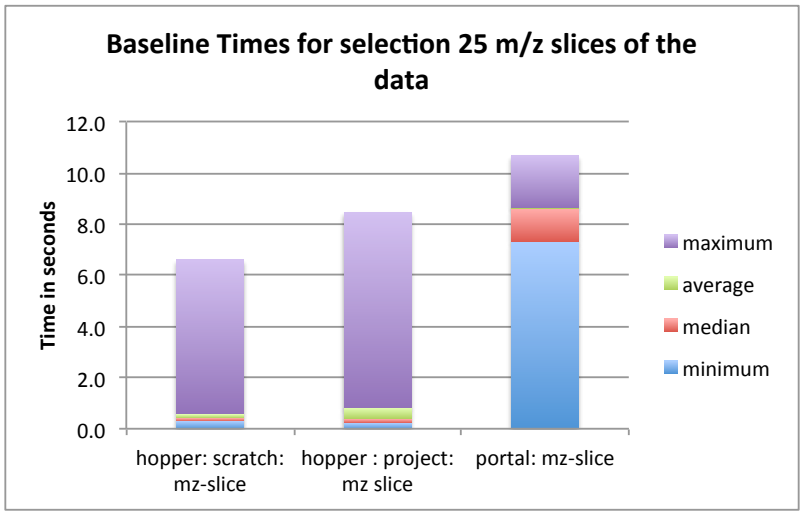


Fig. 8.1: Baseline performance for the slice selection test case

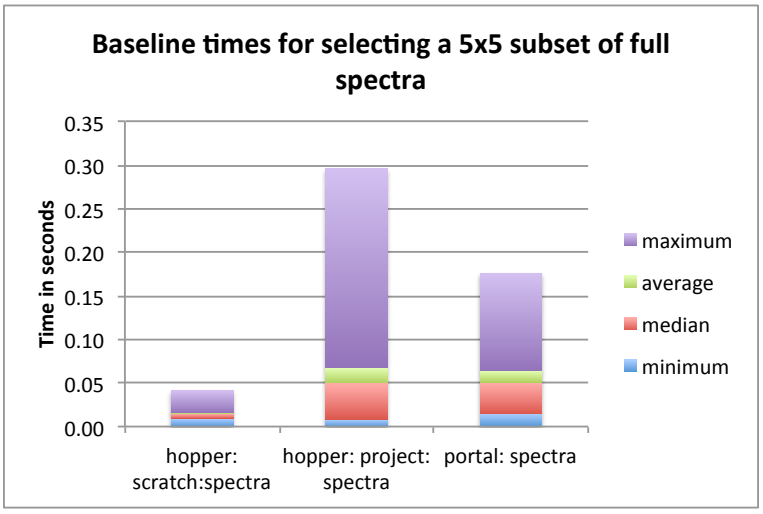


Fig. 8.2: Baseline performance for the spectra selection test case

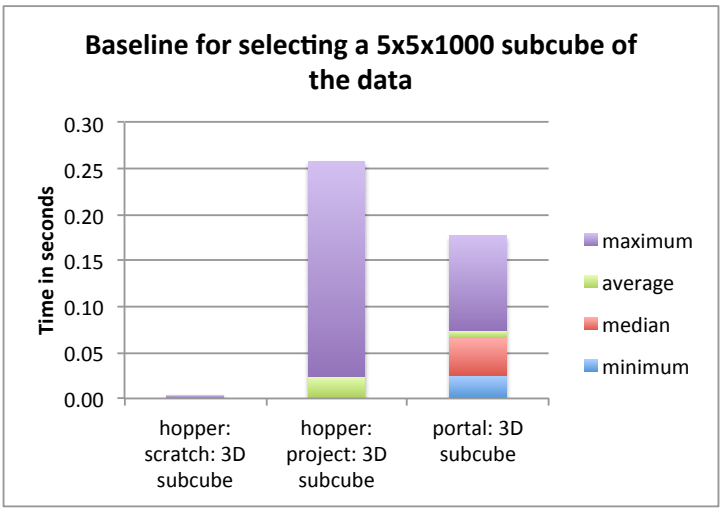


Fig. 8.3: Baseline performance for the subcube selection test

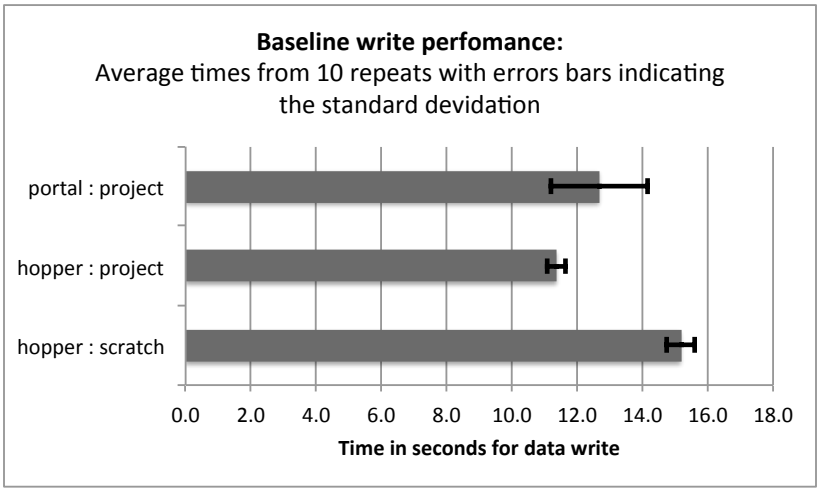


Fig. 8.4: Baseline performance for data write

8.4 Chunking: Part 1

Use of a chunked data layout has many potential advantages. In particular, use of chunking enables independent data I/O operations on individual chunks of the data so that chunking: i) can reduce the amount of data that needs to be read during hyperslab selections, ii) enables parallel independent I/O on a single file, and iii) enables the use of data compression (discussed later in Section *Compression*). The goal of this section is to evaluate the use of chunking to improve I/O performance. Due to the amount of additional metadata and overhead associated with finding chunks, one should avoid the use of too small chunks. At the same time, use of too large chunks should be avoided, because the entire chunk must be read from disk (and decompressed) before performing any operations. When operating on small subsets of the data (and if the cache is too small to hold the chunk), the use of too large chunks can result in large performance penalties. In addition, if the chunk is too large to be held in memory, the operating system may have to page memory to disk, slowing down the entire system. [1]

Choosing a good chunking strategy for MSI data is complicated because: i) the data has a very unconventional shape, with the m/z dimension being three to four orders of magnitude larger than the spatial x/y dimensions and ii) orthogonal data access operations (access to spectra vs. z-slices) are required with good first-time-access performance.

To account for these properties we use odd chunk sizes of $m \times m \times n$ with $n >> m$. Finding a good compromise for choosing a good chunking is challenging. Larger chunk sizes m in x, y are expected to improve z-slice selections but also increase the overhead for spectra selections. Similarly, large chunk sizes n in z (m/z) are expected to improve spectra selections while increasing the overhead for z-slice selections. The goal of this first set of experiments is to find a chunking that provides a good compromise in performance for all three selection test cases.

In the following we compare the performance of a range of different chunking strategies of the form $m \times m \times n$ with $m \in \{1, 2, 4, 8, 16, 32\}$ and $n \in \{128, 256, 512, 1024, 2048, 4096, 8192\}$ using `hopper` using `/scratch`. We first evaluate the effects of the different data layouts on file size (Section *File Size*) and write performance (Section *Data Write*). We then compare the performance for performing the three selection test cases (Section *Selection Performance*). We conclude this chunked layout study with an evaluation of the overall performance of the different chunked data layouts to identify the best-performing data layouts (Section *Selection Performance*)

8.4.1 File Size

The use of chunking effects the size of data files in two main ways. First, storing the additional metadata required for chunking —such as the B-tree used for indexing of data chunks— increases file size. Second, the use of chunking may result in allocation of additional empty data (padding) in case that the chunks do not align with the data. This can result in substantial data overheads. A simple example illustrates this problem. When storing a simple 1D dataset with 101 elements using a chunk size of 100, then we need to allocated two chunks, one chunk to store the first 100 elements and a second chunk to store the last element. In this case we allocated space for 200 elements in order to store 101 elements, nearly twice the amount of storage needed for the raw data. For multi-dimensional data arrays –here 3D– the storage overheads due to padding can increase even faster. It is, therefore, important that we consider the potential storage overhead when evaluating the use of data chunking.

Figure *File sizes using different chunking strategies* illustrates the effects of chunking on the size of data files. The baseline curve indicates the file size using a contiguous data layout. We observe that the file with a chunking of $1 \times 1 \times 128$ is much larger than the other files with a $1 \times 1 \times n$ chunked layout. No padding is applied in the spatial dimensions x, y. When using a z chunk size of 128, 782 chunks are required per spectrum, resulting in a total of 7,820,000 chunks. Due to padding in the z dimension, 96 100×100 slices remain empty. However, this accounts for only $100 * 100 * 96 * 2\text{Bytes} = 1,920,000\text{Bytes} = 1.92\text{MB}$. In comparison, the $1 \times 1 \times 2048$ dataset is much smaller while requiring a much larger z padding of 352 slices (i.e, $\approx 7.04\text{MB}$). The reason for the larger file size for the $1 \times 1 \times 128$ chunking illustrates the large overhead for storing the metadata required for the large number of chunks.

We also observe that the file size increases significantly when using chunk sizes in x, y of $8 \times 8 \times n$ or larger. This behavior is due to the padding required in the spatial dimensions. For example, when using a chunking of

[1] See also http://www.hdfgroup.org/HDF5/doc/Advanced/Chunking/

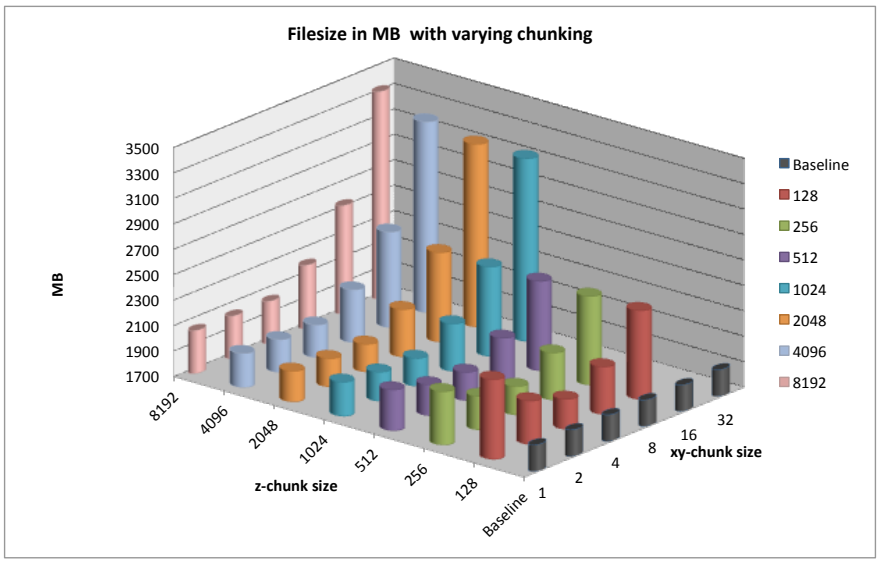


Fig. 8.5: File sizes using different chunking strategies

$32 \times 32 \times n$ we requires 4 chunks in the x and y dimension (i.e., $4 * 32 = 128$ elements). This means, in order to store the $100 \times 100 \times 100,000$ test dataset, we allocate space for at least $128 \times 128 \times 100,000$ records (additional padding may be required in the z dimension). This means that we allocate at least an additional amount of space of $(28*128*100,000)+(28*100*100,000)$ records $= 638,400,000*2$ Bytes $= 1,276,800,000$ Bytes $= 1276.8$ MB. This example illustrates that a bad choice for the chunking can result in substantially larger data files. Since in the case of MSI data, the x, y dimensions of the data are much smaller than the z (mz, mass) dimension, it is important that we keep the padding required in x and y as small as possible, whereas padding in the z dimension typically has a much smaller effect on the size of the data.

8.4.2 Data Write

Traditionally, MSI data is often written one-spectrum-at-a-time. Figure *Write performance using one-spectrum-at-a-time I/O using different chunk sizes (hopper using /scratch)* illustrates the write performance for the different data layouts using a one-spectrum-at-a-time write strategy. It is not surprising that we observes a significant decrease in performance with increasing chunk sizes m in the x and y dimensions, as each data chunk is modified $m*m$ times. For chunkings of $m \times m \times 32$ with $m \in \{1024, 2048, 4096, 8192\}$ the write performance improves possibly due to higher HDF5 chunk-cache hit rates. The write performance data points for data layouts with a chunking of $128 \times 128 \times 32$, $256 \times 256 \times 32$, and $512 \times 512 \times 32$ are missing as we terminated the tests due to the very poor one-spectrum-at-a-time write performance in those cases.

To achieve optimal data write performance, it is important that we reduce the number of times each chunk is modified. Figure *Write performance using different data write strategies and chunk sizes (hopper using /project)* compares the write performance for $m \times m \times 2048$ chunked data layout using a one-spectrum-at-a-time, $m \times m$-spectra-at-a-time, and chunk-at-a-time data write strategy. Using the latter two strategies ensures that each chunk is modified only once. We observe that the chunk-at-a-time write strategy quickly outperforms the other write strategies as the chunk size increases (and the total number of chunks decreases). It is not surprising that the contiguous baseline layout outperforms the chunked layouts in a serial setting. However, the chunked layouts efficiently support parallel data write operations. Using a chunk-at-a-time write strategy, independent parallel tasks can be utilized to write the different chunks.

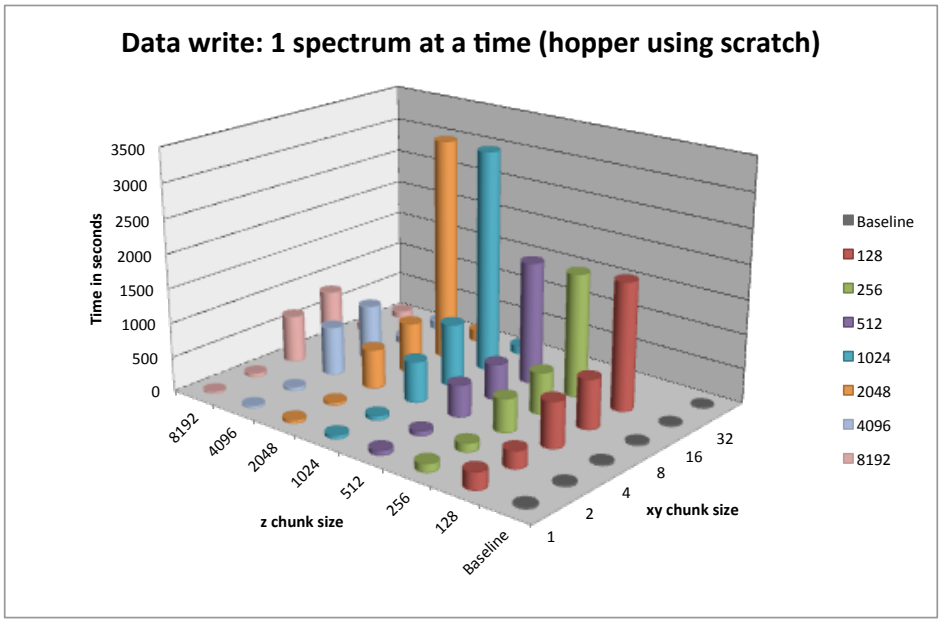


Fig. 8.6: Write performance using one-spectrum-at-a-time I/O using different chunk sizes (`hopper` using `/scratch`)

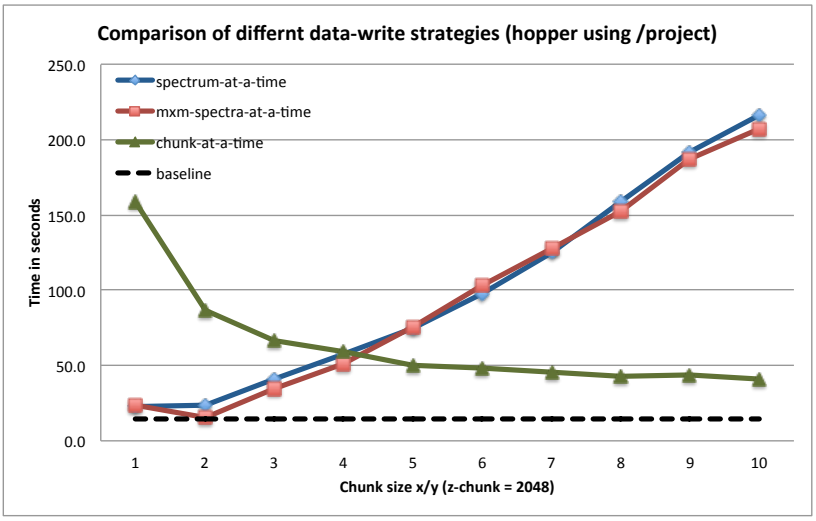


Fig. 8.7: Write performance using different data write strategies and chunk sizes (`hopper` using `/project`)

8.4.3 Selection Performance

In this section we evaluate the selection performance of the different chunked data layouts for the three selection test cases: i) selection of a random set of 25 consecutive z-slices, ii) selection of a random 5×5 set of full spectra, and iii) selection of a random $5 \times 5 \times 1000$ subcube of the data. Figure *Performance results for z-slice selection using varying chunk sizes (hopper using /scratch)* [2] shows the results for the z-slice hyperslap selection. We observe that data layouts with a chunking of $m \times m \times n$ with $m \in \{4, 8, 16\}$ and $n \in \{128, 256, 512, 1024, 2048, 4096\}$ show the best z-slice selection performance. For the mentioned chunking strategies we observe in general best performance for larger values in m and smaller values of n. This behavior is likely due to the reduced amount of data and number of chunks that need to be loaded to fulfill the selection of complete slices in z.

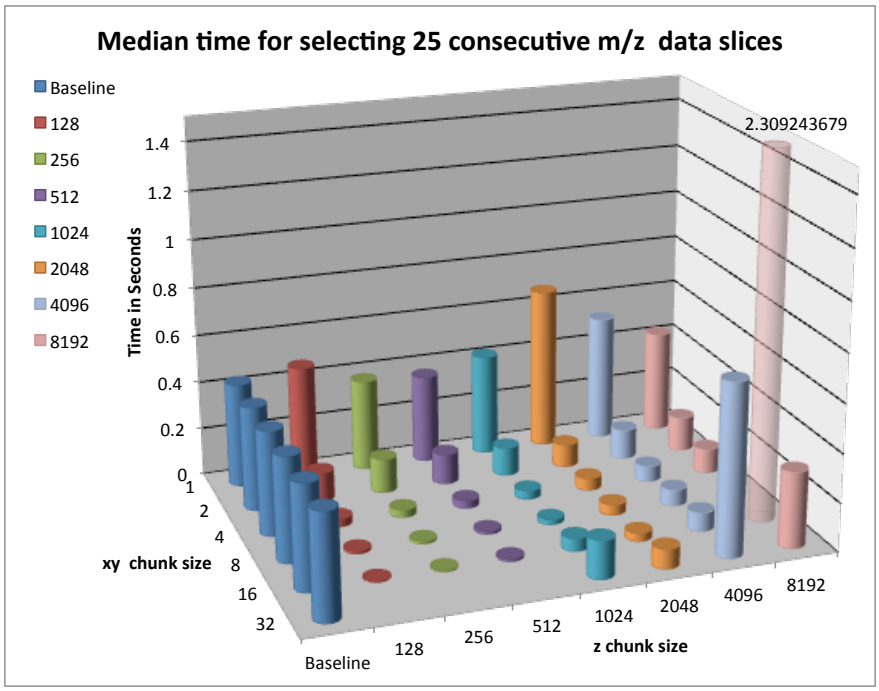


Fig. 8.8: Performance results for z-slice selection using varying chunk sizes (`hopper` using `/scratch`)

For the spectra selections (see Figure *Performance results for spectra selection using varying chunk sizes (hopper using /scratch)*) we observe in most cases a decrease in the median performance compared to the baseline contiguous data layout. This behavior is likely due to the fact that the data is flattened in a z-column order in the contiguous layout, so that a full spectrum can be read via a single seek and contiguous read operation. In contrast, using a chunked data layout requires for the test dataset, loading $100,000/n$ chunks. However, we observe that data layouts with a chunk size in z of 1024 and larger, still provide good performance for the selection of full spectra. In this case, small chunk sizes in x, y of 2 or 4, work well for the test case of loading a 5×5 set of spectra, as the number of chunks that need to be loaded remains constant. For data layouts with a x,y chunking of 8×8, the 5×5 spectra selection can fit into a single x,y chunk, however, it is still likely that the 5×5 selection crosses multiple chunk boarders, requiring the load of a large number of chunks. For x, y chunk sizes of 16 or 32, the 5×5 spectra selection is more likely to fit in a single chunk in x,y, explaining the better performance of those data layouts.

Figure *Performance results for 3D subcube selection using varying chunk sizes (hopper using /scratch)* [2] summarizes the results for the selection of a $5 \times 5 \times 1000$ data subcube. We observe that using chunking generally improves the performance of the selection. In particular, using chunking decreases the time for initial data access compared to the baseline contiguous data layout.

[2] Bars shown transparently indicate that the bars exceed the maximum value shown in the plot. The real value for those bars are indicated via additional text labels.

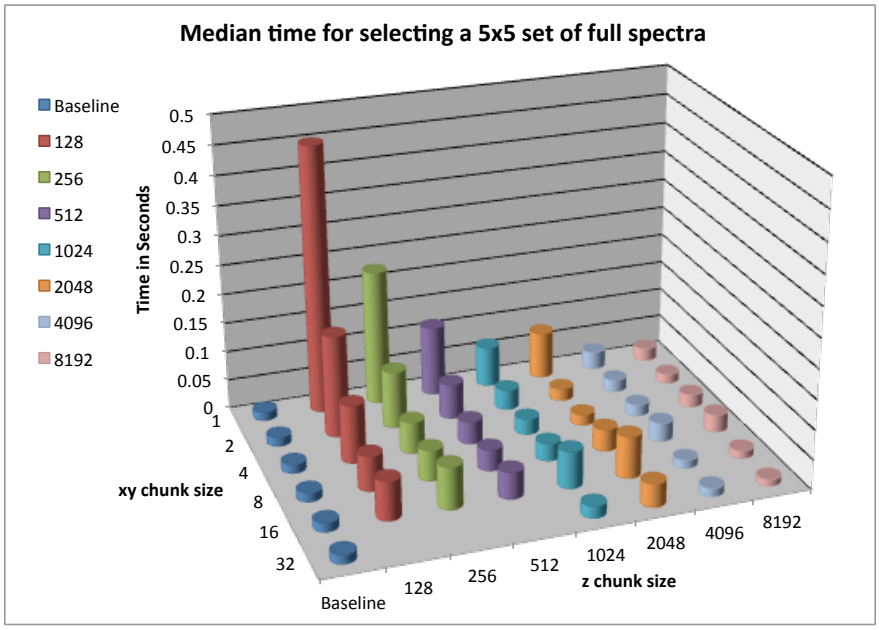


Fig. 8.9: Performance results for spectra selection using varying chunk sizes (`hopper` using `/scratch`)

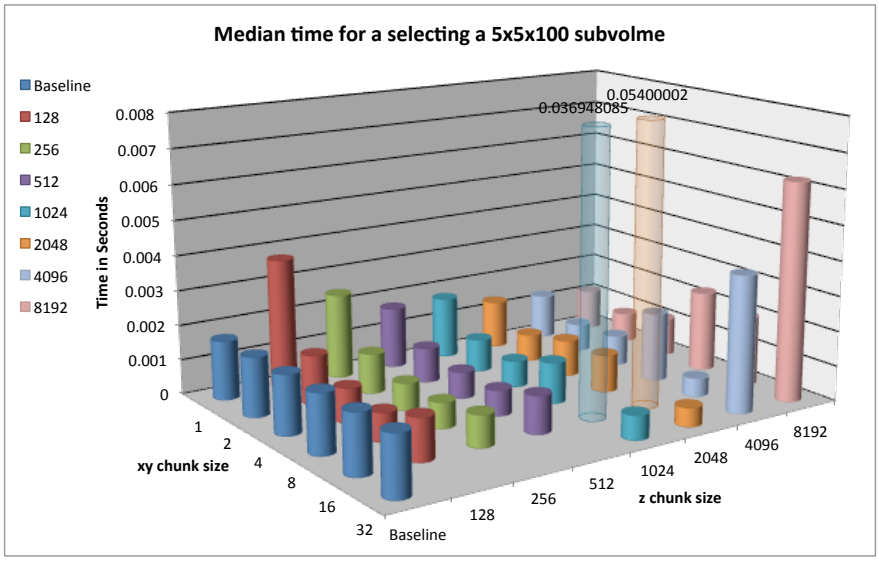


Fig. 8.10: Performance results for 3D subcube selection using varying chunk sizes (`hopper` using `/scratch`)

When comparing the selection performance plots, we observe that — even though the amount of data that is retrieved is only 0.5MB in z-slice selection case compared to 5MB in the spectra selection case— the performance for z-slice selection case is generally lower than for the spectra selection case. The reason for this behavior is that while the z-slice selection returns less data, the number of I/O (seek) operations required and the amount of data that needs to be loaded to fulfill the selection is larger. E.g, using a chunking of $4 \times 4 \times 2048$ each chunk requires $4*4*2048*2\text{Byte} = 65536\text{Byte} = 64\text{kB}$. To retrieve a 5×5 set of spectra, HDF5 needs to load $2*2*49$ Chunks $= 196*64$ kB $= 12.25$ MB, whereas in order retrieve 25 z-slices (without crossing a z-chunk boundary), HDF5 needs to load $25 * 25$ Chunks $= 625$ Chunks $= 39.0625$ MB, i.e, more than three times the data (and that even though the 4×4 x,y chunking does not align well with the 5×5 spectra selection). Similary, in the contiguous data layout, we can load a single spectrum using a single seek and contiguous read operation, whereas in order to load complete a z-slice we requires $m * m$ $(= 100 * 100 = 10,000$ for the test data) seek and load operations.

8.4.4 Summary

To illustrate the overall performance of the different dataset layouts and to identify the "best" layouts, we define the following set of minimum performance criteria a data layout should fulfill:

- The median time for the z-slice selection test case should be `<0.1 s`
- The median time for the spectra selection test case should be `<0.05 s`
- The median time for the 3D subcube selection test case should be `<0.002 s`
- The total file size should be `< 2100 MB` (limiting the overhead in the test case to a maximum of $\approx$ 200MB)
- (We do not take the write performance results shown in Figure *Write performance using one-spectrum-at-a-time I/O using different chunk sizes (hopper using /scratch)* into account in the total score here as a chunk-at-a-time write strategy likely improve the write performance significantly)

Based on these criteria we can determine an overall performance score by evaluating how many of the criteria a particular data layout fulfills (with 4=best (passes all criteria) and 0=worst (does not pass any of the criteria)). We observe a cluster of 8 data layouts that satisfy the four performance conditions.

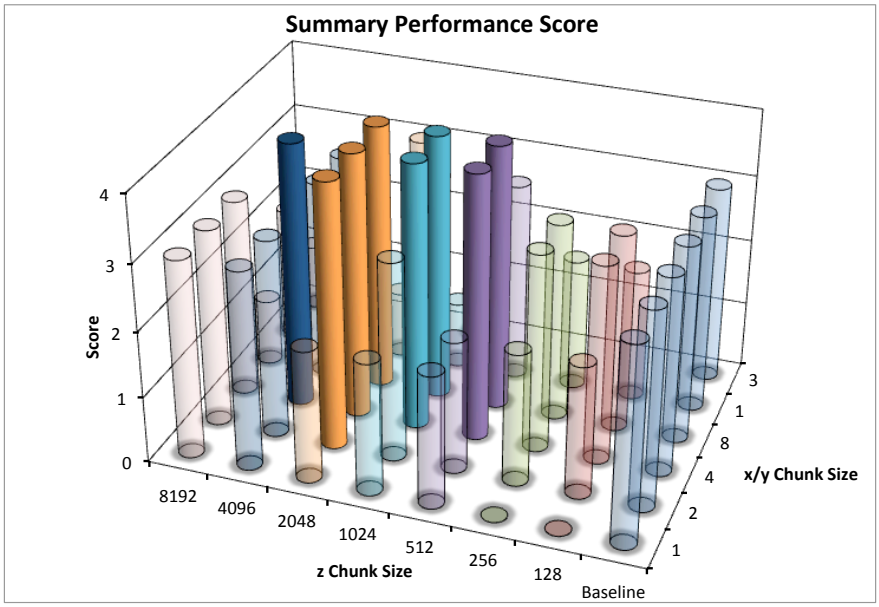


Fig. 8.11: Summary performance score using various different chunk sizes (`hopper` using `/scratch`)

Figure *Summary performance score using various different chunk sizes (hopper using /scratch)* summarizes the performance scores for the different data layouts. Bars with the maximum score of 4 are plotted opaque whereas all other bars are plotted transparently. We observe a cluster of 8 layouts with a performance score of 4. While the overall performance score used here is simple in nature, it illustrates well which data layouts achieve overall the best performance. Overall, the performance experiments indicate that the largest z chunk size for which we observe good performance in our experiments across a large range of x/y chunk sizes is 2048. We, therefore, chose a z chunk size of 2048 for further experiments.

So far our experiments have focused on `hopper` using the `/scratch` file system. In order to evaluate the performance of the permanent data storage system `/project` and the web-hosting system `portal` we performed a series of follow-up tests using a fixed z-chunking of 2048 on `portal` as well as on `hopper` using `/project` (more details are provided in the next section). We generally observed that the `/project` file system provided better serial write performance while the overall performance for selection was not as good as for `/scratch`. While the performance of ``hopper` using `/project` was still acceptable, the performance (and in particular the worst-case maximum times) were poor using `/portal` (see, e.g, Figure *Performance results for z-slice selection (portal using compression)* shown later). We, therefore, next extended our evaluation to also include data compression as an option to possibly improve data I/O performance and storage requirements.

8.5 Chunking: Part 2

In part 1 of the chunking study we were interesting in finding chunked data layouts that provide a good compromise for all three selection use-cases. In part 2 we focus on chunked data layouts that are designed to optimize single selection operations.

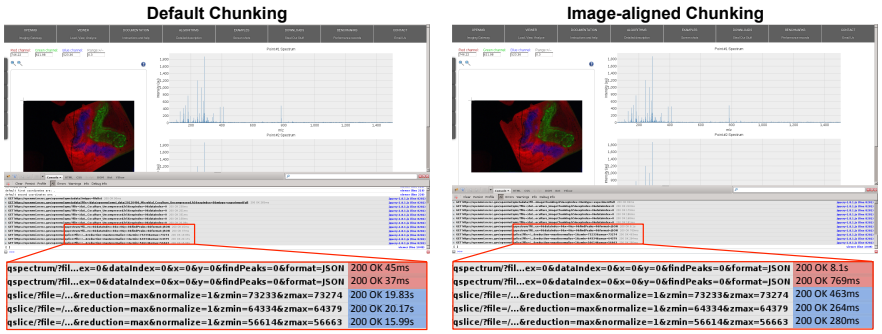
8.5.1 Image-aligned Chunking

Figure *Comparison of the performance of the default chunking with a chunked layout that is better-aligned with the ion-images to improve the performance the z-slice selection.* shows the performance of the z-slice selection in the OpenMSI client when optimizing the chunked data layout to align with the selection of m/z images. Using an image-aligned chunking of $50 \times 80 \times 100$, only 10 chunks containing 100 image slice need to be read in order to retrieve a single image slice, wheras, using the default chunking of $4 \times 4 \times 2048$, HDF5 needs to load 2,520 chunks containing 2048 image slices. The figure shows the performance we achieve in the OpenMSI client using the same data stored without compression using the two different chunked layouts. Using the default chunking it takes $\approx 20s$ to compute the ion-images compared to just $\approx 0.5s$ using the image-aligned chunking. However, not surprisingly, the performance of the orthogonal operation of selecting full spectra decreases significantly (here from 45ms to 8.1s) when optimizing the chunking to improve the selection of z-slices.

Further improvement in performance could be achieved by using a (m/z, x ,y) or (m/z, y, x) layout of the data rather than the commen (x, y, m/z). By transposing the image cube (making m/z the first dimension of the 3D cube) the data will be linearized on disk as $ionimage_0. ionimage_1$, ... , $ionimage_n$ rather than $spectrum_{0,0}$, $spectrum_{0,1}$, ... , $spectrum_{l,m}$. Linearizing the data in image order improves locality of data and reduces the number of seek operations required when loading ion-image. Currently, reordering of data dimensions is not yet supported by HDF5 as a transparent data layout optimization, but rather needs to be performed manually by the user. To remain ease of usability of the OpenMSI file format we, therefore, chose to use a consistent ordering of dimensions in all cases.

8.6 Compression

The primary goal of data compression is to reduce the size of data by providing a more compact encoding of the data. In many cases, compression is used as means to reduce the size of data stored on disk. However, while additional compute time overheads are incurred due to the time required for compression/decompression of the data during



	x	y	z	Total
Image Size	160	250	116151	9.4GB
Chunk Size	4	4	2048	64KB
#Chunks	40	63	57	143,640

	x	y	z	Total
Image Size	160	250	116151	9.3GB
Chunk Size	80	50	100	781.25KB
#Chunks	2	5	1162	11,620

Fig. 8.12: Comparison of the performance of the default chunking with a chunked layout that is better-aligned with the ion-images to improve the performance the z-slice selection.

write/read, compression may also improve the read and/or write performance, as less data needs to be transferred and/or written to disk. This is in particular the case in I/O bound systems (e.g., due to network bottlenecks etc.).

Use of data compression in HDF5 relies on the use of chunking and, hence, shares the same overheads and advantages and disadvantages. Compression is applied to each chunk of the data. The overall compression ratio achieved, therefore, inherently relies on the use of a good chunking strategy. Data compression is implemented via I/O filters in HDF5, which are applied transparently during data read and write operations, i.e., after enabling compression when generating the dataset, data read/write operations are performed using the same API calls whether the data is stored in raw or compressed form.

`HDF5/h5py` typically provides three main compression algorithms: i) `gzip`, standard `HDF5` deflate compression available with most HDF5 installations, ii) `szip`, third-party compression algorithm optionally available with HDF5 (i.e., it may not be available on all systems), iii) `LZF` is a stand-alone compression filter for HDF5 available via `h5py` but may not be available in many other standard (non-Python) installations of HDF5. In the context of OpenMSI it is important that we are able to transfer and use data at different institutes, compute systems and using a larger range of API's for accessing HDF5 data (e.g., matlab, HDF5 C API, h5py etc.). We, therefore, chose the standard `gzip` compression filter as it is typically available with most systems (in contrast to `LZF` and `szip`). The `gzip` filter provides and additional `aggression` parameter. The `aggression` parameter is a number between $[0, 9]$ to indicate the trade-off between speed and compression ratio (zero is fastest, nine is best ratio). Unless indicated otherwise, we here generally set the `aggression` parameter to 4 for all tests to achieve a balance of compression ratio and speed.

8.6.1 Compression Ratio

Using a chunking of $4 \times 4 \times 2,048$, we achieve for dataset A a compression ratio of ≈ 2.9, reducing the data from 3.3GB (including ≈ 100 MB of data for nmf and global peak-finding) to 1.2GB (while only the MSI data is stored in compressed form). Using the same setup, we achieve for dataset B a compression ratio of ≈ 6.3, reducing the dataset from 9.5GB to 1.5GB (again with nmf and global peak-finding results included in the file and stored uncompressed in both cases). An overview of the file sizes using compression and compression ratios achieved using the $100 \times 100 \times 100,000$ test dataset (using dataset *A* as donor MSI dataset) are summarized in Figure *Compression ratios using different chunk sizes*. The compression ratios we achieve are on the order of 2.9 to 3.8 in all cases (comparable to the compression ratio we have seen for the donor dataset A).

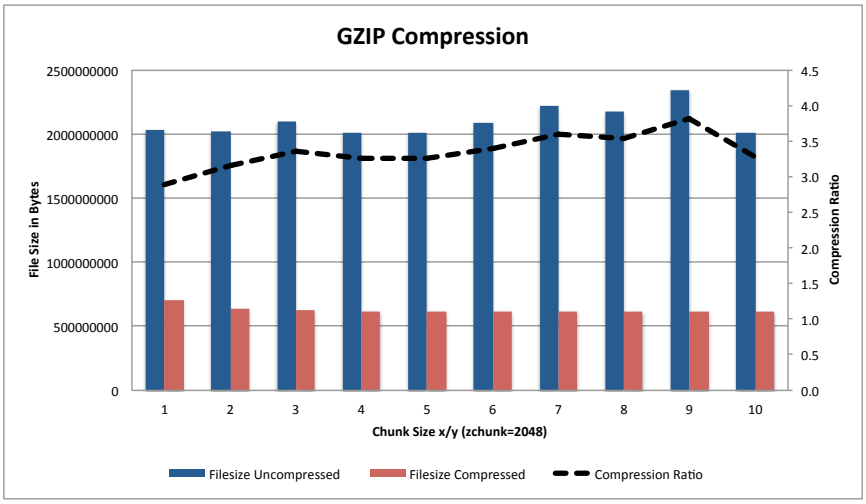


Fig. 8.13: Compression ratios using different chunk sizes

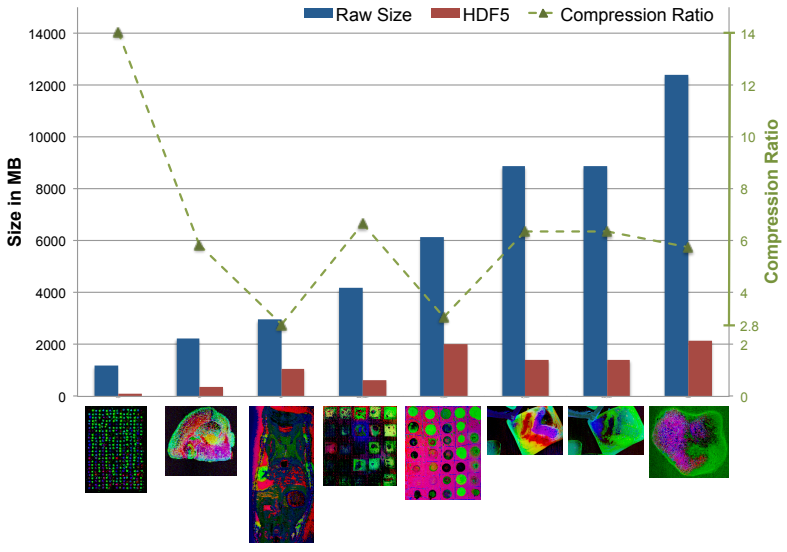


Fig. 8.14: Compression performance on a select set of real MSI datasets.

8.6.2 Data Write

Figure *Serial write performance using compression* compares the write performance results with and without using compression for data layouts with a chunking of $m \times m \times 2048$ with $m \in [1, 10]$. As expected, we observe a general decrease in the write performance when using compression. As mentioned earlier, when using compression it is important that we use a chunk-aligned data write strategy as the compression filter needs to be executed each time a chunk is loaded and/or modified. We, therefore, use the chunk-at-a-time write strategy when writing HDF5 datasets with compression enabled.

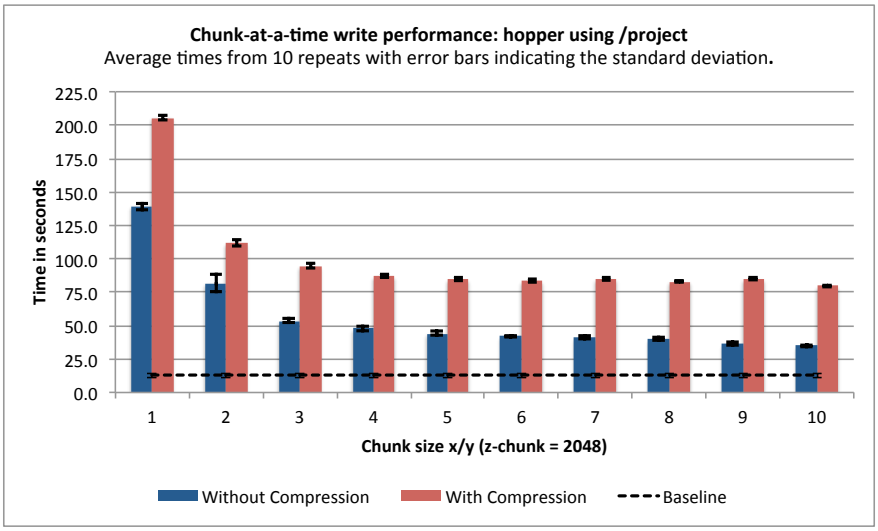


Fig. 8.15: Serial write performance using compression

8.6.3 Selection Performance

In this section we evaluate the selection performance of the different $m \times m \times 2048$ chunked data layouts (with $m \in [1, 10]$) for `portal` and `hopper` using `/project` and `/scratch`. For `portal` we observe that using compression can significantly improve the median selection time for the z-slice selection test case (see Figure *Performance results for z-slice selection (portal using compression)*). In particular, using compression significantly reduces and stabilizes the worst-case maximum time for selecting z-slices of the data [3] . This is especially important in the context of a web-based application, such as, OpenMSI's online data viewer. For the other two selection test cases we observe that we can achieve similar performance for the spectra and 3D subcube selection test cases on `portal` with and without compression (see Figures *Performance results for spectra selection (portal using compression)* and *Performance results for 3D subcube selection (portal using compression)*)

The selection performance results for `hopper` using `/project` and `/scratch` and with and without using compression are shown in Figures: i) *Performance results for z-slice selection (hopper using compression)* , ii) *Performance results for spectra selection (hopper using compression)*, and *Performance results for subcube selection (hopper using compression)*. As baseline we use the performance of the contiguous data layout on `hopper` using `/project`. In contrast to `portal`, we observe on `hopper` a general decrease (of up to 1 order of magnitude) in the selection performance when using compression compared to when storing the data in raw, uncompressed form. Compared to the

[3] **Author comment:** Depending on when the test were run we have seen significant (approximately 1 order of magnitude) differences in the median selection times on `portal`, however, the maximum appeared to not improve between different reruns of the experiments. Using compression, the results on `portal` have been much more stable and, in particular, the maximum times were much better. This indicates that: i) system load, on a highly utilized system like `portal`, has a significant impact on the performance and ii) compression can significantly improve performance the selection performance on I/O bound systems and stabilized the performance results.

baseline contiguous data layout we, however, still observe an improvement in many cases even when using compression. Generally it appears that the use of compression may have stronger negative effect on the selection performance when operating on the `/scratch` filesystem then when using `/project` [4].

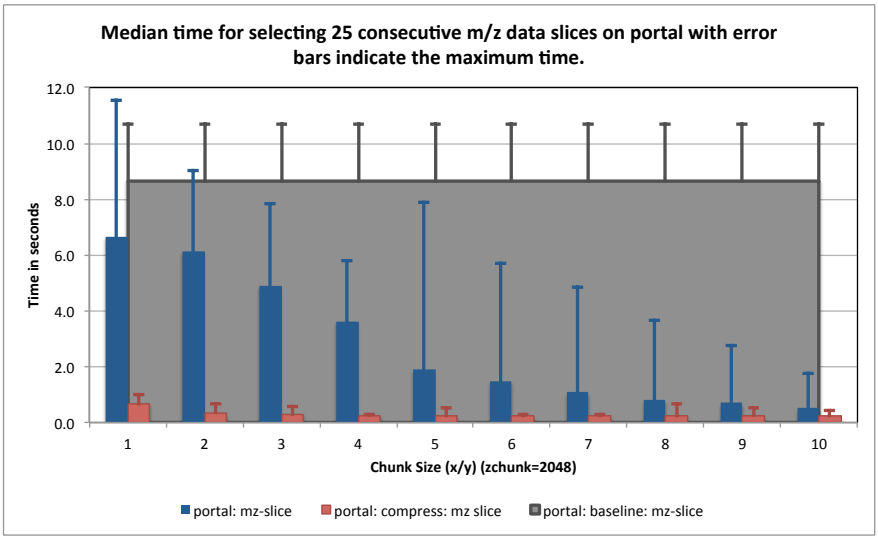


Fig. 8.16: Performance results for z-slice selection (`portal` using compression)

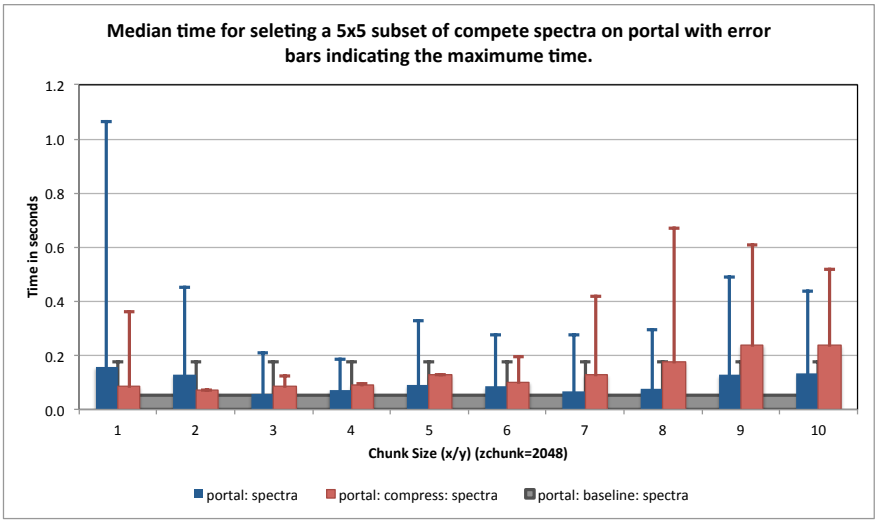


Fig. 8.17: Performance results for spectra selection (`portal` using compression)

8.6.4 Aggression Parameter Study

So far we have focused on the performance using `gzip` with $aggression = 4$, assuming that a medium aggression value provides a good balance of compression ratio and speed. [5] The goal of this section is to determine the influence

[4] **Author comment:** Note, `/scratch` is a parallel, LUSTRE-based file system, whereas `/project` is based on GPFS. Also `hopper` may have a higher bandwidth connection to the `/scratch` file system than `/project`. Overall, accesses to `/project` is likely to be more I/O bound than access to `/scratch`.

[5] The $aggression$ parameter is a number between $[0, 9]$ to indicate the tradeoff between speed and compression ratio (0=fastest, 9=best ratio).

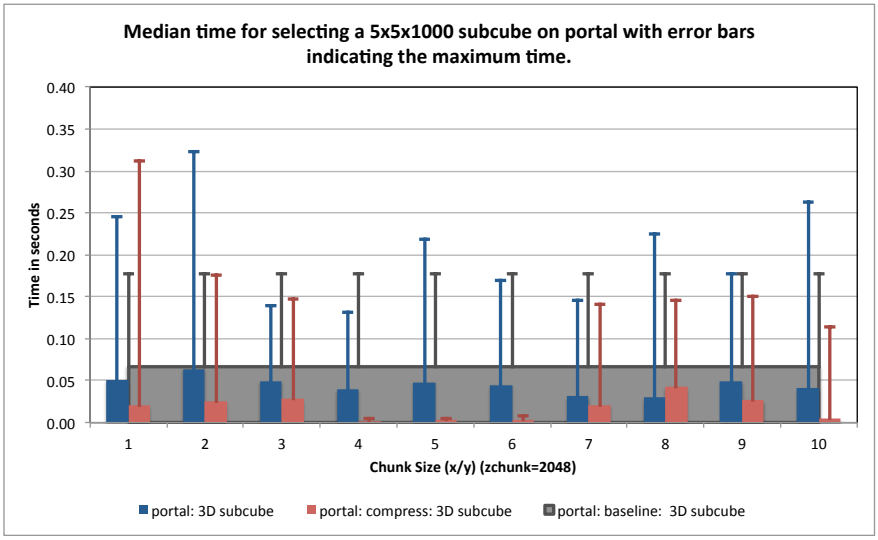


Fig. 8.18: Performance results for 3D subcube selection (`portal` using compression)

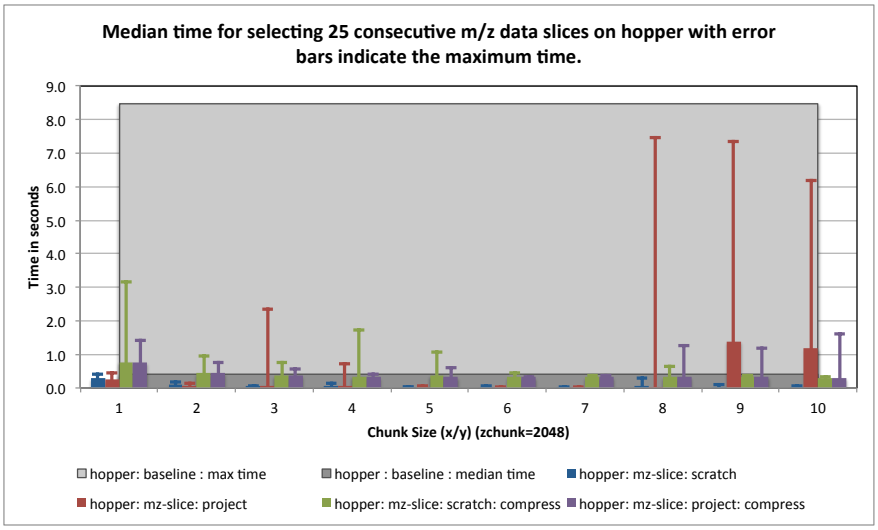


Fig. 8.19: Performance results for z-slice selection (`hopper` using compression)

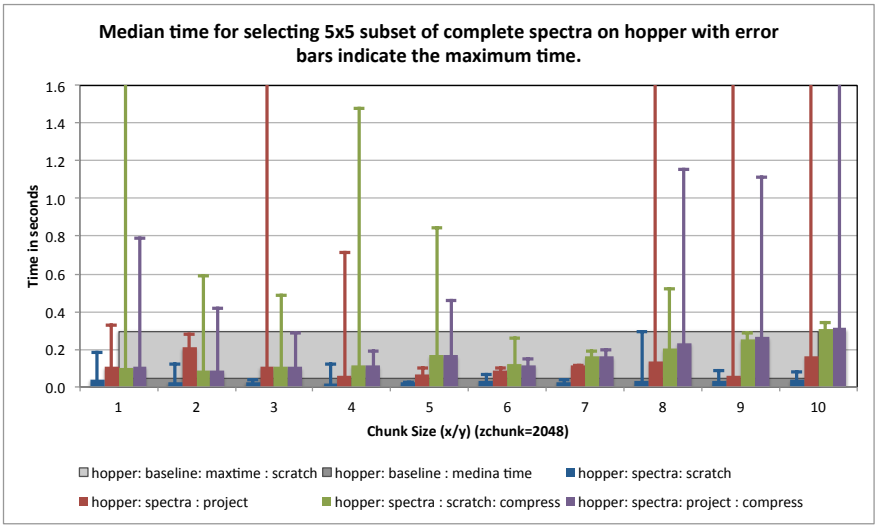


Fig. 8.20: Performance results for spectra selection (`hopper` using compression)

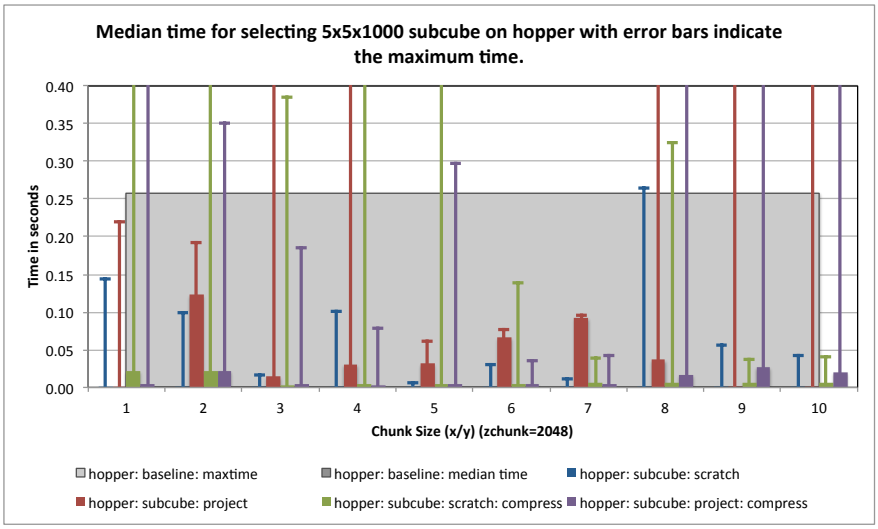


Fig. 8.21: Performance results for subcube selection (`hopper` using compression)

of the $aggression$ setting on the overall performance. Figure *File size and write performance using varying gzip aggression settings* shows that the data compression we achieve for the test $100 \times 100 \times 100,000$ dataset (using dataset A as donor dataset) are comparable for all $aggression \in [1, 8]$ settings (we did not evaluate an aggression setting of 9 as the write performance was very poor). For the data write, we observe that the performance is acceptable for $aggression \in [1, 5]$ and decreases significantly for $aggression > 5$.

For the selection test cases, the performance results are consistent with the results from the previous tests. On `portal`, the performance of the z-slice selection improves significantly when using compression, while the spectra and subcube selection show comparable performance with and without compression (see Figure *Selection performance results using varying gzip aggression settings (portal)*). For `hopper`, we again observe a general strong decrease in the selection performance when enabling compression (while, although much slower, the overall selection performance is still acceptable) (see Figures *Selection performance results using varying gzip aggression settings (hopper using /project)* and *Selection performance results using varying gzip aggression settings (hopper using /scratch)* [6]).

Overall, we find that for the data layouts tested here, increasing the aggression parameter above 1 does not have a large impact on the compression ratio and selection performance, whereas high aggression values may significantly decrease the data write performance. In the context of MSI data, low aggression values of $aggression \in [1, 4]$ may, therefore, be preferable when using `gzip` compression.

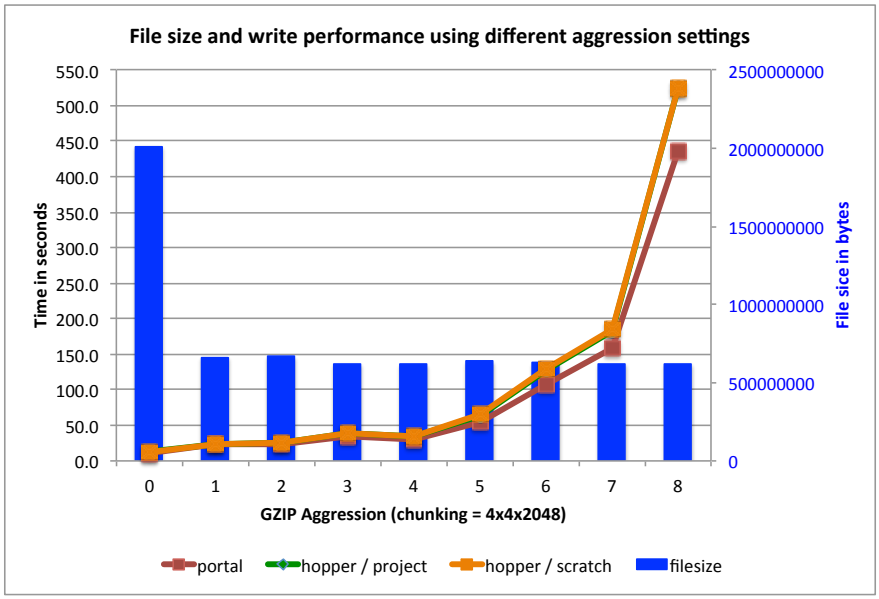


Fig. 8.22: File size and write performance using varying `gzip` aggression settings

8.7 Local Scalability: Multi-processing

Next we tested the local scalability using Python's multiprocessing capabilities (i.e, on a single `hopper` login node and `portal`, and not across multiple compute nodes). We again use a $100 \times 100 \times 100,000$ test dataset (using *A* as donor dataset) and we regenerate the dataset for each experiment (i.e., file layout + system). We repeat each computation 50 times on the same file and report the average times and standard deviations. For this test we select 20,000 z slices (i.e, 20% of the data) and compute the variance of the data values across the slices, i.e.:

- $numpy.var(data[:, :, zstart : (zstart + 20001)])$ with $zstart$ being selected randomly ($zstart \in [0, 79999]$)

[6] Bars shown transparently indicate that the bars exceed the maximum value shown in the plot. The real value for those bars are indicated via additional text labels.

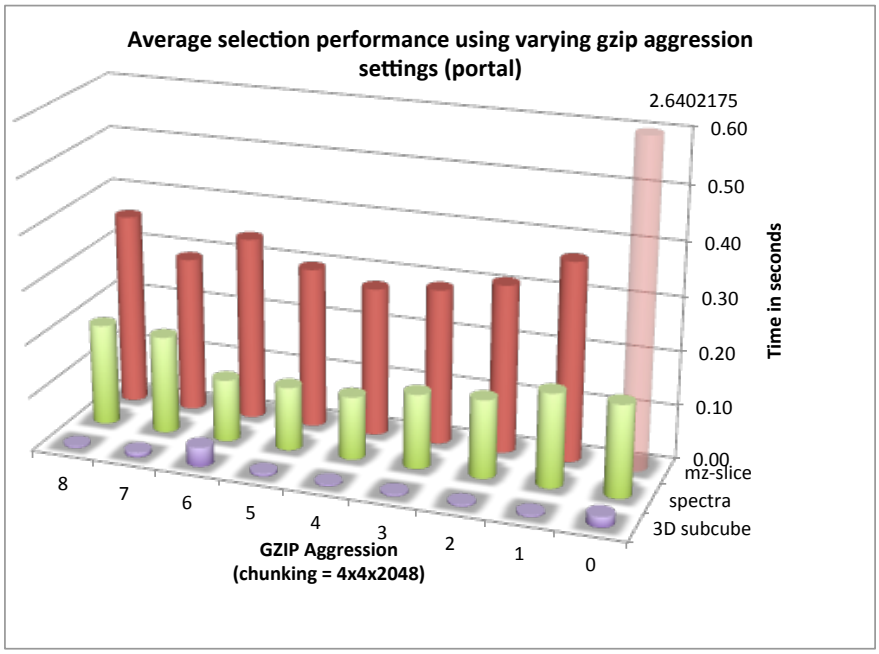


Fig. 8.23: Selection performance results using varying `gzip` aggression settings (`portal`)

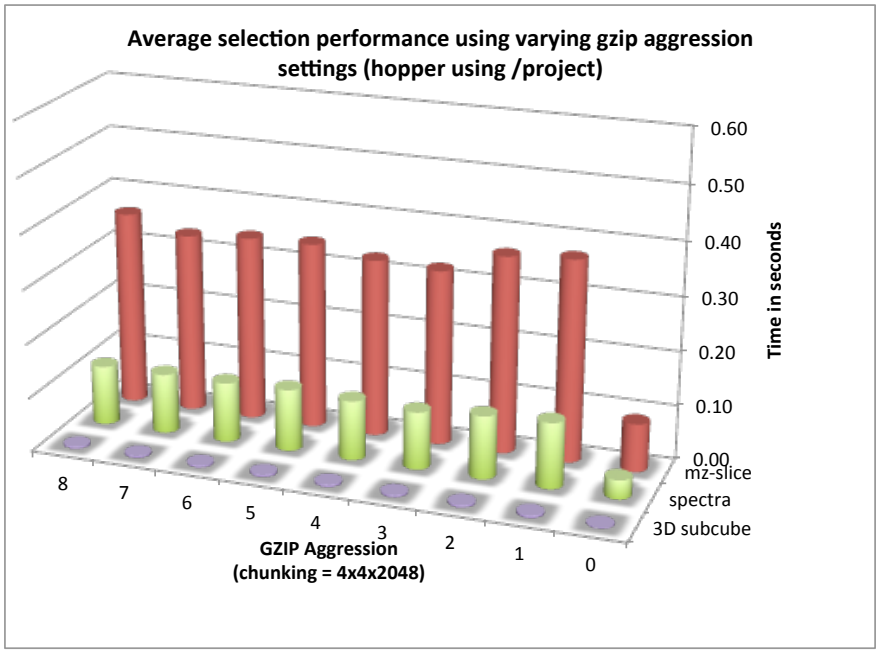


Fig. 8.24: Selection performance results using varying `gzip` aggression settings (`hopper` using `/project`)

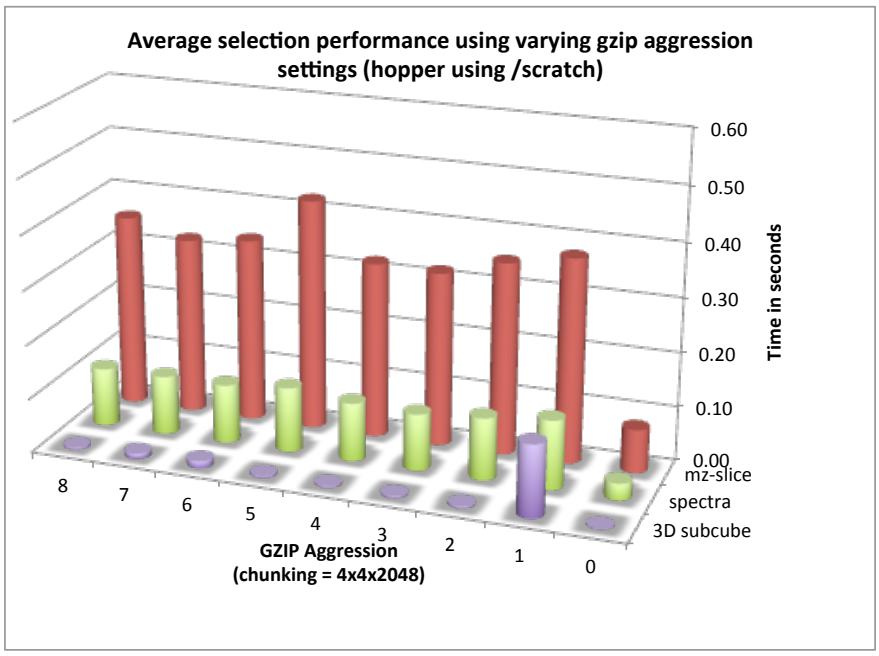


Fig. 8.25: Selection performance results using varying `gzip` aggression settings (`hopper` using `/scratch`)

We parallelize the computation across processes by dividing data along the x axis, i.e., each process computes for its portion of the data:

- $numpy.var(data[xstart : xend, :, zstart : (zstart + 20001)])$

while $xstart$ and $xend$ are determined based on the process id. The result is then stored in a shared array. The average performance (with error bars indicating the standard deviation) for performing this calculation on `hopper` using `project` are shown in Figure *Scaling results for computing the variance for 20000 z-slices (hopper using /project)*. We compute the speed-up by using the time required using 1 process as reference (i.e., the time from the current experiment so that the speed-up using 1 processor is always equal to 1)(see Figure *Speed-up results for computing the variance for 20000 z-slices (hopper using /project)*). We repeated the same tests also on `portal` (again using the `/project` file systems). The results for portal are shown in Figures: i) *Scaling results for computing the variance for 20000 z-slices (portal)* and ii) *Speed-up results for computing the variance for 20000 z-slices (portal)*.

The main bottleneck in this calculation is again the data selection/load. We observe that we can achieve good speed-up for larger numbers of processes using `hopper` compared to `portal`. This behavior is likely due to the better I/O (network) performance of `hopper` compared to `portal`. On `portal` we observe a stable speed-up for up to 5 processes (when using compression) and we achieve a $\approx 3\times$ speed-up. Using `hopper` we observe a linear speed-up for up to 8 processes. Afterwards, we still observe speed-up, however, at a lower and less stable rate. As before, we observe that using compression yields better performance on `portal` while reducing the performance when using `hopper`.

In the context of the OpenMSI web-based data viewer we typically need to extract smaller subsets of the data. We, therefore, next repeated the variance computation for 25 consecutive z slices (similar to the z slice selection use-case used in the previous sections). The timings and speed-up results on `portal` using default setup —i.e., with $4 \times 4 \times 2048$ chunking and `gzip` compression, aggression=4— are shown in Figure *Timings and sppeed-up results for computing the variance for 25 z-slices (portal)*. We observe that even-though the amount of data retrieved is with 0.5MB comparably small —note the data being loaded to fulfill the query is on the order of 39.0625MB—, we can still achieve good speed-ups until 4-7 processes, afterwards the performance degrades again.

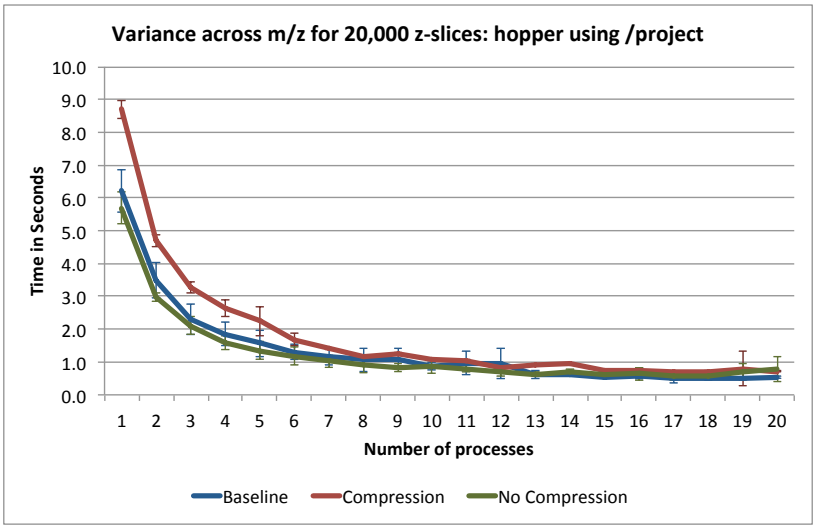


Fig. 8.26: Scaling results for computing the variance for 20000 z-slices (`hopper` using `/project`)

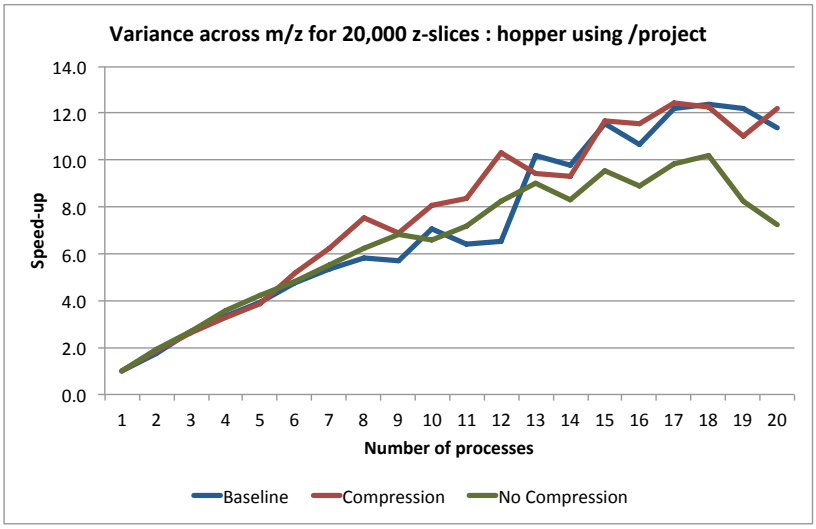


Fig. 8.27: Speed-up results for computing the variance for 20000 z-slices (`hopper` using `/project`)

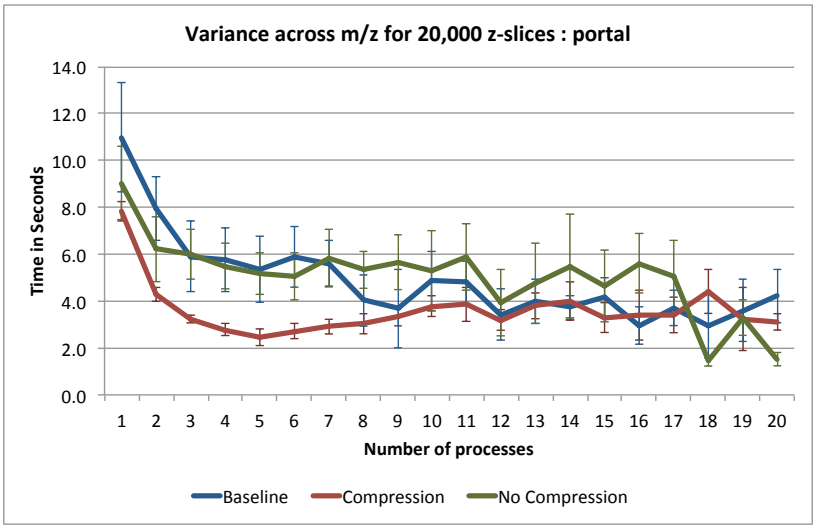


Fig. 8.28: Scaling results for computing the variance for 20000 z-slices (`portal`)

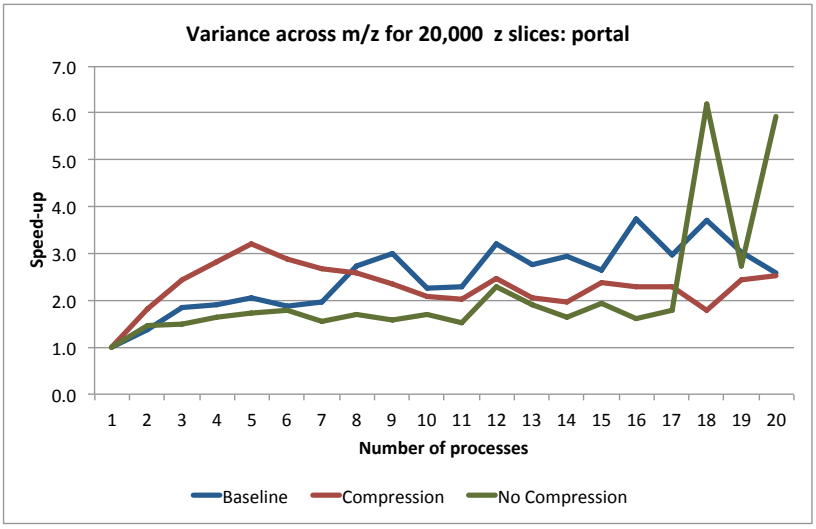


Fig. 8.29: Speed-up results for computing the variance for 20000 z-slices (`portal`)

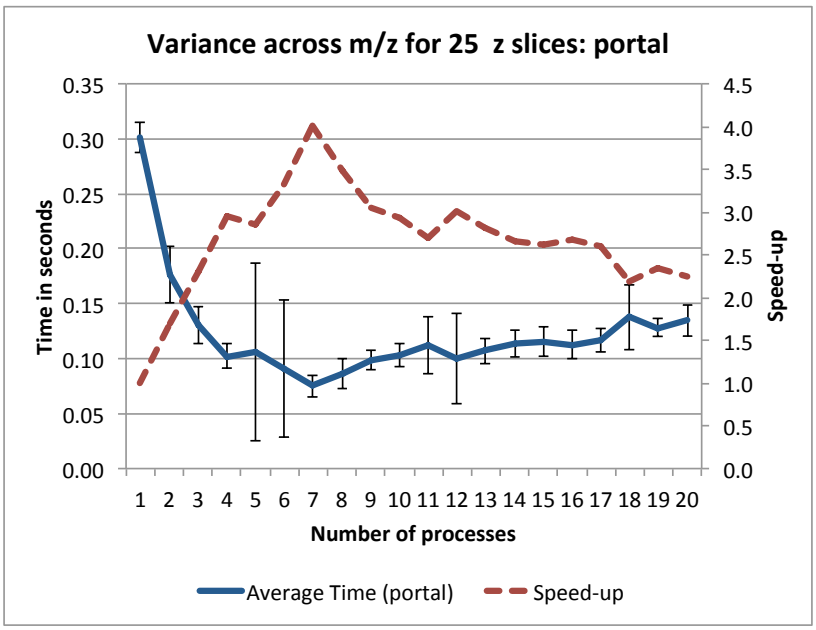


Fig. 8.30: Timings and sppeed-up results for computing the variance for 25 z-slices (`portal`)

8.8 Discussion

8.8.1 Data Layout

Use of chunking has many benefits but choosing the correct chunk size can be complicated. In the context of MSI data, the choice of a good data layout is complicated by: i) the large difference between the size of the spatial x/y and the z (mz, mass) dimension and ii) the need for regularly performing orthogonal data selection operations (namely selection of spectra `[x,y,:]` and full slices in z `[:,:,z]`. Our experiments have shown that a chunking of $4 \times 4 \times 2048$ may work well for most cases, i.e., it provides a good compromise in performance between the different selection operations while maintaining acceptable write performance and limiting the worst-case overhead in file size.

Our experiments have also shown that MSI data lends itself well to compression (we have seen reductions in file size on the order of $3\times$ to $9\times$ on real MSI datasets). We have also seen that the use of data compression (here `gzip`) may also improve the selection performance by reducing the amount of data that needs to be loaded from disk (see results from `portal`). This is particularly true for I/O (and or network) bound systems, such as `portal`. However, we have also seen (on `hopper`) that the use of compression can also decrease the selection performance due to the time required for decompression (see results `hopper`). Having direct access to uncompressed data may, hence, be advantageous for any analyses that require a large number of random accesses to the data from a high-performance compute systems (such as `hopper`) where the time required for decompression is larger than the time saved for data transfer. However, the reduced storage requirements and overall more stable selection performance results suggest that the use of compression may be advantageous.

Based on the results from this study we currently use a data layout of $4 \times 4 \times 2048$ with `gzip` compression and `aggression=4` as default for storing MSI data using the OMSI HDF5 data format.

8.8.2 System Performance

In a serial setting we observe that `hopper`'s `/scratch` filesystem generally provides better selective read performance than the `/project` file system. This is not unexpected and overall the performance of both file systems appears to be sufficient to perform most common MSI analysis tasks. However, based on the test results it appears that

on `portal`: i) the selection performance is highly dependent on system load (which appeared to be high on many occasions) and ii) the selection performance is bound by the performance of the I/O system. Since the performance using `/project` is significantly higher on `hopper` login nodes than on `portal`, it appears that the bandwidth of the network connection of `portal` to the GPFS `/project` file system may be too low to ensure a reliably fast operation of web-applications that require repeated access to large datasets. This, however, is essential for production use of science gateways that aim to make advanced data viewing and analysis capabilities accessible to the application community (such as the OpenMSI science gateway for MSI data). While we were able to achieve usable I/O performance on `portal` through the use of chunking and compression, we have also seen that even from `/project` we can achieve significantly better performance on `hopper` when storing the data in a raw, uncompressed form (i.e., we should be able to get much better selective I/O performance on `portal` using `/project`). While `portal` provides a good platform for development of science gateways and web applications, the question remains whether `portal` is powerful enough —with respect to both compute, I/O and network performance— to provide a reliable, high-performance platform for hosting production science gateways.

8.8.3 Future Work

In future we plan to evaluate the performance of the different data layouts in a: i) local parallel (multi-processing) and ii) distribution parallel (MPI) environment.

While `gzip` is one of the most widely available compression algorithms in HDF5 it is not necessarily one with the best performance. In future we plan to evaluate the use of other compression algorithms —such as, szip [7], LZF [8], HDF5 N-Bit Filter [9] , HDF5 Scale+Offset Filter [10] etc.— to further improve the overall read performance and to reduce the larger overheads for compression we have seen on `hopper`. In addition to compression, HDF5 also provides a shuffle filter [11] which can potentially further improve the effectiveness of data compression [12] .

[7] http://www.hdfgroup.org/doc_resource/SZIP/
[8] http://h5py.alfven.org/lzf/
[9] http://www.hdfgroup.org/HDF5/doc/RM/RM_H5P.html#Property-SetNbit
[10] http://www.hdfgroup.org/HDF5/doc/RM/RM_H5P.html#Property-SetScaleoffset
[11] http://www.hdfgroup.org/HDF5/doc/RM/RM_H5Z.html
[12] http://www.hdfgroup.org/HDF5/doc_resource/H5Shuffle_Perf.pdf ,

CHAPTER

NINE

OMSI PACKAGE

9.1 Subpackages

The omsi package defines the main BASTet software stack used, e.g., by the OpenMSI project. It contains a large range of functionality for interacting analyses, OpenMSI HDF5 data files, analysis workflows and other related infrastructure. The following is a rough overview of the various packages and modules

- **Analysis** *omsi.analysis* Package containing the base classes that facilitate the integration of new analysis with the BASTet software stack (e.g, the file format) and collection of specific analysis functionality.

omsi.analysis	Package containing the base classes that facilitate the integration of new analysis w
omsi.analysis.compound_stats	Package containing shared third-party code modules included here to reduce the ne
omsi.analysis.findpeaks	Package of peak-finding related analysis modules.
omsi.analysis.msi_filtering	Module with third-party modules, functions, classes used by some of the analysis n
omsi.analysis.multivariate_stats	Multivariate statistics analysis

- **Data Format** `omsi.dataformat` Package for implementation and specification of file formats. In particular this package contains the base API for interacting with OpenMSI HDF5 datasets.

`omsi.dataformat`	Package for implementation and specification of file formats.
omsi.dataformat.omsi_file	Module for specification of the OpenMSI file API.

- **Workflow** *omsi.workflow* Package with modules for specification and execution of analysis tasks and complex analysis workflows.

omsi.workflow	Package with modules for specification and execution of analysis tasks and complex analysis work
`omsi.worflow.dirver`	
omsi.workflow.executor	Package with executors of analysis workflows.

- **Data Structures** `omsi.datastructure` Package with a collection of various data structures and related classes used throughout the software stack, e.g., for metadata, analysis parameter data, runtime information data etc.

omsi.datastructures	Package with a collection of various data structures and related classes used throughout t
omsi.datastructures.metadata	Package with metadata datastructures

- **Shared** `omsi.shared` Package used to implement shared functionality and helper functions.

`omsi.shared`	Package used to implement shared functionality and helper functions.
`omsi.shared.thirdparty`	

- **Tools** `omsi.tools` Package for collecting tools (e.g,. command-line programs) to help with particular tasks. This includes, e.g, tools for data conversion, document generation, etc.

`omsi.tools`	Package for collecting tools (e.g,.
`omsi.tools.misc`	Collection of miscellaneous tools.

- **Templates** *`omsi.templates`* This package provides a collection of code templates to ease the development of additional components, e.g., analysis modules. As such, this package is NOT intended for direct usage but is rather just a library of code templates.

`omsi.templates`	This package provides a collection of code templates to ease the development of additional components, e.g.,

- **Examples** `omsi.examples` Package with a collection of various misc. example scripts.

`omsi.examples`	Package with a collection of various misc.

9.1.1 analysis Package

`omsi.analysis`	Package containing the base classes that facilitate the inte
`omsi.analysis.base`	Module specifying the base analysis API for integrating n
`omsi.analysis.generic`	Generic analysis class used to represent analyses of unkn
`omsi.analysis.analysis_views`	Helper module with functions and classes for interfacing
`omsi.analysis.compound_stats`	Package containing shared third-party code modules inclu
`omsi.analysis.compound_stats.omsi_score_compounds`	
`omsi.analysis.findpeaks`	Package of peak-finding related analysis modules.
`omsi.analysis.findpeaks.omsi_findpeaks_global`([...])	Basic global peak detection analysis.
`omsi.analysis.findpeaks.omsi_findpeaks_local`([...])	Class defining a basic gloabl peak finding.
`omsi.analysis.msi_filtering`	Module with third-party modules, functions, classes used
`omsi.analysis.msi_filtering.omsi_tic_norm`([...])	TIC Normalization analysis.
`omsi.analysis.multivariate_stats`	Multivariate statistics analysis
`omsi.analysis.multivariate_stats.omsi_cx`([...])	Class used to implement CX factorization on MSI data.
`omsi.analysis.multivariate_stats.omsi_nmf`([...])	Class defining a basic nmf analysis.

`analysis` Package

Package containing the base classes that facilitate the integration of new analysis with the BASTet software stack (e.g, the file format) and collection of specific analysis functionality.

class `omsi.analysis.`**`analysis_data`**(*name='undefined'*, *data=None*, *dtype='float32'*)

Bases: `dict`

Define an output dataset for the analysis that should be written to the omsi HDF5 file

The class can be used like a dictionary but restricts the set of keys that can be used to the following required keys which should be provided during initalization.

Required Keyword Arguments:

Parameters

- **`name`** – The name for the dataset in the HDF5 format
- **`data`** – The numpy array to be written to HDF5. The data write function omsi_file_experiment.create_analysis used for writing of the data to file can in principal

also handel other primitive data types by explicitly converting them to numpy. However, in this case the dtype is determined based on the numpy conversion and correct behavior is not guaranteed. I.e., even single scalars should be stored as a 1D numpy array here. Default value is None which is mapped to np.empty(shape=(0) , dtype=dtype) in __init__

- **dtype** – The data type to be used during writing. For standard numpy data types this is just the dtype of the dataset, i.e., ['data'].dtype. Other allowed datatypes are:
  - For string: omsi_format.str_type (omsi_format is located in omsi.dataformat.omsi_file)
  - To generate data links: ana_hdf5link (analysis_data)

ana_hdf5link = -1

class omsi.analysis.**analysis_base**

Bases: *omsi.datastructures.analysis_data.parameter_manager*

Base class for omsi analysis functionality. The class provides a large set of functionality designed to facilitate storage of analysis data in the omsi HDF5 file format. The class also provides a set of functions to enable easy intergration of new analysis with the OpenMSI web-based viewer (see Viewer functions below for details).

Slicing:

This class supports basic slicing to access data stored in the main member variables. By default the data is retrieved from __data_list and the __getitem__(key) function. which implements the [..] operator, returns __data_list[key]['data']. The key is a string indicating the name of the parameter to be retrieved. If the key is not found in the __data_list then the function will try to retrieve the data from self.parameters list instead. By adding "parameter/key" or "dependency/key" one may also explicitly retrieve values from the parameters.

Instance Variables:

Variables

- ***analysis_identifier*** – Define the name for the analysis used as key in search operations
- **__data_list** – List of analysis_data to be written to the HDF5 file. Derived classes need to add all data that should be saved for the analysis in the omsi HDF5 file to this dictionary. See omsi.analysis.analysis_data for details.
- **parameters** – List of parameter_data objects of all analysis parameters (including those that may have dependencies).
- **data_names** – List of strings of all names of analysis output datasets. These are the target keys for __data_list.
- **profile_time_and_usage** – Boolean indicating whether we should profile the execute_analysis(...) function when called as part of the execute(...) function. The default value is false. Use the enable_time_and_usage_profiling(..) function to determine which profiling should be performed. The time_and _usage profile uses pythons cProfile (or Profile) to monitor how often and for how long particular parts of the analysis code executed.
- **profile_memory** – Boolean indicating whether we should monitor memory usage (line-by-line) when executing the execute_analysis(...) function. The default value is false. Use the enable_time_and_usage_profiling(..) function to determine which profiling should be performed.
- **omsi_analysis_storage** – List of omsi_file_analysis object where the analysis is stored. The list may be empty.
- **mpi_comm** – In case we are running with MPI, this is the MPI communicator used for runnign the analysis. Default is MPI.Comm_world/

- **mpi_root** – In case we are running with MPI, this is the root rank where data is collected to (e.g., runtime data and analysis results)
- **update_analysis** – If the value is True, then we should execute the analysis before using the outputs. If False, then the analysis has been executed with the current parameter settings.
- ***driver*** – Workflow driver to be used when executing multiple analyses, e.g., via execute_recursive or execute_all. Default value is None in which case a new default driver will be used each time we execute a workflow.

Execution Functions:

- `execute` : Then main function the user needs to call in order to execute the analysis
- "execute_analysis: This function needs to be implemented by child classes of *analysis_base* to implement the specifics of executing the analysis.

I/O functions:

These functions can be optionally overwritten to control how the analysis data should be written/read from the omsi HDF5 file. Default implementations are provided here, which should be sufficient for most cases.

- `add_custom_data_to_omsi_file`: The default implementation is empty as the default data write is managed by the *omsi_file_experiment.create_analysis()* function. Overwrite this function, in case that the analysis needs to write data to the HDF5 omsi file beyond what the defualt omsi data API does.
- `read_from_omsi_file`: The default implementation tries to reconstruct the original data as far as possible, however, in particular in case that a custom add_custom_data_to_omsi_file function has been implemented, the default implementation may not be sufficien. The default implementation reconstructs: i) analysis_identifier and reads all custom data into ii)__data_list. Note, an error will be raised in case that the analysis type specified in the HDF5 file does not match the analysis type specified by get_analysis_type(). This function can be optionally overwritten to implement a custom data read.

Viewer functions:

Several convenient functions are used to allow the OpenMSI online viewer to interact with the analysis and to visualize it. The default implementations provided here simply indicate that the analysis does not support the data access operations required by the online viewer. Overwrite these functions in the derived analysis classes in order to interface them with the viewer. All viewer-related functions start with `v\_...` .

NOTE: the default implementation of the viewer functions defined in `analysis_base` are designed to take care of the common requirement for providing viewer access to data from all dependencies of an analysis. In many cases, the default implementation is often sill called at the end of custom viewer functions.

NOTE: The viewer functions typically support a viewer_option parameter. viewer_option=0 is expected to refer to the analysis itself.

- `v_qslice`: Retrieve/compute data slices as requested via qslice URL requests. The corresponding view of the DJANGO data access server already translates all input parameters and takes care of generating images/plots if needed. This function is only responsible for retrieving the data.
- `v_qspectrum`: Retrieve/compute spectra as requested via qspectrum URL requests. The corresponding view of the DJANGO data access server already translates all input parameters and takes care of generating images/plots if needed. This function is only responsible for retrieving the data.
- `v_qmz`: Define the m/z axes for image slices and spectra as requested by qspectrum URL requests.
- `v_qspectrum_viewer_options`: Define a list of strings, describing the different viewer options available for the analysis for qspectrum requests (i.e., `v_qspectrum`). This feature allows the analysis developer to define multiple different visualization modes for the analysis. For example, when performing a data reduction (e.g., PCA or NMF) one may want to show the raw spectra or the loadings vector of the

projection in the spectrum view (v_qspectrum). By providing different viewer options we allow the user to decide which option they are most interested in.

- `v_qslice_viewer_options`: Define a list of strings, describing the different viewer options available for the analysis for qslice requests (i.e., `v_qslice`). This feature allows the analysis developer to define multiple different visualization modes for the analysis. For example, when performing a data reduction (e.g., PCA or NMF) one may want to show the raw spectra or the loadings vector of the projection in the spectrum view (v_qspectrum). By providing different viewer options we allow the user to decide which option they are most interested in.

Initialize the basic data members

add_custom_data_to_omsi_file(*analysis_group*)

This function can be optionally overwritten to implement a custom data write function for the analysis to be used by the omsi_file API.

Note, this function should be used only to add additional data to the analysis group. The data that is written by default is still written by the *omsi_file_experiment.create_analysis()* function, i.e., the following data is written by default: i) analysis_identifier ,ii) get_analysis_type, iii)__data_list, iv) parameters, v) runinfo . Since the *omsi_file.experiment.create_analysis()* functions takes care of setting up the basic structure of the analysis storage (included the subgroubs for storing parameters and data dependencies) this setup can generally be assumed to exist before this function is called. This function is called automatically at the end omsi_file.experiment.create_analysis() (i.e, actually *omsi_file_analysis.__populate_analysis__(..)* so that this function typically does not need to be called explicitly.

Parameters **analysis_group** – The h5py.Group object where the analysis is stored.

add_parameter(*name*, *help*, *dtype=<type 'unicode'>*, *required=False*, *default=None*, *choices=None*, *data=None*, *group=None*)

Add a new parameter for the analysis. This function is typically used in the constructor of a derived analysis to specify the parameters of the analysis.

Parameters

- **name** – The name of the parameter
- **help** – Help string describing the parameter
- **type** – Optional type. Default is string.
- **required** – Boolean indicating whether the parameter is required (True) or optional (False). Default False.
- **default** – Optional default value for the parameter. Default None.
- **choices** – Optional list of choices with allowed data values. Default None, indicating no choices set.
- **data** – The data assigned to the parameter. None by default.
- **group** – Optional group string used to organize parameters. Default None, indicating that parameters are automatically organized by driver class (e.g. in required and optional parameters)

Raises ValueError is raised if the parameter with the given name already exists.

analysis_identifier_defined()

Check whether the analysis identifier is defined by the user, i.e., set to value different than undefined :return: bool

check_ready_to_execute()

Check if all inputs are ready to determine if the analysis is ready to run.

Returns List of omsi_analysis_parameter objects that are not ready. If the returned list is empty, then the analysis is ready to run.

clear_analysis()
Clear all analysis data—i.e., parameter, dependency data, output results, runtime data

clear_analysis_data()
Clear the list of analysis data

clear_and_restore(*analysis_manager=None*, *resave=False*)
Clear all analysis data and restore the results from file

Parameters

- **analysis_manager** – Instance of omsi_analysis_manager (e.g., an omsi_file_experiment) where the analysis should be saved.
- **resave** – Boolean indicating whether the analysis should be saved again, even if it has been saved before. This parameter only has effect if analysis_manager is given.

Returns self, i.e., the updated analysis object with all data replaced with HDF5 references

clear_parameter_data()
Clear the list of parameter data

clear_run_info_data()
Clear the runtime information data

define_missing_parameters()
Called by the execute function before self.update_analysis_parameters to set any required parameters that have not been defined to their respective default values.

This function may be overwritten in child classes to customize the definition of default parameter values and to apply any modifications (or checks) of parameters before the analysis is executed. Any changes applied here will be recorded in the parameter of the analysis.

enable_memory_profiling(*enable=True*)
Enable or disable line-by-line profiling of memory usage of execute_analysis.

Parameters **enable_memory** (*bool*) – Enable (True) or disable (False) line-by-line profiling of memory usage

Raises ImportError is raised if a required package for profiling is not available.

enable_time_and_usage_profiling(*enable=True*)
Enable or disable profiling of time and usage of code parts of execute_analysis.

Parameters **enable** (*bool*) – Enable (True) or disable (False) profiling

Raises ImportError is raised if a required package for profiling is not available.

execute(***kwargs*)
Use this function to run the analysis.

Parameters **kwargs** – Parameters to be used for the analysis. Parameters may also be set using the __setitem__ mechanism or as batches using the set_parameter_values function.

Returns This function returns the output of the execute analysis function.

Raises AnalysisReadyError in case that the analysis is not ready to be executed. This may be the case, e.g, when a dependent input parameter is not ready to be used.

classmethod **execute_all**(*force_update=False*, *executor=None*)
Execute all analysis instances that are currently defined.

Parameters

- **force_update** – Boolean indicating whether we should force that all analyses are executed again, even if they have already been run with the same settings before. False by default.
- **executor** – Optional workflow executor to be used for the execution of all analyses. The executor will be cleared and then all analyses will be added to executor. Default value is None, in which case the function creates a default executor to be used.

Returns The workflow executor used

execute_analysis()
Implement this function to implement the execution of the actual analysis.

This function may not require any input parameters. All input parameters are recorded in the parameters and dependencies lists and should be retrieved from there, e.g, using basic slicing self[paramName]

Input parameters may be added for internal use ONLY. E.g, we may add parameters that are used internally to help with parallelization of the execute_analysis function. Such parameters are not recorded and must be strictly optional so that analysis_base.execute(...) can call the function.

Returns This function may return any developer-defined data. Note, all output that should be recorded must be put into the data list.

execute_recursive(***kwargs*)
Recursively execute this analysis and all its dependencies if necessary

We use a workflow driver to control the execution. To define the workflow driver we can set the self.driver variable. If no workflow driver is given (i.e, self.driver==None), then the default driver will be created. To change the default driver, see *omsi.workflow.base.workflow_executor_base.DEFAULT_EXECUTOR_CLASS*

Parameters **kwargs** – Parameters to be used for the analysis. Parameters may also be set using the __setitem__ mechanism or as batches using the set_parameter_values function.

Returns Same as execute

get_all_analysis_data()
Get the complete list of all analysis datasets to be written to the HDF5 file

get_all_dependency_data()
Get the complete list of all direct dependencies to be written to the HDF5 file

NOTE: These are only the direct dependencies as specified by the analysis itself. Use get_all_dependency_data_recursive(..) to also get the indirect dependencies of the analysis due to dependencies of the dependencies themselves.

Returns List of parameter_data objects that define dependencies.

get_all_parameter_data(*exclude_dependencies=False*)
Get the complete list of all parameter datasets to be written to the HDF5 file

Parameters **exclude_dependencies** – Boolean indicating whether we should exclude parameters that define dependencies from the list

get_all_run_info()
Get the dict with the complete info about the last run of the analysis

get_analysis_data(*index*)
Given the index return the associated dataset to be written to the HDF5 file

:param index : Retrun the index entry of the private member __data_list.

get_analysis_data_by_name(*dataname*)
Given the key name of the data return the associated analysis_data object.

Parameters **dataname** – Name of the analysis data requested from the private __data_list member.

Returns The analysis_data object or None if not found.

get_analysis_data_names()
Get a list of all analysis dataset names.

get_analysis_identifier()
Return the name of the analysis used as key when searching for a particular analysis

classmethod **get_analysis_instances**()
Generator function used to iterate through all instances of analysis_base. The function creates references for all weak references stored in cls._analysis_instances and returns the references if it exists and cleans up the any invalid references after the iteration is complete. :return: References to analysis_base objects

get_analysis_type()
Return a string indicating the type of analysis performed

static **get_default_dtypes**()
Get a list of available default dtypes used for analyses. Same as *data_dtypes.get_dtypes()*.

static **get_default_parameter_groups**()
Get a list of commonly used parameter groups and associated descriptions.

Use of default groups provides consistency and allows other system to design custom behavior around the semantic of parameter groups

Returns Dictionary where the keys are the short names of the groups and the values are dicts with following keys:value pairs: 'name' , 'description'. Use the 'name' to define the group to be used.

get_help_string()
Get a string describing the analysis.

Returns Help string describing the analysis and its parameters

get_memory_profile_info()
Based on the memory profile of the execute_analysis(..) function get the string describing the line-by-line memory usage.

Returns String describing the memory usage profile. None is returned in case that no memory profiling data is available.

get_num_analysis_data()
Retrun the number of analysis datasets to be wirtten to the HDF5 file

get_num_dependency_data()
Return the number of dependencies to be wirtten to the HDF5 file

get_num_parameter_data()
Return the number of parameter datasets to be wirtten to the HDF5 file

get_omsi_analysis_storage()
Get a list of known locations where this analysis has been saved.

Returns List of *omsi.dataformat.omsi_file.analysis. omsi_file_analysis* objects where the analysis is saved.

get_parameter_data(*index*)
Given the index return the associated dataset to be written to the HDF5 file

:param index : Return the index entry of the private member parameters.

get_parameter_data_by_name(*dataname*)
Given the key name of the data return the associated parameter_data object.

Parameters **dataname** – Name of the parameter requested from the parameters member.

Returns The parameter_data object or None if not found

get_parameter_names()
Get a list of all parameter dataset names (including those that may define dependencies.

get_profile_stats_object(*consolidate=True*, *stream=None*)
Based on the execution profile of the execute_analysis(..) function get `pstats.Stats` object to help with the interpretation of the data.

Parameters

- **consolidate** – Boolean flag indicating whether multiple stats (e.g., from multiple cores) should be consolidated into a single stats object. Default is True.
- **stream** – The optional stream parameter to be used fo the pstats.Stats object.

Returns A single pstats.Stats object if consolidate is True. Otherwise the function returns a list of pstats.Stats objects, one per recorded statistic. None is returned in case that the stats objects cannot be created or no profiling data is available.

has_omsi_analysis_storage()
Check whether a storage location is known where the anlaysis has been saved.

Returns Boolean indicating whether self.omsi_analysis_storage is not empty

keys()
Get a list of all valid keys, i.e., a combination of all input parameter and output names.

Returns List of strings with all input parameter and output names.

classmethod **locate_analysis**(*data_object*, *include_parameters=False*)
Given a data_object try to locate the analysis that creates the object as an output of its execution (and optionally analyses that have the object as an input).

Parameters

- **data_object** – The data object of interest.
- **include_parameters** – Boolean indicating whether also input parameters should be considered in the search in addition to the outputs of an analysis

Returns dependency_dict pointing to the relevant object or None in case the object was not found.

read_from_omsi_file(*analysis_object*, *load_data=True*, *load_parameters=True*, *load_runtime_data=True*, *dependencies_omsi_format=True*, *ignore_type_conflict=False*)
This function can be optionally overwritten to implement a custom data read.

The default implementation tries to reconstruct the original data as far as possible, however, in particular in case that a custom add_custom_data_to_omsi_file function has been implemented, the default implementation may not be sufficient. The default implementation reconstructs: i) analysis_identifier and reads all custom data into iii)__data_list. Note, an error will be raised in case that the analysis type specified in the HDF5 file does not match the analysis type specified by get_analysis_type()

Parameters

- **analysis_object** – The omsi_file_analysis object associated with the hdf5 data group with the analysis data_list
- **load_data** – Should the analysis data be loaded from file (default) or just stored as h5py data objects
- **load_parameters** – Should parameters be loaded from file (default) or just stored as h5py data objects.
- **load_runtime_data** – Should runtime data be loaded from file (default) or just stored as h5py data objects
- **dependencies_omsi_format** – Should dependencies be loaded as omsi_file API objects (default) or just as h5py objects.
- **ignore_type_conflict** – Set to True to allow the analysis to be loaded into the current analysis object even if the type indicated in the file does not match the class. Default value is False. This behavior can be useful when different analysis have compatible data structures or when we want to load the data in to a generic analysis container, e.g, analysis_generic.

Returns bool Boolean indicating whether the data was read successfully

Raise TypeError : A type error will be raised in case that the analysis type specified by the file does not match the analysis type provided by self.get_analysis_type()

record_execute_analysis_outputs(*analysis_output*)

Function used internally by execute to record the output of the custom execute_analysis(...) function to the __data_list.

This function may be overwritten in child classes in order to customize the behavior for recording data outputs. Eg., for some analyses one may only want to record a particular set of outputs, rather than all outputs generated by the analysis.

Parameters analysis_output – The output of the execute_analysis(...) function to be recorded

results_ready()

Check whether the results of the analysis are ready to be used :return: Boolean

set_analysis_identifier(*identifier*)

Set the name of the analysis to identifer

Side Effects: This function modifies self.analysis_identifier

Parameters identifier (*str*) – The new analysis identifier string to be used (should be unique)

set_parameter_values(***kwargs*)

Set all parameters given as input to the function. The inputs are placed in the self.parameters list. If the parameter refers to an existing h5py.Dataset, h5py.Group, managed h5py object, or is an instance of an existing omis_analysi_base object, then a dependency_dict will be created and stored as value instead.

Parameters kwargs – Dictionary of keyword arguments. All keys are expected to be strings. All values are expected to be either i) numpy arrays, ii) int, float, str or unicode variables, iii) h5py.Dataset or h5py.Group, iv) or any the omsi_file API class objects. For iii) and iv) one may provide a tuple consisting of the dataobject t[0] and an additional selection string t[1].

update_analysis_parameters(***kwargs*)

Record the analysis parameters passed to the execute() function.

The default implementation simply calls the set_parameter_values(...) function. This function may be overwritten to customize the behavior of how parameters are recorded by the execute function.

Parameters **kwargs** – Dictionary of keyword arguments with the parameters passed to the execute(..) function

classmethod **v_qmz**(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Get the mz axes for the analysis

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **qslice_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qslice URL pattern.
- **qspectrum_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qspectrum URL pattern.

Returns

The following four arrays are returned by the analysis:

- mzSpectra : Array with the static mz values for the spectra.
- labelSpectra : Label for the spectral mz axis
- mzSlice : Array of the static mz values for the slices or None if identical to the mzSpectra.
- labelSlice : Label for the slice mz axis or None if identical to labelSpectra.
- values_x: The values for the x axis of the image (or None)
- label_x: Label for the x axis of the image
- values_y: The values for the y axis of the image (or None)
- label_y: Label for the y axis of the image
- values_z: The values for the z axis of the image (or None)
- label_z: Label for the z axis of the image

classmethod **v_qslice**(*analysis_object*, *z*, *viewer_option=0*)
Get 3D analysis dataset for which z-slices should be extracted for presentation in the OMSI viewer

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **z** – Selection string indicting which z values should be selected.
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns numpy array with the data to be displayed in the image slice viewer. Slicing will be performed typically like [:,:,zmin:zmax].

Raises NotImplementedError in case that v_qslice is not supported by the analysis.

classmethod **v_qslice_viewer_options**(*analysis_object*)
Get a list of strings describing the different default viewer options for the analysis for qslice. The default implementation tries to take care of handling the spectra retrieval for all the dependencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decission based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qslice requests (i.e., v_qslice(...) is not available).

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)

Get from which 3D analysis spectra in x/y should be extracted for presentation in the OMSI viewer

Developer Note: h5py currently supports only a single index list. If the user provides an index-list for both x and y, then we need to construct the proper merged list and load the data manually, or if the data is small enough, one can load the full data into a numpy array which supports multiple lists in the selection.

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **x** – x selection string
- **y** – y selection string
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns

The following two elements are expected to be returned by this function :

1. 1D, 2D or 3D numpy array of the requested spectra. NOTE: The mass (m/z) axis must be the last axis. For index selection x=1,y=1 a 1D array is usually expected. For indexList selections x=[0]&y=[1] usually a 2D array is expected. For ragne selections x=0:1&y=1:2 we one usually expects a 3D array.
2. None in case that the spectra axis returned by v_qmz are valid for the returned spectrum. Otherwise, return a 1D numpy array with the m/z values for the spectrum (i.e., if custom m/z values are needed for interpretation of the returned spectrum).This may be needed, e.g., in cases where a per-spectrum peak analysis is performed and the peaks for each spectrum appear at different m/z values.

classmethod **v_qspectrum_viewer_options**(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qspectrum. The default implementation tries to take care of handling the spectra retrieval for all the dependencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decision based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qspectrum requests (i.e., v_qspectrum(...) is not available).

write_analysis_data(*analysis_group=None*)

This function is used to write the actual analysis data to file. If not implemented, then the omsi_file_analysis API's default behavior is used instead.

Parameters **analysis_group** – The h5py.Group object where the analysis is stored. May be None on cores that do not perform any writing but which need to participate in communication, e.g., to collect data for writing.

exception omsi.analysis.**AnalysisReadyError**(*value*, *params=None*)
Bases: exceptions.Exception

Custom exception used to indicate that an analysis is not ready to execute.

Initialize the AnalysisReadyError

Parameters

- **value** – Error message string
- **params** – Optional list of dependent parameters that are not ready to be used.

class omsi.analysis.**analysis_generic**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

This analysis class is used if the specific anlaysis type is unknown, e.g., when loading custom user-defined analysis data that may have not be available in the standard omsi package used.

Initialize the basic data members

Parameters **name_key** – The name for the analysis

DEFAULT_OUTPUT_PREFIX = 'output_'

execute(***kwargs*)
Overwrite the default implementation of execute to update parameter specifications/types when wrapping functions where the types are not known a priori.

Parameters **kwargs** – Custom analysis parameters

Returns The result of execute_analysis()

execute_analysis()
Nothing to do here.

classmethod **from_function**(*analysis_function*, *output_names=None*, *parameter_specs=None*, *name_key='undefined'*)
Create a generic analysis class for a given analysis function.

This functionality is useful to ease quick scripting on analyses but should not be used in production.

NOTE: __analysis_function is a reserved parameter name used to store the analysis function and may not be used as an input parameter for the analysis function.

Parameters

- **analysis_function** – The analysis function to be wrapped for provenance tracking and storage
- **output_names** – Optionally, define a list of the names of the outputs
- **parameter_specs** – Optional list of omsi.datastructures.analysis_data.parameter_data with additional information about the parameters of the function.
- **name_key** – The name for the analysis, i.e., the analysis identifier

Returns A new generic analysis class

classmethod **get_analysis_type**()
Return a string indicating the type of analysis performed

get_real_analysis_type()
This class is designed to handle generic (including unkown) types of analysis. In cases, e.g., were this class is used to store analysis data from an HDF5 file we may have an actual analysis type available even if we do not have a special analysis class may not be available in the current installation

read_from_omsi_file(*analysis_object*, *load_data=True*, *load_parameters=True*, *load_runtime_data=True*, *dependencies_omsi_format=True*, *ignore_type_conflict=False*)
See *omsi.analysis.analysis_base.read_from_omsi_file(...)* for details. The function is overwritten here mainly to initialize the self.real_analysis_type instance variable but otherwise uses the default behavior.

classmethod v_qmz(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Implement support for qmz URL requests for the viewer

classmethod v_qslice(*analysis_object*, *z*, *viewer_option=0*)
Implement support for qslice URL requests for the viewer

classmethod v_qslice_viewer_options(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

classmethod v_qspectrum(*analysis_object*, *x*, *y*, *viewer_option=0*)
Implement support for qspectrum URL requests for the viewer

classmethod v_qspectrum_viewer_options(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

write_analysis_data(*analysis_group=None*)
This function is used to write the actual analysis data to file. If not implemented, then the omsi_file_analysis API's default behavior is used instead.

Parameters **analysis_group** – The h5py.Group object where the analysis is stored. May be None on cores that do not perform any writing but which need to participate in communication, e.g., to collect data for writing.

class omsi.analysis.**omsi_findpeaks_global**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Basic global peak detection analysis. The default implementation computes the peaks on the average spectrum and then computes the peak-cube data, i.e., the values for the detected peaks at each pixel.

TODO: The current version assumes 2D data

Initialize the basic data members

execute_analysis()
Execute the global peak finding for the given msidata and mzdata.

classmethod v_qmz(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Implement support for qmz URL requests for the viewer

classmethod v_qslice(*analysis_object*, *z*, *viewer_option=0*)
Implement support for qslice URL requests for the viewer

classmethod v_qslice_viewer_options(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

classmethod v_qspectrum(*analysis_object*, *x*, *y*, *viewer_option=0*)
Implement support for qspectrum URL requests for the viewer

classmethod v_qspectrum_viewer_options(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

class omsi.analysis.**omsi_findpeaks_local**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Class defining a basic gloabl peak finding. The default implementation computes the peaks on the average spectrum and then computes the peak-cube data, i.e., the values for the detected peaks at each pixel.

TODO: The current version assumes 2D data

Initialize the basic data members

execute_analysis(*msidata_subblock=None*)
Execute the local peak finder for the given msidata.

Parameters **msidata_subblock** – Optional input parameter used for parallel execution of the analysis only. If msidata_subblock is set, then the given subblock will be processed in SERIAL instead of processing self['msidata'] in PARALLEL (if available). This parameter is strictly optional and intended for internal use only.

classmethod **v_qmz**(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Implement support for qmz URL requests for the viewer

classmethod **v_qslice**(*analysis_object*, *z*, *viewer_option=0*)
Implement support for qslice URL requests for the viewer

classmethod **v_qslice_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)
Implement support for qspectrum URL requests for the viewer

classmethod **v_qspectrum_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

write_analysis_data(*analysis_group=None*)
This function is used to write the actual analysis data to file. If not implemented, then the omsi_file_analysis API's default behavior is used instead.

Parameters **analysis_group** – The h5py.Group object where the analysis is stored.

class omsi.analysis.**omsi_nmf**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Class defining a basic nmf analysis.

The function has primarily been tested we MSI datasets but should support arbitrary n-D arrays (n>=2). The last dimension of the input array must be the spectrum dimnensions.

Initalize the basic data members

execute_analysis()
Execute the nmf for the given msidata

classmethod **v_qmz**(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Implement support for qmz URL requests for the viewer

classmethod **v_qslice**(*analysis_object*, *z*, *viewer_option=0*)
Implement support for qslice URL requests for the viewer

classmethod **v_qslice_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)
Implement support for qspectrum URL requests for the viewer

classmethod **v_qspectrum_viewer_options** (*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

class omsi.analysis.**omsi_cx** (*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Class used to implement CX factorization on MSI data.

Initalize the basic data members

classmethod **comp_lev_exact** (*A*, *k*, *axis*)
This function computes the column or row leverage scores of the input matrix.

Parameters

- **A** – n-by-d matrix
- **k** – rank parameter, k <= min(n,d)
- **axis** – 0: compute row leverage scores; 1: compute column leverage scores.

Returns 1D array of leverage scores. If axis = 0, the length of lev is n. otherwise, the length of lev is d.

dimension_index = {'pixelDim': 1, 'imageDim': 0}

execute_analysis ()
EDIT_ME:

Replace this text with the appropriate documentation for the analysis. Describe what your analysis does and how a user can use it. Note, a user will call the function execute(...) which takes care of storing parameters, collecting execution data etc., so that you only need to implement your analysis, the rest is taken care of by analysis_base. omsi uses Sphynx syntax for the documentation.

Keyword Arguments:

Parameters **mydata** – ...

classmethod **v_qmz** (*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Get the mz axes for the analysis

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **qslice_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qslice URL pattern.
- **qspectrum_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qspectrum URL pattern.

Returns

The following four arrays are returned by the analysis:

- mz_spectra : Array with the static mz values for the spectra.
- label_spectra : Lable for the spectral mz axis
- mz_slice : Array of the static mz values for the slices or None if identical to the mz_spectra.
- label_slice : Lable for the slice mz axis or None if identical to label_spectra.

classmethod **v_qslice**(*analysis_object*, *z*, *viewer_option=0*)
Get 3D analysis dataset for which z-slices should be extracted for presentation in the OMSI viewer

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **z** – Selection string indicting which z values should be selected.
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns numpy array with the data to be displayed in the image slice viewer. Slicing will be performed typically like [:,:,zmin:zmax].

classmethod **v_qslice_viewer_options**(*analysis_object*)
Get a list of strings describing the different default viewer options for the analysis for qslice. The default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decision based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qslice requests (i.e., v_qslice(...) is not available).

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)
Get from which 3D analysis spectra in x/y should be extracted for presentation in the OMSI viewer

Developer Note: h5py currently supports only a single index list. If the user provides an index-list for both x and y, then we need to construct the proper merged list and load the data manually, or if the data is small enough, one can load the full data into a numpy array which supports mulitple lists in the selection.

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **x** – x selection string
- **y** – y selection string
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns

The following two elemnts are expected to be returned by this function :

1. 1D, 2D or 3D numpy array of the requested spectra. NOTE: The mass (m/z) axis must be the last axis. For index selection x=1,y=1 a 1D array is usually expected. For indexList selections x=[0]&y=[1] usually a 2D array is expected. For ragne selections x=0:1&y=1:2 we one usually expects a 3D array.
2. None in case that the spectra axis returned by v_qmz are valid for the returned spectrum. Otherwise, return a 1D numpy array with the m/z values for the spectrum (i.e., if custom m/z values are needed for interpretation of the returned spectrum).This may be needed,

e.g., in cases where a per-spectrum peak analysis is performed and the peaks for each spectrum appear at different m/z values.

classmethod **v_qspectrum_viewer_options**(*analysis_object*)
Get a list of strings describing the different default viewer options for the analysis for qspectrum. The default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decission based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qspectrum requests (i.e., v_qspectrum(...) is not available).

class omsi.analysis.**omsi_kmeans**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Class defining a basic nmf analysis for a 2D MSI data file or slice of the data

Initalize the basic data members

execute_analysis()
Execute the kmeans clustering for the given msidata

class omsi.analysis.**omsi_tic_norm**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

TIC Normalization analysis.

Initalize the basic data members

execute_analysis()
Normalize the data based on the total intensity of a spectrum or the intensities of a select set of ions.

Calculations are performed using a memory map approach to avoid loading all data into memory. TIC normalization can as such be performed even on large files (assuming sufficient disk space).

Keyword Arguments:

Parameters

- **msidata** (*h5py.dataset or numpu array (3D)*) – The input MSI dataset
- **mzdata** – The mz axsis do the dataset
- **maxCount** – ...
- **mzTol** – ...
- **infIons** – List of informative ions

record_execute_analysis_outputs(*analysis_output*)
We are not returning any outputs here, but we are going to record them manually. :param analysis_output: The output of the execute_analysis(...) function.

classmethod **v_qmz**(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Get the mz axes for the analysis

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **qslice_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qslice URL pattern.
- **qspectrum_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qspectrum URL pattern.

Returns

The following four arrays are returned by the analysis:

- mz_spectra : Array with the static mz values for the spectra.
- label_spectra : Lable for the spectral mz axis
- mz_slice : Array of the static mz values for the slices or None if identical to the mz_spectra.
- label_slice : Lable for the slice mz axis or None if identical to label_spectra.

classmethod v_qslice(*analysis_object*, *z*, *viewer_option=0*)

Get 3D analysis dataset for which z-slices should be extracted for presentation in the OMSI viewer

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **z** – Selection string indicting which z values should be selected.
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns numpy array with the data to be displayed in the image slice viewer. Slicing will be performed typically like [:,:,zmin:zmax].

classmethod v_qslice_viewer_options(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qslice. The default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decision based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qslice requests (i.e., v_qslice(...) is not available).

classmethod v_qspectrum(*analysis_object*, *x*, *y*, *viewer_option=0*)

Get from which 3D analysis spectra in x/y should be extracted for presentation in the OMSI viewer

Developer Note: h5py currently supports only a single index list. If the user provides an index-list for both x and y, then we need to construct the proper merged list and load the data manually, or if the data is small enough, one can load the full data into a numpy array which supports multiple lists in the selection.

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **x** – x selection string
- **y** – y selection string
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns

The following two elements are expected to be returned by this function :

1. 1D, 2D or 3D numpy array of the requested spectra. NOTE: The mass (m/z) axis must be the last axis. For index selection x=1,y=1 a 1D array is usually expected. For indexList selections x=[0]&y=[1] usually a 2D array is expected. For ragne selections x=0:1&y=1:2 we one usually expects a 3D array/
2. None in case that the spectra axis returned by v_qmz are valid for the returned spectrum. Otherwise, return a 1D numpy array with the m/z values for the spectrum (i.e., if custom m/z values are needed for interpretation of the returned spectrum).This may be needed, e.g., in cases where a per-spectrum peak analysis is performed and the peaks for each spectrum appear at different m/z values.

classmethod v_qspectrum_viewer_options(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qspectrum. The default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

param analysis_object The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decission based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qspectrum requests (i.e., v_qspectrum(...) is not available).

base Module

Module specifying the base analysis API for integrating new analysis with the toolkit and the OpenMSI science gateway.

exception omsi.analysis.base.**AnalysisReadyError**(*value*, *params=None*)

Bases: exceptions.Exception

Custom exception used to indicate that an analysis is not ready to execute.

Initialize the AnalysisReadyError

Parameters

- **value** – Error message string
- **params** – Optional list of dependent parameters that are not ready to be used.

class omsi.analysis.base.**analysis_base**

Bases: *omsi.datastructures.analysis_data.parameter_manager*

Base class for omsi analysis functionality. The class provides a large set of functionality designed to facilitate storage of analysis data in the omsi HDF5 file format. The class also provides a set of functions to enable easy intergration of new analysis with the OpenMSI web-based viewer (see Viewer functions below for details).

Slicing:

This class supports basic slicing to access data stored in the main member variables. By default the data is retrieved from __data_list and the __getitem__(key) function. which implements the [..] operator, returns __data_list[key]['data']. The key is a string indicating the name of the parameter to be retrieved. If the key is not found in the __data_list then the function will try to retrieve the data from self.parameters list instead. By adding "parameter/key" or "dependency/key" one may also explicitly retrieve values from the parameters.

Instance Variables:

Variables

- ***analysis_identifier*** – Define the name for the analysis used as key in search operations
- **__data_list** – List of analysis_data to be written to the HDF5 file. Derived classes need to add all data that should be saved for the analysis in the omsi HDF5 file to this dictionary. See omsi.analysis.analysis_data for details.
- **parameters** – List of parameter_data objects of all analysis parameters (including those that may have dependencies).
- **data_names** – List of strings of all names of analysis output datasets. These are the target keys for __data_list.
- **profile_time_and_usage** – Boolean indicating whether we should profile the execute_analysis(...) function when called as part of the execute(...) function. The default value is false. Use the enable_time_and_usage_profiling(..) function to determine which profiling should be performed. The time_and _usage profile uses pythons cProfile (or Profile) to monitor how often and for how long particular parts of the analysis code executed.
- **profile_memory** – Boolean indicating whether we should monitor memory usage (line-by-line) when executing the execute_analysis(...) function. The default value is false. Use the enable_time_and_usage_profiling(..) function to determine which profiling should be performed.
- **omsi_analysis_storage** – List of omsi_file_analysis object where the analysis is stored. The list may be empty.
- **mpi_comm** – In case we are running with MPI, this is the MPI communicator used for runnign the analysis. Default is MPI.Comm_world/
- **mpi_root** – In case we are running with MPI, this is the root rank where data is collected to (e.g., runtime data and analysis results)
- **update_analysis** – If the value is True, then we should execute the analysis before using the outputs. If False, then the analysis has been executed with the current parameter settings.
- ***driver*** – Workflow driver to be used when executing multiple analyses, e.g., via execute_recursive or execute_all. Default value is None in which case a new default driver will be used each time we execute a workflow.

Execution Functions:

- `execute` : Then main function the user needs to call in order to execute the analysis
- "execute_analysis: This function needs to be implemented by child classes of *analysis_base* to implement the specifics of executing the analysis.

I/O functions:

These functions can be optionally overwritten to control how the analysis data should be written/read from the omsi HDF5 file. Default implementations are provided here, which should be sufficient for most cases.

- `add_custom_data_to_omsi_file`: The default implementation is empty as the default data write is managed by the *omsi_file_experiment.create_analysis()* function. Overwrite this function, in case that the analysis needs to write data to the HDF5 omsi file beyond what the defualt omsi data API does.
- `read_from_omsi_file`: The default implementation tries to reconstruct the original data as far as possible, however, in particular in case that a custom add_custom_data_to_omsi_file function has been implemented, the default implementation may not be sufficien. The default implementation reconstructs: i) analysis_identifier and reads all custom data into ii)__data_list. Note, an error will be raised in case that the analysis type specified in the HDF5 file does not match the analysis type specified by get_analysis_type(). This function can be optionally overwritten to implement a custom data read.

Viewer functions:

Several convenient functions are used to allow the OpenMSI online viewer to interact with the analysis and to visualize it. The default implementations provided here simply indicate that the analysis does not support the data access operations required by the online viewer. Overwrite these functions in the derived analysis classes in order to interface them with the viewer. All viewer-related functions start with `v\_...` .

NOTE: the default implementation of the viewer functions defined in `analysis_base` are designed to take care of the common requirement for providing viewer access to data from all dependencies of an analysis. In many cases, the default implementation is often sill called at the end of custom viewer functions.

NOTE: The viewer functions typically support a viewer_option parameter. viewer_option=0 is expected to refer to the analysis itself.

- `v_qslice`: Retrieve/compute data slices as requested via qslice URL requests. The corresponding view of the DJANGO data access server already translates all input parameters and takes care of generating images/plots if needed. This function is only responsible for retrieving the data.
- `v_qspectrum`: Retrieve/compute spectra as requested via qspectrum URL requests. The corresponding view of the DJANGO data access server already translates all input parameters and takes care of generating images/plots if needed. This function is only responsible for retrieving the data.
- `v_qmz`: Define the m/z axes for image slices and spectra as requested by qspectrum URL requests.
- `v_qspectrum_viewer_options`: Define a list of strings, describing the different viewer options available for the analysis for qspectrum requests (i.e., `v_qspectrum`). This feature allows the analysis developer to define multiple different visualization modes for the analysis. For example, when performing a data reduction (e.g., PCA or NMF) one may want to show the raw spectra or the loadings vector of the projection in the spectrum view (v_qspectrum). By providing different viewer options we allow the user to decide which option they are most interested in.
- `v_qslice_viewer_options`: Define a list of strings, describing the different viewer options available for the analysis for qslice requests (i.e., `v_qslice`). This feature allows the analysis developer to define multiple different visualization modes for the analysis. For example, when performing a data reduction (e.g., PCA or NMF) one may want to show the raw spectra or the loadings vector of the projection in the spectrum view (v_qspectrum). By providing different viewer options we allow the user to decide which option they are most interested in.

Initialize the basic data members

add_custom_data_to_omsi_file(*analysis_group*)

This function can be optionally overwritten to implement a custom data write function for the analysis to be used by the omsi_file API.

Note, this function should be used only to add additional data to the analysis group. The data that is written by default is still written by the *omsi_file_experiment.create_analysis()* function, i.e., the following data is written by default: i) analysis_identifier ,ii) get_analysis_type, iii)__data_list, iv) parameters, v) runinfo . Since the *omsi_file.experiment.create_analysis()* functions takes care of setting up the basic structure of the analysis storage (included the subgroubs for storing parameters and data dependencies) this setup can generally be assumed to exist before this function is called. This function is called automatically at the end omsi_file.experiment.create_analysis() (i.e, actually *omsi_file_analysis.__populate_analysis__(..)* so that this function typically does not need to be called explicitly.

Parameters **analysis_group** – The h5py.Group object where the analysis is stored.

add_parameter(*name*, *help*, *dtype=<type 'unicode'>*, *required=False*, *default=None*, *choices=None*, *data=None*, *group=None*)

Add a new parameter for the analysis. This function is typically used in the constructor of a derived analysis to specify the parameters of the analysis.

Parameters

- **name** – The name of the parameter
- **help** – Help string describing the parameter
- **type** – Optional type. Default is string.
- **required** – Boolean indicating whether the parameter is required (True) or optional (False). Default False.
- **default** – Optional default value for the parameter. Default None.
- **choices** – Optional list of choices with allowed data values. Default None, indicating no choices set.
- **data** – The data assigned to the parameter. None by default.
- **group** – Optional group string used to organize parameters. Default None, indicating that parameters are automatically organized by driver class (e.g. in required and optional parameters)

Raises ValueError is raised if the parameter with the given name already exists.

analysis_identifier_defined()

Check whether the analysis identifier is defined by the user, i.e., set to value different than undefined :return: bool

check_ready_to_execute()

Check if all inputs are ready to determine if the analysis is ready to run.

Returns List of omsi_analysis_parameter objects that are not ready. If the returned list is empty, then the analysis is ready to run.

clear_analysis()

Clear all analysis data—i.e., parameter, dependency data, output results, runtime data

clear_analysis_data()

Clear the list of analysis data

clear_and_restore(*analysis_manager=None*, *resave=False*)

Clear all analysis data and restore the results from file

Parameters

- **analysis_manager** – Instance of omsi_analysis_manager (e.g., an omsi_file_experiment) where the analysis should be saved.

- **resave** – Boolean indicating whether the analysis should be saved again, even if it has been saved before. This parameter only has effect if analysis_manager is given.

Returns self, i.e., the updated analysis object with all data replaced with HDF5 references

clear_parameter_data()
Clear the list of parameter data

clear_run_info_data()
Clear the runtime information data

define_missing_parameters()
Called by the execute function before self.update_analysis_parameters to set any required parameters that have not been defined to their respective default values.

This function may be overwritten in child classes to customize the definition of default parameter values and to apply any modifications (or checks) of parameters before the analysis is executed. Any changes applied here will be recorded in the parameter of the analysis.

enable_memory_profiling(*enable=True*)
Enable or disable line-by-line profiling of memory usage of execute_analysis.

Parameters **enable_memory** (*bool*) – Enable (True) or disable (False) line-by-line profiling of memory usage

Raises ImportError is raised if a required package for profiling is not available.

enable_time_and_usage_profiling(*enable=True*)
Enable or disable profiling of time and usage of code parts of execute_analysis.

Parameters **enable** (*bool*) – Enable (True) or disable (False) profiling

Raises ImportError is raised if a required package for profiling is not available.

execute(***kwargs*)
Use this function to run the analysis.

Parameters **kwargs** – Parameters to be used for the analysis. Parameters may also be set using the __setitem__ mechanism or as batches using the set_parameter_values function.

Returns This function returns the output of the execute analysis function.

Raises AnalysisReadyError in case that the analysis is not ready to be executed. This may be the case, e.g, when a dependent input parameter is not ready to be used.

classmethod **execute_all**(*force_update=False*, *executor=None*)
Execute all analysis instances that are currently defined.

Parameters

- **force_update** – Boolean indicating whether we should force that all analyses are executed again, even if they have already been run with the same settings before. False by default.
- **executor** – Optional workflow executor to be used for the execution of all analyses. The executor will be cleared and then all analyses will be added to executor. Default value is None, in which case the function creates a default executor to be used.

Returns The workflow executor used

execute_analysis()
Implement this function to implement the execution of the actual analysis.

This function may not require any input parameters. All input parameters are recorded in the parameters and dependencies lists and should be retrieved from there, e.g, using basic slicing self[paramName]

Input parameters may be added for internal use ONLY. E.g, we may add parameters that are used internally to help with parallelization of the execute_analysis function. Such parameters are not recorded and must be strictly optional so that analysis_base.execute(...) can call the function.

Returns This function may return any developer-defined data. Note, all output that should be recorded must be put into the data list.

execute_recursive(***kwargs*)
Recursively execute this analysis and all its dependencies if necessary

We use a workflow driver to control the execution. To define the workflow driver we can set the self.driver variable. If no workflow driver is given (i.e, self.driver==None), then the default driver will be created. To change the default driver, see *omsi.workflow.base.workflow_executor_base.DEFAULT_EXECUTOR_CLASS*

Parameters **kwargs** – Parameters to be used for the analysis. Parameters may also be set using the __setitem__ mechanism or as batches using the set_parameter_values function.

Returns Same as execute

get_all_analysis_data()
Get the complete list of all analysis datasets to be written to the HDF5 file

get_all_dependency_data()
Get the complete list of all direct dependencies to be written to the HDF5 file

NOTE: These are only the direct dependencies as specified by the analysis itself. Use get_all_dependency_data_recursive(..) to also get the indirect dependencies of the analysis due to dependencies of the dependencies themselves.

Returns List of parameter_data objects that define dependencies.

get_all_parameter_data(*exclude_dependencies=False*)
Get the complete list of all parameter datasets to be written to the HDF5 file

Parameters **exclude_dependencies** – Boolean indicating whether we should exclude parameters that define dependencies from the list

get_all_run_info()
Get the dict with the complete info about the last run of the analysis

get_analysis_data(*index*)
Given the index return the associated dataset to be written to the HDF5 file

:param index : Retrun the index entry of the private member __data_list.

get_analysis_data_by_name(*dataname*)
Given the key name of the data return the associated analysis_data object.

Parameters **dataname** – Name of the analysis data requested from the private __data_list member.

Returns The analysis_data object or None if not found.

get_analysis_data_names()
Get a list of all analysis dataset names.

get_analysis_identifier()
Return the name of the analysis used as key when searching for a particular analysis

classmethod **get_analysis_instances**()
Generator function used to iterate through all instances of analysis_base. The function creates references for all weak references stored in cls._analysis_instances and returns the references if it exists and cleans up the any invalid references after the iteration is complete. :return: References to analysis_base objects

get_analysis_type()
Return a string indicating the type of analysis performed

static get_default_dtypes()
Get a list of available default dtypes used for analyses. Same as *data_dtypes.get_dtypes()*.

static get_default_parameter_groups()
Get a list of commonly used parameter groups and associated descriptions.

Use of default groups provides consistency and allows other system to design custom behavior around the semantic of parameter groups

Returns Dictionary where the keys are the short names of the groups and the values are dicts with following keys:value pairs: 'name' , 'description'. Use the 'name' to define the group to be used.

get_help_string()
Get a string describing the analysis.

Returns Help string describing the analysis and its parameters

get_memory_profile_info()
Based on the memory profile of the execute_analysis(..) function get the string describing the line-by-line memory usage.

Returns String describing the memory usage profile. None is returned in case that no memory profiling data is available.

get_num_analysis_data()
Retrun the number of analysis datasets to be wirtten to the HDF5 file

get_num_dependency_data()
Return the number of dependencies to be wirtten to the HDF5 file

get_num_parameter_data()
Return the number of parameter datasets to be wirtten to the HDF5 file

get_omsi_analysis_storage()
Get a list of known locations where this analysis has been saved.

Returns List of *omsi.dataformat.omsi_file.analysis. omsi_file_analysis* objects where the analysis is saved.

get_parameter_data(*index*)
Given the index return the associated dataset to be written to the HDF5 file

:param index : Return the index entry of the private member parameters.

get_parameter_data_by_name(*dataname*)
Given the key name of the data return the associated parameter_data object.

Parameters **dataname** – Name of the parameter requested from the parameters member.

Returns The parameter_data object or None if not found

get_parameter_names()
Get a list of all parameter dataset names (including those that may define dependencies.

get_profile_stats_object(*consolidate=True*, *stream=None*)
Based on the execution profile of the execute_analysis(..) function get `pstats.Stats` object to help with the interpretation of the data.

Parameters

- **consolidate** – Boolean flag indicating whether multiple stats (e.g., from multiple cores) should be consolidated into a single stats object. Default is True.
- **stream** – The optional stream parameter to be used fo the pstats.Stats object.

Returns A single pstats.Stats object if consolidate is True. Otherwise the function returns a list of pstats.Stats objects, one per recorded statistic. None is returned in case that the stats objects cannot be created or no profiling data is available.

has_omsi_analysis_storage()
Check whether a storage location is known where the anlaysis has been saved.

Returns Boolean indicating whether self.omsi_analysis_storage is not empty

keys()
Get a list of all valid keys, i.e., a combination of all input parameter and output names.

Returns List of strings with all input parameter and output names.

classmethod locate_analysis(*data_object*, *include_parameters=False*)
Given a data_object try to locate the analysis that creates the object as an output of its execution (and optionally analyses that have the object as an input).

Parameters

- **data_object** – The data object of interest.
- **include_parameters** – Boolean indicating whether also input parameters should be considered in the search in addition to the outputs of an analysis

Returns dependency_dict pointing to the relevant object or None in case the object was not found.

read_from_omsi_file(*analysis_object*, *load_data=True*, *load_parameters=True*, *load_runtime_data=True*, *dependencies_omsi_format=True*, *ignore_type_conflict=False*)
This function can be optionally overwritten to implement a custom data read.

The default implementation tries to reconstruct the original data as far as possible, however, in particular in case that a custom add_custom_data_to_omsi_file function has been implemented, the default implementation may not be sufficient. The default implementation reconstructs: i) analysis_identifier and reads all custom data into iii)__data_list. Note, an error will be raised in case that the analysis type specified in the HDF5 file does not match the analysis type specified by get_analysis_type()

Parameters

- **analysis_object** – The omsi_file_analysis object associated with the hdf5 data group with the analysis data_list
- **load_data** – Should the analysis data be loaded from file (default) or just stored as h5py data objects
- **load_parameters** – Should parameters be loaded from file (default) or just stored as h5py data objects.
- **load_runtime_data** – Should runtime data be loaded from file (default) or just stored as h5py data objects
- **dependencies_omsi_format** – Should dependencies be loaded as omsi_file API objects (default) or just as h5py objects.
- **ignore_type_conflict** – Set to True to allow the analysis to be loaded into the current analysis object even if the type indicated in the file does not match the class. Default value is False. This behavior can be useful when different analysis have compatible

data structures or when we want to load the data in to a generic analysis container, e.g, analysis_generic.

Returns bool Boolean indicating whether the data was read successfully

Raise TypeError : A type error will be raised in case that the analysis type specified by the file does not match the analysis type provided by self.get_analysis_type()

record_execute_analysis_outputs(*analysis_output*)
Function used internally by execute to record the output of the custom execute_analysis(...) function to the __data_list.

This function may be overwritten in child classes in order to customize the behavior for recording data outputs. Eg., for some analyses one may only want to record a particular set of outputs, rather than all outputs generated by the analysis.

Parameters **analysis_output** – The output of the execute_analysis(...) function to be recorded

results_ready()
Check whether the results of the analysis are ready to be used :return: Boolean

set_analysis_identifier(*identifier*)
Set the name of the analysis to identifer

Side Effects: This function modifies self.analysis_identifier

Parameters **identifier** (*str*) – The new analysis identifier string to be used (should be unique)

set_parameter_values(***kwargs*)
Set all parameters given as input to the function. The inputs are placed in the self.parameters list. If the parameter refers to an existing h5py.Dataset, h5py.Group, managed h5py object, or is an instance of an existing omis_analysi_base object, then a dependency_dict will be created and stored as value instead.

Parameters **kwargs** – Dictionary of keyword arguments. All keys are expected to be strings. All values are expected to be either i) numpy arrays, ii) int, float, str or unicode variables, iii) h5py.Dataset or h5py.Group, iv) or any the omsi_file API class objects. For iii) and iv) one may provide a tuple consisting of the dataobject t[0] and an additional selection string t[1].

update_analysis_parameters(***kwargs*)
Record the analysis parameters passed to the execute() function.

The default implementation simply calls the set_parameter_values(...) function. This function may be overwritten to customize the behavior of how parameters are recorded by the execute function.

Parameters **kwargs** – Dictionary of keyword arguments with the parameters passed to the execute(..) function

classmethod **v_qmz**(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Get the mz axes for the analysis

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **qslice_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qslice URL pattern.
- **qspectrum_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qspectrum URL pattern.

Returns

The following four arrays are returned by the analysis:

- mzSpectra : Array with the static mz values for the spectra.
- labelSpectra : Label for the spectral mz axis
- mzSlice : Array of the static mz values for the slices or None if identical to the mzSpectra.
- labelSlice : Label for the slice mz axis or None if identical to labelSpectra.
- values_x: The values for the x axis of the image (or None)
- label_x: Label for the x axis of the image
- values_y: The values for the y axis of the image (or None)
- label_y: Label for the y axis of the image
- values_z: The values for the z axis of the image (or None)
- label_z: Label for the z axis of the image

classmethod **v_qslice**(*analysis_object*, *z*, *viewer_option=0*)

Get 3D analysis dataset for which z-slices should be extracted for presentation in the OMSI viewer

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **z** – Selection string indicting which z values should be selected.
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns numpy array with the data to be displayed in the image slice viewer. Slicing will be performed typically like [:,:,zmin:zmax].

Raises NotImplementedError in case that v_qslice is not supported by the analysis.

classmethod **v_qslice_viewer_options**(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qslice. The default implementation tries to take care of handling the spectra retrieval for all the dependencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decission based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qslice requests (i.e., v_qslice(...) is not available).

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)

Get from which 3D analysis spectra in x/y should be extracted for presentation in the OMSI viewer

Developer Note: h5py currently supports only a single index list. If the user provides an index-list for both x and y, then we need to construct the proper merged list and load the data manually, or if the data is small enough, one can load the full data into a numpy array which supports multiple lists in the selection.

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **x** – x selection string
- **y** – y selection string
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns

The following two elements are expected to be returned by this function :

1. 1D, 2D or 3D numpy array of the requested spectra. NOTE: The mass (m/z) axis must be the last axis. For index selection x=1,y=1 a 1D array is usually expected. For indexList selections x=[0]&y=[1] usually a 2D array is expected. For ragne selections x=0:1&y=1:2 we one usually expects a 3D array.
2. None in case that the spectra axis returned by v_qmz are valid for the returned spectrum. Otherwise, return a 1D numpy array with the m/z values for the spectrum (i.e., if custom m/z values are needed for interpretation of the returned spectrum).This may be needed, e.g., in cases where a per-spectrum peak analysis is performed and the peaks for each spectrum appear at different m/z values.

classmethod v_qspectrum_viewer_options(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qspectrum. The default implementation tries to take care of handling the spectra retrieval for all the dependencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decision based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qspectrum requests (i.e., v_qspectrum(...) is not available).

write_analysis_data(*analysis_group=None*)

This function is used to write the actual analysis data to file. If not implemented, then the omsi_file_analysis API's default behavior is used instead.

Parameters **analysis_group** – The h5py.Group object where the analysis is stored. May be None on cores that do not perform any writing but which need to participate in communication, e.g., to collect data for writing.

generic Module

Generic analysis class used to represent analyses of unknown type, e.g., when loading a custom user-defined analysis from file for which the indicate class may not be available with the local installation. In this case we want to at least be able to load and investigate the data.

class omsi.analysis.generic.**analysis_generic**(*name_key='undefined'*)

Bases: *omsi.analysis.base.analysis_base*

This analysis class is used if the specific anlaysis type is unknown, e.g., when loading custom user-defined analysis data that may have not be available in the standard omsi package used.

Initialize the basic data members

Parameters **name_key** – The name for the analysis

DEFAULT_OUTPUT_PREFIX = 'output_'

execute(***kwargs*)
Overwrite the default implementation of execute to update parameter specifications/types when wrapping functions where the types are not known a priori.

Parameters **kwargs** – Custom analysis parameters

Returns The result of execute_analysis()

execute_analysis()
Nothing to do here.

classmethod **from_function**(*analysis_function*, *output_names=None*, *parameter_specs=None*, *name_key='undefined'*)
Create a generic analysis class for a given analysis function.

This functionality is useful to ease quick scripting on analyses but should not be used in production.

NOTE: __analysis_function is a reserved parameter name used to store the analysis function and may not be used as an input parameter for the analysis function.

Parameters

- **analysis_function** – The analysis function to be wrapped for provenance tracking and storage
- **output_names** – Optionally, define a list of the names of the outputs
- **parameter_specs** – Optional list of omsi.datastructures.analysis_data.parameter_data with additional information about the parameters of the function.
- **name_key** – The name for the analysis, i.e., the analysis identifier

Returns A new generic analysis class

classmethod **get_analysis_type**()
Return a string indicating the type of analysis performed

get_real_analysis_type()
This class is designed to handle generic (including unkown) types of analysis. In cases, e.g., were this class is used to store analysis data from an HDF5 file we may have an actual analysis type available even if we do not have a special analysis class may not be available in the current installation

read_from_omsi_file(*analysis_object*, *load_data=True*, *load_parameters=True*, *load_runtime_data=True*, *dependencies_omsi_format=True*, *ignore_type_conflict=False*)
See *omsi.analysis.analysis_base.read_from_omsi_file(...)* for details. The function is overwritten here mainly to initialize the self.real_analysis_type instance variable but otherwise uses the default behavior.

classmethod **v_qmz**(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Implement support for qmz URL requests for the viewer

classmethod **v_qslice**(*analysis_object*, *z*, *viewer_option=0*)
Implement support for qslice URL requests for the viewer

classmethod **v_qslice_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)
Implement support for qspectrum URL requests for the viewer

classmethod **v_qspectrum_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

write_analysis_data(*analysis_group=None*)
This function is used to write the actual analysis data to file. If not implemented, then the omsi_file_analysis API's default behavior is used instead.

Parameters **analysis_group** – The h5py.Group object where the analysis is stored. May be None on cores that do not perform any writing but which need to participate in communication, e.g., to collect data for writing.

omsi.analysis.generic.**bastet_analysis**(*output_names=None*, *parameter_specs=None*, *name_key='undefined'*)
Decorator used to wrap a function and replace it with an analysis_generic object that behaves like a function but adds the ability for saving the analysis to file and tracking provenance

This is essentially the same as analysis_generic.from_function(....).

Parameters

- **func** – The function to be wrapped
- **output_names** – Optional list of strings with the names of the outputs
- **parameter_specs** – Optional list of omsi.datastructures.analysis_data.parameter_data with additional information about the parameters of the function.
- **name_key** – Optional name for the analysis, i.e., the analysis identifier

Returns analysis_generic instance for the wrapped function

analysis_views Module

Helper module with functions and classes for interfacing with different analysis algorithms. Many of these functions are used to ease interaction with the analysis module in a generic fashion, without having to explicitly know about all the different available modules, e.g., we can just look up modules by name and interact with them directly.

class omsi.analysis.analysis_views.**analysis_views**
Bases: object

Helper class for interfacing different analysis algorithms with the web-based viewer

Nothing to do here.

classmethod **analysis_name_to_class**(*class_name*)
Convert the given string indicating the class to a python class.

Parameters **class_name** – Name of the analysis class. This may be a fully qualified name, e.g., *omsi.analysis.multivariate_stat.omsi_nmf* or a name relative to the omis.analysis module, e.g, *multivariate_stat.omsi_nmf*.

Raises Attribute error in case that the class cannot be restored.

classmethod **available_analysis**()
Get all available analysis, i.e., all analysis that are subclasses of analysis_base.

Returns Dictionary where the dict-keys are the full qualified name of the module and the values are the analysis class corresponding to that module.

classmethod **available_analysis_descriptions**()
Get all available analysis, i.e., all analysis that are subclasses of analysis_base. For each analysis compile the list of input parameters, outputs, the corresponding class etc.

Returns Dictionary where the dict-keys are the full qualified name of the module and the values are dicts with class, list of analysis paremeter names, list of analysis outputs.

classmethod **get_axes**(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Get the mz axes for the analysis

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **qslice_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qslice URL pattern.
- **qspectrum_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qspectrum URL pattern.

Returns

The following four arrays are returned by the analysis:

- mz_spectra : Array with the static mz values for the spectra.
- label_spectra : Lable for the spectral mz axis
- mz_slice : Array of the static mz values for the slices or None if identical to the mz_spectra.
- label_slice : Lable for the slice mz axis or None if identical to label_spectra.
- values_x: The values for the x axis of the image (or None)
- label_x: Label for the x axis of the image
- values_y: The values for the y axis of the image (or None)
- label_y: Label for the y axis of the image
- values_z: The values for the z axis of the image (or None)
- label_z: Label for the z axis of the image

classmethod **get_qslice_viewer_options**(*analysis_object*)
Get a list of strings describing the different default viewer options for qslice.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed.

Returns Array of strings indicating the different available viewer options. The array may be empty if now viewer_options are available, i.e., get_slice and get_spectrum are undefined for the given analysis.

classmethod **get_qspectrum_viewer_options**(*analysis_object*)
Get a list of strings describing the different default viewer options for qspectrum.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed.

Returns Array of strings indicating the different available viewer options. The array may be empty if now viewer_options are available, i.e., get_slice and get_spectrum are undefined for the given analysis.

classmethod **get_slice**(*analysis_object*, *z*, *operations=None*, *viewer_option=0*)
Get 3D analysis dataset for which z-slices should be extracted for presentation in the OMSI viewer

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **z** – Selection string indicting which z values should be selected.
- **operations** – JSON string with list of dictionaries or a python list of dictionaries. Each dict specifies a single data transformation or data reduction that are applied in order. See omsi.shared.omsi_data_selection.transform_and_reduce_data(...) for details.
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns numpy array with the data to be displayed in the image slice viewer. Slicing will be performed typically like [:,:,zmin:zmax].

classmethod get_spectra(*analysis_object*, *x*, *y*, *operations=None*, *viewer_option=0*)

Get from which 3D analysis spectra in x/y should be extracted for presentation in the OMSI viewer

Developer Note: h5py currently supports only a single index list. If the user provides an index-list for both x and y, then we need to construct the proper merged list and load the data manually, or if the data is small enough, one can load the full data into a numpy array which supports multiple lists in the selection.

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **x** – x selection string
- **y** – y selection string
- **operations** – JSON string with list of dictionaries or a python list of dictionaries. Each dict specifies a single data transformation or data reduction that are applied in order. See omsi.shared.omsi_data_selection.transform_and_reduce_data(...) for details.
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns 2D or 3D numpy array of the requested spectra. The mass (m/z) axis must be the last axis.

classmethod supports_slice(*analysis_object*)

Get whether a default slice selection behavior is defined for the analysis.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed

Returns Boolean indicating whether get_slice(...) is defined for the analysis object.

classmethod supports_spectra(*analysis_object*)

Get wheter a default spectra selection behavior is defined for the analysis.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed.

Returns Boolean indicating whether get_spectra(...) is defined for the analysis object.

Subpackages

findpeaks Package

findpeaks Package Package of peak-finding related analysis modules.

class omsi.analysis.findpeaks.**omsi_findpeaks_global**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Basic global peak detection analysis. The default implementation computes the peaks on the average spectrum and then computes the peak-cube data, i.e., the values for the detected peaks at each pixel.

TODO: The current version assumes 2D data

Initialize the basic data members

execute_analysis()
Execute the global peak finding for the given msidata and mzdata.

classmethod v_qmz(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Implement support for qmz URL requests for the viewer

classmethod v_qslice(*analysis_object*, *z*, *viewer_option=0*)
Implement support for qslice URL requests for the viewer

classmethod v_qslice_viewer_options(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

classmethod v_qspectrum(*analysis_object*, *x*, *y*, *viewer_option=0*)
Implement support for qspectrum URL requests for the viewer

classmethod v_qspectrum_viewer_options(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

class omsi.analysis.findpeaks.**omsi_findpeaks_local**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Class defining a basic gloabl peak finding. The default implementation computes the peaks on the average spectrum and then computes the peak-cube data, i.e., the values for the detected peaks at each pixel.

TODO: The current version assumes 2D data

Initialize the basic data members

execute_analysis(*msidata_subblock=None*)
Execute the local peak finder for the given msidata.

Parameters **msidata_subblock** – Optional input parameter used for parallel execution of the analysis only. If msidata_subblock is set, then the given subblock will be processed in SERIAL instead of processing self['msidata'] in PARALLEL (if available). This parameter is strictly optional and intended for internal use only.

classmethod v_qmz(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Implement support for qmz URL requests for the viewer

classmethod v_qslice(*analysis_object*, *z*, *viewer_option=0*)
Implement support for qslice URL requests for the viewer

classmethod v_qslice_viewer_options(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

classmethod v_qspectrum(*analysis_object*, *x*, *y*, *viewer_option=0*)
Implement support for qspectrum URL requests for the viewer

classmethod v_qspectrum_viewer_options(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

write_analysis_data(*analysis_group=None*)
This function is used to write the actual analysis data to file. If not implemented, then the omsi_file_analysis API's default behavior is used instead.

Parameters **analysis_group** – The h5py.Group object where the analysis is stored.

omsi_findpeaks_global Module Global peak finder computing peaks and associated ion-images for the full MSI data.

class omsi.analysis.findpeaks.omsi_findpeaks_global.**omsi_findpeaks_global**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Basic global peak detection analysis. The default implementation computes the peaks on the average spectrum and then computes the peak-cube data, i.e., the values for the detected peaks at each pixel.

TODO: The current version assumes 2D data

Initialize the basic data members

execute_analysis()
Execute the global peak finding for the given msidata and mzdata.

classmethod **v_qmz**(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Implement support for qmz URL requests for the viewer

classmethod **v_qslice**(*analysis_object*, *z*, *viewer_option=0*)
Implement support for qslice URL requests for the viewer

classmethod **v_qslice_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)
Implement support for qspectrum URL requests for the viewer

classmethod **v_qspectrum_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

omsi_findpeaks_local Module Local peak finding analysis module.

class omsi.analysis.findpeaks.omsi_findpeaks_local.**omsi_findpeaks_local**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Class defining a basic gloabl peak finding. The default implementation computes the peaks on the average spectrum and then computes the peak-cube data, i.e., the values for the detected peaks at each pixel.

TODO: The current version assumes 2D data

Initialize the basic data members

execute_analysis(*msidata_subblock=None*)
Execute the local peak finder for the given msidata.

Parameters **msidata_subblock** – Optional input parameter used for parallel execution of the analysis only. If msidata_subblock is set, then the given subblock will be processed in SERIAL instead of processing self['msidata'] in PARALLEL (if available). This parameter is strictly optional and intended for internal use only.

classmethod **v_qmz**(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Implement support for qmz URL requests for the viewer

classmethod **v_qslice**(*analysis_object*, *z*, *viewer_option=0*)
Implement support for qslice URL requests for the viewer

classmethod **v_qslice_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)
Implement support for qspectrum URL requests for the viewer

classmethod **v_qspectrum_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

write_analysis_data(*analysis_group=None*)
This function is used to write the actual analysis data to file. If not implemented, then the omsi_file_analysis API's default behavior is used instead.

Parameters **analysis_group** – The h5py.Group object where the analysis is stored.

findpeaks.third_party Package

findpeaks.third_party Package Package containing shared third-party code modules included here to reduce the need for external dependencies when only small parts of external code are used.

findpeaks Module

class omsi.analysis.findpeaks.third_party.findpeaks.**findpeaks**(*x*, *y*, *sizesmooth*, *slwindow*, *peakheight*)

Name = 'findpeaks'

display()

peakdet()
Converted from MATLAB script at http://billauer.co.il/peakdet.html

Currently returns two lists of tuples, but maybe arrays would be better

function [maxtab, mintab]=peakdet(v, delta, x) %PEAKDET Detect peaks in a vector % [MAXTAB, MINTAB] = PEAKDET(V, DELTA) finds the local % maxima and minima ("peaks") in the vector V. % MAXTAB and MINTAB consists of two columns. Column 1 % contains indices in V, and column 2 the found values. % % With [MAXTAB, MINTAB] = PEAKDET(V, DELTA, X) the indices % in MAXTAB and MINTAB are replaced with the corresponding % X-values. % % A point is considered a maximum peak if it has the maximal % value, and was preceded (to the left) by a value lower by % DELTA.

% Eli Billauer, 3.4.05 (Explicitly not copyrighted). % This function is released to the public domain; Any use is allowed.

sliding_window_minimum()
A iterator which takes the size of the window, *k*, and an iterable, *li*. Then returns an iterator such that the ith element yielded is equal to min(list(li)[max(i - k + 1, 0):i+1]).

Each yield takes amortized O(1) time, and overall the generator takes O(k) space.

smoothListGaussian()

findpeaks.experimental Package

findpeaks.experimental Package Module with experimental analysis code, i.e., code that is not (yet) used in production but is under development. Often this is code that is used in a specific research.

omsi_peakcube Module

omsi.analysis.findpeaks.experimental.omsi_peakcube.**main**(*argv=None*)

class omsi.analysis.findpeaks.experimental.omsi_peakcube.**omsi_peakcube**(*name_key='undefined'*)

Bases: *omsi.analysis.base.analysis_base*

Initalize the basic data members

execute_analysis()

getGlobalMz(*peaksBins*, *peaksMZdata*, *HCpeaksLabels*, *HCLabelsList*)

getPeakCube(*peaksIntensities*, *peaksArrayIndex*, *HCpeaksLabels*, *HCLabelsList*)

record_execute_analysis_outputs(*analysis_output*)

We are recording our outputs manually as part of the execute function

classmethod v_qmz(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)

Implement support for qmz URL requests for the viewer

classmethod v_qslice(*analysis_object*, *z*, *viewer_option=0*)

Implement support for qslice URL requests for the viewer

classmethod v_qslice_viewer_options(*analysis_object*)

Define which viewer_options are supported for qspectrum URL's

classmethod v_qspectrum(*analysis_object*, *x*, *y*, *viewer_option=0*)

Implement support for qspectrum URL requests for the viewer

classmethod v_qspectrum_viewer_options(*analysis_object*)

Define which viewer_options are supported for qspectrum URL's

omsi.analysis.findpeaks.experimental.omsi_peakcube.**stop**()

pfrun Module

omsi.analysis.findpeaks.experimental.pfrun.**generateScript**(*scriptfile*, *PFcontent=None*, *repo=None*)

omsi.analysis.findpeaks.experimental.pfrun.**main**(*argv*)

omsi.analysis.findpeaks.experimental.pfrun.**printHelp**(*thisfilename*)

omsi.analysis.findpeaks.experimental.pfrun.**queuePCjob**(*pcstring*, *therepo=None*)

omsi.analysis.findpeaks.experimental.pfrun.**run_lpf**(*omsiInFile*, *expIndex*, *dataIndex*, *ph*, *slw*, *smw*)

omsi.analysis.findpeaks.experimental.pfrun.**run_npg**(*omsiInFile*, *expIndex*, *dataIndex*, *LPFIndex*, *mzth*, *tcut*)

omsi.analysis.findpeaks.experimental.pfrun.**run_peakcube**(*omsiInFile*, *expIndex*, *dataIndex*, *LPFIndex*, *NPGIndex*)

omsi.analysis.findpeaks.experimental.pfrun.**stop**()

omsi_lpf Module

omsi.analysis.findpeaks.experimental.omsi_lpf.**cl_peakfind**(*self*, *msidt*, *smoothsize*, *slwindow*, *peakheight*)

omsi.analysis.findpeaks.experimental.omsi_lpf.**execute_analysis**(*self*)

omsi.analysis.findpeaks.experimental.omsi_lpf.**main**(*argv=None*)

Then main function

class omsi.analysis.findpeaks.experimental.omsi_lpf.**omsi_lpf**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

omsi.analysis.findpeaks.experimental.omsi_lpf.**v_qmz**
classmethod(function) -> method

Convert a function to be a class method.

A class method receives the class as implicit first argument, just like an instance method receives the instance. To declare a class method, use this idiom:

class C: def f(cls, arg1, arg2, ...): ... f = classmethod(f)

It can be called either on the class (e.g. C.f()) or on an instance (e.g. C().f()). The instance is ignored except for its class. If a class method is called for a derived class, the derived class object is passed as the implied first argument.

Class methods are different than C++ or Java static methods. If you want those, see the staticmethod builtin.

omsi.analysis.findpeaks.experimental.omsi_lpf.**v_qslice**
classmethod(function) -> method

Convert a function to be a class method.

A class method receives the class as implicit first argument, just like an instance method receives the instance. To declare a class method, use this idiom:

class C: def f(cls, arg1, arg2, ...): ... f = classmethod(f)

It can be called either on the class (e.g. C.f()) or on an instance (e.g. C().f()). The instance is ignored except for its class. If a class method is called for a derived class, the derived class object is passed as the implied first argument.

Class methods are different than C++ or Java static methods. If you want those, see the staticmethod builtin.

omsi.analysis.findpeaks.experimental.omsi_lpf.**v_qslice_viewer_options**
classmethod(function) -> method

Convert a function to be a class method.

A class method receives the class as implicit first argument, just like an instance method receives the instance. To declare a class method, use this idiom:

class C: def f(cls, arg1, arg2, ...): ... f = classmethod(f)

It can be called either on the class (e.g. C.f()) or on an instance (e.g. C().f()). The instance is ignored except for its class. If a class method is called for a derived class, the derived class object is passed as the implied first argument.

Class methods are different than C++ or Java static methods. If you want those, see the staticmethod builtin.

omsi.analysis.findpeaks.experimental.omsi_lpf.**v_qspectrum**
classmethod(function) -> method

Convert a function to be a class method.

A class method receives the class as implicit first argument, just like an instance method receives the instance. To declare a class method, use this idiom:

class C: def f(cls, arg1, arg2, ...): ... f = classmethod(f)

It can be called either on the class (e.g. C.f()) or on an instance (e.g. C().f()). The instance is ignored except for its class. If a class method is called for a derived class, the derived class object is passed as the implied first argument.

Class methods are different than C++ or Java static methods. If you want those, see the staticmethod builtin.

omsi.analysis.findpeaks.experimental.omsi_lpf.**v_qspectrum_viewer_options**
classmethod(function) -> method

Convert a function to be a class method.

A class method receives the class as implicit first argument, just like an instance method receives the instance. To declare a class method, use this idiom:

class C: def f(cls, arg1, arg2, ...): ... f = classmethod(f)

It can be called either on the class (e.g. C.f()) or on an instance (e.g. C().f()). The instance is ignored except for its class. If a class method is called for a derived class, the derived class object is passed as the implied first argument.

Class methods are different than C++ or Java static methods. If you want those, see the staticmethod builtin.

omsi_npg Module

class omsi.analysis.findpeaks.experimental.omsi_npg.**Node**(*label*)
omsi.analysis.findpeaks.experimental.omsi_npg.**main**(*argv=None*)

class omsi.analysis.findpeaks.experimental.omsi_npg.**omsi_npg**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Initalize the basic data members

Find(*x*)

MakeSet(*x*)

Union(*x*, *y*)

execute_analysis()

getClustersInfo(*GpeaksLabels*, *GLabelsList*)

getCoordIdxB(*xCoord*, *yCoord*)

getCoordInfoB(*xCoord*, *yCoord*, *peaksLabels*)

getCoordPeaksB(*xCoord*, *yCoord*)

getNearestPeakIndex(*myPeaksArray*, *myPeak*)

getPixelMap(*Nx*, *Ny*)

classmethod getnpgimage(*PeaksLabels*, *LabelsList*, *peaksArrayIndex*, *peaksIntensities*, *z*)

classmethod getnpgspec(*PeaksLabels*, *LabelsList*, *peaksArrayIndex*, *peaksIntensities*, *xCoord*, *yCoord*)

myHC(*labelsMMz*, *TreeCut*)

record_execute_analysis_outputs(*analysis_output*)
We are recording our outputs manually as part of the execute function

splitLabelsList(*LabelData*, *Thres*, *SplitMax*)

classmethod v_qmz(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Implement support for qmz URL requests for the viewer

classmethod v_qslice(*analysis_object*, *z*, *viewer_option=0*)
Implement support for qslice URL requests for the viewer

classmethod v_qslice_viewer_options(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)
Implement support for qspectrum URL requests for the viewer

classmethod **v_qspectrum_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

omsi.analysis.findpeaks.experimental.omsi_npg.**stop**()

mypeakfinder Module

omsi.analysis.findpeaks.experimental.mypeakfinder.**generateScript**(*scriptfile*, *PFcontent=None*, *repo=None*)

omsi.analysis.findpeaks.experimental.mypeakfinder.**getJobOutput**(*jobname*, *runtype*)

omsi.analysis.findpeaks.experimental.mypeakfinder.**getPFcmd**(*pfstring*, *lpfstring*, *npgstring*, *LPFIndex*, *NPGIndex*, *SkipNPG*, *SkipPeakCube*, *IndexFile=None*)

omsi.analysis.findpeaks.experimental.mypeakfinder.**main**(*argv*)

omsi.analysis.findpeaks.experimental.mypeakfinder.**monitorJob**(*jobid*, *jobname*, *runtype='pf'*)

omsi.analysis.findpeaks.experimental.mypeakfinder.**printHelp**(*thisfilename*)

omsi.analysis.findpeaks.experimental.mypeakfinder.**stop**()

multivariate_stats Package

multivariate_stats Package Multivariate statistics analysis

class omsi.analysis.multivariate_stats.**omsi_nmf**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Class defining a basic nmf analysis.

The function has primarily been tested we MSI datasets but should support arbitrary n-D arrays (n>=2). The last dimension of the input array must be the spectrum dimnensions.

Initalize the basic data members

execute_analysis()
Execute the nmf for the given msidata

classmethod **v_qmz**(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Implement support for qmz URL requests for the viewer

classmethod **v_qslice**(*analysis_object*, *z*, *viewer_option=0*)
Implement support for qslice URL requests for the viewer

classmethod **v_qslice_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)
Implement support for qspectrum URL requests for the viewer

classmethod **v_qspectrum_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

class omsi.analysis.multivariate_stats.**omsi_cx**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Class used to implement CX factorization on MSI data.

Initalize the basic data members

classmethod comp_lev_exact(*A*, *k*, *axis*)
This function computes the column or row leverage scores of the input matrix.

Parameters

- **A** – n-by-d matrix
- **k** – rank parameter, k <= min(n,d)
- **axis** – 0: compute row leverage scores; 1: compute column leverage scores.

Returns 1D array of leverage scores. If axis = 0, the length of lev is n. otherwise, the length of lev is d.

dimension_index = {'pixelDim': 1, 'imageDim': 0}

execute_analysis()
EDIT_ME:

Replace this text with the appropriate documentation for the analysis. Describe what your analysis does and how a user can use it. Note, a user will call the function execute(...) which takes care of storing parameters, collecting execution data etc., so that you only need to implement your analysis, the rest is taken care of by analysis_base. omsi uses Sphynx syntax for the documentation.

Keyword Arguments:

Parameters **mydata** – ...

classmethod v_qmz(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Get the mz axes for the analysis

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **qslice_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qslice URL pattern.
- **qspectrum_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qspectrum URL pattern.

Returns

The following four arrays are returned by the analysis:

- mz_spectra : Array with the static mz values for the spectra.
- label_spectra : Lable for the spectral mz axis
- mz_slice : Array of the static mz values for the slices or None if identical to the mz_spectra.
- label_slice : Lable for the slice mz axis or None if identical to label_spectra.

classmethod v_qslice(*analysis_object*, *z*, *viewer_option=0*)
Get 3D analysis dataset for which z-slices should be extracted for presentation in the OMSI viewer

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **z** – Selection string indicting which z values should be selected.
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns numpy array with the data to be displayed in the image slice viewer. Slicing will be performed typically like [:,:,zmin:zmax].

classmethod v_qslice_viewer_options(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qslice. The default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decision based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qslice requests (i.e., v_qslice(...) is not available).

classmethod v_qspectrum(*analysis_object*, *x*, *y*, *viewer_option=0*)

Get from which 3D analysis spectra in x/y should be extracted for presentation in the OMSI viewer

Developer Note: h5py currently supports only a single index list. If the user provides an index-list for both x and y, then we need to construct the proper merged list and load the data manually, or if the data is small enough, one can load the full data into a numpy array which supports mulitple lists in the selection.

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **x** – x selection string
- **y** – y selection string
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns

The following two elemnts are expected to be returned by this function :

1. 1D, 2D or 3D numpy array of the requested spectra. NOTE: The mass (m/z) axis must be the last axis. For index selection x=1,y=1 a 1D array is usually expected. For indexList selections x=[0]&y=[1] usually a 2D array is expected. For ragne selections x=0:1&y=1:2 we one usually expects a 3D array.
2. None in case that the spectra axis returned by v_qmz are valid for the returned spectrum. Otherwise, return a 1D numpy array with the m/z values for the spectrum (i.e., if custom m/z values are needed for interpretation of the returned spectrum).This may be needed, e.g., in cases where a per-spectrum peak analysis is performed and the peaks for each spectrum appear at different m/z values.

classmethod v_qspectrum_viewer_options(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qspectrum. The

default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decission based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qspectrum requests (i.e., v_qspectrum(...) is not available).

class omsi.analysis.multivariate_stats.**omsi_kmeans**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Class defining a basic nmf analysis for a 2D MSI data file or slice of the data

Initalize the basic data members

execute_analysis()
Execute the kmeans clustering for the given msidata

omsi_nmf Module Module for performing non-negative matrix factorization (NMF) for MSI data.

class omsi.analysis.multivariate_stats.omsi_nmf.**omsi_nmf**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Class defining a basic nmf analysis.

The function has primarily been tested we MSI datasets but should support arbitrary n-D arrays (n>=2). The last dimension of the input array must be the spectrum dimnensions.

Initalize the basic data members

execute_analysis()
Execute the nmf for the given msidata

classmethod **v_qmz**(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Implement support for qmz URL requests for the viewer

classmethod **v_qslice**(*analysis_object*, *z*, *viewer_option=0*)
Implement support for qslice URL requests for the viewer

classmethod **v_qslice_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)
Implement support for qspectrum URL requests for the viewer

classmethod **v_qspectrum_viewer_options**(*analysis_object*)
Define which viewer_options are supported for qspectrum URL's

multivariate_stats.third_party Package

multivariate_stats.third_party Package Package containing shared third-party code modules included here to reduce the need for external dependencies when only small parts of external code are used.

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omsi.analysis.multivariate_stats.third_party.nmf.**nlssubprob**(*V*, *W*, *Hinit*, *tol*, *maxiter*)

H, grad: output solution and gradient iter: #iterations used V, W: constant matrices Hinit: initial solution tol: stopping tolerance maxiter: limit of iterations

omsi.analysis.multivariate_stats.third_party.nmf.**nmf**(*V*, *Winit*, *Hinit*, *tol*, *timelimit*, *maxiter*)

(W,H) = nmf(V,Winit,Hinit,tol,timelimit,maxiter) W,H: output solution Winit,Hinit: initial solution tol: tolerance for a relative stopping condition timelimit, maxiter: limit of time and iterations

multivariate_stats.experimental Package

multivariate_stats.experimental Package Module with experimental analysis code, i.e., code that is not (yet) used in production but is under development. Often this is code that is used in a specific research.

msi_filtering Package

msi_filtering Package Module with third-party modules, functions, classes used by some of the analysis modules in the containing package.

class omsi.analysis.msi_filtering.**omsi_tic_norm**(*name_key='undefined'*)

Bases: *omsi.analysis.base.analysis_base*

TIC Normalization analysis.

Initalize the basic data members

execute_analysis()

Normalize the data based on the total intensity of a spectrum or the intensities of a select set of ions.

Calculations are performed using a memory map approach to avoid loading all data into memory. TIC normalization can as such be performed even on large files (assuming sufficient disk space).

Keyword Arguments:

Parameters

- **msidata** (*h5py.dataset or numpu array (3D)*) – The input MSI dataset
- **mzdata** – The mz axsis do the dataset
- **maxCount** – ...
- **mzTol** – ...
- **infIons** – List of informative ions

record_execute_analysis_outputs (*analysis_output*)
We are not returning any outputs here, but we are going to record them manually. :param analysis_output: The output of the execute_analysis(...) function.

classmethod v_qmz (*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Get the mz axes for the analysis

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **qslice_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qslice URL pattern.
- **qspectrum_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qspectrum URL pattern.

Returns

The following four arrays are returned by the analysis:

- mz_spectra : Array with the static mz values for the spectra.
- label_spectra : Lable for the spectral mz axis
- mz_slice : Array of the static mz values for the slices or None if identical to the mz_spectra.
- label_slice : Lable for the slice mz axis or None if identical to label_spectra.

classmethod v_qslice (*analysis_object*, *z*, *viewer_option=0*)
Get 3D analysis dataset for which z-slices should be extracted for presentation in the OMSI viewer

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **z** – Selection string indicting which z values should be selected.
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns numpy array with the data to be displayed in the image slice viewer. Slicing will be performed typically like [:,:,zmin:zmax].

classmethod v_qslice_viewer_options (*analysis_object*)
Get a list of strings describing the different default viewer options for the analysis for qslice. The default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decision based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qslice requests (i.e., v_qslice(...) is not available).

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)

Get from which 3D analysis spectra in x/y should be extracted for presentation in the OMSI viewer

Developer Note: h5py currently supports only a single index list. If the user provides an index-list for both x and y, then we need to construct the proper merged list and load the data manually, or if the data is small enough, one can load the full data into a numpy array which supports multiple lists in the selection.

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **x** – x selection string
- **y** – y selection string
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns

The following two elements are expected to be returned by this function :

1. 1D, 2D or 3D numpy array of the requested spectra. NOTE: The mass (m/z) axis must be the last axis. For index selection x=1,y=1 a 1D array is usually expected. For indexList selections x=[0]&y=[1] usually a 2D array is expected. For ragne selections x=0:1&y=1:2 we one usually expects a 3D array/
2. None in case that the spectra axis returned by v_qmz are valid for the returned spectrum. Otherwise, return a 1D numpy array with the m/z values for the spectrum (i.e., if custom m/z values are needed for interpretation of the returned spectrum).This may be needed, e.g., in cases where a per-spectrum peak analysis is performed and the peaks for each spectrum appear at different m/z values.

classmethod **v_qspectrum_viewer_options**(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qspectrum. The default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

param analysis_object The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decission based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qspectrum requests (i.e., v_qspectrum(...) is not available).

omsi_tic_norm Module Module with the TIC normalization analysis.

class omsi.analysis.msi_filtering.omsi_tic_norm.**omsi_tic_norm**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

TIC Normalization analysis.

Initalize the basic data members

execute_analysis()
Normalize the data based on the total intensity of a spectrum or the intensities of a select set of ions.

Calculations are performed using a memory map approach to avoid loading all data into memory. TIC normalization can as such be performed even on large files (assuming sufficient disk space).

Keyword Arguments:

Parameters

- **msidata** (*h5py.dataset or numpu array (3D)*) – The input MSI dataset
- **mzdata** – The mz axsis do the dataset
- **maxCount** – ...
- **mzTol** – ...
- **infIons** – List of informative ions

record_execute_analysis_outputs(*analysis_output*)
We are not returning any outputs here, but we are going to record them manually. :param analysis_output: The output of the execute_analysis(...) function.

classmethod v_qmz(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Get the mz axes for the analysis

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **qslice_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qslice URL pattern.
- **qspectrum_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qspectrum URL pattern.

Returns

The following four arrays are returned by the analysis:

- mz_spectra : Array with the static mz values for the spectra.
- label_spectra : Lable for the spectral mz axis
- mz_slice : Array of the static mz values for the slices or None if identical to the mz_spectra.
- label_slice : Lable for the slice mz axis or None if identical to label_spectra.

classmethod v_qslice(*analysis_object*, *z*, *viewer_option=0*)
Get 3D analysis dataset for which z-slices should be extracted for presentation in the OMSI viewer

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **z** – Selection string indicting which z values should be selected.
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns numpy array with the data to be displayed in the image slice viewer. Slicing will be performed typically like [:,:,zmin:zmax].

classmethod v_qslice_viewer_options (*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qslice. The default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decision based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qslice requests (i.e., v_qslice(...) is not available).

classmethod v_qspectrum (*analysis_object*, *x*, *y*, *viewer_option=0*)

Get from which 3D analysis spectra in x/y should be extracted for presentation in the OMSI viewer

Developer Note: h5py currently supports only a single index list. If the user provides an index-list for both x and y, then we need to construct the proper merged list and load the data manually, or if the data is small enough, one can load the full data into a numpy array which supports multiple lists in the selection.

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **x** – x selection string
- **y** – y selection string
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns

The following two elements are expected to be returned by this function :

1. 1D, 2D or 3D numpy array of the requested spectra. NOTE: The mass (m/z) axis must be the last axis. For index selection x=1,y=1 a 1D array is usually expected. For indexList selections x=[0]&y=[1] usually a 2D array is expected. For ragne selections x=0:1&y=1:2 we one usually expects a 3D array/
2. None in case that the spectra axis returned by v_qmz are valid for the returned spectrum. Otherwise, return a 1D numpy array with the m/z values for the spectrum (i.e., if custom m/z values are needed for interpretation of the returned spectrum).This may be needed, e.g., in cases where a per-spectrum peak analysis is performed and the peaks for each spectrum appear at different m/z values.

classmethod v_qspectrum_viewer_options (*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qspectrum. The

default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

param analysis_object The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decission based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qspectrum requests (i.e., v_qspectrum(...) is not available).

msi_filtering.third_party Package

msi_filtering.third_party Package Package containing shared third-party code modules included here to reduce the need for external dependencies when only small parts of external code are used.

msi_filtering.experimental Package

msi_filtering.experimental Package Module with experimental analysis code, i.e., code that is not (yet) used in production but is under development. Often this is code that is used in a specific research.

omsi_filter_by_mask Module Module for performing masking for MSI data.

class omsi.analysis.msi_filtering.experimental.omsi_filter_by_mask.**omsi_filter_by_mask**(*name_ke*
Bases: *omsi.analysis.base.analysis_base*

Class defining a basic mask creation a 2D MSI data file or slice of the data

Initalize the basic data members

execute_analysis()

classmethod v_qmz(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Get the mz axes for the analysis

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **qslice_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qslice URL pattern.
- **qspectrum_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qspectrum URL pattern.

Returns

The following four arrays are returned by the analysis:

- mz_spectra : Array with the static mz values for the spectra.
- label_spectra : Lable for the spectral mz axis
- mz_slice : Array of the static mz values for the slices or None if identical to the mz_spectra.

- label_slice : Lable for the slice mz axis or None if identical to label_spectra.

classmethod **v_qslice**(*analysis_object*, *z*, *viewer_option=0*)

Get 3D analysis dataset for which z-slices should be extracted for presentation in the OMSI viewer

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **z** – Selection string indicting which z values should be selected.
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns numpy array with the data to be displayed in the image slice viewer. Slicing will be performed typically like [:,:,zmin:zmax].

classmethod **v_qslice_viewer_options**(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qslice. The default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decision based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qslice requests (i.e., v_qslice(...) is not available).

classmethod **v_qspectrum**(*analysis_object*, *x*, *y*, *viewer_option=0*)

Get from which 3D analysis spectra in x/y should be extracted for presentation in the OMSI viewer

Developer Note: h5py currently supports only a single index list. If the user provides an index-list for both x and y, then we need to construct the proper merged list and load the data manually, or if the data is small enough, one can load the full data into a numpy array which supports mulitple lists in the selection.

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **x** – x selection string
- **y** – y selection string
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns

The following two elemnts are expected to be returned by this function :

1. 1D, 2D or 3D numpy array of the requested spectra. NOTE: The mass (m/z) axis must be the last axis. For index selection x=1,y=1 a 1D array is usually expected. For indexList selections x=[0]&y=[1] usually a 2D array is expected. For ragne selections x=0:1&y=1:2 we one usually expects a 3D array.
2. None in case that the spectra axis returned by v_qmz are valid for the returned spectrum. Otherwise, return a 1D numpy array with the m/z values for the spectrum (i.e., if custom

m/z values are needed for interpretation of the returned spectrum).This may be needed, e.g., in cases where a per-spectrum peak analysis is performed and the peaks for each spectrum appear at different m/z values.

classmethod v_qspectrum_viewer_options(*analysis_object*)
Get a list of strings describing the different default viewer options for the analysis for qspectrum. The default implementation tries to take care of handling the spectra retrieval for all the dependencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

param analysis_object The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decission based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qspectrum requests (i.e., v_qspectrum(...) is not available).

omsi_mask_by_cluster Module Module for performing making a mask from cluster matrix for MSI data.

class omsi.analysis.msi_filtering.experimental.omsi_mask_by_cluster.**omsi_mask_by_cluster**(*name*
Bases: *omsi.analysis.base.analysis_base*

Class defining a basic mask creation a 2D MSI data file or slice of the data

Initalize the basic data members

execute_analysis()

classmethod v_qmz(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Get the mz axes for the analysis

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **qslice_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qslice URL pattern.
- **qspectrum_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qspectrum URL pattern.

Returns

The following four arrays are returned by the analysis:

- mz_spectra : Array with the static mz values for the spectra.
- label_spectra : Lable for the spectral mz axis
- mz_slice : Array of the static mz values for the slices or None if identical to the mz_spectra.
- label_slice : Lable for the slice mz axis or None if identical to label_spectra.

classmethod v_qslice(*analysis_object*, *z*, *viewer_option=0*)
Get 3D analysis dataset for which z-slices should be extracted for presentation in the OMSI viewer

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **z** – Selection string indicting which z values should be selected.
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns numpy array with the data to be displayed in the image slice viewer. Slicing will be performed typically like [:,:,zmin:zmax].

classmethod v_qslice_viewer_options(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qslice. The default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decision based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qslice requests (i.e., v_qslice(...) is not available).

classmethod v_qspectrum(*analysis_object*, *x*, *y*, *viewer_option=0*)

Get from which 3D analysis spectra in x/y should be extracted for presentation in the OMSI viewer

Developer Note: h5py currently supports only a single index list. If the user provides an index-list for both x and y, then we need to construct the proper merged list and load the data manually, or if the data is small enough, one can load the full data into a numpy array which supports mulitple lists in the selection.

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **x** – x selection string
- **y** – y selection string
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns

The following two elemnts are expected to be returned by this function :

1. 1D, 2D or 3D numpy array of the requested spectra. NOTE: The mass (m/z) axis must be the last axis. For index selection x=1,y=1 a 1D array is usually expected. For indexList selections x=[0]&y=[1] usually a 2D array is expected. For ragne selections x=0:1&y=1:2 we one usually expects a 3D array.
2. None in case that the spectra axis returned by v_qmz are valid for the returned spectrum. Otherwise, return a 1D numpy array with the m/z values for the spectrum (i.e., if custom m/z values are needed for interpretation of the returned spectrum).This may be needed, e.g., in cases where a per-spectrum peak analysis is performed and the peaks for each spectrum appear at different m/z values.

classmethod v_qspectrum_viewer_options(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qspectrum. The

default implementation tries to take care of handling the spectra retrieval for all the dependencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

param analysis_object The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decission based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qspectrum requests (i.e., v_qspectrum(...) is not available).

compound_stats Package

compound_stats Package Package containing shared third-party code modules included here to reduce the need for external dependencies when only small parts of external code are used.

omsi_score_midas Module MIDAS spectrum analysis

class omsi.analysis.compound_stats.omsi_score_midas.**omsi_score_midas**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Class for executing midas on an MSI or local peak finding dataset.

Initialize the basic data members

execute_analysis(*spectrum_indexes=None*, *compound_list=None*)
Execute the local peak finder for the given msidata.

Parameters

- **spectrum_indexes** – List with a list of integer indicies of the subset of sepctra that should be processed by this MPI task. If spectrum_indexes is set, then the given subblock will be processed in SERIAL instead of processing self['fpl_data'] in PARALLEL (if available). This parameter is strictly optional and intended for internal use only to facilitate the efficient parallel implementation.
- **compound_list** – List of the compounds from the database file. This parameter is used to avoid having to read the compound database on every compute task that calls this function when running in parallel. This parameter is strictly optional and intended for internal use only to facilitate the efficient parallel implementation.

Returns

A tuple with an array of hit_tables with the scores for each pixel and a 2D array of pixel indices describing for each spectrum the (x,y) pixel location in the image. The hit_table is an array of (#spectra x #compounds). The hit_table is a structured numpy array with the following columns:

- 'score', float, MIDAS score of row
- 'id', str, database ID e.g. 'MetaCyC_7884'
- 'name', str, database name, e.g. 'glycine'
- 'mass', float, mass in Da of IDed compound
- 'n_peaks', int, number of peaks in data

- 'n_match', int, number of peaks in data matched

omsi_score_pactolus Module MIDAS spectrum analysis

class omsi.analysis.compound_stats.omsi_score_pactolus.**omsi_score_pactolus**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Class for executing Pactolus on a local peak finding dataset.

Initialize the basic data members

execute_analysis(*spectrum_indexes=None*, *file_lookup_table=None*)
Execute the local peak finder for the given msidata.

Parameters

- **spectrum_indexes** – List with a list of integer indicies of the subset of sepctra that should be processed by this MPI task. If spectrum_indexes is set, then the given subblock will be processed in SERIAL instead of processing self['fpl_data'] in PARALLEL (if available). This parameter is strictly optional and intended for internal use only to facilitate the efficient parallel implementation.
- **file_lookup_table** – The Pactolus lookup table with the list of tree files and their mass.

Returns

A series of numpy arrays with the score data for each pixel and a 2D array of pixel indices describing for each spectrum the (x,y) pixel location in the image.

['pixel_index', 'score', 'id', 'name', 'mass', 'n_peaks', 'n_match']

- 'pixel_index' , int, 2D array of pixel indices describing for each spectrum the (x,y) pixel location in the imag
- 'score', float, MIDAS score of row
- 'id', str, database ID e.g. 'MetaCyC_7884'
- 'name', str, database name, e.g. 'glycine'
- 'mass', float, mass in Da of IDed compound
- 'n_peaks', int, number of peaks in data
- 'n_match', int, number of peaks in data matched

compound_stats.third_party Package

compound_stats.third_party Package Package containing shared third-party code modules included here to reduce the need for external dependencies when only small parts of external code are used.

compound_stats.experimental Package

compound_stats.experimental Package Module with experimental analysis code, i.e., code that is not (yet) used in production but is under development. Often this is code that is used in a specific research.

9.1.2 dataformat Package

Main module for specification of data formats. This module also contains the *omsi_file* module which specifies the OpenMSI HDF5 data format. In addition it defines the base class for third-party file readers (i.e, *file_reader_base*) and implements various basic file readers for third-party formats, e.g, *img_file* and *mzml_file* for IMG and MZML data files respectively (among others).

omsi.dataformat.omsi_file	Module for specification of the OpenMSI file API.
omsi.dataformat.omsi_file.analysis	Module for managing custom analysis data in OMSI HDF5 file
omsi.dataformat.omsi_file.common	Module for common data format classes and functionality.
omsi.dataformat.omsi_file.dependencies	Base module for managing of dependencies between data in Op
omsi.dataformat.omsi_file.experiment	OMSI file module for management of experiment data.
omsi.dataformat.omsi_file.format	This module defines the basic format for storing mass spectrom
omsi.dataformat.omsi_file.instrument	Module for managing instrument related data in OMSI files.
omsi.dataformat.omsi_file.main_file	Module for managing OpenMSI HDF5 data files.
omsi.dataformat.omsi_file.metadata_collection	Module for management of general metadata storage entities.
omsi.dataformat.omsi_file.methods	Module for management of method specific data in OMSI data
omsi.dataformat.omsi_file.msidata	Module for managing MSI data in OMSI data files
omsi.dataformat.file_reader_base	Module for base classes for implementation and integration of t
omsi.dataformat.bruckerflex_file	This module provides functionality for reading bruker flex mass
omsi.dataformat.img_file	This module provides functionality for reading img mass spectr
omsi.dataformat.imzml_file	
omsi.dataformat.mzml_file	

OMSI Dataformat Package

Main module for specification of the OpenMSI HDF5-based data format. The module contains various sub-modules, with the main goal to organize different categories of data.

Naming conventions for objects inside the HDF5 file are defined in the *omsi_file.format* module. These are used by the manager API classes to then implement the specific format.

The basic idea behind the design of the OpenMSI file format is the concept of managed objects. Managed objects are objects in an HDF5 file (usually HDF5 Groups –similar to directories just within a file) that have a corresponding interface class in the API. These classes in the API always start with the prefix *omsi_file_* and inherit from *omsi_file.common.omsi_file_common*.

To make it easy to nest different objects, we also have the concept of manager helper classes, which encapsulate common functionality for creation and interaction with the objects when they are contained in another object. Manager helper classes follow the following naming convection *omsi_<objectname>_manager*, where objectname is name of the object to be managed. E.g, *omsi_instrument_manager* is used to help place instrument groups inside another managed object. This is done by inheriting from the given manager helper class.

This means, multiple inheritance is used in order to nest other managed modules with other interfaces. This allows us to easily encapsulate common interaction features in centralized locations and construct more complex containers simply via inheritance.

The user of multiple inheritance and *super* can be tricky in python. To simplify the use and ensure stability we use the following conventions:

- All *omsi_file_** manager classes must except the h5py.Group object they manage as input and call *super(..)__init__(managed_group)* with the managed group as parameter in their *__init__*.
- All *omsi_<objectname>_manager* manager helper classes must except the h5py.Group that contains the object(s) that should be managed using the helper class as input and call *super(..)__init__(managed_group)* with the managed group as parameter in their in *__init__*.

- All *omsi_file_** manager classes must inherit from *omsi_file.common.omsi_file_common*
- All *omsi_<objectname>_manager* manager helper classes must inherit from *object* (i.e., we use new-style classes).

omsi_file Package

Module for specification of the OpenMSI file API.

format Module

This module defines the basic format for storing mass spectrometry imaging data, metadata, and analysis in HDF5 in compliance with OpenMSI file format.

class omsi.dataformat.omsi_file.format.**omsi_format_analysis**
Bases: *omsi.dataformat.omsi_file.format.omsi_format_common*

Specification for storing analysis related data.

Variables

- ***analysis_groupname*** – *analysis_* : Group with additional analysis results
- ***analysis_identifier*** – *analysis_identifier* : Identifier for the analysis to enable look-up by analysis id
- ***analysis_type*** – *analysis_type* : Dataset used to store the analysis type descriptor string
- ***analysis_parameter_group*** – Group for storing analysis parameters. Dependent parameters are stored separately using a omsi_format_dependencies group.
- ***analysis_runinfo_group*** – Group for storing run information, e.g., where was the analysis run, how long did it take etc.

analysis_groupname = 'analysis_'

analysis_identifier = 'analysis_identifier'

analysis_parameter_group = 'parameter'

analysis_parameter_help_attr = 'help'

analysis_runinfo_group = 'runinfo'

analysis_type = 'analysis_type'

current_version = '0.2'

class omsi.dataformat.omsi_file.format.**omsi_format_common**
Bases: object

Specification of common attributes, and names for the file format.

Variables

- ***str_type*** – *str_type = h5py.new_vlen(str)* : Datatype used for storing strings in hdf5
- ***type_attribute*** – Name of the optional type attribute indicating which omsi_file_* class should be used to interact with a given group.

current_version = '0.1'

str_type = dtype('O')

str_type_unicode = True

timestamp_attribute = 'timestamp'

type_attribute = 'omsi_type'

version_attribute = 'version'

class omsi.dataformat.omsi_file.format.**omsi_format_data**
Bases: *omsi.dataformat.omsi_file.format.omsi_format_common*

Specification for storing raw data information.

Variables

- ***data_groupname*** – The base name for the hdf5 group containing the imaging data
- ***dataset_name*** – The base name for storing raw data. In the case of MSI data, this is the 3D data cube stored as 3D (full_cube), 2D (partial_cube) or 1D (partial_spectra) dataset, depending on the format_type.
- **data_dependency_group** – Optional group for storing data dependencies

current_version = '0.1'

data_groupname = 'data_'

dataset_name = 'data_'

class omsi.dataformat.omsi_file.format.**omsi_format_dependencies**
Bases: *omsi.dataformat.omsi_file.format.omsi_format_common*

Specification for the management of a collection of dependencies.

Variables ***dependencies_groupname*** – *dependency* : Name of the group the dependencies are stored in.

current_version = '0.1'

dependencies_groupname = 'dependency'

class omsi.dataformat.omsi_file.format.**omsi_format_dependencydata**
Bases: *omsi.dataformat.omsi_file.format.omsi_format_common*

Specification for the storage of a single dependency.

This type of group does not have specific name to allow the user to specify a specific link_name to ease retrieval of the data.

Variables

- ***dependency_parameter*** – *parameter_name* : Name of string dataset used to store the name of the dependent parameter
- ***dependency_selection*** – *selection* : Name of the string dataset used to store a selection string if needed.
- ***dependency_mainname*** – *main_name* : Name of the string dataset used to store the description of the link to the object that this depends on.
- ***dependency_datasetname*** – 'data_name' : Name fo the string dataset used to store the name of dataset within the mainname highlevel object.

current_version = '0.3'

dependency_datasetname = 'data_name'

dependency_mainname = 'main_name'

dependency_parameter = 'parameter_name'

dependency_parameter_help_attr = 'help'

dependency_selection = 'selection'

dependency_typename = 'dependency_type'

class omsi.dataformat.omsi_file.format.**omsi_format_experiment**
Bases: *omsi.dataformat.omsi_file.format.omsi_format_common*

Specification of file format specific name conventions

Variables

- ***exp_groupname*** – *entry_* : The base name for a group containing data about an experiment
- ***exp_identifier_name*** – *experiment_identifier* : The identifier dataset for an experiment

current_version = '0.1'

exp_groupname = 'entry_'

exp_identifier_name = 'experiment_identifier'

class omsi.dataformat.omsi_file.format.**omsi_format_file**
Bases: *omsi.dataformat.omsi_file.format.omsi_format_common*

Specification of main-file related specific name conventions

current_version = '0.1'

class omsi.dataformat.omsi_file.format.**omsi_format_instrument**
Bases: *omsi.dataformat.omsi_file.format.omsi_format_metadata_collection*

Specification for storing instrument related information

Variables

- ***instrument_groupname*** – *instrument* : Group with information about the intrument used
- ***instrument_mz_name*** – *mz* : Name of the dataset for the intrument's mz data values
- ***instrument_name*** – *name* : The dataset with the name of the instrument

current_version = '0.2'

instrument_groupname = 'instrument'

instrument_mz_name = 'mz'

instrument_name = 'name'

class omsi.dataformat.omsi_file.format.**omsi_format_metadata_collection**
Bases: *omsi.dataformat.omsi_file.format.omsi_format_common*

Specification of the basic format for a general-purpose metadata storage

Variables

- ***metadata_collection_groupname_default*** – Default name for the group where the collection of metadata is stored.
- ***description_value_attribute*** – The attribute to be associated with each metadata value describing the content in a human-readable form

- ***unit_value_attribute*** – The attribute to be associated with each metatdata value describing the unit
- ***ontology_value_attribute*** – Optional ontology associated with a metadata value

current_version = '0.1'

description_value_attribute = 'description'

metadata_collection_groupname_default = 'metadata'

ontology_value_attribute = 'ontology'

unit_value_attribute = 'unit'

class omsi.dataformat.omsi_file.format.**omsi_format_methods**
Bases: *omsi.dataformat.omsi_file.format.omsi_format_metadata_collection*

Specification of the basic format for storing method-related information

Variables

- ***methods_groupname*** – *methods* : The group storing all the information about the method
- ***methods_old_groupname*** – *method* : The group object was refactored to methods. To ensure that old files can still be read, this variable was added and is checked as well if needed.
- ***methods_name*** – *name* : The dataset with the name of the method

current_version = '0.3'

methods_groupname = 'methods'

methods_name = 'name'

methods_old_groupname = 'sample'

class omsi.dataformat.omsi_file.format.**omsi_format_msidata**
Bases: *omsi.dataformat.omsi_file.format.omsi_format_data*

Specification of the basic format for storing an MSI dataset consisting of a complete 3D cube (or a 3D cube completed with 0s for missing data)

Variables

- ***format_types*** – Data layout types supported for storing MSI data.
- ***mzdata_name*** – Global mz axis for the MSI data cube.
- ***format*** – Dataset in HDF5 with the format_type descriptor.

current_version = '0.1'

format_name = 'format'

format_types = {'full_cube': 1, 'partial_cube': 2, 'partial_spectra': 3}

mzdata_name = 'mz'

class omsi.dataformat.omsi_file.format.**omsi_format_msidata_partial_cube**
Bases: *omsi.dataformat.omsi_file.format.omsi_format_msidata*

Specification of the basic format for storing an MSI datasets that define a partial cube with full spectra

Variables

- ***xy_index_name*** – 2D dataset indicating for each spectrum its start location in the the main dataset
- ***inv_xy_index_name*** – 2D dataset with n rows and 2 columns indicating for each spectrum i the (x,y) pixel index the spectrum belongs to. This index is stored for convenience purposes but is not actually needed for data access.
- ***shape_name*** – Simple [3] indicating the true image size in x,y,mz

inv_xy_index_name = 'inv_xy_index'

shape_name = 'shape'

xy_index_name = 'xyindex'

class omsi.dataformat.omsi_file.format.**omsi_format_msidata_partial_spectra**
Bases: *omsi.dataformat.omsi_file.format.omsi_format_msidata_partial_cube*

Specification of the basic format for storing an MSI dataset of a full or partial cube with partial spectra

Variables

- ***mz_index_name*** – 1D dataset of the same size as the spectrum data, indicating the indices into the global m/z list
- ***xy_index_end_name*** – 2D dataset indicating for each spectrum its end location (index not included) in the the main dataset

mz_index_name = 'mz_index'

xy_index_end_name = 'xyindexend'

common Module

Module for common data format classes and functionality.

class omsi.dataformat.omsi_file.common.**omsi_file_common**(*managed_group*)
Bases: object

Base class for definition of file format modules for the OpenMSI data format.

Use of super()

This class inherits only from object and calls super in the __init__ without parameters. In the standard design pattern of the *omsi.dataformat.omsi_file module*, it is, therefore, the last class we inherit from in the case of multiple inheritance.

Multiple inheritance is used in *omsi.dataformat.omsi_file module* when a class contains other managed objects and uses the manager classes, e.g, omsi_instrument_mangager etc. to get all the features needed to manage those objects.

All child classes of omsi_file_common also call super(..).__init__(manager_group) but using a single input parameter indicating the manager h5py.Group object that contains the given object.

Variables

- **managed_group** – The h5py.Group object managed by the class
- **name** – The path to the object in the hdf5 file. Same as managed_group.name
- **file** – The h5py.File object the managed_group is associated with. Same as managed_group.file

static create_path_string(*filename*, *objectname*)
Given the name of the file and the object path within the file, create a string describing the external reference to the datra

Parameters

- **filename** – The full or relative path to the file
- **objectname** – The object path in the HDF5 file

Returns String describing the path to the object

classmethod get_h5py_object(*omsi_object*, *resolve_dependencies=False*)
This static method is a convenience function used to retrieve the corresponding h5py interface object for any omsi file API object.

Parameters

- **omsi_object** – omsi file API input object for which the corresponding h5py.Group, h5py.File, or h5py.Dataset object should be retrieved. The omsi_object input may itself also be a h5py.Group, h5py.File, or h5py.Dataset, in which case omsi_object itself is returned by the function.
- **resolve_dependencies** – Set to True if omsi_file_dependencydata objects should be resolved to retrieve the dependent object the dependency is pointing to. Dependencies are resolved recursively, i.e., if a dependency points to another dependency then that one will be resolved as well. Default value is False, i.e., the omis_file_dependency object itself is returned.

Returns h5py.Group, h5py.File, or h5py.Dataset corresponding to the given omsi_object.

Raises **ValueError** – A ValueError is raised in case that an unsupported omsi_object object is given, i.e., the input object is not a omsi_file API object nor a h5py Group, File, or Dataset object.

get_managed_group()
Return the h5py object with the analysis data.

The returned object can be used to read data directly from the HDF5 file. Write operations to the analysis group can be performed only if the associated omsi_file was opened with write permissions.

Returns h5py object for the analysis group.

classmethod get_num_items(*file_group*, *basename=''*)
Get the number of object with the given basename at the given path

Parameters

- **file_group** – The h5py object to be examined
- **basename** – The name that should be searched for.

Returns Number of objects with the given basename at the given path

classmethod get_omsi_object(*h5py_object*, *resolve_dependencies=False*)
This static method is convenience function used to retrieve the corresponding interface class for a given h5py group object.

Parameters

- **h5py_object** – h5py object for which the corresponding omsi_file API object should be generated. This may also be a string describing the requested object based on a combination of the path to the file and a path ot the object <filename.h5>:<object_path>

- **resolve_dependencies** – Set to True if omsi_file_dependencydata objects should be resolved to retrieve the dependent object the dependency is pointing to. Dependencies are resolved recursively, i.e., if a dependency points to another dependency then that one will be resolved as well. Default value is False, i.e., the omis_file_dependency object itself is returned.

Returns

None in case no corresponding object was found. Otherwise an instance of:

- omsi_file : If the given object is a h5py.File object
- omsi_file_experiment : If the given object is an experiment groupt
- omsi_file_methods : If the given object is a method group
- omsi_file_instrument : If the given object is an instrument group
- omsi_file_analysis : If the given object is an analysis group
- omsi_file_msidata : If the given object is a MSI data group
- omsi_file_dependencydata : If the fiven object is a dependency group
- The input h5py_object: If the given object is a h5py.Dataset or h5py.Group
- None: In case that an unknown type is given.

get_timestamp()
Get the timestamp when the analysis group was created in the HDF5 file.

Returns Python timestamp string generated using time.ctime(). None may be returned in case that the timestamp does not exists or cannot be retrieved from the file for some reason.

get_version()
Get the omsi version for the representation of this object in the HDF5 file

classmethod is_managed(*in_object*)
Check whether the given object is managed by any omsi API class.

Parameters **in_object** (*Any omsi_file API object or h5py.Dataset or h5py.Group or h5py.File object.*) – The object to be checked

items()
Get the list of items associdated with the h5py.Group object managed by this object

static parse_path_string(*path*)
Given a string of the form <filename.h5>:<object_path> retrieve the name of the file and the object path.

Parameters **path** – The string defining the file and object path.

Returns Tuple with the filename and the object path. Both may be None depending on whether an object_path is given and whether the path string is valid.

Raises ValueError in case that an invalid string is given

static same_file(*filename1*, *filename2*)
Check whether two files are the same.

This function uses the os.path.samefile(...) method to compare files and falls back to comparing the absolute paths of files if samefile should fail or cannot be imported.

Parameters

- **filename1** – The name of the first file
- **filename2** – The name of the second file

Returns

class omsi.dataformat.omsi_file.common.**omsi_file_object_manager**(**args*, ***kwargs*)
Bases: object

Base class used to define manager helper classes used to manage contained managed objects. Managed objects are HDF5.Groups (or Datasets) with a corresponding manager API class and may be nested within other Managed objects.

What is a manager helper class?

Manager classes are used in the design of *omsi.dataformat.omsi_file* to encapsulate functionality needed for management of other manager objects. The expected use of this class, hence, is through multiple inheritance where the main base class is *omsi.dataformat.omsi_file.common.omsi_file_common*. This is important due to the use of super to accomodate multiple inheritance to allow object to manage an arbitrary number of other object and inherit from other object as well.

Use of super()

This class inherits only from object but calls super in the __init__(manager_group) with the manager_group as only input parameter, in the expectation that this class is used using multiple inheritance with *omsi_file_common* as main base class .

Multiple inheritance is used in *omsi.dataformat.omsi_file module* when a class contains other managed objects and uses the manager classes (such as this one) to get all the features needed to manage those objects.

All child classes of omsi_file_common call super(..).__init__(manager_group) and all manager helper classes (such as this one) use a single input parameter indicating the manager h5py.Group object that contains the given object.

main_file Module

Module for managing OpenMSI HDF5 data files.

class omsi.dataformat.omsi_file.main_file.**omsi_file**(*filename*, *mode='a'*, ***kwargs*)
Bases: *omsi.dataformat.omsi_file.experiment.omsi_experiment_manager*, *omsi.dataformat.omsi_file.common.omsi_file_common*

API for creating and managing a single OpenMSI data file.

Use of supe()r

This class inherits from *omsi.dataformat.omsi_file.common.omsi_file_common* . Consistent with the design pattern for multiple inheritance of the *omsi.dataformat.omsi_file* module, the *__init__* function calls *super(...).__init__(manager_group)* with a single parameter indicating the parent group.

Inherited Instance Variables

Variables

- **managed_group** – The group that is managed by this object
- **name** – Name of the managed group

Open the given file or create it if does not exit.

The creation of the object may fail if the file does not exist, and the selected mode is 'r' or 'r+'.

Keyword arguments:

Parameters

- **filename** – string indicating the name+path of the OpenMSI data file. Alternatively this may also be an h5py.File instance (or an h5py.Group, h5py.Dataset instance from which we can get the file)
- **mode** – read/write mode. One of :

  r = readonly, file must exist.

  r+ = read/write, file must exist.

  w = Create file, truncate if exists.

  w- = create file, fail if exists.

  a = read/write if exists, create otherwise (default)
- ****kargs** – Other keyword arguments to be used for opening the file using h5py. See the h5py.File documentation for details. For example to use parallel HDF5, the following additional parameters can be given driver='mpio', comm:MPI.COMM_WORLD.

close_file()
Close the msi data file

flush()
Flush all I/O

get_filename()
Get the name of the omsi file

Returns String indicating the filename (possibly including the full path, depending on how the object has been initalized)

get_h5py_file()
Get the h5py object for the omsi file

Returns h5py redernce to the HDF5 file

classmethod is_valid_dataset(*name*)
Perform basic checks for the given filename, whether it is a valid OMSI file.

Parameters **name** – Name of the file to be checked.

Returns Boolean indicating whether the file is valid

write_xdmf_header(*xdmf_filename*)
Write XDMF header file for the current HDF5 datafile

Parameters **xdmf_filename** – The name of the xdmf XML header file to be created for the HDF5 file.

experiment Module

OMSI file module for management of experiment data.

class omsi.dataformat.omsi_file.experiment.**omsi_experiment_manager**(*experiment_parent*)
Bases: *omsi.dataformat.omsi_file.common.omsi_file_object_manager*

Experiment manager helper class used to define common functionality needed for experiment-related data. Usually, a class that defines a format that contains an omsi_file_experiment object will inherit from this class (in addition to omsi_file_common) to acquire the common features.

For more details see: *omsi.dataforamt.omsi_file.omsi_common.omsi_file_object_manager*

Variables **experiment_parent** – The h5py.Group parent object containing the instrument object to be managed.

create_experiment(*exp_identifier=None*, *flush_io=True*)
Create a new group in the file for a new experiment and return the omsi_file_experiment object for the new experiment.

Parameters

- **exp_identifier** (*string or None (default)*) – The string used to identify the analysis
- **flush_io** – Call flush on the HDF5 file to ensure all HDF5 bufferes are flushed so that all data has been written to file.

Returns omsi_file_experiment object for the newly created group for the experiment

get_experiment(*exp_index*)
Get the omsi_format_experiment object for the experiment with the given index

Parameters **exp_index** (*uint*) – The index of the requested experiment

Returns h5py reference to the experiment with the given index. Returns None in case the experiment does not exist.

get_experiment_by_identifier(*exp_identifier_string*)
Get the omsi_format_experiment object for the experiment with the given identifier.

Parameters **exp_identifier_string** (*string*) – The string used to identify the analysis

Returns Returns h5py object of the experiment group or None in case the experiment is not found.

static get_experiment_path(*exp_index=None*)
Based on the index of the experiment return the full path to the hdf5 group containing the data for an experiment.

Parameters **exp_index** – The index of the experiment.

Returns String indicating the path to the experiment.

get_num_experiments()
Get the number of experiments in this file.

Returns Integer indicating the number of experiments.

class omsi.dataformat.omsi_file.experiment.**omsi_file_experiment**(*exp_group*)
Bases: *omsi.dataformat.omsi_file.methods.omsi_methods_manager*, *omsi.dataformat.omsi_file.instrument.omsi_instrument_manager*, *omsi.dataformat.omsi_file.analysis.omsi_analysis_manager*, *omsi.dataformat.omsi_file.msidata.omsi_msidata_manager*, *omsi.dataformat.omsi_file.common.omsi_file_common*

Class for managing experiment specific data

Use of super():

This class inherits from *omsi.dataformat.omsi_file.common.omsi_file_common*. Consistent with the design pattern for multiple inheritance of the *omsi.dataformat.omsi_file* module, the __init__ function calls super(...).__init__(manager_group) with a single parameter indicating the parent group.

Inherited instance variable:

Variables

- **managed_group** – The group that is managed by this object
- **methods_parent** – The parent group containing the methods object (same as managed_group)
- **instrument_parent** – The parent group containing the instrument object (same as managed_group)
- **name** – Name of the managed group

Initalize the experiment object given the h5py object of the experiment group

Parameters **exp_group** – The h5py object with the experiment group of the omsi hdf5 file.

get_experiment_identifier()
Get the HDF5 dataset with the identifier description for the experiment.

Returns h5py object of the experiment identifier or None in case not present

get_experiment_index()
Determine the index of the experiment based on the name of the group :return: Integer index of the experiment

get_instrument_info(*check_parent=False*)
Inherited from omsi_instrument_manager parent class. Overwritten here to change the default parameter setting for check_parent. See *omsi.dataformat.omsi_file.instrument.omsi_instrument_manager* for details.

get_method_info(*check_parent=False*)
Inherited from omsi_method_manager parent class. Overwritten here to change the default parameter setting for check_parent. See *omsi.dataformat.omsi_file.methods.omsi_method_manager* for details

set_experiment_identifier(*identifier*)
Overwrite the current identfier string for the experiment with the given string

Parameters **identifier** – The new experiment identifier string.

metadata_collection Module

Module for management of general metadata storage entities. These are often specialized —e.g., omsi_file_instrument, omsi_file_sample—to store specific metadata and add more functionality.

class omsi.dataformat.omsi_file.metadata_collection.**omsi_file_metadata_collection**(*metadata_group*
Bases: *omsi.dataformat.omsi_file.common.omsi_file_common*

Class for managing method specific data.

Use of super():

This class inherits from *omsi.dataformat.omsi_file.common.omsi_file_common*. Consistent with the design pattern for multiple inheritance of the *omsi.dataformat.omsi_file* module, the __init__ function calls super(...).__init__(manager_group) with a single parameter indicating the parent group.

Inherited Instance Variables

Variables

- **managed_group** – The group that is managed by this object
- **name** – Name of the managed group

Initialize the metadata collection object given the h5py object of the metadata collection

Parameters **metadata_group** – The h5py object with the metadata collection group of the omsi hdf5 file.

add_metadata(*metadata*)
Add a new metadata entry

Parameters **metadata** – Instance of *omsi.shared.metadata_data.metadata_value* or describing *omsi.shared.metadata_data.metadata_dict* with the metadata to be added.

get_metadata(*key=None*)
Get dict with the full description of the metadata for the given key or all metadata if no key is given.

Returns *omsi.shared.metadata_data.metadata_value* object if a key is given or a *omsi.shared.metadata_data.metadata_dict* with all metadata if no key is specified.

Raises KeyError is raised in case that the specified key does not exist

keys()
Get a list of all metadata keys

Returns List of string with the metadata keys

values()
Convenience function returning a list of all metadata objects. This is equivilant get_metadata(key=None).values(), however, for consistency with other dict-like interfaces this function returns a list of *omsi.shared.metadata_data.metadata_value* objects rather than the *omsi.shared.metadata_data.metadata_dict*

Returns List of *omsi.shared.metadata_data.metadata_value* with all metadata

class omsi.dataformat.omsi_file.metadata_collection.**omsi_metadata_collection_manager**(*metadata_p*
Bases: *omsi.dataformat.omsi_file.common.omsi_file_object_manager*

This is a file format manager helper class used to define common functionality needed for management of metadata-related data. Usually, a class that defines a format that contains an omsi_file_metadata object will inherit from this class (in addition to omsi_file_common) to acquire the common features.

For more details see: *omsi.dataforamt.omsi_file.omsi_common.omsi_file_object_manager*

Variables **metadata_parent** – The parent h5py.Group object containing the method object to be managed

create_metadata_collection(*group_name=None*, *metadata=None*, *flush_io=True*)
Add a new group for managing metadata

Parameters

- **group_name** (*str, None*) – Optional name of the new metadata group. If None is given then the omsi_format_metadata_collection.metadata_collection_groupname_default will be used
- **metadata** (*None, omsi.shared.metadata_data.metadata_value, omsi_shared.metadata_data.metadata_dict*) – Additional metadata to be added to the collection after creation
- **flush_io** – Call flush on the HDF5 file to ensure all HDF5 buffers are flushed so that all data has been written to file

Returns *omsi_file_metadata_collection* object

get_default_metadata_collection(*omsi_object=None*)
Get the default metadata collection object if it exists

Parameters **omsi_object** – The omsi file API object or h5py.Group object that we should check. If set to None (default) then the self.metadata_parent will be used

Returns None, omsi_file_metadata_collection

get_metadata_collections(*omsi_object=None*, *name=None*)
Get all metadata_collections defined for given OpenMSI file API object or h5py.Group.

Parameters

- **omsi_object** – The omsi file API object or h5py.Group object that we should check. If set to None (default) then the self.metadata_parent will be use
- **name** – If name is specified, then only retrieve collections with the given name

Returns List of omsi_file_metadata_collection objects for the requested group. The function returns None in case that the h5py.Group for the omsi_object could not be determined.

has_default_metadata_collection(*omsi_object*)
Check whether the omsi API object (or h5py.Group) contains any a metadata collection with the default name.

Returns bool

has_metadata_collections(*omsi_object=None*)
Check whether the given omsi API object (or h5py.Group) contains any metadata collections

Parameters **omsi_object** – The omsi file API object or h5py.Group object that we should check. If set to None (default) then the self.metadata_parent will be used

Returns Boolean indicating whether metadata collections were found

instrument Module

Module for managing instrument related data in OMSI files.

class omsi.dataformat.omsi_file.instrument.**omsi_file_instrument**(*instrument_group*)
Bases: *omsi.dataformat.omsi_file.metadata_collection.omsi_file_metadata_collection*

Class for managing instrument specific data

Use of super():

This class inherits from *omsi.dataformat.omsi_file.common.omsi_file_common*. Consistent with the design pattern for multiple inheritance of the *omsi.dataformat.omsi_file* module, the __init__ function calls super(...).__init__(manager_group) with a single parameter indicating the parent group.

Inherited Instance Variables

Variables

- **managed_group** – The group that is managed by this object
- **name** – Name of the managed group

Initalize the instrument object given the h5py object of the instrument group

Parameters **instrument_group** – The h5py object with the instrument group of the omsi hdf5 file.

get_instrument_mz()
Get the HDF5 dataset with the mz data for the instrument.

To get the numpy array of the full mz data use: get_instrument_mz()[:]

Returns Returns the h5py object with the instrument mz data. Returns None in case no mz data was found for the instrument.

get_instrument_name()
Get the HDF5 dataset with the name of the instrument.

To get the string of the instrument name use: get_instrument_name()[...]

Returns h5py object to the dataset with the instrument name. Returns None in case no method name is found.

has_instrument_name()
Check whether a name has been saved for the instrument

Returns bool

set_instrument_name(*name*)
Overwrite the current identifier string for the experiment with the given string.

Parameters **name** (*string.*) – The new instrument name.

class omsi.dataformat.omsi_file.instrument.**omsi_instrument_manager**(*instrument_parent*)
Bases: *omsi.dataformat.omsi_file.metadata_collection.omsi_metadata_collection_manager*

Instrument manager helper class used to define common functionality needed for instrument-related data. Usually, a class that defines a format that contains an omsi_file_methods object will inherit from this class (in addition to omsi_file_common) to acquire the common features.

For more details see: *omsi.dataforamt.omsi_file.omsi_common.omsi_file_object_manager*

Variables **instrument_parent** – The h5py.Group parent object containing the instrument object to be managed.

create_instrument_info(*instrument_name=None*, *mzdata=None*, *flush_io=True*)
Add information about the instrument used for creating the images for this experiment.

Parameters

- **instrument_name** (*string, None*) – The name of the instrument
- **mzdata** (*numpy array or None*) – Numpy array of the mz data values of the instrument
- **flush_io** – Call flush on the HDF5 file to ensure all HDF5 bufferes are flushed so that all data has been written to file

Returns The function returns the h5py HDF5 handler to the instrument info group created for the experiment.

get_instrument_info(*check_parent=True*)
Get the HDF5 group opbject with the instrument information.

Parameters **check_parent** – If no method group is available for this dataset should we check whether the parent object (i.e., the experiment group containing the dataset) has information about the method. (default=True)

Returns omsi_file_instrument object for the requested instrument info. The function returns None in case no instrument information was found for the experiment

has_instrument_info(*check_parent=False*)
Check whether custom instrument information is available for this dataset.

Parameters **check_parent** – If no instrument group is available for this dataset should we check whether the parent object (i.e., the experiment group containing the dataset) has information about the instrument. (default=False)

Returns Boolean indicating whether instrument info is available.

methods Module

Module for management of method specific data in OMSI data files

class omsi.dataformat.omsi_file.methods.**omsi_file_methods**(*method_group*)
Bases: *omsi.dataformat.omsi_file.metadata_collection.omsi_file_metadata_collection*

Class for managing method specific data.

Use of super():

This class inherits from *omsi.dataformat.omsi_file.common.omsi_file_common*. Consistent with the design pattern for multiple inheritance of the *omsi.dataformat.omsi_file* module, the __init__ function calls super(...).__init__(manager_group) with a single parameter indicating the parent group.

Inherited Instance Variables

Variables

- **managed_group** – The group that is managed by this object
- **name** – Name of the managed group

Initialize the method object given the h5py object of the method group

Parameters **method_group** – The h5py object with the method group of the omsi hdf5 file.

get_method_name()
Get the HDF5 dataset with the name of the method.

To retrieve the name string use get_method_name()[...]

Returns h5py object where the method name is stored. Returns None in case no method name is found.

has_method_name()
Check whether an object has a method name

Returns bool

set_method_name(*name_string*)
Overwrite the name string for the method with the given name string

Parameters **name_string** (*string*) – The new method name.

class omsi.dataformat.omsi_file.methods.**omsi_methods_manager**(*methods_parent=None*)
Bases: *omsi.dataformat.omsi_file.metadata_collection.omsi_metadata_collection_manager*

This is a file format manager helper class used to define common functionality needed for methods-related data. Usually, a class that defines a format that contains an omsi_file_methods object will inherit from this class (in addition to omsi_file_common) to acquire the common features.

For more details see: *omsi.dataforamt.omsi_file.omsi_common.omsi_file_object_manager*

Variables **method_parent** – The parent h5py.Group object containing the method object to be managed

create_method_info(*method_name=None*, *metadata=None*, *flush_io=True*)
Add information about the method imaged to the experiment. Note, if a methods group already exists, then that group will be used. If method_name is not None, then the existing name will be overwritten by the new value.

Parameters

- **method_name** (*str, None*) – Optional name of the method

- **metadata** (*metadata_value, metadata_dict*) – Additional metadata to be stored with the methods
- **flush_io** – Call flush on the HDF5 file to ensure all HDF5 buffers are flushed so that all data has been written to file

Returns h5py object of the newly created method group.

get_method_info(*check_parent=True*)
Get the omsi_file_methods object with the method information.

Parameters **check_parent** – If no method group is available for this dataset should we check whether the parent object (i.e., the experiment group containing the dataset) has information about the method. (default=True)

Returns omsi_file_methods object for the requested method info. The function returns None in case no method information was found for the experiment

has_method_info(*check_parent=False*)
Check whether custom method information is available for this dataset.

Parameters **check_parent** – If no method group is available for this dataset should we check whether the parent object (i.e., the experiment group containing the dataset) has information about the method. (default=False)

Returns Boolean indicating whether method info is available.

msidata Module

Module for managing MSI data in OMSI data files

class omsi.dataformat.omsi_file.msidata.**omsi_file_msidata**(*data_group*, *fill_space=True*, *fill_spectra=True*, *preload_mz=False*, *preload_xy_index=False*)

Bases: *omsi.dataformat.omsi_file.dependencies.omsi_dependencies_manager*, *omsi.dataformat.omsi_file.methods.omsi_methods_manager*, *omsi.dataformat.omsi_file.instrument.omsi_instrument_manager*, *omsi.dataformat.omsi_file.metadata_collection.omsi_metadata_collection_manager*, *omsi.dataformat.omsi_file.common.omsi_file_common*

Interface for interacting with mass spectrometry imaging datasets stored in omis HDF5 files. The interface allows users to interact with the data as if it where a 3D cube even if data is missing. Full spectra may be missing in cases where only a region of interest in space has been imaged. Spectra may further be pre-processed so that each spectrum has only information about its peaks so that each spectrum has it's own mz-axis.

To load data ue standard array syntax, e.g., [1,1,:] can be used to retrieve the spectrums at location (1,1).

Use of super():

This class inherits from *omsi.dataformat.omsi_file.common.omsi_file_common*. Consistent with the design pattern for multiple inheritance of the *omsi.dataformat.omsi_file* module, the __init__ function calls super(...).__init__(manager_group) with a single parameter indicating the parent group.

Current limitations:

•The estimates in def __best_dataset__(self,keys) are fairly crude at this point

•The __getitem__ function for the partial_spectra case is not implemented yet.

- The __setitem__ function for the partial spectra case is not implemented yet (Note, it should also support dynamic expansion of the cube by adding previously missing spectra).
- For the partial cube case, assignement using __setitem__ function is only supported to valid spectra, i.e., spectra that were specified as occupied during the intital creation process.

Public object variables:

Variables

- **shape** – Define the full 3D shape of the dataset (i.e., even if the data is stored in sparse manner)
- **dtype** – The numpy datatyp of the main MSI data. This is the same as dataset.dtype
- **name** – The name of the corresponding groupt in the HDF5 file. Used to generate hard-links to the group.
- **format_type** – Define according to which standard the data is stored in the file
- **datasets** – List of h5py objects containing possibly multiple different version of the same MSI data (spectra). There may be multiple versions stored with different layouts in order to optimize the selection process.
- **mz** – dataset with the global mz axis information. If prelaod_mz is set in the constructor, then this is a numpy dataset with the preloaded data. Otherwise, this is the h5py dataset pointing to the data on disk.
- **xy_index** – None if format_type is 'full_cube'. Otherwise, this is the 2D array indicating for each x/y location the index of the spectrum in dataset. If prelaod_xy_index is set in the constructor, then this is a numpy dataset with the preloaded data. Otherwise, this is the h5py dataset pointing to the data on disk. Negative (-1) entries indicate that no spectrum has been recored for the given pixel.
- **inv_xy_index** – 2D dataset with n rows and 2 columns indicating for each spectrum i the (x,y) pixel index the spectrum belongs to. This index is stored for convenience purposes but is not actually needed for data access.
- **mz_index** – None if format_type is not 'partial_spectra'. Otherwise this is a dataset of the same size as the spectra data stored in dataset. Each entry indicates an index into the mz dataset to determine the mz_data value for a spectrum. This means mz[mx_index] gives the true mz value.
- **xy_index_end** – None if format_type is not 'partial_spectra'. Otherwise this is a 2D array indicating for each x/y location the index where the given spectrum ends in the dataset. If prelaod_xy_index is set in the constructor, then this is a numpy dataset with the preloaded data. Otherwise, this is the h5py dataset pointing to the data on disk. Negative (-1) entries indicate that no spectrum has been recored for the given pixel.

Private object variables:

Variables

- **_data_group** – Store the pointer to the HDF5 group with all the data
- **_fill_xy** – Define whether the data should be reconstructed as a full image cube Set using the set_fill_space function(..)
- **_fill_mz** – Define whether spectra should be remapped onto a global m/z axis. Set using the set_fill_spectra function(..)

Initialize the omsi_msidata object.

The fill options are provided to enable a more convenient access to the data independent of how the data is stored in the file. If the fill options are enabled, then the user can interact with the data as if it where a 3D cube while missing is data is filled in by the given fill value.

The prelaod options provided here refer to generally smaller parts of the data for which it may be more efficient to load the data and keep it around rather than doing repeated reads. If the object is used only for a single read and destroyed afterwards, then disabling the preload options may give a slight advantage but in most cases enabling the preload should be Ok (default).

Parameters

- **data_group** – The h5py object for the group with the omsi_msidata.
- **fill_space** – Define whether the data should be padded in space (filled with 0's) when accessing the data using [..] operator so that the data behaves like a 3D cube.
- **fill_spectra** – Define whether the spectra should completed by adding 0's so that all spectra retrieved via the [..] operator so that always spectra of the full length are returned. This option is provided to ease extension of the class to cases where only partial spectra are stored in the file but is not used at this point.
- **preload_mz** – Should the data for the mz axis be kept in memory or loaded on the fly when needed.
- **preload_xy_index** – Should the xy index (if available) be preloaderd into memory or should the required data be loaded on the fly when needed.

copy_dataset(*source*, *destination*, *print_status=False*)

Helper function used to copy a source msi dataset one chunk at a time to the destination dataset. The data copy is done one destination chunk at a time to achieve chunk-aligned write.

Parameters

- **source** – The source h5py dataset
- **destination** – The h5py desitnation h5py dataset.
- **print_status** – Should the function print the status of the conversion process to the command line?

create_optimized_chunking(*chunks=None*, *compression=None*, *compression_opts=None*, *copy_data=True*, *print_status=False*, *flush_io=True*)

Helper function to allow one to create optimized copies of the dataset with different internal data layouts to speed up selections. The function expects that the original data has already been written to the data group. The function takes

Parameters

- **chunks** – Specify whether chunking should be used (True,False), or specify the chunk sizes to be used explicitly.
- **compression** – h5py compression option. Compression strategy. Legal values are 'gzip', 'szip', 'lzf'. Can also use an integer in range(10) indicating gzip.
- **compression_opts** – h5py compression settings. This is an integer for gzip, 2-tuple for szip, etc.. For gzip (H5 deflate filter) this is the aggression paramter. The agression parameter is a number between zero and nine (inclusive) to indicate the tradeoff between speed and compression ratio (zero is fastest, nine is best ratio).
- **copy_data** – Should the MSI data be copied by this function to the new dataset or not. If False, then it is up to the user of the function to copy the appropriate data into the returned h5py dataset (not recommended but may be useful for performance optimization).

- **print_status** – Should the function print the status of the conversion process to the command line?
- **flush_io** – Call flush on the HDF5 file to ensure all HDF5 bufferes are flushed so that all data has been written to file

Returns h5py dataset with the new copy of the data

get_h5py_datasets(*index=0*)
Get the h5py dataset object for the given dataset.

Parameters **index** – The index of the dataset.

Returns h5py object for the requested dataset.

Raises and Index error is generated in case an invalid index is given.

get_h5py_mzdata()
Get the h5py object for the mz datasets.

Returns h5py object of the requested mz dataset.

set_fill_space(*fill_space*)
Define whether spatial selection should be filled with 0's to retrieve full image slices

Parameters **fill_space** – Boolean indicating whether images should be filled with 0's

set_fill_spectra(*fill_spectra*)
Define whether spectra should be filled with 0's to map them to the global mz axis when retrieved.

Parameters **fill_spectra** – Define whether m/z values should be filled with 0's.

class omsi.dataformat.omsi_file.msidata.**omsi_msidata_manager**(*msidata_parent*)
Bases: *omsi.dataformat.omsi_file.common.omsi_file_object_manager*

MSI-data manager helper class used to define common functionality needed for msidata-related data. Usually, a class that defines a format that contains an omsi_file_msidata object will inherit from this class (in addition to omsi_file_common) to acquire the common features.

For more details see: *omsi.dataforamt.omsi_file.omsi_common.omsi_file_object_manager*

Variables **msidata_parent** – The h5py.Group parent object containing the instrument object to be managed.

Initatize the manger object.

Parameters **msidata_parent** – The h5py.Group parent object for the msi data.

create_msidata_full_cube(*data_shape*, *data_type='f'*, *mzdata_type='f'*, *chunks=None*, *compression=None*, *compression_opts=None*, *flush_io=True*)
Create a new mass spectrometry imaging dataset for the given experiment written as a full 3D cube.

Parameters

- **data_shape** – Shape of the dataset. Eg. shape=(10,10,10) creates a 3D dataset with 10 entries per dimension
- **data_type** – numpy style datatype to be used for the dataset.
- **mzdata_type** – numpy style datatype to be used for the mz data array.
- **chunks** – Specify whether chunkning should be used (True,False), or specify the chunk sizes to be used in x,y, and m/z explicitly.
- **compression** – h5py compression option. Compression strategy. Legal values are 'gzip', 'szip', 'lzf'. Can also use an integer in range(10) indicating gzip.

- **compression_opts** – h5py compression settings. This is an integer for gzip, 2-tuple for szip, etc.. For gzip (H5 deflate filter) this is the aggression paramter. The agression parameter is a number between zero and nine (inclusive) to indicate the tradeoff between speed and compression ratio (zero is fastest, nine is best ratio).
- **flush_io** – Call flush on the HDF5 file to ensure all HDF5 bufferes are flushed so that all data has been written to file

Returns

The following two empty (but approbriately sized) h5py datasets are returned in order to be filled with data:

- `data_dataset` : Primary h5py dataset for the MSI data with shape data_shape and dtype data_type.
- `mz_dataset` : h5py dataset for the mz axis data with shape [data_shape[2]] and dtype mzdata_type.

Returns `data_group` : The h5py object with the group in the HDF5 file where the data should be stored.

create_msidata_partial_cube(*data_shape*, *mask*, *data_type='f'*, *mzdata_type='f'*, *chunks=None*, *compression=None*, *compression_opts=None*, *flush_io=True*)

Create a new mass spectrometry imaging dataset for the given experiment written as a partial 3D cube of complete spectra.

Parameters

- **data_shape** – Shape of the dataset. Eg. shape=(10,10,10) creates a 3D dataset with 10 entries per dimension
- **mask** – 2D boolean NumPy array used as mask to indicate which (x,y) locations have spectra associated with them.
- **data_type** – numpy style datatype to be used for the dataset.
- **mzdata_type** – numpy style datatype to be used for the mz data array.
- **chunks** – Specify whether chunkning should be used (True,False), or specify the chunk sizes to be used in x,y, and m/z explicitly.
- **compression** – h5py compression option. Compression strategy. Legal values are 'gzip', 'szip', 'lzf'. Can also use an integer in range(10) indicating gzip.
- **compression_opts** – h5py compression settings. This is an integer for gzip, 2-tuple for szip, etc.. For gzip (H5 deflate filter) this is the aggression paramter. The agression parameter is a number between zero and nine (inclusive) to indicate the tradeoff between speed and compression ratio (zero is fastest, nine is best ratio).
- **flush_io** – Call flush on the HDF5 file to ensure all HDF5 bufferes are flushed so that all data has been written to file

Returns

The following two empty (but approbriately sized) h5py datasets are returned in order to be filled with data:

- `data_dataset` : Primary h5py dataset for the MSI data with shape data_shape and dtype data_type.

- `mz_dataset` : h5py dataset for the mz axis data with shape [data_shape[2]] and dtype mzdata_type.

Returns

The following already complete dataset

- `xy_index_dataset` : This dataset indicates for each xy location to which index in `data_dataset` the location corresponds to. This dataset is needed to identify where spectra need to be written to.

Returns `data_group` : The h5py object with the group in the HDF5 file where the data should be stored.

create_msidata_partial_spectra(*spectra_length*, *len_global_mz*, *data_type='f'*, *mzdata_type='f'*, *chunks=None*, *compression=None*, *compression_opts=None*, *flush_io=True*)

Create a new mass spectrometry imaging dataset for the given experiment written as a partial 3D cube of partial spectra.

Parameters

- **spectra_length** – 2D boolean NumPy array used indicating for each (x,y) locations the length of the corresponding partial spectrum.
- **len_global_mz** – The total number of m/z values in the global m/z axis for the full 3D cube
- **data_type** – The dtype for the MSI dataset
- **mzdata_type** – The dtype for the mz dataset
- **mzdata_type** – numpy style datatype to be used for the mz data array.
- **chunks** – Specify whether chunkning should be used (True,False), or specify the chunk sizes to be used in x,y, and m/z explicitly.
- **compression** – h5py compression option. Compression strategy. Legal values are 'gzip', 'szip', 'lzf'. Can also use an integer in range(10) indicating gzip.
- **compression_opts** – h5py compression settings. This is an integer for gzip, 2-tuple for szip, etc.. For gzip (H5 deflate filter) this is the aggression paramter. The agression parameter is a number between zero and nine (inclusive) to indicate the tradeoff between speed and compression ratio (zero is fastest, nine is best ratio).
- **flush_io** – Call flush on the HDF5 file to ensure all HDF5 bufferes are flushed so that all data has been written to file

Returns

The following two empty (but approbriatelu sized) h5py datasets are returned in order to be filled with data:

- `data_dataset` : The primary h5py dataset for the MSI data with shape data_shape and dtype data_type.
- `mz_index_dataset` : h5py dataset with the mz_index values
- `mz_dataset` : h5py dataset for the mz axis data with shape [data_shape[2]] and dtype mzdata_type.

Returns

The following already complete dataset

- **xy_index_dataset** [This dataset indicates for each xy location at which index in `data_dataset`] the corresponding spectrum starts. This dataset is needed to identify where spectra need to be written to.
- **xy_index_end_dataset** [This dataset indicates for each xy location at which index in] `data_dataset` the corresponding spectrum ends (exclusing the given value). This dataset is needed to identify where spectra need to be written to.

Returns `data_group` : The h5py object with the group in the HDF5 file where the data should be stored.

get_msidata(*data_index*, *fill_space=True*, *fill_spectra=True*, *preload_mz=True*, *preload_xy_index=True*)

Get the dataset with the given index for the given experiment.

For more detailed information about the use of the fill_space and fill_spectra and preload_mz and preload_xy_index options, see the init function of omsi.dataformat.omsi_file_msidata.

Parameters

- **data_index** (*unsigned int*) – Index of the dataset.
- **fill_space** – Define whether the data should be padded in space (filled with 0's) when accessing the data using [..] operator so that the data behaves like a 3D cube.
- **fill_spectra** – Define whether the spectra should completed by adding 0's so that all spectra retrived via the [..] opeator so that always spectra of the full length are returned.
- **preload_mz** – Should the data for the mz axis be kept in memory or loaded on the fly when needed.
- **preload_xy_index** – Should the xy index (if available) be preloaderd into memory or should the required data be loaded on the fly when needed.

Returns omsi_file_msidata object for the given data_index or None in case the data with given index does not exist or the access failed for any other reason.

get_msidata_by_name(*data_name*)

Get the h5py data object for the the msidata with the given name.

Parameters **data_name** (*string*) – The name of the dataset

Returns h5py object of the dataset or None in case the dataset is not found.

get_num_msidata()

Get the number of raw mass spectrometry images stored for a given experiment

Returns Integer indicating the number of msi datasets available for the experiment.

analysis Module

Module for managing custom analysis data in OMSI HDF5 files.

class omsi.dataformat.omsi_file.analysis.**omsi_analysis_manager**(*analysis_parent*)

Bases: *omsi.dataformat.omsi_file.common.omsi_file_object_manager*

Analysis manager helper class used to define common functionality needed for analysis-related data. Usually, a class that defines a format that contains an omsi_file_analysis object will inherit from this class (in addition to omsi_file_common) to acquire the common features.

For more details see: *omsi.dataforamt.omsi_file.omsi_common.omsi_file_object_manager*

Variables **analysis_parent** – The h5py.Group parent object containing the instrument object to be managed.

create_analysis(*analysis*, *flush_io=True*, *force_save=False*, *save_unsaved_dependencies=True*, *mpi_root=0*, *mpi_comm=None*)

Add a new group for storing derived analysis results for the current experiment

Create the analysis group using omsi_file_analysis.__create___ which in turn uses omsi_file_analysis.__populate_analysis__(...) to populate the group with the appropriate data.

NOTE: Dependencies are generally resolved to point to file objects. However, if save_unsaved_dependencies is set to False and a given in-memory dependency has not been saved yet, then the value associated with that dependency will be saved instead as part of the parameters and, hence, only the value of the dependency is persevered in that case and not the full dependency chain.

NOTE: Dependencies if they only exists in memory are typically saved recursively unless save_unsaved_dependencies is set to False. I.e, calling create_analysis may result in the creating of multiple other dependent analyses if they have not been saved before.

Parameters

- **analysis** (*omsi.analysis.analysis_base:*) – Instance of omsi.analysis.analysis_base defining the analysis
- **flush_io** (*bool*) – Call flush on the HDF5 file to ensure all HDF5 bufferes are flushed so that all data has been written to file
- **force_save** (*bool*) – Should we save the analysis even if it has been saved in the same location before? If force_save is False (default) and the self.omsi_analysis_storage parameter of the analysis object contains a matching storage location—i.e., same file and experiment—, then the analysis will not be saved again, but the object will only be retrieved from file. If force_save is True, then the analysis will be saved either way and the self.omsi_analysis_storage parameter will be extended.
- **save_unsaved_dependencies** (*bool*) – If there are unsaved (in-memory) dependencies, then should those be saved to file as well? Default value is True, i.e, by default all in-memory dependencies that have not been saved yet, i.e, for which the self.omsi_analysis_storage of the corresponding **omsi_analysis_** base object is empty, are saved as well. If in-memory dependencies have been saved before, then a link to those dependencies will be established, rather than re-saving the dependency.
- **mpi_root** – The root MPI process that should perform the writing. This is to allow all analyses to call the function and have communication in the analysis.write_analysis_data function be handled.
- **mpi_comm** – The MPI communicator to be used. None if default should be used (ie., MPI.COMM_WORLD

Returns The omsi_file_analysis object for the newly created analysis group and the integer index of the analysis. NOTE: if force_save is False (default), then the group returned may not be new but may be simply the first entry in the list of existing storage locations for the given analysis. NOTE: If we are in MPI parallel and we are on a core that does not write any data, then None is returned instead.

static **create_analysis_static**(*analysis_parent*, *analysis*, *flush_io=True*, *force_save=False*, *save_unsaved_dependencies=True*, *mpi_root=0*, *mpi_comm=None*)

Same as create_analysis(...) but instead of relying on object-level, this function allows additional parameters (specifically the analysis_parent) to be provided as input, rather than being determined based on self

Parameters

- **analysis_parent** – The h5py.Group object or omsi.dataformat.omsi_file.common.omsi_file_common object where the analysis should be created
- **kwargs** – Additional keyword arguments for create_analysis(...). See create_analysis(...) for details.

Returns The output of create_analysis

get_analysis(*analysis_index*)
Get the omsi_format_analysis analysis object for the experiment with the given index.

Parameters **analysis_index** (*Unsigned integer*) – The index of the analysis

Returns omsi_file_analysis object for the requested analysis. The function returns None in case the analysis object was not found.

get_analysis_by_identifier(*analysis_identifier_string*)
Get the omsi_format_analysis analysis object for the the analysis with the given identifier.

Parameters **analysis_identifier_string** (*string*) – The string used as identifier for the analysis.

Returns h5py obejct of the analysis or None in case the analysis is not found.

get_analysis_identifiers()
Get a list of all identifiers for all analysis stored for the experiment

Returns List of strings of analysis identifiers.

get_num_analysis()
Get the number of raw mass spectrometry images stored for a given experiment

Returns Integer indicating the number of analyses available for the experiment.

class omsi.dataformat.omsi_file.analysis.**omsi_file_analysis**(*analysis_group*)
Bases: *omsi.dataformat.omsi_file.dependencies.omsi_dependencies_manager*, *omsi.dataformat.omsi_file.common.omsi_file_common*

Class for managing analysis specific data in omsi hdf5 files

Initialize the analysis object given the h5py object of the analysis group.

Parameters **analysis_group** – The h5py object with the analysis group of the omsi hdf5 file.

get_all_analysis_data(*load_data=False*)
Get all analysis data associated with the analysis.

Parameters **load_data** – load_data: Should the data be loaded or just the h5py objects be stored in the dictionary.

Returns List of analysis_data objects with the names and h5py or numpy objects. Access using [index]['name'] and [index]['data'].

get_all_parameter_data(*load_data=False*, *exclude_dependencies=False*)
Get all parameter data associated with the analysis.

Parameters **load_data** – Should the data be loaded or just the h5py objects be stored in the dictionary.

Returns List of parameter_data objects with names and h5py or numpy object. Access using [index]['name'] and [index]['data'].

get_all_runinfo_data(*load_data=False*)
Get a dict of all runtime information stored in the file

Returns omsi.shared.run_info_data.run_info_dict type python dict with the runtime information restored.

get_analysis_data_names()
This function returns all dataset names (and groups) that are custom to the analysis, i.e., that are not part of the omsi file standard.

Returns List of analysis-specific dataset names.

get_analysis_data_shapes_and_types()
This function returns two dictionaries with all dataset names (and groups) that are custom to the analysis, i.e., that are not part of the omsi file standard, and idenifies the shape of the analysis data objects.

Returns Dictonary indicating for each analysis-specific dataset its name (key) and shape (value). And a second dictionariy indicating the name (key) and dtype of the dataset.

get_analysis_identifier()
Get the identifier name of the analysis.

Use get_analysis_identifier()[...] to retrive the identifier string.

Returns h5py object for the dataset with the identifier string. Returns None, in case no identifer exisits. This should not be the case for a valid OpenMSI file.

get_analysis_index()
Based on the name of the group, get the index of the analysis.

Returns Integer index of the analysis in the file.

get_analysis_type()
Get the type for the analysis.

Use get_analysis_type()[...] tor retrieve the type string.

Returns h5py object with the dataset of the analysis string. Returns, None in case no analysis type exists. This should not be the case in a valid omsi file.

recreate_analysis(***kwargs*)
Load an analysis from file and re-execute it. This is equivalent to omsi_analysis.base.restore_analysis().execute()

Parameters **kwargs** – Additional keyword arguments to be passed to the execute function of the analysis

Returns Instance of the specific analysis object (e.g, omsi_nmf) that inherits from omsi.analysis.analysis_base with the input parameters and dependencies restored from file. The output, however, is the result from re-executing the analysis. None is returned in case the analysis object cannot be created.

restore_analysis(*load_data=True*, *load_parameters=True*, *load_runtime_data=True*, *dependencies_omsi_format=True*)
Load an analysis from file and create an instance of the appropriate analysis object defined by the analysis type (i.e., a derived class of *omsi.analysis. analysis_base*)

Parameters

- **load_data** – Should the analysis data be loaded from file (default) or just stored as h5py data objects
- **load_parameters** – Should parameters be loaded from file (default) or just stored as h5py data objects.

- **load_runtime_data** – Should runtime data be loaded from file (default) or just stored as h5py data objects.
- **dependencies_omsi_format** – Should dependencies be loaded as omsi_file API objects (default) or just as h5py objects.

Returns Instance of the specific analysis object (e.g, omsi_nmf) that inherits from omsi.analysis.analysis_base with the input parameters, output result, and dependencies restored. We can call execute(..) on the returned object to rerun an analysis. May return analysis_generic in case that the specific analysis is not known.

dependencies Module

Base module for managing of dependencies between data in OpenMSI HDF5 files

class omsi.dataformat.omsi_file.dependencies.**omsi_dependencies_manager**(*dependencies_parent*)
Bases: *omsi.dataformat.omsi_file.common.omsi_file_object_manager*

Dependencies manager helper class used to define common functionality needed for managing dependencies. Usually, a class that defines a format that contains an omsi_file_dependencies object will inherit from this class (in addition to omsi_file_common) to acquire the common features.

For more details see: *omsi.dataforamt.omsi_file.omsi_common.omsi_file_object_manager*

Variables

- **dependencies_parent** – h5py.Group object containing the dependencies object(s) to be managed
- ***dependencies*** – omsi_file_dependencies object managed by this object or None

Parameters **dependencies_parent** – Parent group containing the dependencies object to be managed

add_dependency(*dependency*, *flush_io=True*)
Create a new dependency for this dataset

Parameters

- **dependency** – omsi.shared.dependency_dict object describing the data dependency
- **flush_io** – Call flush on the HDF5 file to ensure all HDF5 bufferes are flushed so that all data has been written to file

Returns omsi_file_dependencydata object with the dependency data or None in case that an error occurred and the dependency has not been generated.

create_dependencies(*dependencies_data_list=None*)
Create a managed group for storing data dependencies if none exists and store the given set of dependencies in it. If a self.dependencies object already exists, then the given dependencies will be added.

This is effectively a shortcut to omsi_file_dependencies.__create___(...) with specific settings for the current dependencies object managed by self.

Parameters **dependencies_data_list** – List of dependency_dict objects to be stored as dependencies. Default is None which is mapped to an empty list []

Returns omsi_file_dependencies object created by the function.

get_all_dependency_data(*omsi_dependency_format=True*)
Get all direct dependencies associated with the data object.

This is convenience function providing access to self.dependencies.get_all_dependency_data(...) which is a function of omsi_file_dependencies class.

Parameters **omsi_dependency_format** – Should the dependencies be retrieved as omsi_analysis_dependency object (True) or as an omsi_file_dependencydata object (False).

Returns List dependency_dict objects containing either omsi file API objects or h5py objects for the dependencies. Access using [index]['name'] and [index]['data'].

get_all_dependency_data_graph(*include_omsi_dependency=False*, *include_omsi_file_dependencydata=False*, *recursive=True*, *level=0*, *name_key='name'*, *prev_nodes=None*, *prev_links=None*, *parent_index=None*, *metadata_generator=None*, *metadata_generator_kwargs=None*)

Get all direct and indirect dependencies associated with the analysis in form of a graph describing all nodes and links in the provenance hierarchy.

This is convenience function providing access to self.dependencies.get_all_dependency_data_graph(...) which is a function of omsi_file_dependencies class.

Parameters

- **include_omsi_dependency** – Should the dependency_dict object be included in the entries in the nodes dict?
- **include_omsi_file_dependencydata** – Should the omsi_file_dependencydata object be included in the entries in the nodes dict?
- **recursive** – Should we trace dependencies recursively to construct the full graph, or only the direct dependencies. Default true (ie., trace recursively)
- **name_key** – Which key should be used in the dicts to indicate the name of the object? Default value is 'name'
- **level** – Integer used to indicated the recursion level. Default value is 0.
- **prev_nodes** – List of nodes that have been previously generated. Note, this list will be modified by the call. Note, each node is represented by a dict which is expected to have at least the following keys defined, path, name_key, level (name_key refers to the key defined by the input parameter name_key.
- **prev_links** – Previouly established links in the list of nodes. Note, this list will be modified by the call.
- **parent_index** – Index of the parent node in the list of prev_nodes for this call.
- **metadata_generator** – Optional parameter. Pass in a function that generates additional metadata about a given omsi API object. Note, the key's level and path and name (i.e., name_key) are already set by this function. The metadata_generator may overwrite these key's, however, the path has to be unique as it is used to identify duplicate nodes. Overwriting the path with a non-unique value, hence, will lead to errors (missing entries) when generating the graph. Note, the metadata_generator function needs to support the following keyword arguments:
  - inDict : The dictionary to which the metadata should be added to.
  - obj : The omsi file API object for which metadata should be generated
  - name : A qualifying name for the object
  - name_key : The key to be used for storing the name

- **metadata_generator_kwargs** – Dictionary of additional keyword arguments that should be passed to the metadata_generator function.

Returns

Dictionary containing two lists. 1) nodes [List of dictionaries, describing the elements] in the dependency graph. 2) links : List of tuples with the links in the graph. Each tuple consists of two integer indices for the nodes list. For each node the following entries are given:

- **dependency_dict: Optional key used to store the corresponding dependency_dict object.** Used only of include_omsi_dependency is True.
- **omsi_file_dependencydata: Optional key used to store the corresponding** omsi_file_dependencydata object. Used only of include_omsi_file_dependencydata is True.
- name : Name of the dependency. The actual key is sepecified by name_key
- level : The recursion level at which the object occurs.
- ... : Any other key/value pairs from the dependency_dict dict.

get_all_dependency_data_recursive(*omsi_dependency_format=True*, *omsi_main_parent=None*, *dependency_list=None*)

Get all direct and indirect dependencies associated with the data object.

This is convenience function providing access to self.dependencies.get_all_dependency_data_recursive(...) which is a function of omsi_file_dependencies class.

NOTE: omsi_main_parent and omsi_main_parent are used primarily to ensure that the case of circular dependencies are supported properly. Circular dependencies may occur in the case of semantic dependencies (rather than pure use dependencies), e.g., two datasets that are related modalities may reference each other, e.g., MS1 pointing to related MS2 data and the MS2 datasets referencing the corresponding MS1 datasets.

Parameters

- **omsi_dependency_format** – Should the dependencies be retrieved as dependency_dict object (True) or as an omsi_file_dependencydata object (False)
- **omsi_main_parent** – The main parent for which the dependencies are calculated. This is needed to avoid recursion back into the main parent for which we are computing dependencies and avoiding that it is added itself as a dependency for itself. If set to None, then we will use our own self.dependencies_parent object
- **dependency_list** – List of previously visited/created dependencies. This is needed only to avoid deep recursion and duplication due to circular dependencies

Returns List analysis_data objects containing either omsi file API interface objects or h5py objects for the dependcies. Access using [index]['name'] and [index]['data'].

has_dependencies()

Check whether any dependencies exists for this datasets

class omsi.dataformat.omsi_file.dependencies.**omsi_file_dependencies**(*dependencies_group*)

Bases: *omsi.dataformat.omsi_file.common.omsi_file_common*

Class for managing collections of dependencies.

** Use of super()**

This class inherits from *omsi.dataformat.omsi_file.common.omsi_file_common*. Consistent with the design pattern for multiple inheritance of the *omsi.dataformat.omsi_file* module, the __init__ function calls super(...).__init__(manager_group) with a single parameter indicating the parent group.

static _omsi_file_dependencies__create_dependency_graph_node(*level*, *name*, *path*, *dependency_object*, *omsi_object*, *include_omsi_dependency=False*, *include_omsi_file_dependencydata=False*, *name_key='name'*, *metadata_generator=None*, *metadata_generator_kwargs=None*)

Internal helper function used to create a new node in the graph

Parameters

- **level** – The recursion level at which the node exists
- **name** – The name of the node
- **path** – The path of the node
- **dependency_object** – The omsi_file_dependencydata object. May be None in case a node to a specific object is set
- **omsi_object** – The OpenMSI file API object. This is required and may NOT be None.
- **include_omsi_dependency** – Should the dependency_dict object be included in the entries in the nodes dict?
- **include_omsi_file_dependencydata** – Should the omsi_file_dependencydata object be included in the entries in the nodes dict?
- **name_key** – Which key should be used in the dicts to indicate the name of the object? Default value is 'name'
- **metadata_generator** – Optional parameter. Pass in a function that generates additional metadata about a given omsi API object. Note, the key's level and path and name (i.e., name_key) are already set by this function. The metadata_generator may overwrite these key's, however, the path has to be unique as it is used to identify duplicate nodes. Overwriting the path with a non-unique value, hence, will lead to errors (missing entries) when generating the graph. Note, the metadata_generator function needs to support the following keyword arguments:
  - in_dict : The dictionary to which the metadata should be added to.
  - obj : The omsi file API object for which metadata should be generated
  - name : A qualifying name for the object
  - name_key : The key to be used for storing the name
- **metadata_generator_kwargs** – Dictionary of additional keyword arguments that should be passed to the metadata_generator function.

Returns Dict describing the new node, containing the 'name', 'level', and 'path' and optionally 'dependency_dict' and/or 'omsi_file_dependencydata' and any additional data generated by the metadata_generator function

add_dependency(*dependency_data*)
Add a new dependency to the collection.

Parameters **dependency_data** (*omsi.shared.omsi_dependency_data*) – The analysis dependency specification.

Returns the newly created omsi_file_dependencydata object

Raises KeyError in case that a dependency with the same name already exists

get_all_dependency_data(*omsi_dependency_format=True*)
Get all direct dependencies associated with the analysis.

Parameters **omsi_dependency_format** – Should the dependencies be retrieved as omsi_analysis_dependency object (True) or as an omsi_file_dependencydata object (False).

Returns List dependency_dict objects containing either omsi file API objects or h5py objects for the dependencies. Access using [index]['name'] and [index]['data'].

get_all_dependency_data_graph(*include_omsi_dependency=False*, *include_omsi_file_dependencydata=False*, *recursive=True*, *level=0*, *name_key='name'*, *prev_nodes=None*, *prev_links=None*, *parent_index=None*, *metadata_generator=None*, *metadata_generator_kwargs=None*)
Get all direct and indirect dependencies associated with the analysis in form of a graph describing all nodes and links in the provenance hierarchy.

Parameters

- **include_omsi_dependency** – Should the dependency_dict object be included in the entries in the nodes dict?
- **include_omsi_file_dependencydata** – Should the omsi_file_dependencydata object be included in the entries in the nodes dict?
- **recursive** – Should we trace dependencies recursively to construct the full graph, or only the direct dependencies. Default true (ie., trace recursively)
- **name_key** – Which key should be used in the dicts to indicate the name of the object? Default value is 'name'
- **level** – Integer used to indicated the recursion level. Default value is 0.
- **prev_nodes** – List of nodes that have been previously generated. Note, this list will be modified by the call. Note, each node is represented by a dict which is expected to have at least the following keys defined, path, name_key, level (name_key refers to the key defined by the input parameter name_key.
- **prev_links** – Previously established links in the list of nodes. Note, this list will be modified by the call.
- **parent_index** – Index of the parent node in the list of prev_nodes for this call. May be None in case the parent we are calling this function for is not yet in the list. If None, then we will add our own parent that contains the dependencies to the list.
- **metadata_generator** – Optional parameter. Pass in a function that generates additional metadata about a given omsi API object. Note, the key's level and path and name (i.e., name_key) are already set by this function. The metadata_generator may overwrite these key's, however, the path has to be unique as it is used to identify duplicate nodes. Overwriting the path with a non-unique value, hence, will lead to errors (missing entries) when generating the graph. Note, the metadata_generator function needs to support the following keyword arguments:

- in_dict : The dictionary to which the metadata should be added to.
- obj : The omsi file API object for which metadata should be generated
- name : A qualifying name for the object
- name_key : The key to be used for storing the name

- **metadata_generator_kwargs** – Dictionary of additional keyword arguments that should be passed to the metadata_generator function.

Returns

Dictionary containing two lists. 1) nodes [List of dictionaries, describing the elements] in the dependency graph. 2) links : List of tuples with the links in the graph. Each tuple consists of two integer indices for the nodes list. For each node the following entries are given:

- **dependency_dict: Optional key used to store the corresponding dependency_dict object.** Used only of include_omsi_dependency is True.
- **omsi_file_dependencydata: Optional key used to store the corresponding** omsi_file_dependencydata object. Used only of include_omsi_file_dependencydata is True.
- name : Name of the dependency. The actual key is sepecified by name_key
- level : The recursion level at which the object occurs.
- path : The full path to the object
- filename : The full path to the file
- ... : Any other key/value pairs from the dependency_dict dict.

get_all_dependency_data_recursive(*omsi_dependency_format=True*, *omsi_main_parent=None*, *dependency_list=None*)

Get all direct and indirect dependencies associated with the analysis.

NOTE: omsi_main_parent and omsi_main_parent are used primarily to ensure that the case of circular dependencies are supported properly. Circular dependencies may occur in the case of semantic dependencies (rather than pure use dependencies), e.g., two datasets that are related modalities may reference each other, e.g., MS1 pointing to related MS2 data and the MS2 datasets referencing the corresponding MS1 datasets.

Parameters

- **omsi_dependency_format** – Should the dependencies be retrieved as dependency_dict object (True) or as an omsi_file_dependencydata object (False)
- **omsi_main_parent** – The main parent for which the dependencies are calculated. This is needed to avoid recursion back into the main parent for which we are computing dependencies and avoiding that it is added itself as a dependency for itself. If set to None, then we will use the omsi_object associated with the parent group of the dependency group.
- **dependency_list** – List of previously visited/created dependencies. This is needed only to avoid deep recursion and duplication due to circular dependencies

Returns List analysis_data objects containing either omsi file API interface objects or h5py objects for the dependcies. Access using [index]['name'] and [index]['data'].

get_dependency_omsiobject(*name*, *recursive=True*)

Get the omsi file API object corresponding to the object the dependency is pointing to.

Parameters

- **name** – Name of the dependency opbject to be loaded .
- **recursive** – Should the dependency be resolved recursively, i.e., if the dependeny points to another dependencies. Default=True.

Returns An omsi file API object (e.g., omsi_file_analysis or omsi_file_msidata) if the link points to a group or the h5py.Dataset the link is pointing to.

get_omsi_file_dependencydata(*name*)
Retrieve the omsi_file_dependencydata object for the dependency with the given name.

class omsi.dataformat.omsi_file.dependencies.**omsi_file_dependencydata**(*dependency_group*)
Bases: *omsi.dataformat.omsi_file.common.omsi_file_common*

Class for managing data groups used for storing data dependencies

Create a new omsi_file_dependencydata object for the given h5py.Group

Parameters **dependency_group** (*h5py.Group with a corresponding omsi type*) – h5py.Group object with the dependency data

get_dataset_name()
Get the string indicating the name of dataset. This may be empty as it is only used if the dependency points to an objec within a managed omsi API object.

Returns String indicating the name of the optional dataset.

get_dependency_objecttype(*recursive=True*)
Indicated the type of the object the dependency is pointing to.

Parameters **recursive** – Should dependencies be resolved recursively, i.e., if the dependency points to another dependencies. Default=True.

Returns String indicating the class of the omsi file API class that is suited to manage the dependency link or the name of the corresponding h5py class.

get_dependency_omsiobject(*recursive=True*, *external_mode=None*)
Get the omsi file API object corresponding to the object the dependency is pointing to.

Parameters

- **recursive** – Should dependencies be resolved recursively, i.e., if the dependency points to another dependencies. Default=True.
- **external_mode** – The file open mode (e.g., 'r', 'a') to be used when we encounter external dependencies, i.e., dependencies that are stored in external files. By default this is set to None, indicating that the same mode should be used in which this (i.e,. the current file describing the dependency) was opened. Allowed modes are 'r', 'r+', and 'a'. The modes 'w', 'w+, 'x' are prohibited to ensure that we do not break external files.

Returns An omsi file API object (e.g., omsi_file_analysis or omsi_file_msidata) if the link points to a group or the h5py.Dataset the link is pointing to.

get_dependency_type()
Get the string describing the type of the dependency

NOTE: If the type is missing in the file but we have a parameter name specified, then the default type 'parameter' will be returned other None is returned.

Returns String indicating the type of the dependency or None if the type is not known.

get_link_name()
Get the name of the dependency link

Returns String indicating the name of the dependency link.

get_mainname()
Get the main name string describing the name of the object (and possibly path of the file if external)

Returns String indicating the main name of the object that we link to

get_omsi_dependency()
Get the dependency information as an omsi.shared.dependency_dict object (as defined in the omsi.shared.dependency_dict module)

Returns dependency_dict object with all the dependency data.

get_parameter_help()
Get the help string for the parameter name if available.

get_parameter_name()
Get the string indicating the name of the dependend parameter of the analysis.

Returns String of the parameter name that has the dependency.

get_selection_string()
String indicating the applied selection. This is an empty string in case no selection was applied.

Returns Selection string. See the omsi.shared.omsi_data_selection for helper functions to deal with selection strings.

file_reader_base Module

Module for base classes for implementation and integration of third-party file readers.

ToDo:

- get_number_of_regions(...) should be updated to return a list of regions, one per dataset
- Need to add base class for multi dataset formats
- Need to add base class for multi dataset+region formats
- Need to implement new file format for combined raw data file (ie., multiple raw files in one folder).

class omsi.dataformat.file_reader_base.**file_reader_base**(*basename*, *requires_slicing=True*)

Bases: object

Base-class used to define the basic interface that file-readers for a new format need to implement.

__init__ interface:

To avoid the need for custom code subclasses should be able to be constructed by providing just the basename parameter and optional requires_slicing parameter. If additional inputs are needed, then file conversion and management scripts may need to be modified to account for the custom requirements. **Required Attributes:**

Variables

- **data_type** – String indicating the data type to be used (e.g., uint16)
- **shape** – Tuple indicating the shape of the data
- **mz** – Numpy array with the m/z axis data. In the case of multi-data this is a list of numpy arrays, one per dataset.

- **basename** – The basename provided for opening the file.

Required Interface Functions:

- `close_file` : Close any opened files
- `is_valid_dataset` : Check whether a given dir/file is valid under the current format
- `spectrum_iter` : Generator function that iterates over all the spectra in the current data cube and yield the numpy array with the intensity and integer x, y position of the spectrum

Optional Interface Functions:

- **__getitem__** [Implement array slicing for files. Reuqired if the requires_slicing parameter] should be supported.
- `supports_regions` : Specify whether the format supports multiple regions (default=False)
- `supports_multidata`: Specify whether the format supports multiple datasets (default=False)
- `supports_multiexperiment`: Specify whether the format supports multiple experiments (default=False)

Construct the base class and define required attributes.

Parameters

- **basename** – The name of the file or directory with the file to be opened by the reader
- **requires_slicing** – Boolean indicating whether the user requires array slicing via the __getitem__ function to work or not. This is an optimization, because many MSI data formats do not easily support arbitrary slicing of data but rather only iteration over spectra.

static available_formats()
Get dictionary of all available file formats that implement the file_format_base API.

Returns Dictionary where the keys are the names of the formats and the values are the corresponding file reader classes.

close_file()
Close the file.

classmethod format_name()
Define the name of the format.

Returns String indicating the name of the format.

get_dataset_metadata()
Get dict of additional metadata associated with the current dataset

NOTE: In the case that multiple regions and/or datasets are supported, this function should return the metadata of the currently selected dataset only. If no particular dataset is selected, then all should be returned.

Returns Instance of omsi.shared.metadata_data.metadata_dict

get_number_of_datasets()
File readers with multi dataset support must overwrite this function to retrieve the true number of raw datasets in the file. Default implementation returns 1.

get_number_of_regions()
File readers with multi region support must overwrite this function to retrieve the true number of regions in the file. Default implementation returns 1.

classmethod **is_valid_dataset**(*name*)
Classmethod used to check whether a given directory (or file) defines as valid data file of the file format specified by the current child class

Parameters **name** (*String*) – Name of the dir or file.

Returns Boolean indicating whether the given file or folder is a valid file.

classmethod **size**(*name*)
Classmethod used to check the estimated size for the given file/folder.

Parameters **name** (*String*) – Name of the dir or file.

Returns Integer indicating the size in byte or None if unknown.

spectrum_iter()
Enable iteration of the spectra of the current data cube.

Iterate over all the spectra in the current data cube and yield the numpy array with the intensity and integer x, y position of the spectrum.

NOTE: As this is a generator one needs to use yield.

Returns

The function yields for each spectrum the following information:

- tuple of (x,y) or (x,y,z) position of the spectrum
- Numpy array with the spectrum

classmethod **supports_multidata**()
Define whether the file format support multiple independent datasets.

classmethod **supports_multiexperiment**()
Define whether the file format supports multiple independent experiments, each of which may contain multiple datasets.

classmethod **supports_regions**()
Define whether the file format support multiple regions.

class omsi.dataformat.file_reader_base.**file_reader_base_multidata**(*basename*, *requires_slicing*)
Bases: *omsi.dataformat.file_reader_base.file_reader_base*

Base-class used to define the basic interface for file-readers used to implement new file formats with support for multiple dataset (e.g, MSI dataset with multiple spectrum types). This class extends file_reader_base, and accordingly all required attributes and functions of file_reader_base must be implemented by subclasses.

In addition to the file_reader_base functions we need to implement the get_number_of_datasets(...) and get_dataset_dependencies(...) functions.

Variables **select_dataset** – Unsigned integer indicating the currently selected dataset

Construct the base class and define required attributes.

get_dataset_dependencies()
Get the dependencies between the current dataset and any of the other datasets stored in the current file. If self.select_dataset is not set, then the function is expected to return a list of lists with all dependencies for all datasets.

Returns

List of dependencies (or list of lists of dependencies if self.select_dataset is None) where each dependency is a dict of the following form:

- 'omsi_object': None, # The omsi file API object where the data is stored. Often None.
- 'link_name': ms2_link_name, # Name for the dependency link to be used
- 'basename': basename, # Basename of the file
- 'region': None, # Index of the region in the dataset or None
- 'dataset': ind2, # Index of the dataset withing the file or None
- 'help':scan_types[ms1scan], # Help describing the depdency
- dependency_type': ... } # Type of dependency see dependency_dict.dependency_type for available types

get_number_of_datasets()
Get the number of available datasets.

set_dataset_selection(*dataset_index*)
Define the current dataset to be read.

classmethod supports_multidata()
Define whether the file format supports multiple data blocks.

class omsi.dataformat.file_reader_base.**file_reader_base_with_regions**(*basename*, *requires_slicing*)
Bases: *omsi.dataformat.file_reader_base.file_reader_base*

Base-class used to define the basic interface for file-readers used to implement new file formats with support for multiple imaging regions per file. This class extends file_reader_base, and accordingly all required attributes and functions of file_reader_base must be implemented by subclasses.

Additional required attributes:

- `select_region` : Integer indicating which region should be selected. If set to None, indicates that the data should be treated as a whole. If set to a region index, then the data should be treated by the reader as if it only pertains to that region, ie., the shape of the data should be set accordingly and __getitem__ should behave as such as well.
- `region_dicts` : List of dictionaries, where each dictionary describes a given region (e.g,. the origin and extend for rectangular regions.

Construct the base class and define required attributes.

get_dataset_dependencies()
Get the dependencies between the current region and any of the other region datasets stored in the current file. If self.select_region is not set, then the function is expected to return a list of lists with all dependencies for all datasets.

Returns

List of dependencies (or list of lists of dependencies if self.select_dataset is None) where each dependency is a dict of the following form:

- 'omsi_object': None, # The omsi file API object where the data is stored. Often None.
- 'link_name': ms2_link_name, # Name for the dependency link to be used
- 'basename': basename, # Basename of the file
- 'region': None, # Index of the region in the dataset or None
- 'dataset': ind2, # Index of the dataset withing the file or None
- 'help':scan_types[ms1scan], # Help describing the depdency

- dependency_type': ... } # Type of dependency see dependency_dict.dependency_type for available types

get_number_of_regions()
Get the number of available regions

get_region_selection()
Get the index of the selected region

get_regions()
Get list of all region dictionaries defining for each region the origin and extend of the region. See also self.region_dicts.

set_region_selection(*region_index=None*)
Define which region should be selected for local data reads.

Parameters **region_index** – The index of the region that should be read. The shape of the data will be adjusted accordingly. Set to None to select all regions and treat the data as a single full 3D image.

classmethod supports_regions()
Define whether the file format support multiple regions.

img_file Module

This module provides functionality for reading img mass spectrometry image files

class omsi.dataformat.img_file.**img_file**(*hdr_filename=None*, *t2m_filename=None*, *img_filename=None*, *basename=None*, *requires_slicing=True*)
Bases: *omsi.dataformat.file_reader_base.file_reader_base*

Interface for reading a single 2D img file

The img format consists of three different files: i) hdr header file, ii) t2m which contains the m/z data, iii) img data file.

Open an img file for data reading.

Parameters

- **hdr_filename** (*string*) – The name of the hdr header file
- **t2m_filename** (*string*) – The name of the t2m_filename
- **img_filename** (*string*) – The name of the img data file
- **basename** (*string*) – Instead of img_filename, t2m_filename, and hdr_filename one may also supply just a single basename. The basename is completed with the .img, .t2m, .hdr extension to load the data.
- **requires_slicing** (*Boolean*) – Unused here. Slicing is always supported by this reader.

Raises **ValueError** – In case that basename and hdr_filename, t2m_filename, and img_filename are specified.

close_file()
Close the img file

classmethod get_files_from_dir(*dirname*)
Get a list of all basenames of all img files in a given directory. Note: The basenames include the dirname.

classmethod is_valid_dataset(*name*)
Check whether the given file or directory points to a img file.

Parameters **name** (*unicode*) – Name of the dir or file.

Returns Boolean indicating whether the given file or folder is a valid img file.

classmethod size(*name*)
Classmethod used to check the estimated size for the given file/folder.

Parameters **name** (*unicode*) – Name of the dir or file.

Returns Integer indicating the size in byte or None if unknown.

spectrum_iter()
Enable iteration over the spectra in the file

Returns tuple of ((x , y) , intensities), i.e., the tuple of (x, y) integer index of the spectrum and the numpy array of the intensities

mzml_file Module

bruckerflex_file Module

This module provides functionality for reading bruker flex mass spectrometry image files

Limitations:

1. Currently the reader assumes a single global m/z axis for all spectra.
2. The read of acqu files does not convert <..> entries to python values but leaves them as strings.
3. __read_spotlist__ converts the regions to start with a 0 index. This is somewhat inconsistent in the spot list file. The spotname seems to number regions starting with 0 while the region list numbers them starting with 1.
4. __read_spotlist__ computes the folder where the spots are located based on the filename of the spotlist. The question is whether this is always the case??? The advantage is that we do not rely on the regions.xml file which contains absolute paths which are in most cases invalid as the data has been copied between different machines in many cases and is stored in different locations on each of the machines.
5. __read_spotlist__ currenly assumes that there is only one fid file per spot
6. __read_spotlist__ currenlty only looks at where the acqu and fid file is located for the spot. Other files are currently ignored.
7. __read_spotlist__ (and hence the reader at large) currently assumes that we have 2D images only.
8. __read_spotlist__ currently generates maps for the image that assume that x and y pixel indices start at 0. Not all images may record data until the border, so that this strategy may add empty spectra rather than generating a new bounding box for the image.
9. __read_spotlist__ assumes in the variable spotname_encoding a maximum of 24 characters in the spotname R01X080Y013. This should in general be more than sufficient as this allows for 7 characters for each R, X, Y entry, however, if this is not enough then this behaviour needs ot be changed.
10. __getitem__ currently only works if we have read the full data into memory. An on-demand load should be supported as well.
11. We can currently only selected either a single region or the full data but we cannot selected multiple regions at once. E.g. if a dataset contains 3 regions then we can either select all regions at once or region 1,2, or 3 but one cannot selected region 1+2, 1+3, or 2+3.

import bruckerflex_file spotlist = "/Users/oruebel/Devel/msidata/Bruker_Data/UNC IMS Data/20130417 Bmycoides Paenibacillus Early SN03130/" + "2013 Bmyc Paeni Early LP/2013 Bmyc Paeni Early LP Spot List.txt" exppath ="/Users/oruebel/Devel/msidata/Bruker_Data/UNC IMS Data/20130417 Bmycoides Paenibacillus Early SN03130/" + "2013 Bmyc Paeni Early LP/2013 Bmyc Paeni Early LP/0_R00X012Y006/1/1SLin" f = bruckerflex_file.bruckerflex_file(spotlist_filename = spotlist) f.s_read_fid(exppath+"/fid" , f.data_type) testacqu = f.s_read_acqu(exppath+"/acqu") testmz = f.s_mz_from_acqu(testacqu) testspotlist = f.s_read_spotlist(spotlist)

a = bruckerflex_file(dirname)

class omsi.dataformat.bruckerflex_file.**bruckerflex_file**(*basename*, *fid_encoding='int32'*, *requires_slicing=True*)

Bases: *omsi.dataformat.file_reader_base.file_reader_base_with_regions*

Interface for reading a single bruker flex image file.

The reader supports standard array slicing for data read. I.e., to read a spectrum use [x,y,:] to read an ion image using [:,:,mz].

The reader supports multiple regions, i.e., reading of different independent regions that were imaged as part of the same dataset. Using the get_regions, get_number_of_regions, set_region_selection and get_region_selection the user can interact with the region settings. Using the set_region_selection the user can define whether the data of the complete image should be read (set_region(None), default) or whether data from a single region should be read. When a region is selected, then the reader acts as if the region were the complete dataset, i.e., the shape variable is addjusted to fit the selected region and the __get_item__ method (which is used to implement array-like slicing (e.g., [1,1,:])) behaves as if the selected region where the full data.

Open an img file for data reading.

Parameters

- **basename** (*string*) – Name of the textfile with the spotlist. Alternatively this may also be the folder with the spots.
- **requires_slicing** (*bool*) – Should the complete data be read into memory (this makes slicing easier). (default is True)
- **fid_encoding** (*string*) – String indicating in which binary format the intensity values (fid files) are stored. (default value is 'int32')

Variables

- **self.basename** – Name of the file with the spotlist
- **self.pixel_dict** – dictionary with the pixel array metadata (see also s_read_spotlist(...)). Some of the main keys of the dictionary are, e.g. (see also s_read_spotlist(...)) :
  - 'spotfolder' : String indicating the folder where all the spot-data is located
  - 'fid' : 2D numpy masked array of strings indicating for (x,y) pixel the fid file with the intensity values.
  - 'acqu' : 2D numpy masked array of strings indicating for each (x,y) pixel the acqu file with the metadata for that pixel.
  - 'regions' : 2D numpy masked array of integers indicating for each pixels the index of the region it belongs to.
  - 'xpos' : 2D numpy masked array of integers indicated for each pixel its x position.
  - 'ypos' : 2D numpy masked array of integers indicated for each pixel its x position.

- 'spotname' : 2D masked numpy array of strings with the names of the spot corresponding to a pixel.

- **self.data_type** – the encoding used for intensity values
- **self.shape** – The 3D shape of the MSI data volume for the currently selected region.
- **self.full_shape** – Shape of the full 3D MSI dataset including all regions imaged.
- **self.metadata** – Dictionary with metadata from the acqu file
- **self.mz** – The 1D numpy array with the m/z axis information
- **self.data** – If requires_slicing is set to true then this 3D array includes the complete data of the MSI data cube. Missing data values (e.g., from regions not imaged during the aquistion processes) are completed with zero values.
- **self.region_dicts** – Dictionary with description of the imaging regions

Raises **ValueError** – In case that no valid data is found.

close_file()
Close the img file

get_dataset_dependencies()
Get the dependencies between the current region and any of the other region datasets stored in the current file. If self.select_region is not set, then the function is expected to return a list of lists with all dependencies for all datasets.

Returns

List of dependencies (or list of lists of dependencies if self.select_dataset is None) where each dependency is a dict of the following form:

- 'omsi_object': None, # The omsi file API object where the data is stored. Often None.
- 'link_name': ms2_link_name, # Name for the dependency link to be used
- 'basename': basename, # Basename of the file
- 'region': None, # Index of the region in the dataset or None
- 'dataset': ind2, # Index of the dataset withing the file or None
- 'help':scan_types[ms1scan], # Help describing the depdency
- dependency_type': ... } # Type of dependency see dependency_dict.dependency_type for available types

classmethod **is_valid_dataset**(*name*)
Determine whether the given file or name specifies a bruckerflex file

Parameters **name** (*string*) – name of the file or dir

Returns Boolean indicating whether the name is a valid bruckerflex

static **s_mz_from_acqu**(*acqu_dict*)
Construct the m/z axis from the data stored in the acqu_dict dictionary. See also s_read_acqu

Parameters **acqu_dict** – Python dictionary with the complete information from the acqu file. See s_read_acqu(...).

returns 1D Numpy array of floats with the mz axis data.

static **s_read_acqu**(*filename*)
Construct an m/z axis for the given acqu file.

Parameters **filename** (*string*) – String with the name+path for the acqu file.

Returns Return dictonary with the parsed metadata information

static s_read_fid(*filename*, *data_type='int32'*, *selection=slice(None*, *None*, *None)*)
Read data from an fid file

Parameters

- **filename** (*string*) – String indicating the name+path to the fid file.
- **data_type** – The numpy datatype encoding used for the fid files. (default is 'int32'). In the instance of this class this is encoded in the data_type variable associated with the instance.
- **selection** (*slice or list, i.e., a selection that numpy understands*) – This may be a python slice or a list of indecies to be read. Default value is to read all (i.e., slice(None,None,None))

Returns 1D numpy array of intensity values read from the file.

static s_read_spotlist(*spotlist_filename*)
Parse the given spotlist file.

Parameters **spotlist_filename** (*string*) – Name of the textfile with the spotlist

Returns

The function returns a number of different items in from of a python dictionary. Most data is stored as 2D spatial maps, indicting for each (x,y) location the corresponding data. Most data is stored as 2D masked numpy arrays. The masked of the array indicated whether data has been recorded for a given pixel or not. The dict contains the following keys:

- 'spotfolder' : String indicating the folder where all the spot-data is located
- 'fid' : 2D numpy masked array of strings with fid file name for each (x,y) pixel (intensities).
- 'acqu' : 2D numpy masked array of strings with acqu file name for each (x,y) (metadata).
- 'regions' : 2D numpy masked array of integers with region index for each (x,y) pixel.
- 'xpos' : 2D numpy masked array of integers indicated for each pixel its x position.
- 'ypos' : 2D numpy masked array of integers indicated for each pixel its x position.
- 'spotname' : 2D masked numpy array of strings with spot name for each (x,y) pixel.

static s_spot_from_dir(*in_dir*, *spot_folder_only=False*)
Similar to s_read_spotlist but instead of using a spotlist file the structure of the data is parsed directly from the structure of the direcory containint all spots.

param in_dir Name of the directory with all spots

type in_dir string

param spot_folder_only If set to True, then the function only constructs the spot folders but does not check for acqu files etc. If set to True, only the spotfolder list will be returned.

returns

The function returns None in case that no valid spots were found. Returns a list of strings with the spotfolders if spot_folder_only is set to True. Otherwise, the function returns a number of different items in from of a python dictionary. Most data is stored as 2D spatial maps, indicting for each (x,y) location the corresponding data. Most data is stored as 2D masked numpy arrays. The masked of the array indicated whether data has been recorded for a given pixel or not. The dict contains the following keys:

- 'spotfolder' : String indicating the folder where all the spot-data is located
- 'fid' : 2D numpy masked array of strings with fid file name for each (x,y) pixel (intensities)
- 'acqu' : 2D numpy masked array of strings with acqu file name for each (x,y) pixel (metadata)
- 'regions' : 2D numpy masked array of integers with the index of the region for each (x,y) pixel.
- 'xpos' : 2D numpy masked array of integers indicated for each pixel its x position.
- 'ypos' : 2D numpy masked array of integers indicated for each pixel its x position.
- 'spotname' : 2D masked numpy array of strings with the name of the spot corresponding to a pixel.

set_region_selection(*region_index=None*)

Define which region should be selected for local data reads.

Parameters **region_index** – The index of the region that should be read. The shape of the data will be adjusted accordingly. Set to None to select all regions and treat the data as a single full 3D image.

9.1.3 datastructures Package

omsi.datastructures	Package with a collection of various data structures and rel
omsi.datastructures.metadata	Package with metadata datastructures
omsi.datastructures.metadata.metadata_data	Define infrastructure for describing metadata (in memory)
omsi.datastructures.metadata.metadata_ontologies	Define ontologies for metadata
omsi.datastructures.analysis_data	Helper module with data structures for managing analysis-r
omsi.datastructures.dependency_data	Define a dependency to another omsi object
omsi.datastructures.run_info_data	Module with helper data structures for recording runtime p

datastructures Package

Package with a collection of various data structures and related classes used throughout the software stack, e.g., for metadata, analysis parameter data, runtime information data etc.

analysis_data Module

Helper module with data structures for managing analysis-related data.

class omsi.datastructures.analysis_data.**analysis_data**(*name='undefined'*, *data=None*, *dtype='float32'*)

Bases: dict

Define an output dataset for the analysis that should be written to the omsi HDF5 file

The class can be used like a dictionary but restricts the set of keys that can be used to the following required keys which should be provided during initalization.

Required Keyword Arguments:

Parameters

- **name** – The name for the dataset in the HDF5 format
- **data** – The numpy array to be written to HDF5. The data write function omsi_file_experiment.create_analysis used for writing of the data to file can in principal also handel other primitive data types by explicitly converting them to numpy. However, in this case the dtype is determined based on the numpy conversion and correct behavior is not guaranteed. I.e., even single scalars should be stored as a 1D numpy array here. Default value is None which is mapped to np.empty(shape=(0) , dtype=dtype) in __init__
- **dtype** – The data type to be used during writing. For standard numpy data types this is just the dtype of the dataset, i.e., ['data'].dtype. Other allowed datatypes are:
  - For string: omsi_format.str_type (omsi_format is located in omsi.dataformat.omsi_file)
  - To generate data links: ana_hdf5link (analysis_data)

ana_hdf5link = -1
Value used to indicate that a hard link to another dataset should be created when saving an analysis object

class omsi.datastructures.analysis_data.**data_dtypes**
Bases: dict

Class specifying basic function for specifying common data types used as part of an analysis.

static bool_type(*argument*)
Implement conversion of boolean input parameters since arparse (or bool, depending on the point of view), do not handle bool as a type in an intuitive fashion.

Parameters **argument** – The argument to be parsed to a boolean

Returns The converted value

static get_dtypes()
Get a list of available data type specifications

static ndarray(*argument*)
This dtype may be used to indicate numpy ndarrays as well as h5py arrays or omsi_dependencies

Parameters **argument** – The argument to be parsed to ndarray

Returns The converted ndarray

class omsi.datastructures.analysis_data.**parameter_data**(*name*, *help=''*, *dtype=None*, *required=False*, *default=None*, *choices=None*, *data=None*, *group=None*)
Bases: dict

Define a single input parameter for an analysis.

Variables ***default_keys*** – List of allowed dictionary keys:

Required keys:

•*name* : The name of the parameter

•*help* : Help string describing the parameter

- *type* : Optional type. Default is None, indicating a dynamically typed dataset that the analysis will convert
- *required* : Boolean indicating whether the parameter is required (True) or optional (False). Default False
- *default* : Optional default value for the parameter. Default None.
- *choices* : Optional list of choices with allowed data values. Default None, indicating no choices set.
- *data* : The data assigned to the parameter. None by default.
- 'group' : Optional group string used to organize parameters. This may also be a dict of {'name':<group>, 'description':<description>}

In the context of the argparse package the default keys have the following mapping:

- *argparse.name = name*
- *argparse.action* –> The action is constant and set to save value
- *argparse.nargs* –> Left as default
- 'argparse.const –> Not used as action is always save value
- *argparse.type = type*
- *argparse.choices = 'choices*
- *argparse.required = 'required*
- *argparse.help = 'help*
- 'argparse.metavar –> Not used. Positional arguments are not allowed for analyses
- *argparse.destination –> Automatically determined by the 'name* of the parameter
- *argparse.add_argument_group(...) –> Automatically determined based on the required parameter and the 'group* parameter if set.

Initialize a new parameter description.

Parameters

- **name** – Required name for the parameter
- **help** – Required help string for the parameter
- **dtype** – Type argument. Default unicode.
- **required** – Boolean indicating whether the parameter is required (default=True)
- **default** – Optional default value for the parameter. Default None.
- **choices** – Optional list of choices with allowed data values. Default None, indicating no choices set.
- **data** – The data assigned to the parameter. None by default.
- **group** – The parameter group to be used. None by default.

clear_data()
Remove the currently assigned data.

copy()
Return a new parameter_data object with the same data as stored in the current object

Returns dependency_dict object

data_ready()
This function check if the data points to a dependency and if so, then check if the dependency can be resolved or not

data_set()
Check if a data has been assigned for the parameter.

default_keys = ['name', 'default', 'dtype', 'choices', 'required', 'help', 'data', 'group']
List of allowed keys for the parameter dict.

get_data_or_default()
Get the data of the parameter if set, otherwise get the default value if available.

Returns The data to be used for the parameter.

Raises KeyError is raised in case that neither 'default' nor 'data' are available. This should never be the case if the object was created properly.

get_group_description()
Get the description for the group if available.

Returns String with the group description or None.

get_group_name()
Get the name of the group to be used.

Returns String with the name of the group of None if not set

is_dependency()
Check whether the parameter defines a dependency.

Returns Boolean indicating whether the parameter defines a dependency.

class omsi.datastructures.analysis_data.**parameter_manager**
Bases: object

Base class for objects that manage their own parameters.

Parameters are set and their values retrieved by name using dict-like slicing. Derived classes may overwrite __getitem__ and __setitem__ to implement their own behavior but we exepct that the functionality of the interface is preserved, i.e., others should still be able set parameter value and retrieve values via dict slicing.

add_parameter(*name*, *help*, *dtype=<type 'unicode'>*, *required=False*, *default=None*, *choices=None*, *data=None*, *group=None*)
Add a new parameter for the analysis. This function is typically used in the constructor of a derived analysis to specify the parameters of the analysis.

Parameters

- **name** – The name of the parameter
- **help** – Help string describing the parameter
- **dtype** – Optional type. Default is string.
- **required** – Boolean indicating whether the parameter is required (True) or optional (False). Default False.
- **default** – Optional default value for the parameter. Default None.
- **choices** – Optional list of choices with allowed data values. Default None, indicating no choices set.
- **data** – The data assigned to the parameter. None by default.

- **group** – Optional group string used to organize parameters. Default None, indicating that parameters are automatically organized by driver class (e.g. in required and optional parameters)

Raises ValueError is raised if the parameter with the given name already exists.

clear_parameter_data()
Clear the list of parameter data

define_missing_parameters()
Set any required parameters that have not been defined to their respective default values.

This function may be overwritten in child classes to customize the definition of default parameter values and to apply any modifications (or checks) of parameters before the analysis is executed. Any changes applied here will be recorded in the parameter of the analysis.

get_all_dependency_data()
Get the complete list of all direct dependencies to be written to the HDF5 file

NOTE: These are only the direct dependencies as specified by the analysis itself. Use get_all_dependency_data_recursive(..) to also get the indirect dependencies of the analysis due to dependencies of the dependencies themselves.

Returns List of parameter_data objects that define dependencies.

get_all_parameter_data(*exclude_dependencies=False*)
Get the complete list of all parameter datasets to be written to the HDF5 file

Parameters **exclude_dependencies** – Boolean indicating whether we should exclude parameters that define dependencies from the list

get_num_dependency_data()
Return the number of dependencies defined as part of the parameters

get_num_parameter_data()
Return the number of parameter datasets to be wirtten to the HDF5 file

get_parameter_data(*index*)
Given the index return the associated dataset to be written to the HDF5 file

:param index [Return the index entry of the private member parameters. If a] string is given, then get_parameter_data_by_name(...) will be used instead.

Raises IndexError is raised when the index is out of bounds

get_parameter_data_by_name(*dataname*)
Given the key name of the data return the associated parameter_data object.

Parameters **dataname** – Name of the parameter requested from the parameters member.

Returns The parameter_data object or None if not found

get_parameter_names()
Get a list of all parameter dataset names (including those that may define dependencies.

keys()
Get a list of all valid keys, i.e., a list of all parameter names.

Returns List of strings with all input parameter and output names.

set_parameter_default_value(*name*, *value*)
Set the default value of the parameter with the given name

Parameters

- **name** – Name of the parameter
- **value** – New value

Raises KeyError if parameter not found

dependency_data Module

Define a dependency to another omsi object

class omsi.datastructures.dependency_data.**dependency_dict**(*param_name=None*, *link_name=None*, *omsi_object=None*, *selection=None*, *dataname=None*, *help=None*, *dependency_type=None*)

Bases: dict

Define a dependency to another omsi file-based data object or in-memory analysis_base object

Required Keyword Arguments:

Variables

- **param_name** – The name of the parameter that has the depency
- **link_name** – The name of for the link to be created in the HDF5 file.
- **omsi_object** – The object to which a link should be established to. This must be either an h5py.Dataset or the omsi_file_analysis or omsi_file_msidata or any of the other omsi_file API interface ojects.
- **selection** – Optional string type parameter indicating a python selection for the dependency
- **dataname** – String indicating the dataset within the omsi_object. If the omsi_object is an h5py object within a managed Group, then the omsi_object is automatically split up into the parent object and dataname.
- **_data** – Private key used to store the data associated with the dependency object.

Optional Keyword arguments:

Variables **dependency_type** – The type of the dependency being modeled. If not defined then the default value of 'parameter' is assumed.

Initialize the allowed set of keys.

Parameters

- **param_name** – The name of the parameter that has the dependency
- **link_name** – The name of for the link to be created in the HDF5 file.
- **omsi_object** – The object to which a link should be established to. This must be either an h5py.Dataset or the omsi_file_analysis or omsi_file_msidata or any of the other omsi_file API interface objects.
- **selection** – Optional string type parameter indicating a python selection for the dependency

- **dataname** – String indicating the dataset within the omsi_object. If the omsi_object is an h5py object within a managed Group, then the omsi_object is automatically split up into the parent object and dataname.
- **help** – Optional string describing the object

copy()
Return a new dependency_dict object with the same data as stored in the current object

Returns dependency_dict object

dependency_types = {'subset': 'subset', 'undefined': None, 'contains': 'contains', 'link': 'link', 'parameter': 'parame

get_data()
Get the data associated with the dependency.

Returns If a selection is applied and the dependency object supports array data load (e.g., h5py.Dataset, omsi_file_msidata), then the selected data will be loaded and returned as numpy array. Otherwise the ['omsi_object'] is returned.

run_info_data Module

Module with helper data structures for recording runtime provenance data

class omsi.datastructures.run_info_data.**run_info_dict**(**args*, ***kwargs*)
Bases: dict

Simple dictionary class for collecting runtime information

The typical use is as follows:

>> my_run_info = run_info_dict() >> my_run_info(my_function)(my_parameters)

With this, all runtime information is automatically collected in my_run_info. We can enable time-and-usage and memory profiling simply by calling enable_profile_time_and_usage(...) or enable_profile_memory(...), respectively, before we run our function.

We can also use the data structure directly and control the population ourselves, however, memory profiling is not supported by default in this case but we need to set and run the memory profiler ourselves, since memory_profiler expects that it can wrap the function

DEFAULT_TIME_FORMAT = '%Y-%m-%d %H:%M:%S.%f'

clean_up()
Clean up the runinfo object. In particular remove empty keys that either recorded None or recorded just an empty string.

This function may be overwritten to also do clean-up needed due to additional custom runtime instrumentation.

When overwriting this function we should call super(..., self).runinfo_clean_up() at the end of the function to ensure that the runinfo dictionary is clean, i.e., does not contain any empty entries.

clear()
Clear the dictionary and other internal parameters

Side Effects

•Remove all key/value pairs from the dict

•Set self.__time_and_use_profiler to None

•Set self.__memory_profiler to None

•Set self.__profile_memory to False if invalid (i.e, if set to True but memory profiling is unavailable)

•Set self.__profile_time_and_usage to False if invalid (i.e., if set to True but profiling is unavailable)

enable_profile_memory(*enable=True*)
Enable/disable profiling of memory usage

Parameters **enable** – boolean to enable (True) or disable (False) memory profiling

enable_profile_time_and_usage(*enable=True*)
Enable/disable time and usage profiling

Parameters **enable** – boolean to enable (True) or disable (False) time and usage profiling

gather()
Simple helper function to gather the runtime information—that has been collected on multiple processes when running using MPI—on a single root process

Returns If we have more than one processes then this function returns a dictionary with the same keys as usual for the run_info but the values are now lists with one entry per mpi processes. If we only have a single process, then the run_info object will be returned without changes. NOTE: Similar to mpi gather, the function only collects information on the root. All other processes will return just their own private runtime information.

get_profile_memory()
Check whether profiling of memory usage is enabled

Returns Boolean indicating whether memory profiling is enabled

get_profile_stats_object(*consolidate=True*, *stream=None*)
Based on the execution profile of the execute_analysis(..) function get `pstats.Stats` object to help with the interpretation of the data.

Parameters

- **consolidate** – Boolean flag indicating whether multiple stats (e.g., from multiple cores) should be consolidated into a single stats object. Default is True.
- **stream** – The optional stream parameter to be used fo the pstats.Stats object.

Returns A single pstats.Stats object if consolidate is True. Otherwise the function returns a list of pstats.Stats objects, one per recorded statistic. None is returned in case that the stats objects cannot be created or no profiling data is available.

get_profile_time_and_usage()
Check whether time and usage profiling is enabled

Returns Boolean indicating whether time and usage profiling is enabled

record_postexecute(*execution_time=None*)
Function used to record runtime information after the task we want to track is comleted, e.g. the *execute_analysis(...)* function of a standard analysis.

The function may be overwritten in child classes to add recording of additional runtime information.

When overwriting the function we should call super(...,self).runinfo_record_postexecute(execution_time) in the custom version to ensure that the execution and end_time are properly recorded.

Parameters

- **execution_time** – The total time it took to execute the analysis. May be None, in which case the function will attempt to compute the execution time based on the start_time (if available) and the the current time.

- **comm** – Used for logging only. The MPI communicator to be used. Default value is None, in which case MPI.COMM_WORLD is used.

record_preexecute()
Record basic runtime information in this dict before the exeuction is started.

Function used to record runtime information prior to executing the process we want to track, e.g., the *execute_analysis(...)* of a standard analysis.

The function may be overwritten in child classes to add recording of additional runtime information. All runtime data should be recorded in the main dict (i.e, self). This ensures in the case of standard analysis that the data is stored in the HDF5 file. Other data should be stored in separate variables that we may add to the object.

When overwriting the function we should typically call super(...,self).runinfo_record_pretexecute() last in the custom version to ensure that the start_time is properly recorded right before the execution of the analysis.

static string_to_structime(*time_string*, *time_format=None*)
Covert a time string to a time.struct_time using time.strptime

Parameters

- **time_string** – String with the time, e.g, with the start time of a program.
- **time_format** – The time format to be used or None in which case run_info_dict.DEFAULT_TIME_FORMAT will be used.

static string_to_time(*time_string*, *time_format=None*)
Convert a time string to local time object using time.mktime.

Parameters

- **time_string** – String with the time, e.g, with the start time of a program.
- **time_format** – The time format to be used or None in which case run_info_dict.DEFAULT_TIME_FORMAT will be used.

Subpackages

metadata Package

metadata Package Package with metadata datastructures

metadata_data Module Define infrastructure for describing metadata (in memory)

class omsi.datastructures.metadata.metadata_data.**metadata_dict**
Bases: dict

Dictionary's for storing metadata information. The values in the dict must be of type omsi_metadata_value and the keys must be strings.

get_metadata_descriptions()
Get a list of all metadata descriptions

get_metadata_units()
Get a list of all metadata units

get_metadata_values()
Get a list of all metadata values.

class omsi.datastructures.metadata.metadata_data.**metadata_value**(*name*, *value*, *description*, *unit=None*, *ontology=None*)

Bases: dict

A single metadata value

•*name* The name of the metadata value

•*value* The actual value associated with the metadata object

•*description* The text description of the metadata object

•*unit* The unit string

•*ontology* Optional ontology

Parameters

- **name** – The name of the metadata value. Name may be None if the metadata_value is added to a metadata_dict as it will be set (if missing) when adding it to the metadata_dict
- **value** – The actual value associated with the metadata object
- **description** – The text description of the metadata object
- **unit** – The unit string
- **ontology** – Optional ontology

metadata_ontologies Module Define ontologies for metadata

var METADATA_ONTOLOGIES

Description of simple ontologies for metadata. This is a dict where the values are the descriptions of the ontologies and the key is the commonly used name of the variable associated with the ontology, however, in practice an ontology may be associated with many different metadata values (the purpose of th ontology is to standardize the values not the names of metadata variables). Available ontologies include:

- *polarity* : Description of the polarity of the instrument
- *msn_value_of_n* : Numeric level of mass spectrometry used (e.g., 1 for MS1 etc).

An ontology can be many things. In general an ontology is a mechanism to formally name and define the types, properties, and interrelationships of entities. We here refer broadly to the concept of ontologies as a means to standardize the names of things. To define an ontology we use simple dicts with the following key/value entries:

- *name*: The name of the ontology
- *value* : Python dict describing the actual ontology. Often this is simply a dict where the the keys are the allowed values and the value is the textual description of the meaning of that value. In many cases this may be a more complete description of an ontology.
- *unit* : The standard unit associated with the values (or None if not unit is available)
- *description* : Human-readable textual description of the ontology
- *version* : The version of the ontology used
- 'uri' : The Universal Remote Identifier (often a URL) associated with the ontology (or None)

Ontologies are stored in the OpenMSI data format as JSON attributes associated with the metadata, i.e., one main restriction is that ontologies should be JSON serializable (which in most cases should be a problem).

class omsi.datastructures.metadata.metadata_ontologies.**metadata_ontologies**
Bases: dict

Helper class for interacting with ontologies

9.1.4 shared Package

omsi.shared	Package used to implement shared functionality and helper functions.
omsi.shared.data_selection	Module for defining and processing data selections.
omsi.shared.log	Module providing functionality for logging based on the python logging modu
omsi.shared.mpi_helper	Module used to ease the use of MPI and distributed parallel implementations u
omsi.shared.omsi_web_helper	Module with helper functions for interactions with the OpenMSI web infrastru
omsi.shared.spectrum_layout	This module provides capabilities for computing different layouts for spectra
omsi.shared.third_party	Package containing shared third-party code modules included here to reduce th
omsi.shared.thirs_party.cloudpickle	

data_selection Module

Module for defining and processing data selections. This includes the definition of selections using strings as well as transformation and reduction of data.

TODO: We may want to expose some of the following numpy functions currently not yet

supported through the transform and reduce data operations:

- array2string
- array_equal
- array_equiv
- array_repr
- array_split
- array_str
- asanyarray
- asarray
- asarray_chkfinite
- ascontiguousarray
- asfarray
- asfortranarray
- asmatrix
- asscalar
- atleast_1d
- atleast_2d
- atleast_3d
- binary_repr
- convolve

- conjugate
- cross
- dot
- extract
- fft.*
- histogram, histogram2D, histogramdd
- kron
- linalg.*
- swapaxes(a, axis1, axis2)
- transpose

#Simple data transformation and reduction example from omsi.shared.omsi_data_selection import * import numpy as np import json t = [{'transformation':'threshold', 'threshold':60} , {'reduction':'max', 'axis':2}] tj = json.dumps(t) tj a = np.arange(125).reshape((5,5,5)) apro = transform_and_reduce_data(data=a, operations=tj, http_error=True) apro

#Another simple example from omsi.shared.omsi_data_selection import * import numpy as np import json a = np.arange(10)+5 print a # 1) substract minimum # 2) divide by the maximum value with the maximum value converted to float # NOTE: The conversion to float is to avoid division of integers, i.e., # 5/10 = 0, whereas 5/float(10) = 0.5 # NOTE: The specification of 'x1':'data' can be omitted as this is the default. # 'x1':'data' simply explicitly specifies that the input data should be # assigned to the first operand of the arithmetic operation. t = [{'transformation':'dualDataTransform' , 'operation':'subtract', 'x1':'data', 'x2':[{'reduction':'min'}]} ,

{'transformation':'dualDataTransform' , 'operation':'divide' , 'x1':'data', 'x2':[{'reduction':'max'} ,
{'transformation':'astype', 'dtype':'float'}]}]

b = transform_and_reduce_data(data=a, operations=t) print b t = [{'transformation':'threshold' , 'threshold':[{'reduction':'median'}]}] print t c = transform_and_reduce_data(data=a, operations=t) print c

#Construct a JSON description of a transformation/reduction from omsi.shared.omsi_data_selection import * #Construct the different pieces of the transformation and reduction pipeline #1) Compute the maximum data value and convert it to float #1.1) Compute the maximum value max_value = construct_reduce_dict(reduction_type='max' , axis=None) #1.2) Convert data to float value_as_float = construct_transform_dict(trans_type='astype' , dtype='float') #1.3) Merge the two steps to compute the maximum data value as float max_value_as_float = construct_transform_reduce_list(max_value, value_as_float) #2) Normalize the data by dividing by the maximum value divide_by_max_value = construct_transform_dict(trans_type='dualDataTransform',

operation='divide' , axes=None , x2=max_value_as_float)

#3) Project along the last axis (i.e., the mz axis) to compute a maximum project image max_projection = construct_reduce_dict(reduction_type='max' , axis=-1) #4) Merge the different steps and construct the json string json_string = transform_reduce_description_to_json(divide_by_max_value , max_projection) #Just copy the result of the following print statement as your JSON description print json_string

omsi.shared.data_selection.**check_selection_string**(*selection_string*)

Check whether the given selection string is valid, and indicate which type of selection the string defined. Checking the selection string is meant as a safeguard to prevent attackers from being able to insert malicious code.

Parameters **selection_string** – String given by the user with the desired selection

Returns

String indicating the type of selection as defined in selection_type:

- 'indexlist' : Selection of the form [1,2,3]
- 'all' : Selection of the form ':'

- 'range: Selection of the form 'a:b'
- 'index: A single index selection, e.g., '1'
- 'invalid': An unsupported selection

omsi.shared.data_selection.**construct_reduce_dict**(*reduction_type*, ***kwargs*)

Helper function used to construct reduction dictionary.

Required Keyword arguments:

Parameters **reduction_type** – The reduction type to be used.

Optional Keyword arguments:

Parameters

- **axis** – Some reduction functions support the axis parameters, describing along which axis the reduction should be performed.
- **x1** – By default the reductions are performed on the output of the previous data operation (x1='data'). We may reference the output of, e.g., the fifth data operation by setting x1='data5'. x1 itself may also specify a separate data transformation and reduction pipeline that operates on 'data'.
- **min_dim** – Minimum number of dimensions the input data should have in order for the reduction should be applied.

Returns Dictionary with the description of the reduction operation.

omsi.shared.data_selection.**construct_transform_dict**(*trans_type*, *axes=None*, ***kwargs*)

Helper function used to construct a dictionary describing a data transformation.

Parameters

- **trans_type** – The transformation type to be used. See transformation_type dict.
- **axes** – The axes along which the data should be split. Default is None.
- **kwargs** – Additional keyword parameters for the transformation functions.

Returns Dictionary with the description of the transformation.

Raises KeyError is raised in case that a parameter is missing. ValueError is raised in case that a given parameter value is invalid.

omsi.shared.data_selection.**construct_transform_reduce_list**(**args*)

Merge a series of transformations and reductions into a single list describing a pipeline of transformation and reduction operations to be performed.

Args Ordered series of dictionaries describing transformation and reduction operations.

Returns List of all transformation and reduction operations

omsi.shared.data_selection.**evaluate_transform_parameter**(*parameter*, *data=None*, *secondary_data=None*)

Evaluate the given query parameter. This function is used to enable the use of data transformation and reductions as part of transformation parameters. E.g., a user may want to substract the minimum, or divide by the maximum etc.

Parameters

- **parameter** – The parameter to be evaluated. This may be a JSON string or list/dictionary-based description of a data transformation. Or any other valid data parameter. If the parameter describes as data reduction or transformation then the transformation will be evaluated and the result is returned, otherwise the parameter itself is returned.
- **data** – The input numpy array that should be transformed.
- **secondary_data** – Other data from previous data iterations a user may reference.

Returns The evaluated parameter result.

omsi.shared.data_selection.**is_transform_or_reduce**(*parameter*)
Check if the given parameter defines a description of a data transformation or data reduction

Parameters **parameter** (*JSON string, dict or list of dicts with transformation parameter.*) – The parameter to be checked.

Returns Boolean

omsi.shared.data_selection.**json_to_transform_reduce_description**(*json_string*)
Convert the json string to the transformation/reduction dict.

Parameters **json_string** – The json string to be converted.

Returns Python list or dict with the description

omsi.shared.data_selection.**perform_reduction**(*data*, *reduction*, *secondary_data*, *min_dim=None*, *http_error=False*, ***kwargs*)
Helper function used reduce the data of a given numpy array.

Parameters

- **data** – The input numpy array that should be reduced
- **reduction** (*String*) – Data reduction to be applied to the input data. Reduction operations are defined as strings indicating the numpy function to be used for reduction. Valid reduction operations include e.g.: mins, max, mean, median, std, var etc.
- **axis** – The axis along which the reduction should be applied
- **secondary_data** – Other data from previous data iterations a user may reference.
- **http_error** – Define which type of error message the function should return. If false then None is returned in case of error. Otherwise a DJANGO HttpResponse is returned.
- **min_dim** – Minimum number of dimensions the input data must have in order for the reduction to be applied.
- **kwargs** – Additional optional keyword arguments.

Returns Reduced numpy data array or in case of error None or HttpResonse with a description of the error that occurred (see http_error option).

omsi.shared.data_selection.**reduction_allowed_numpy_function = ['all', 'alltrue', 'amax', 'amin', 'angle', 'a**
List of allowed numpy data reduction operations. Reduction operations are any single data operations that may change the shape of the data. NOTE: Some operations may have additional optional or required keyword arguments. HELP: For full documentation of the different functions see the numpy documentation.

Additional input parameters are often:

•**'x1'** [The data operand specifying the data the reduction should be performed on. \] The input data will be used by default if x1 is not specified. You may also specify 'data' to explicitly indicate that the input data should be assigned to x1. You may specify data0 to indicate that the output of another data operation should be used. Note, data0 here refers to the input to the full data operation pipeline. Data

from other parts of the pipeline, are then indexed using 1-based indices. E.g,. to access the output of the first data operation set x1='data0'

- **'axis'** [Integer indicating the axis along which the data should be reduced. \] The default behavior, if axis is not specified, depends on the behavior of the corresponding numpy function. However, in most cases (if not all cases) the data operation will be applied to the full input data if no axis is specified.
- **'min_dim'** [Integer specifying the minimum number of data dimensions the input data \] must have in order for the reduction operation to be applied.

Here the list of allowed data reduction operations.

- 'all' : out = numpy.all(data, axis)
- 'amax' : out = numpy.amax(data, axis)
- 'amin' : out = numpy.amin(data, axis)
- 'alltrue' : out = numpy.alltrue(data, axis)
- 'angle' : out = numpy.angle(z, deg)
- 'any' : out = numpy.any(data, axis)
- 'append' : out = numpy.append(data, values, axis)
- 'argmax' : out = numpy.argmax(data, axis)
- 'argmin' : out = numpy.argmin(data, axis)
- 'argwhere' : out = numpy.argwhere(data)
- 'average' : out = numpy.average(data, axis)
- 'bincount' : out = numpy.bincount(x, weights=None, minlength=None)
- 'corrcoef' : out = numpy.corrcoef(data)
- 'count_nonzero' : out = numpy.count_nonzero(data)
- 'cumprod' : out = numpy.cumprod(data,axis)
- 'cumproduct': out = numpy.cumproduct(data,axis)
- 'cumsum' : out = numpy.cumsum(data,axis)
- 'diag' : out = numpy.diag(data,k=0)
- 'diag_indices: out = numpu.diag_indices(data, ndim=2)
- 'diagflat' : out = numpy.diagflat(data, k=0)
- 'diagonal' : out = numpy.diagonal(data, offset=0, axis1=0, axis2=1)
- 'diff' : out = numpy.diff(a, n=1, axis=-1)
- 'max' : out = numpy.max(data, axis)
- 'min' : out = numpy.min(data, axis)
- 'median' : out = numpy.median(data, axis)
- 'mean' : out = numpy.mean(data, axis)
- 'percentile': out = numpy.percentile(data, q, axis)
- 'product' : out = numpy.product(data, axis)
- 'prod' : out = numpy.prod(data,axis)

- 'ptp' : out = numpy.ptp(data,axis)
- 'squeeze' : out = numpy.squeeze(data)
- 'std' : out = numpy.std(data, axis)
- 'swapaxes: out = numpy.swapaxes(x1, axis1, axis2)
- 'var' : out = numpy.var(data, axis)
- 'transpose' : out = numpy.transpose(data)
- 'sum' : out = numpy.sum(data, axis)

None-numpy data reduction operations:

- 'select_values' : out = data[selection]

omsi.shared.data_selection.**selection_string_to_object**(*selection_string*, *list_to_index=False*)

Convert the given selection string to a python selection object, i.e., either a slice, list or integer index.

Parameters

- **selection_string** – A selection string of the type indexlist
- **list_to_index** – Should we turn the list into an index if the list contains only a single value. Default value is False, i.e., the list is not modified.

Returns

- An integer index if an index selection is specified
- A python list of indices if a list specified in the string
- A python slice object if a slice operation is specified by the string

omsi.shared.data_selection.**selection_to_indexlist**(*selection_string*, *axis_size=0*)

Parse the indexlist selection string and return a python list of indices

Parameters

- **selection_string** – A selection string of the type indexlist
- **axis_size** – Size of the dimensions for which the selection is defined. Only needed in case that a range selection is given. This should be a list of sizes, in case that a multiaxis selection is given.

Returns

- A python list of point indices for the selection.
- None in case the list is empty or in case an error occurred.

omsi.shared.data_selection.**selection_to_string**(*selection*)

Convert the given selection, which may be either an int, a list of ints, a slice object or a tuple of the mentioned types which is used to define a selection along multiple axes. :param selection: The selection to be converted to a string :type selection: int, list, slice, or a tuple of int, list, slice objects :return: The selection string

omsi.shared.data_selection.**selection_type = {'index': 0, 'all': 3, 'indexlist': 2, 'invalid': -1, 'range': 4, 'multiaxi**

This an extended list of types indicated by the check_selection_string function. Indices <0 are assumed to be invalid selections.

omsi.shared.data_selection.**transform_and_reduce_data**(*data*, *operations*, *secondary_data=None*, *http_error=False*)

Helper function used to apply a series of potentially multiple operations to a given numpy dataset. This function

uses the transform_data_single(...) function to apply each indicated transformation to the data. This function uses the perform_reduction function to perform data reduction operations.

Parameters

- **data** – The input numpy array that should be transformed.
- **operations** – JSON string with list of dictionaries or a python list of dictionaries. Each dict specifies a single data transformation or data reduction. The operations are applied in order, i.e., operations[0] is applied first, then operations[1] and so on. The dicts must be structured according to one of the following specifications:
  - *{'transformation':<op>}* : Single transformation applied to all data at once.
  - *{'transformation':<op>, 'axes':[..]}* : Apply a single transformation to data chunks defined by the axes parameter. The data is split into chunks along the dimensions defined by the axes parameter. E.g., if we have a 3D MSI dataset and we want to op ion images independently, then we need to set axes=[2]. Accordingly, if we want to op spectra individually, then we need to split the two image dimensions into chunks by setting axes=[0,1].
  - *{'reduction':<reduction>, 'axis':int}* : Define the reduction operations to be applied and the axis along which the data should be reduced. If reduction along all axis should be done then set axis ot None (in python) or null in JSON.
- **secondary_data** – Other data from previous data iterations a user may reference.
- **http_error** – Define which type of error message the function should return. If false then None is returned in case of error. Otherwise a DJANGO HttpResponse is returned.

Returns Reduced numpy data array or HttpResonse with a description of the error that occurred.

omsi.shared.data_selection.**transform_data_single**(*data*, *transformation='minusMinDivideMax'*, *axes=None*, *secondary_data=None*, *http_error=False*, *transform_kwargs=None*)

Helper function used to transform data of a numpy array. The function potentially splits the array into independent chunks that are normalized separately (depending on how the axes parameter is defined). The actual data transformations are implemented by transform_datachunk(...).

Parameters

- **data** – The input numpy array that should be transformed.
- **transformation** – Data transformation option to be used. Available options are: 'minusMinDivideMax' ,...
- **axes** – List of data axis that should be split into chunks that are treated independently during the transformation. By default transformation is applied based on the full dataset (axes=None). E.g, if transformation should be performed on a per image basis, then we need to split the m/z dimension into individual chunks and set axes=[2]. If we want to transform spectra individually, then we need to split the two image dimensions into chunks by setting axes=[0,1].
- **secondary_data** – Other data from previous data iterations a user may reference.
- **http_error** – Define which type of error message the function should return. If false then None is returned in case of error. Otherwise a DJANGO HttpResponse is returned.
- **transform_kwargs** – Dictionary of additional keyword arguments to be passed to the transform_datachunk(...) function.

Returns Reduced numpy data array or HttpResonse with a description of the error that occurred.

omsi.shared.data_selection.**transform_datachunk**(*data*, *transformation='minusMinDivideMax'*, *secondary_data=None*, ***kwargs*)

Helper function used to transform a given data chunk. In contrast to transform_data, this function applies the transformation directly to the data provided, without consideration of axis information. This function is used by transform_data(...) to implement the actual normalization for independent data chunks that need to be normalized.

Required keyword arguments:

Parameters

- **data** – The input numpy array that should be transformed.
- **transformation** – Data transformation option to be used. For available options see the transformation_type dictionary.
- **secondary_data** – Other data from previous data iterations a user may reference.

Additional transformation-dependent keyword arguments:

Parameters **kwargs** – Additional keyword arguments that are specific for different data transformation. Below a list of additional keyword arguments used for different transformation options

- **transformation: 'threshold'**

  ** **'threshold'** [The threshold parameter to be used for] the thresold operation. If threshold is not specified, then the 5th %tile will be used as threshold value instead, ie., the bottom 5% of the data are set to 0.

Returns This function returns the normalized data array. If an unsupported transformation option is given, then the function simply return the unmodified input array.

omsi.shared.data_selection.**transform_reduce_description_to_json**(**args*)

Convert the dictionary describing the transformation/reduction operations to a JSON string.

Parameters **args** – The list or dictionaries with the description of the transformation and reduction operations.

Returns JSON string

omsi.shared.data_selection.**transformation_allowed_numpy_dual_data = ['add', 'arctan2', 'bitwise_and', '**

List of allowed dual data transformations. Dual data transformation, are operation that operate on a two data input datasets but which do not change the shape of the data. Below a list of available numpy function options. NOTE: Some operations may have additional optional or required keyword arguments. HELP: For full documentation of the different functions see the numpy documentation.

- 'add' : out = x1 + x2 = numpy.add(x1,x2)
- 'arctan2' : out = numpy.arctan2(x1,x2)
- 'bitwise_and' : out = x1 && x2 = numpy.bitwise_and(x1,x2)
- 'bitwise_not' : out = numpy.bitwise_not(x1,x2)
- 'bitwise_or', : out = x1 || x2 = numpy.bitwise_or(x1,x2)
- 'bitwise_xor' : out = numpy.bitwise_xor(x1,x2)
- 'corrcoef' : out = numpy.corrcoef(x1,x2)
- 'cov' : out = numpy.cov(x1, x2, rowvar=1, bias=0, ddof=None)
- 'divide' : out = x1 / x2 = numpy.divide(x1,x2)

- 'equal' : out = x1 == x2 = numpy.equal(x1,x2)
- 'fmax' : out = numpy.fmax(x1,x2)
- 'fmin' : out = numpy.fmin(x1,x2)
- 'fmod' : out = numpy.fmod(x1,x2)
- 'greater' : out = x1 > x2 = numpy.greater(x1,x2)
- 'greater_equal' : out = x1 >= x2 = numpy.greater_equal(x1,x2)
- 'left_shift' : out = numpy.left_shift(x1,x2)
- 'less' : out = x1 < x2 = numpy.less(x1,x2)
- 'less_equal' : out = x1 <= x2 = numpy.less_equal(x1,x2)
- 'logical_and' : out = numpy.logical_and(x1,x2)
- 'logical_not' : See transformation_allowed_numpy_single_data instead.
- 'logical_or' : out = numpy.logical_or(x1,x2)
- 'logical_xor' : out = numpy.logical_xor(x1,x2)
- 'mod' : out = numpy.mod(x1,x2)
- 'multiply' : out = x1 * x2 = numpy.multiply(x1,x2)
- 'not_equal' : out = x1 != x2 = numpy.not_equal(x1,x2)
- 'power' : out = numpy.power(x1,x2)
- 'subtract' : out = x1 - x2 = numpy.subtract(x1,x2)
- 'right_shift : out = np.right_shift(x1,x2)

omsi.shared.data_selection.**transformation_allowed_numpy_single_data = ['abs', 'arccos', 'arccosh', 'arc**

List of allowed single data transformations. Single data transformation, are operations that operate on a single data input and which do not change the shape of the data. Below a list of available numpy options. NOTE: Some operations may have additional optional or required keyword arguments. HELP: For full documentation of the different functions see the numpy documentation.

- 'abs' : out = numpy.abs(x1)
- 'arccos' : out = numpy.arccos(x1)
- 'arccosh': out = numpy.arccosh(x1)
- 'arcsin' : out = numpy.arcsin(x1)
- 'arcsinh': out = numpy.arcsinh(x1)
- 'arctan' : out = numpy.arctan(x1)
- 'arctanh': out = numpy.arctanh1(x1)
- 'argsort' : out = numpy.argsort(data, axis, kind='quicksort', order=None)
- 'around' : out = numpy.around(x1, decimals)
- 'ceil' : out = numpy.ceil(x1)
- 'cos' : out = numpy.cos(x1)
- 'cosh' : out = numpy.cosh(x1)
- 'clip' : out = numpy.clip(x1, a_min, a_max)

- 'deg2rad': out = numpy.deg2rad(x1)
- 'degrees : out = numpy.degrees(x1)
- 'exp' : out = numpy.exp(x1)
- 'exp2' : out = numpy.exp2(x1)
- 'fabs' : out = numpy.fabs(x1)
- 'floor' : out = numpy.floor(x1)
- 'hypot' : out = numpy.hypot(x1)
- 'invert' : out = numpy.invert(x1)
- **'log'** [out[x1>0] = log(x1[x1>0]) \] out[x1<0] = log(x1[x1<0]*-1)*-1 out[x1==0] = 0
- **'log2 ': out[x1>0] = log2(x1[x1>0])** out[x1<0] = log2(x1[x1<0]*-1)*-1 out[x1==0] = 0
- **'log10': out[x1>0] = log10(x1[x1>0])** out[x1<0] = log10(x1[x1<0]*-1)*-1 out[x1==0] = 0
- 'logical_not' : out = numpy.logical_not(x1)
- 'negative' : out = np.negative(x1)
- 'round' : out = numpy.round(x1, decimals)
- **'sqrt'** [out[x1>0] = sqrt(x1[x1>0]) \] out[x1<0] = sqrt(x1[x1<0]*-1)*-1 out[x1==0] = 0
- 'sign' : out = numpy.sign(x1)
- 'sin' : out = numpy.sin(x1)
- 'sinc' : out = numpy.sinc(x1)
- 'sinh' : out = numpy.sinh(x1)
- 'sort' : out = numpy.sort(x1, axis=-1, kind='quicksort', order=None)
- 'swapaxes: out = numpy.swapaxes(x1, axis1, axis2)
- 'tan' : out = numpy.tan(x1)
- 'tanh' : out = numpy.tanh(x1)

omsi.shared.data_selection.**transformation_type = {'singleDataTransform': 'singleDataTransform', 'scale': 'sc**

Dictionary of available data transformation options. Available options are:

- 'arithmetic' : Same as 'dualDataTransform'. See 'dualDataTransform' below for details.
- 'divideMax' : Divide the data by the current maximum value.
- **'minusMinDivideMax'** [Substract the minimum value from the data and \] then divide the data by maximum of the data (with the minimum already substracted.
- **'dualDataTransform'** [Apply arbitrary arithmetic operation to the data. Additional parameter \] required for this option are:
  - *operation* : String defining the arithmetic operations to be applied. Supported operations are: 'add', 'divide', 'greater', 'greater_equal', 'multiply', 'subtract'
  - **'x1'** [The first data operand of the arithmetic operation. \] The input data will be used by default if x1 is not specified. You may also specify 'data' to explicitly indicate that the input data should be assigned to x1. You may specify data0 to indicate that the output of another data operation should be used. Note, data0 here refers to the input to the full data operation pipeline. Data from other parts of the pipeline, are then indexed using 1-based indices. E.g,. to access the output of the first data operation set x1='data0'

- **'x2'** [The second data operand of the arithmetic operation. \] The input data will be used by default if x2 is not specified. You may also specify 'data' to explicitly indicate that the input data should be assigned to x2. You may specify data0 to indicate that the output of another data operation should be used. Note, data0 here refers to the input to the full data operation pipeline. Data from other parts of the pipeline, are then indexed using 1-based indices. E.g,. to access the output of the first data operation set x2='data0'
- ... any additional parameters needed for the numpy function.

- **'singleDataTransform'** [Apply scaling transformation to the data. Additional parameters \] required for this options are. NOTE: operation=='log or operation=='sqrt': If the minimum value is 0 then the transformation is applied topositive values only and 0 values remain as is. If the minimum value is larger then 0, then the log-scale is applied as is, i.e., np.log(data). If the minimum data value is negative, then the log scale is applied independently to the positive values and the negative values, ie., outdata[posvalues] = np.log(data[posvalues]) outdata[negvalues] = np.log(data[negvalues]*-1.)*-1.
  - 'operation' : String defining the scaling operations to be applied. See the transformation_allowed_numpy_single_data list for a complete list of allowed scaling operations. Some of the more commonly used scalingoperations include: 'abs', 'log', 'sqrt', 'around' etc.
  - **'x1'** [The first data operand for the scaling.] The input data will be used by default if x1 is not specified. You may also specify 'data' to explicitly indicate that the input data should be assigned to x1.

  Additional optional keyword arguments depending on the used operation:
  - **'decimals'** [Number of decimal places to round to when using numpy.around or numpy.round \] (default: 0). If decimals is negative, it specifies the number of positions to the left of the decimal point.
  - 'a_min', 'a_max' : Lower and upper bound when using numpy.clip.
  - 'axis', 'kind', 'order' : Additional optional arguments for numpy.argsort and numpy.sort.
  - ...

- 'scale' : Same as 'singleDataTransform'. See 'singleDataTransform' for details.
- **'threshold'** [Threshold the data. Set all values that are smaller than threshold \] to 0. Additional parameters required for this option are:
  - 'threshold'. If threshold is missing, then the threshold will be

    set ot the 5%'ile so that the bottom 5% of the data will be set to 0.

- 'astype' : Change the type of the data. Additional required parameters are:
  - 'dtype' : The numpy data type to be used. Default dtype='float'.

omsi_web_helper Module

Module with helper functions for interactions with the OpenMSI web infrastructure, e.g. update job status, explicitly add a file to the OpenMSI database, update file permissions so that Apache can access it etc.

class omsi.shared.omsi_web_helper.**UserInput**

Bases: object

Collection of helper functions used to collect user input

static userinput_with_timeout (*timeout*, *default=''*)
Read user input. Return default value given after timeout. This function decides which platform-dependent version should be used to retrieve the user input.

Parameters

- **timeout** – Number of seconds till timeout
- **default** (*String*) – Default string to be returned after timeout

Returns String

static userinput_with_timeout_default (*timeout*, *default=''*)
Read user input. Return default value given after timeout.

Parameters

- **timeout** – Number of seconds till timeout
- **default** (*String*) – Default string to be returned after timeout

Returns String

static userinput_with_timeout_windows (*timeout*, *default=''*)

Read user input. Return default value given after timeout. This function is used when running on windows-based systems.

Parameters

- **timeout** – Number of seconds till timeout
- **default** (*String*) – Default string to be returned after timeout

Returns String

class omsi.shared.omsi_web_helper.**WebHelper**
Bases: object

Class providing a collection of functions for web-related file conversion tasks, e.g, : i) adding files to the web database, ii) notifying users via email, iii) setting file permissions for web-access.

allowed_nersc_locations = ['/project/projectdirs/openmsi/omsi_data_private', '/global/project/projectdirs/openms

default_db_server_url = 'https://openmsi.nersc.gov/'

static register_file_with_db (*filepath*, *db_server*, *file_user_name*, *jobid=None*, *check_add_nersc=True*)
Function used to register a given file with the database

Parameters

- **filepath** – Path of the file to be added to the database
- **db_server** – The database server url
- **file_user_name** – The user to be used, or None if the user should be determined based on the file URL.
- **jobid** – Optional input parameter defining the jobid to be updated. If the jobid is given then the job will be updated with the database instead of adding the file explicitly. I.e., instead of register_filer_with_db the update_job_status call is executed.

Returns Boolean indicating whether the operation was successful

static send_email(*subject*, *body*, *sender='convert@openmsi.nersc.gov'*, *email_type='success'*, *email_success_recipients=None*, *email_error_recipients=None*)
Send email notification to users.

Parameters

- **subject** – Subject line of the email
- **body** – Body text of the email.
- **sender** – The originating email address
- **email_type** – One of 'success, 'error', 'warning'. Error messages are sent to ConvertSettings.email_error_recipients, success messages to ConvertSettings.email_success_recipients and warning messages are sent to both lists.
- **email_success_recipients** – List of user that should receive an email if the status is success or warning.
- **email_error_recipients** – List of users that should receive an email if the status is error or warning.

static set_apache_acl(*filepath*)
Helper function used to set acl permissions for apache to make the given file accesible to Apache at NERSC. This necessary to make the file readable for adding it to the database.

super_users = ['bpb', 'oruebel']

static update_job_status(*filepath*, *db_server*, *jobid*, *status='complete'*)
Function used to update the status of the job on the server

Parameters

- **filepath** – Path of the file to be added to the database (only needed update file permissions)
- **db_server** – The database server url
- **jobid** – The id of the current job.
- **status** – One of 'running', 'complete' or 'error'

spectrum_layout Module

This module provides capabilities for computing different layouts for spectra

omsi.shared.spectrum_layout.**compute_hilbert_spectrum**(*original_coords*, *original_intensities*, *left=0*, *right=0*)
Given a 1D spectrum, interpolate the spectrum onto the closest 2D hilbert curve.

Parameters

- **original_coords** (*1D numpy array in increasing order.*) – The original coordinate values (m/z). Values must be increasing.
- **original_intensities** (*1D numpy array of same length as original_coords*) – The original intensity values. Same length as original_coords.
- **left** – Optional. Value to be used for padding data at the lower bound during interpolation
- **right** – Optional. Value to be used for padding data at the upper bound during interpolation

Type float

Type float

Returns 2D numpy array with the coordinate (m/z) values for the hilbert spectrum and separate 2D numpy array for the interpolated intensity values.

Raises ValueError If original_coords and original_intensities have different length.

omsi.shared.spectrum_layout.**hilbert_curve**(*order=2*)
Compute a 2D hilbert curve.

Parameters **order** (*Integer that defines a power of 2 (>=2)*) – The order of the hilber curve. This is the length of the sides of the square, i.e., the number of points in x and y.

Returns Returns two numpy arrays of integers x,y, indicating the locations of the vertices of the hilbert curve.

omsi.shared.spectrum_layout.**plot_2d_spectrum_as_image**(*hilbert_intensities*, *show_plot=False*, *show_axis=False*)
Plot image with pixels colored according to hilbert_intensities.

Parameters

- **hilbert_intensities** (*2D numpy array.*) – 2D numpy array with the intensity values for the spectrum.
- **show_plot** (*Boolean*) – Show the generated plot in a window.
- **show_axis** (*Boolean*) – Show x,y axis for the plot. Default is False.

Returns matplotlib image plot or None in case that the plotting failed.

omsi.shared.spectrum_layout.**reinterpolate_spectrum**(*coords*, *original_coords*, *original_intensitities*, *left=0*, *right=0*)
Given a 1D spectrum, interpolate the spectrum onto a new axis.

Parameters

- **coords** – The coordinate values (m/z) for which intensities should be computed.
- **original_coords** – The original coordinate values (m/z). Values must be increasing.
- **original_intensitities** – The original intensity values. Same length as orignal_coords.
- **left** – Optional. Value to be used if coords < orignal_coords
- **right** – Optional. Value to be used if coords > orignal_coords

Returns y : {float, ndarray} The interpolated values, same shape as coords.

Raises ValueError If original_coords and original_intensities have different length.

log Module

Module providing functionality for logging based on the python logging module. The module is intended toease the use of logging while a developer can still access the standard python logging mechanism if needed.

class omsi.shared.log.**log_helper**
Bases: object

BASTet helper module to ease the use of logging

Class Variables:

Variables ***log_levels*** – Dictionary describing the different available logging levels.

classmethod **critical**(*module_name*, *message*, *root=0*, *comm=None*, **args*, ***kwargs*)
Create a critical log entry. This function is typically called as:

log_helper.critical(module_name=__name__, message="your message")

Parameters

- **module_name** – __name__ of the calling module or None in case the ROOT logger should be used.
- **message** – The message to be added to the log
- **root** – The root process to be used for output when running in parallel. If None, then all calling ranks will perform logging. Default is 0.
- **comm** – The MPI communicator to be used to determin the MPI rank. None by default, in which case mpi.comm_world is used.
- **args** – Additional positional arguments for the python logger.debug function. See the python docs.
- **kwargs** – Additional keyword arguments for the python logger.debug function. See the python docs.

classmethod **debug**(*module_name*, *message*, *root=0*, *comm=None*, **args*, ***kwargs*)
Create a debug log entry. This function is typically called as:

log_helper.debug(module_name=__name__, message="your message")

Parameters

- **module_name** – __name__ of the calling module or None in case the ROOT logger should be used.
- **message** – The message to be added to the log
- **root** – The root process to be used for output when running in parallel. If None, then all calling ranks will perform logging. Default is 0.
- **comm** – The MPI communicator to be used to determin the MPI rank. None by default, in which case mpi.comm_world is used.
- **args** – Additional positional arguments for the python logger.debug function. See the python docs.
- **kwargs** – Additional keyword arguments for the python logger.debug function. See the python docs.

classmethod **error**(*module_name*, *message*, *root=0*, *comm=None*, **args*, ***kwargs*)
Create a error log entry. This function is typically called as:

log_helper.error(module_name=__name__, message="your message")

Parameters

- **module_name** – __name__ of the calling module or None in case the ROOT logger should be used.
- **message** – The message to be added to the log
- **root** – The root process to be used for output when running in parallel. If None, then all calling ranks will perform logging. Default is 0.
- **comm** – The MPI communicator to be used to determin the MPI rank. None by default, in which case mpi.comm_world is used.

- **args** – Additional positional arguments for the python logger.debug function. See the python docs.
- **kwargs** – Additional keyword arguments for the python logger.debug function. See the python docs.

classmethod exception(*module_name*, *message*, *root=0*, *comm=None*, **args*, ***kwargs*)
Create a exception log entry. This function is typically called as:

log_helper.exception(module_name=__name__, message="your message")

Parameters

- **module_name** – __name__ of the calling module or None in case the ROOT logger should be used.
- **message** – The message to be added to the log
- **root** – The root process to be used for output when running in parallel. If None, then all calling ranks will perform logging. Default is 0.
- **comm** – The MPI communicator to be used to determin the MPI rank. None by default, in which case mpi.comm_world is used.
- **args** – Additional positional arguments for the python logger.debug function. See the python docs.
- **kwargs** – Additional keyword arguments for the python logger.debug function. See the python docs.

classmethod get_default_format()
Get default formatting string.

classmethod get_logger(*module_name*)
Get the logger for a particular module. The module_name should always be set to the __name__ variable of the calling module.

Parameters **module_name** – __name__ of the calling module or None in case the ROOT logger should be used.

Returns Python logging.Logger retrieved via logging.getLogger.

global_log_level = 20

classmethod info(*module_name*, *message*, *root=0*, *comm=None*, **args*, ***kwargs*)
Create a info log entry. This function is typically called as:

log_helper.info(module_name=__name__, message="your message")

Parameters

- **module_name** – __name__ of the calling module or None in case the ROOT logger should be used.
- **message** – The message to be added to the log
- **root** – The root process to be used for output when running in parallel. If None, then all calling ranks will perform logging. Default is 0.
- **comm** – The MPI communicator to be used to determin the MPI rank. None by default, in which case mpi.comm_world is used.
- **args** – Additional positional arguments for the python logger.debug function. See the python docs.

- **kwargs** – Additional keyword arguments for the python logger.debug function. See the python docs.

initialized = False

classmethod log(*module_name*, *message*, *root=0*, *comm=None*, *level=None*, **args*, ***kwargs*)
Convenience function used to select the log message level using an input parameter rathern than by selecting the approbriate function.

Parameters

- **module_name** – __name__ of the calling module or None in case the ROOT logger should be used.
- **message** – The message to be added to the log
- **root** – The root process to be used for output when running in parallel. If None, then all calling ranks will perform logging. Default is 0.
- **comm** – The MPI communicator to be used to determine the MPI rank. None by default, in which case mpi.comm_world is used.
- **level** – To which logging level should we send the message
- **args** – Additional positional arguments for the python logger.debug function. See the python docs.
- **kwargs** – Additional keyword arguments for the python logger.debug function. See the python docs.

log_levels = {'INFO': 20, 'WARNING': 30, 'CRITICAL': 50, 'ERROR': 40, 'DEBUG': 10, 'NOTSET': 0}

classmethod log_var(*module_name*, *root=0*, *comm=None*, *level=None*, ***kwargs*)
Log one or more variable values

Parameters

- **module_name** – __name__ of the calling module or None in case the ROOT logger should be used.
- **message** – The message to be added to the log
- **root** – The root process to be used for output when running in parallel. If None, then all calling ranks will perform logging. Default is 0.
- **comm** – The MPI communicator to be used to determin the MPI rank. None by default, in which case mpi.comm_world is used.
- **kwargs** – Variables+values to be logged

classmethod set_log_level(*level*)
Set the logging level for all BASTet loggers

Parameters level – The logging levels to be used, one of the values specified in log_helper.log_levels.

classmethod setup_logging(*level=None*)
Call this function at the beginning of your code to initiate logging.

Parameters level – The default log level to be used. One of `log_helper.log_level`.

classmethod warning(*module_name*, *message*, *root=0*, *comm=None*, **args*, ***kwargs*)
Create a warning log entry. This function is typically called as:

log_helper.warning(module_name=__name__, message="your message")

Parameters

- **module_name** – __name__ of the calling module or None in case the ROOT logger should be used.
- **message** – The message to be added to the log
- **root** – The root process to be used for output when running in parallel. If None, then all calling ranks will perform logging. Default is 0.
- **comm** – The MPI communicator to be used to determin the MPI rank. None by default, in which case mpi.comm_world is used.
- **args** – Additional positional arguments for the python logger.debug function. See the python docs.
- **kwargs** – Additional keyword arguments for the python logger.debug function. See the python docs.

mpi_helper Module

Module used to ease the use of MPI and distributed parallel implementations using MPI

omsi.shared.mpi_helper.**barrier**(*comm=None*)
MPI barrier operation or no-op when running without MPI

Parameters **comm** – MPI communicator. If None, then MPI.COMM_WORLD will be used.

omsi.shared.mpi_helper.**broadcast**(*data*, *comm=None*, *root=0*)
MPI broadcast operation to broadcast data from one rank to all other ranks

Parameters

- **data** – The data to be gathered
- **comm** – MPI communicator. If None, then MPI.COMM_WORLD will be used.
- **root** – The rank where the data is sned from

Returns The data object

omsi.shared.mpi_helper.**gather**(*data*, *comm=None*, *root=0*)
MPI gather operation or return a list with just [data,] if MPI is not available

Parameters

- **data** – The data to be gathered
- **comm** – MPI communicator. If None, then MPI.COMM_WORLD will be used.
- **root** – The rank where the data should be collected to. Default value is 0

Returns List of data objects from all the ranks

omsi.shared.mpi_helper.**get_comm_world**()
Get MPI.COMM_WORLD :return: mpi communicator or None if MPI is not available

omsi.shared.mpi_helper.**get_rank**(*comm=None*)
Get the current process rank :param comm: MPI communicator. If None, then MPI.COMM_WORLD will be used. :return: The integer index of the rank

omsi.shared.mpi_helper.**get_size**(*comm=None*)
Get the size of the current communication domain/ :param comm: MPI communicator. If None, then MPI.COMM_WORLD will be used. :return: The integer index of the rank

omsi.shared.mpi_helper.**imports_mpi**(*python_object*)
Check whether the given class import mpi

The implementation inspects the source code of the analysis to see if MPI is imported by the code.

omsi.shared.mpi_helper.**is_mpi_available**()
Check if MPI is available. Same as MPI_AVAILABLE :return: bool indicating whether MPI is available

omsi.shared.mpi_helper.**mpi_type_from_dtype**(*dtype*)
Ge the the corresponding MPI type for the given basic numpy dtype

Parameters **dtype** – Basic numpy dtype to be mapped to the MPI type

Returns The MPI type or None if not found

class omsi.shared.mpi_helper.**parallel_over_axes**(*task_function*, *task_function_params*, *main_data*, *split_axes*, *main_data_param_name*, *schedule='STATIC_1D'*, *root=0*, *comm=None*)
Bases: object

Helper class used to parallelize the execution of a function using MPI by splitting the input data into sub-blocks along a given set of axes.

Variables

- **task_function** – The function we should run.
- **task_function_params** – Dict with the input parameters for the function. may be None or {} if no parameters are needed.
- **main_data** – Dataset over which we should parallelize
- **split_axes** – List of integer axis indicies over which we should parallelize
- **main_data_param_name** – The name of data input parameter of the task function
- **root** – The master MPI rank (Default=0)
- **schedule** – The task scheduling schema to be used (see parallel_over_axes.SCHEDULES
- **collect_output** – Should we collect all the output from the ranks on the master rank?
- **schedule** – The parallelization schedule to be used. See also parallel_over_axes.schedule
- **result** – The result form the task_function. If self.__data_collected is set and we are the root then this will a list with the the output of all tasks
- **blocks** – List with tuples describing the selected subset of data processed by the given block task. If self.__data_collected is set and we are the root rank then this is a list of all the blocks processed by each rank.
- **block_times** – List of times in seconds used to process the data block with the given index. NOTE: The block times include also any required communications and other operations to initialize and complete the task, and not just the execution of the task function itself.
- **run_time** – Float time in seconds for executing the run function.
- **comm** – The MPI communicator used for the parallelization. Default value is MPI.COMM_WORLD

Parameters

- **task_function** – The function we should run.

- **task_function_params** – Dict with the input parameters for the function. May be None or {} if no parameters are needed.
- **main_data** – Dataset over which we should parallelize
- **split_axes** – List of integer axis indicies over which we should parallelize
- **main_data_param_name** – The name of data input parameter of the task function
- **root** – The master MPI rank (Default=0)
- **schedule** – The task scheduling schema to be used (see parallel_over_axes.SCHEDULES
- **comm** – The MPI communicator used for the parallelization. Default value is None, in which case MPI.COMM_WORLD is used

MPI_MESSAGE_TAGS = {'BLOCK_MSG': 12, 'COLLECT_MSG': 13, 'RANK_MSG': 11}

SCHEDULES = {'DYNAMIC': 'DYNAMIC', 'STATIC_1D': 'STATIC_1D', 'STATIC': 'STATIC'}

collect_data(*force_collect=False*)

Collect the results from the parallel execution to the self.root rank.

NOTE: On the root the self.result, self.blocks, and self.block_times variables are updated with the collected data as well and self.__data_collected will be set

NOTE: If the data has already been collected previously (ie., collect_data has been called before), then the collection will not be performed again, unless force_collect is set.

Parameters **force_collect** – Set this parameter to force that data collection is performed again. By default the collect_data is performed only once for each time the run(..) function is called and the results are reused to ensure consistent data structures. We can force that collect will be reexecuted anyways by setting force_collect.

Returns On worker ranks (i.e., MPI_RANK!=self.root) this is simply the self.result and self.blocks containing the result created by run function. On the root rank (i.e., MPI_RANK!=self.root) this is a tuple of two lists containing the combined data of all self.result and self.blocks from all ranks respectively.

run()

Call this function to run the function in parallel.

Returns

Tuple with the following elements:

1. List with the results from the local execution of the task_function. Each entry is the result from one return of the task_function. In the case of static execution, this is always a list of length 1.
2. List of block_indexes. Each block_index is a tuple with the selection used to divide the data into sub-blocks. In the case of static decomposition we have a range slice object along the axes used for decomposition whereas in the case of dynamic scheduling we usually have single integer point selections for each task.

omsi.shared.mpi_helper.**test_mpi_available**()

This function import MPI in a seperate process to safely check if MPI is available. This precaution is necessary as on Cray systems importing MPI can lead to a crash on, e.g., login nodes where the use of MPI is not permitted. By executing the import in a separate process we avoid crashing the main process and we can safely check whether the process aborted or not.

Returns False if the import failed, otherwise return True

9.1.5 workflow Package

omsi.workflow	Package with modules for specification and execution of analysis tasks a
omsi.workflow.common	Module defining basic data structures used by workflows.
omsi.workflow.driver	Package with drivers for analyses and workflows.
omsi.workflow.driver.base	Module with base classes for workflow drivers.
omsi.workflow.driver.cl_analysis_driver	Module used to help with driving the execution of omsi-based analyses.
omsi.workflow.driver.cl_workflow_driver	Module used to help with driving the execution of analysis workflows
omsi.workflow.executor	Package with executors of analysis workflows.
omsi.workflow.executor.base	Module containing base classes for workflow executors.
omsi.workflow.executor.greedy_executor	Module used to help with the execution of complex analyses workflows

workflow Package

Package with modules for specification and execution of analysis tasks and complex analysis workflows.

common Module

Module defining basic data structures used by workflows.

class omsi.workflow.common.**RawDescriptionDefaultHelpArgParseFormatter**(*prog*, *indent_increment=2*, *max_help_position=24*, *width=None*)

Bases: argparse.ArgumentDefaultsHelpFormatter, argparse.RawDescriptionHelpFormatter

Simple derived formatter class for use with argparse used by the cl_analysis_driver class. This formatter combines the default argparse.ArgumentDefaultsHelpFormatter and argparse.RawDescriptionHelpFormatter for formatting arguments and help descriptions.

class omsi.workflow.common.**analysis_task_list**(*analysis_objects=None*)

Bases: list

Define a python list of analyses to be executed as a workflow. The list allows only for storage of analysis_base objects and ensures uniqueness of elements in the list.

Initialize the set of analysis tasks to be performed as part of the workflow

Parameters **analysis_objects** – Set or list of unique analysis objects to be added. Duplicates will be removed.

add(*analysis_object*)

Same as append

add_all()

Add all known analyses to the workflow list

Returns The updated analysis_task_list with all analyses added

add_analysis_dependencies()

Add the dependencies of all analyses to the workflow list in case they are missing.

This function is recursive, step-by-step adding all dependencies of the workflow to the list of tasks to be executed, until no more dependencies are found.

Usually this function is called by the workflow executor itself before running the analysis and should not need to be called by the user.

Returns Integer indicating the number of dependencies added to the list of tasks

classmethod **all**()
Get an analysis_task_list of all current analysis_base objects

Returns New analysis_task_list of all current analysis objects

analysis_identifiers_unique()
Check whether all identifiers of the analyses in the this list are unique. :return: bool

append(*analysis_object*)
Add a given analysis to the set of object to be executed by the workflow

This is the same as set.add() but we ensure that only analysis_base objects are added.

Parameters **analysis_object** (omsi.analysis.base.analysis_base) – Analysis object to be added to the execution. All dependencies of the analysis will also be executed as part of the execution.

Raises ValueError is raised if the given analysis_object is invalid

clear()
Remove all elements from the list

enable_memory_profiling(*enable=True*)
Enable or disable line-by-line profiling of memory usage of execute_analysis.

Parameters **enable_memory** (*bool*) – Enable (True) or disable (False) line-by-line profiling of memory usage

Raises ImportError is raised if a required package for profiling is not available.

enable_time_and_usage_profiling(*enable=True*)
Enable or disable profiling of time and usage of code parts of execute_analysis for all analyses.

Parameters **enable** (*bool*) – Enable (True) or disable (False) profiling

Raises ImportError is raised if a required package for profiling is not available.

classmethod **from_script_files**(*script_files*)
Same as from_script, but the script is read from the given files.

Parameters **script_files** – List of strings with the paths to the script files. If only a single script is used, then a single string may be used as well.

Returns An instance of workflow_base with the specification of the workflow to be executed

classmethod **from_scripts**(*scripts*)
Evaluate the workflow script to extract all analyses to be run.

NOTE: This function executes using eval(..), i.e., there are NO safeguards against malicious codes.

Parameters **scripts** – The script with the setup of the workflow. This should only include the definition of analyses and their inputs.

Returns An instance of workflow_base with the specification of the workflow to be executed

get_additional_analysis_dependencies()
Compute a list of all dependencies of the current list of analyses (excluding analyses that are already in the the list of tasks.

Returns analysis_task_list of all analysis dependencies

get_all_analysis_data()
Get a list of all output data objects for all analysis

Returns List of omsi.analysis.analysis_data.analysis_data objects, one for each analysis

get_all_analysis_identifiers()
Get a list of all analysis identifiers

Returns List of strings with the analysis identifier of each analysis

get_all_dependency_data()
Get the complete list of all direct and indirect dependencies of all analysis tasks.

NOTE: These are only the direct dependencies as specified by the analysis itself. Use get_all_dependency_data_recursive(..) to also get the indirect dependencies of the analysis due to dependencies of the dependencies themselves.

Returns List of parameter_data objects that define dependencies.

get_all_parameter_data(*exclude_dependencies=False*)
Get the complete list of all parameters

Parameters **exclude_dependencies** – Boolean indicating whether we should exclude parameters that define dependencies from the list

Returns List of omsi.analysis.analysis_data.parameter_data objects with the description of the parameters

get_all_run_info()
Get a list of dict with the complete info about the last run of each of the analysis analysis

Returns List of run_info_dict objects, one for each analysis

insert(*index*, *analysis_object*)
Insert a given analysis object at the given location

Parameters

- **index** – Location where the obejct should be inserted
- **analysis_object** – The analysis object to be inserted

make_analysis_identifiers_unique()
Update analysis identifiers to be unique.

Side effects: This function updates the analysis tasks stored in the set

Returns self, i.e., the modified object with identifiers updated

set_undefined_analysis_identifiers()
Check that all analysis descriptors are set to a value different than "undefined" and set the descriptor based on their index in the list if necessary.

update(*analysis_objects*)
Return the set with elements added from the given set of analysis_objects.

This is the same as set.update() but we ensure that only analysis_base objects are added.

Parameters **analysis_objects** – List or set of analysis_base objects to be added to workflow set

Raise ValueError is raised in case that objects that are not instances of analysis_base are to be added.

Returns self with elements added to self.

Subpackages

driver Package

driver Package Package with drivers for analyses and workflows. Drivers are intented to control the set up —i.e., creation and initialization—of workflows. The execution of workflows itself is typically performed by a workflow executor.

base Module Module with base classes for workflow drivers.

Workflow drivers are responsible for the creation and initialization of workflows. The execution of workflows is then controlled by the workflow executor.

class omsi.workflow.driver.base.**analysis_driver_base**(*analysis_class*)
Bases: *omsi.workflow.driver.base.driver_base*

Base class defining the minimal interface for drivers of a single analysis based on the type/class of the analysis.

This is a class-based execution, i.e, the user defines only the type of analysis and inputs but does not actually create the analysis.

Derived classes must implement the main(...) function where the analysis is created and executed.

Variables **analysis_class** – The analysis class for which we want to execute the analysis. The analysis class must derive from omsi.analysis.analysis_base. May be None in case that we use other means to set the analysis_class, e.g., via the command-line.

Initialize the analysis driver

Variables **analysis_class** – The analysis class for which we want to execute the analysis. The analysis class must derive from omsi.analysis.analysis_base. May be None in case that we use other means to set the analysis_class, e.g., via the command-line.

main()
The main function for running the analysis.

class omsi.workflow.driver.base.**driver_base**
Bases: object

Primitve base class for driving the execution of an object

execute()
Same as main

main()
The main function for running the analysis.

class omsi.workflow.driver.base.**workflow_driver_base**(*workflow_executor*)
Bases: object

Base class defining the minimal interface for drivers of complex analysis workflows.

Workflows may be specified via scripts or given via a set of analysis objects.

Derived classes must implement the main(...) function where the analysis is created and executed.

Variables **workflow_executor** – The executor of the workflow.

Initalize the workflow driver

Parameters **workflow_executor** – The executor of the workflow we want to drive.

main()
The main function for running the analysis.

cl_analysis_driver Module Module used to help with driving the execution of omsi-based analyses.

class omsi.workflow.driver.cl_analysis_driver.**cl_analysis_driver**(*analysis_class*, *add_analysis_class_arg=False*, *add_output_arg=True*, *add_log_level_arg=True*)

Bases: *omsi.workflow.driver.base.analysis_driver_base*

Command-line analysis driver.

Variables

- ***analysis_class_arg_name*** – The name for the argument where the positional argument for defining the analysis class should be stored.
- ***output_save_arg_name*** – Name of the optional keyword argument for specifying the name and target for the analysis
- ***analysis_class_arg_name*** – Name of the optional first positional argument to be used to define the analysis class to be used.
- ***log_level_arg_name*** – Name of the keyword cl argument to define the level of logging ot be used.
- **analysis_class** – The class (subclass of analysis_base) defining the analysis to be executed
- **analysis_object** – Instance of the analysis object to be executed
- **add_analysis_class_arg** – Boolean indicating whether an optional positional command line argument should be used to determine the analysis class (or whether the analysis class will be set explicitly)
- **add_output_arg** – Boolean indicating whether an optional keyword argument should be added to define the output target for the analysis.
- **add_log_level_arg** – Boolean indicating whether the –loglevel argument should be added to the command line
- **parser** – The argparse.ArgumentParser instance used for defining command-line arguments
- **required_argument_group** – argparse.ArgumentParser argument group used to define required command line arguments
- **custom_argument_groups** – Dict of custom argparse.ArgumentParser argument groups specified by the analysis
- **output_target** – Specification of the output target where the analysis result should be stored
- **analysis_arguments** – Dictionary defining the input arguments to be used for the analysis
- **mpi_root** – Integer indicating the root rank when running using MPI
- **mpi_comm** – Integer indicating the MPI communicator to be used when running in parallel using MPI

Parameters

- **analysis_class** (omsi.analysis.base.analysis_base) – The analysis class for which we want to execute the analysis. The analysis class must derive from omsi.analysis.analysis_base. May be None in case that we use the command-line to define the analysis class via the optional positional argument for the command class (i.e., set add_analysis_class_arg to True).
- **add_analysis_class_arg** – Boolean indicating whether we will use the positional command-line argument to determine the analysis class name
- **add_output_arg** – Boolean indicating whether we should add the optional keyword argument for defining the output target for the analysis.
- **add_log_level_arg** – Boolean indicating wither we should add the option keyword argument to specify the logging level via the command line.

Raises A ValueError is raised in the case of conflicting inputs, i.e., if i) analysis_class==None and add_analysis_class_arg=False, i.e., the analysis class is not determined or ii) analysis_class!=None and add_analysis_class_arg=False, i.e, the analysis class is determined via two separate mechanisms.

add_and_parse_analysis_arguments()
The function assumes that the command line parser has been setup using the initialize_argument_parser(..)

This function is responsible for adding all command line arguments that are specific to the analysis and to then parse those argument and save the relevant data in the self.analysis_arguments dictionary. Command-line arguments that are specific to the command line driver are removed, so that only arguments that can be consumed by the analysis are handed to the analysis.

Side effects: The function sets `self.analysis_arguments`

analysis_class_arg_name = '__analysis_class'
The name where the positional argument for defining the analysis class will be stored.

create_analysis_object()
Initialize the analysis object, i.e., set self.analysis_object

get_analysis_class_from_cl()
Internal helper function used to get the analysis class object based on the analysis_class_arg_name positional argument from the command line.

Side effects: The function sets ‘‘self.analysis_class‘

Raises ImportError in case that the analysis module cannot be loaded

Raises AttributeError in case that the analysis class cannot be extracted from the module

initialize_argument_parser()
Internal helper function used to initialize the argument parser. NOTE: self.analysis_class must be set before calling this function.

Side effects: The function sets `self.parser` and `self.required_argument_group`

log_level_arg_name = 'loglevel'
Name of the keyword argument used to specify the level of logging to be used

main()
Default main function for running an analysis from the command line. The default implementation exposes all specified analysis parameters as command line options to the user. The default implementation also provides means to print a help text for the function.

Raises ValueError is raised in case that the analysis class is unknown

output_save_arg_name = 'save'
Name of the key-word argument used to define

parse_cl_arguments()
The function assumes that the command line parser has been setup using the initialize_argument_parser(..)

This function parses all arguments that are specific to the command-line parser itself. Analysis arguments are added and parsed later by the add_and_parse_analysis_arguments(...) function. The reason for this is two-fold: i) to separate the parsing of analysis arguments and arguments of the command-line driver and ii) if the same HDF5 file is used as input and output target, then we need to open it first here in append mode before it gets opened in read mode later by the arguments.

Side effects: The function sets `self.output_target` and `self.profile_analysis`

print_settings()
Print the analysis settings.

remove_output_target()
This function is used to delete any output target files created by the command line driver. This is done in case that an error occurred and we do not want to leave garbage files left over.

Side effects The function modifies `self.output_target`

Returns Boolean indicating whether we succesfully cleaned up the output

reset_analysis_object()
Clear the analysis object and recreate it, i.e., delete self.analysis_object and set it again.

cl_workflow_driver Module Module used to help with driving the execution of analysis workflows

class omsi.workflow.driver.cl_workflow_driver.**cl_workflow_driver**(*workflow_executor=None*, *add_script_arg=False*, *add_output_arg=True*, *add_log_level_arg=True*, *add_profile_arg=False*, *add_mem_profile_arg=False*)

Bases: *omsi.workflow.driver.base.workflow_driver_base*

Command-line workflow driver.

Variables

- ***script_arg_name*** – Name of the optional keyword cl argument for defining workflow scripts to be executed
- ***output_save_arg_name*** – Name of the optional keyword argument for specifying the name and target for the workflow. This may be a folder or an HDF5 file ending with .h5
- ***profile_arg_name*** – Name of the keyword argument used to enable profiling of the analysis
- ***profile_mem_arg_name*** – Name of the keyword argument used to enable profiling of memory usage of an analysis
- ***log_level_arg_name*** – Name of the keyword cl argument to define the level of logging ot be used.
- **workflow_executor** – The workflow executor object used to execute the analysis workflow. The workflow executor must derive from omsi.workflow.executor.base.workflow_executor_base. May be None in case that we use the command-line to define workflow executor or if the default executor should be used. The default executur class is defined by omsi.workflow.executor.base.workflow_executor_base.

- **script_files** – List of strings with the paths to files with workflow scripts to be executed.
- **add_script_arg** – Boolean indicating whether the –script keyword argument should be added to the command-line, to define the workflow scripts via the CL (or whether the scripts will be set explicitly)
- **add_output_arg** – Boolean indicating whether an optional keyword argument should be added to define the output target for the analysis.
- **add_profile_arg** – Add the optional –profile keyword argument for profiling the analysis
- **add_mem_profile_arg** – Boolean indicating whether we should add the optional keyword argument for enabling memory profiling of the analysis.
- **add_log_level_arg** – Boolean indicating wither we should add the option keyword argument to specify the logging level via the command line.
- **parser** – The argparse.ArgumentParser instance used for defining command-line arguments
- **required_argument_group** – argparse.ArgumentParser argument group used to define required command line arguments
- **optional_argument_group** – argparse.ArgumentParser argument group used to define optional command line arguments
- **custom_argument_groups** – Dict of custom argparse.ArgumentParser argument groups specified by the analysis
- **identifier_argname_seperator** – String used to seperate the analysis identifier and argument name when creating custom command-line options for the individual analyses of the workflow
- **output_target** – Specification of the output target where the analysis result should be stored
- **profile_analyses** – Boolean indicating whether we should profile the analysis for time and usage
- **profile_analyses_mem** – Boolean indicating whether we should profile the memory usage of the individual analyses
- **analysis_arguments** – Dictionary defining the custom input arguments to be used for the analysis
- **workflow_executor_arguments** – Dictionary defining the custom input arguments routed to the workflow executor
- **__output_target_self** – Private member variable used to store the output files created by this object.
- **user_log_level** – The custom logging level specified by the user (or None)
- **mpi_root** – The root rank used when running in parallel
- **mpi_comm** – The mpit communicator to be used when running in parallel

Parameters

- **workflow_executor** (omsi.analysis.base.analysis_base) – The workflow executor object used to execute the analysis workflow. The workflow executor must derive from omsi.workflow.executor.base.workflow_executor_base. May

be None in case that we use the command-line to define workflow executor or if the default executor should be used. The default executur class is defined by omsi.workflow.executor.base.workflow_executor_base.

- **add_script_arg** – Boolean indicating whether the –script keyword argument should be added to the command-line, to define the workflow scripts via the CL (or whether the scripts will be set explicitly)
- **add_output_arg** – Boolean indicating whether we should add the optional keyword argument for defining the output target for the analysis.
- **add_log_level_arg** – Boolean indicating wither we should add the option keyword argument to specify the

logging level via the command line. :param add_profile_arg: Boolean indicating whether we should add the optional keyword

argument for enabling profiling of the analysis.

Parameters **add_mem_profile_arg** – Boolean indicating whether we should add the optional keyword argument for enabling memory profiling of the analysis.

Raises A ValueError is raised in the case of conflicting inputs, i.e., if i) workflow_executor==None and add_script_arg=False, i.e., the analysis class is not determined or ii) workflow_executor!=None and add_script_arg=False, i.e, the analysis class is determined via two separate mechanisms.

add_and_parse_workflow_arguments()

The function assumes that the command line parser has been setup using the initialize_argument_parser(..)

This function is responsible for adding all command line arguments that are specific to the workflow and to then parse those arguments and save the relevant data in the self.analysis_arguments dictionary. Command-line arguments that are specific to the command line driver are removed, so that only arguments that can be consumed by the analysis are handed to the analysis.

Side effects: **The function sets `self.analysis_arguments` and updates the analysis parameters of the** analyses stored in `self.workflow_executor.analysis_tasks`

create_workflow_executor_object()

Initialize the workflow executor object, i.e., set self.workflow_executor

Side effects This function potentially modifies self.workflow_executor

initialize_argument_parser()

Internal helper function used to initialize the argument parser.

Side effects: The function sets:

- `self.parser`
- `self.required_argument_group`
- `self.opitonal_argument_group`

log_level_arg_name = 'loglevel'

Name of the keyword argument used to specify the level of logging to be used

main()

Default main function for running an analysis from the command line. The default implementation exposes all specified analysis parameters as command line options to the user. The default implementation also provides means to print a help text for the function.

Raises ValueError is raised in case that the analysis class is unknown

output_save_arg_name = 'save'
Name of the key-word argument used to define

parse_cl_arguments()
The function assumes that the command line parser has been setup using the initialize_argument_parser(..)

This function parses all arguments that are specific to the command-line parser itself. Analysis workflow arguments are added and parsed later by the add_and_parse_workflow_arguments(...) function. The reason for this is two-fold: i) to separate the parsing of analysis arguments and arguments of the command-line driver and ii) if the same HDF5 file is used as input and output target, then we need to open it first here in append mode before it gets opened in read mode later by the arguments.

Side effects: The function sets:

- `self.output_target`
- `self.profile_analyses`

print_memory_profiles()
Print the memory profiles if available

print_settings()
Print the analysis settings.

print_time_and_usage_profiles()
Print the profiling data for time and usage if available

profile_arg_name = 'profile'
Name of the keyword argument used to enable profiling of the analysis

profile_mem_arg_name = 'memprofile'
Name of the keyword argument used to enable profiling of memory usage of an analysis

remove_output_target()
This function is used to delete any output target files created by the command line driver. This is done in case that an error occurred and we do not want to leave garbage files left over.

Side effects The function modifies `self.output_target`

Returns Boolean indicating whether we succesfully cleaned up the output

reset_workflow_executor_object()
Remove and recreate the workflow executor object

script_arg_name = 'script'
The name where the positional argument for defining the analysis class will be stored.

executor Package

executor Package Package with executors of analysis workflows. Executors perform and control the execution of workflows. The setup of workflows is often performed by the user or via dedicated workflow drivers.

base Module Module containing base classes for workflow executors.

Workflow executors control the execution of workflows. The setup of workflows is often controlled either by a workflow driver or the user.

class omsi.workflow.executor.base.**workflow_executor_base**(*analysis_objects=None*)
Bases: *omsi.datastructures.analysis_data.parameter_manager*

Base class used to execute a workflow of one or many analyses. This is an object-based execution, i.e., the user defines a set of analyses to be executed.

We are given a set of existing analysis objects for which we need to coordinate the execution.

Variables

- **analysis_objects** – Private set of analysis objects to be executed
- ***DEFAULT_EXECUTOR_CLASS*** – Define the derived workflow_executor_base class to be used as default executor The default value is None, in which case the greedy_workflow_executor is used. This variable is used by the get_default_executor function to instantiate a default workflow executor on request. Using this variable we can change the default executor to our own preferred executor, e.g., to change the executor used by the omsi.analysis.base.analysis_base functions execute_all(...) and execute_recursive(...)

To implement a derived workflow executor, we need to implement a derived class that implements the main() function.

Initialize the workflow executor

Parameters **analysis_objects** – A list of analysis objects to be executed

DEFAULT_EXECUTOR_CLASS = None
The default executor class to be used

add_analysis(*analysis_object*)
Add a given analysis to the set of object to be executed by the workflow

Shorthand for: self.analysis_tasks.add(analysis_object)

add_analysis_all()
Add all known analyses to the workflow.

Shorthand for: self.analysis_tasks.add_analysis_all()

add_analysis_dependencies()
Add the dependencies of all analyses to the workflow in case they are missing.

This function is recursive, step-by-step adding all dependencies of the workflow to the list of tasks to be executed, until no more dependencies are found.

Usually this function is called by the workflow executor itself before running the analysis and should not need to be called by the user.

Returns Integer indicating the number of dependencies added to the list of tasks

add_analysis_from_scripts(*script_files*)
Evaluate the list of scripts and add all (i.e., zero, one, or multiple) analyses to this workflow

NOTE: This function executes scripts using exec(..), i.e., there are NO safeguards against malicious codes.

Parameters **script_files** – List of strings with the paths to the script files. If only a single script is used, then a single string may be used as well.

clear()
Remove all analyses from the workflow.

Shorthand for: self.analysis_tasks.clear()

execute()
Execute the workflow. This uses the main() function to run the actual workflow.

classmethod **from_script_files**(*script_files*)
Same as from_script, but the scripts are read from the given list of files.

NOTE: This function executes scripts using exec(..), i.e., there are NO safeguards against malicious codes.

Parameters **script_files** – List of strings with the paths to the script files. If only a single script is used, then a single string may be used as well.

Returns Instance of the current workflow executor class for running the given workflow

classmethod from_scripts(*scripts*)
Create and initalize a worklflow executor of the current class type to execute the workflow defined in the given set of scripts.

This function using analysis_task_list.from_scripts to evaluate the workflow scripts to extract all analyses to be created.

NOTE: This function executes scripts using exec(..), i.e., there are NO safeguards against malicious codes.

Parameters **scripts** – The script with the setup of the workflow. This should only include the definition of analyses and their inputs.

Returns Instance of the current workflow executor class for running the given workflow

get_analyses()
Get the list of analyses to be run.

Shorthand for: self.analysis_tasks

get_analysis(*index*)
Get the analysis with the given index

Shorthand for: self.analysis_tasks[index]

Parameters **index** – Integer index of the analysis

Returns omsi.analysis.base.analysis_base object

Raises IndexError in case that the index is invalid

classmethod get_default_executor(*analysis_objects=None*)
Create an instance of the default workflow executor to be used.

Parameters **analysis_objects** – A set or unique list of analysis objects to be executed by the workflow

Returns Instance of the default workflow executor

classmethod get_default_executor_class()
Get the default executor class

Returns Derived class of workflow_executor_base

main()
Implement the execution of the workflow. We should always call execute(..) or __call__(..) to run the workflow. This function is intended to implementd the executor-specific exeuction behavior and must be implemented in child classes.

greedy_executor Module Module used to help with the execution of complex analyses workflows

class omsi.workflow.executor.greedy_executor.**greedy_executor**(*analysis_objects=None*)
Bases: *omsi.workflow.executor.base.workflow_executor_base*

Execute a set of analysis objects and their dependencies

Variables

- **run_info** – The runtime information dictionary for the overall workflow
- **mpi_comm** – The MPI communicator to be used when running in parallel
- **mpi_root** – The MPI root rank when running in parallel

Additional parameters:

Parameters **reduce_memory_usage** – Boolean indicating whether we should reduce memory usage by pushing analysis data to file after an analysis has been completed. This reduces the amount of data we keep in memory but results in additional overhead for I/O and temporary disk storage.

Initalize the workflow driver

Parameters **analysis_objects** – A list of analysis objects to be executed

main()
Execute the analysis workflow

9.1.6 tools Package

omsi.tools	Package for collecting tools (e.g,.
omsi.tools.convertToOMSI	Tool used to convert img files to OpenMSI HDF5 files.
omsi.tools.run_analysis	Simple helper tool to run an analysis.
omsi.tools.run_workflow	Simple helper tool to run a workflow.
omsi.tools.misc	Collection of miscellaneous tools.
omsi.tools.misc.create_peak_cube_overview	Simple helper tool used to generate a set of PNG images for a global
omsi.tools.misc.make_thumb	Simple script to generate thumbnail images
omsi.tools.experimental	Collection of experimental tools and tools under development.

convertToOMSI Module

Tool used to convert img files to OpenMSI HDF5 files.

For usage information execute: python convertToOMSI –help

class omsi.tools.convertToOMSI.**ConvertFiles**
Bases: object

Class providing a number of functions for converting various file types to OMSI, including a number of helper functions related to the data conversion.

static check_format(*name*, *format_type*)
Helper function used to determine the file format that should be used

Parameters

- **name** – Name of the folder/file that we should read
- **format_type** – String indicating the format-option given by the user. If the format is not determined (i.e., "auto") then this function tries to determine the appropriate format. Otherwise this option is returned as is, as the user explicitly said which format should be used.

Returns String indicating the appropriate format. Returns None in case no valid option was found.

static convert_files()
Convert all files in the given list of files with their approbriate conversion options

static create_dataset_list(*input_filenames*, *format_type=None*, *data_region_option='split+merge'*)
Based on the list of input_filenames, generate the ConvertSettings.dataset_list, which contains a dictionary describing each conversion job

Parameters

- **input_filenames** – List of names of files to be converted.
- **format_type** – Define which file-format should be used. Default value is 'auto' indicating the function should determine for each file the format to be used. See also ConvertSettings.available_formats parameter.
- **data_region_option** – Define how different regions defined for a file should be handled. E.g., one may want to split all regions into indiviudal datasets ('split'), merge all regions into a single dataset ('merge'), or do both ('split+merge'). See also the ConvertSettings.available_region_options parameter for details. By default the function will do 'split+merge'.

Returns

List of dictionaries describing the various conversion jobs. Each job is described by a dict with the following keys:

- 'basename' : The base name of the file or directory with the data
- 'format' : The data format to be used
- 'dataset' : The index of the dataset to be converted if the input stores multiple data cubes
- 'region' : The index of the region to be converted if the input defines multiple regions
- 'exp' : One of 'previous' or 'new', defining whether a new experiment should be created or whether the experiment from the previous conversion(s) should be reused.

static suggest_chunking(*xsize*, *ysize*, *mzsize*, *dtype*, *print_results=False*)
Helper function used to suggest god chunking strategies for a given data cube

Parameters

- **xsize** – Size of the dataset in x.
- **ysize** – Size o the dataset in y.
- **mzsize** – Size of the dataset in mz.
- **print_results** – Print the results to the console.

Returns

Three tuples:

- `spectrum_chunk` : The chunking to be used to optimize selection of spectra.
- `slice_chunk` : The chunking to be used to optimize selection of image slices.
- `balanced_chunk` : The chunking that would provide a good balance in performance for different selection strategies.

static suggest_chunkings_for_files(*in_dataset_list*)
Helper function used to suggest good chunking strategies for a given set of files.

Parameters **in_dataset_list** – Python list of dictionaries describing the settings to be used for the file conversion

Returns This function simply prints results to standard-out but does not return anything.

static **write_data**(*input_file*, *data*, *data_io_option='spectrum'*, *chunk_shape=None*, *write_progress=True*)

Helper function used to implement different data write options.

Parameters

- **input_file** – The input data file
- **data** – The output dataset (either an h5py dataset or omsi_file_msidata object.
- **data_io_option** – String indicating the data write method to be used. One of:
  - `spectrum`: Write the data one spectrum at a time
  - `all` : Write the complete dataset at once.
  - `chunk` : Write the data one chunk at a time.
- **chunk_shape** – The chunking used by the data. Needed to decide how the data should be written when a chunk-aligned write is requested.
- **write_progress** (*bool*) – Write progress in % to standard out while data is being written.

class omsi.tools.convertToOMSI.**ConvertSettings**

Bases: object

This class is used specify the settings for the data conversion

add_file_to_db = True

auto_chunk = True

available_error_options = ['terminate-and-cleanup', 'terminate-only', 'continue-on-error']

available_formats = {'bruckerflex_file': <class 'omsi.dataformat.bruckerflex_file.bruckerflex_file'>, 'img_file': <cla

available_io_options = ['chunk', 'spectrum', 'all']

available_region_options = ['split', 'merge', 'split+merge']

check_add_nersc = True

chunks = (4, 4, 2048)

compression = 'gzip'

compression_opts = 4

dataset_list = []

Parameters **dataList** – List of python dictionaries describing specific conversion settings for each conversion task. Each dictionary contains the following keys:

- 'basename' : Name of the file to be converted
- 'format' : File format to be used (see ConvertSettings.available_formats)
- 'exp' : Indicate the experiment the dataset should be stored with. Valid values are
  - 'new' : Generate a new experiment for the dataset
  - 'previous' : Use the same experiment as used for the previous dataset
  - 1, 2,3... : Integer value indicating the index of the experiment to be used.

•'region' : Optional key with index of the region to be converted. None to merge all regions.

- 'dataset' : Optional key with index of the dataset to be converted.
- 'omsi_object': Optional key used to save a pointer to the omsi data object with the converted data
- 'dependencies': Additional dependencies that should be added for the dataset

db_server_url = 'https://openmsi.nersc.gov/'

email_error_recipients = []

email_success_recipients = []

error_handling = 'terminate-and-cleanup'

execute_fpg = True

execute_fpl = False

execute_nmf = True

execute_ticnorm = False

file_user = 'oruebel'

format_option = None

generate_thumbnail = False

generate_xdmf = False

io_block_size_limit = 524288000

io_option = 'spectrum_to_image'

job_id = None

metadata = {}

nmf_num_component = 20

nmf_num_iter = 2000

nmf_timeout = 600

nmf_tolerance = 0.0001

nmf_use_raw_data = False

omsi_output_file = None

classmethod parse_input_args (*argv*)
Process input parameters and define the script settings.

Parameters **argv** – The list of input arguments

Returns

This function returns the following four values:

- 'input_error' : Boolean indicating whether an error has occurred during the processing of the inputs
- 'inputWarning' : Boolean indicating whether a warning occurred during the processing of the inputs
- 'output_filename' : Name for the output HDF5 file
- 'input_filenames' : List of strings indicating the list of input filenames

classmethod print_help()
Function used to print the help for this script

recorded_warnings = []

region_option = 'split+merge'

suggest_file_chunkings = False

user_additional_chunks = []

omsi.tools.convertToOMSI.**main**(*argv=None*)
The main function defining the control flow for the conversion

run_analysis Module

Simple helper tool to run an analysis. This is essentially just a short-cut to the omsi/workflow/analysis_driver/omsi_cl_diver module

run_workflow Module

Simple helper tool to run an analysis. This is essentially just a short-cut to the omsi/workflow/analysis_driver/omsi_cl_diver module

Subpackages

tools.experimental Package

tools.experimental Package Collection of experimental tools and tools under development.

tools.misc Package

tools.misc Package Collection of miscellaneous tools.

make_thumb Module Simple script to generate thumbnail images

omsi.tools.misc.make_thumb.**main**(*argv=None*)
Then main function

create_peak_cube_overview Module Simple helper tool used to generate a set of PNG images for a global peak analysis (one per global peak) as well as a LaTeX document that summarizes all the images in a single document.

NOTE: The module will try to build the LaTeX document using pdflatex, i.e, it is assumed that pdflatex is available.

omsi.tools.misc.create_peak_cube_overview.**main**(*argv=None*)
Then main function

omsi.tools.misc.create_peak_cube_overview.**print_help**()
Print the user help information to standard out.

9.1.7 examples Package

omsi.examples	Package with a collection of various misc.

simple_viewer Module

Simple viewer for OpenMSI data

class omsi.examples.simple_viewer.**MyViewer**(*data*, *mzdata*)
Create a simple viewer with image of the data and a cruve plot for a spectrum.

Parameters

- **data** – Reference to the hdf5 dataset of the image
- **mzdata** – mz values of the instrument to be displayed as axis in the curve plot. may be None in case the mz data is unknown

omsi.examples.simple_viewer.**main**(*argv=None*)
Then main function

testHDF5Optimization Module

Simple test script used to test the performance of different HDF5 optimizations (using chunking) to improve the performance of hyperslap selections

omsi.examples.testHDF5Optimization.**generateTestFile**(*omsiOutFile*, *xdim*, *ydim*, *zdim*, *xchunk*, *ychunk*, *zchunk*)

omsi.examples.testHDF5Optimization.**main**(*argv=None*)
Then main function

omsi.examples.testHDF5Optimization.**printHelp**()
Print the help explaining the usage of testHDF5Optimiation

testHDF5Optimization_alignedWrite Module

omsi.examples.testHDF5Optimization_alignedWrite.**generateTestFile**(*omsiOutFile*, *xdim*, *ydim*, *zdim*, *xchunk*, *ychunk*, *zchunk*)

omsi.examples.testHDF5Optimization_alignedWrite.**main**(*argv=None*)
Then main function

omsi.examples.testHDF5Optimization_alignedWrite.**printHelp**()
Print the help explaining the usage of testHDF5Optimiation

test_multiprocess_slice Module

omsi.examples.test_multiprocess_slice.**create_process**(*argv*)

omsi.examples.test_multiprocess_slice.**generateBaseTestFile**(*omsiOutFile*, *xdim*, *ydim*, *zdim*)

omsi.examples.test_multiprocess_slice.**generateChunkedTestFile**(*omsiOutFile*, *xdim*, *ydim*, *zdim*, *xchunk*, *ychunk*, *zchunk*, *compress=False*, *donorFile='/project/projectdirs/openmsi/omsi_d*

omsi.examples.test_multiprocess_slice.**main**(*argv=None*)
Then main function

omsi.examples.test_multiprocess_slice.**sliceSelect**(*args*)

omsi.examples.test_multiprocess_slice.**spectraSelect**(*args*)

test_par Module

omsi.examples.test_par.**create_process**(*argv*)

omsi.examples.test_par.**generateBaseTestFile**(*omsiOutFile*, *xdim*, *ydim*, *zdim*)

omsi.examples.test_par.**generateChunkedTestFile**(*omsiOutFile*, *xdim*, *ydim*, *zdim*, *xchunk*, *ychunk*, *zchunk*, *compress=False*, *donorFile='/project/projectdirs/openmsi/omsi_data/old/TEST.h5'*)

omsi.examples.test_par.**main**(*argv=None*)
Then main function

omsi.examples.test_par.**sliceSelect**(*args*)

omsi.examples.test_par.**spectraSelect**(*args*)

test_peakcube Module

omsi.examples.test_peakcube.**main**(*argv=None*)
Then main function

omsi.examples.test_peakcube.**printHelp**()

testhdf5_file_read Module

Simple test script used to test the performance of different HDF5 optimizations (using chunking) to improve the performance of hyperslap selections

omsi.examples.testhdf5_file_read.**main**(*argv=None*)
Then main function

omsi.examples.testhdf5_file_read.**printHelp**()
Print the help explaining the usage of testHDF5Optimiation

9.1.8 templates Package

omsi.templates	This package provides a collection of code templates to ease the development of ad
omsi.templates.analysis_template	Template intended to help with the development of new analysis modules.

templates Package

This package provides a collection of code templates to ease the development of additional components, e.g., analysis modules. As such, this package is NOT intended for direct usage but is rather just a library of code templates.

analysis_template Module

Template intended to help with the development of new analysis modules.

class omsi.templates.analysis_template.**analysis_template**(*name_key='undefined'*)
Bases: *omsi.analysis.base.analysis_base*

Template intended to help with the development of new analysis classes.

Search for EDIT_ME to find locations that need to be changed.

EDIT_ME Search for analysis_template and replace it with your classname throughout

EDIT_ME Replace this doc-string with your class documentation

Initalize the basic data members

execute_analysis()
EDIT_ME Implement this function to implement the execution of the actual analysis.

This function may not require any input parameters. All input parameters are recoded in the parameters and dependencies lists and should be retrieved from there, e.g, using basic slicing self[paramName]

EDIT_ME Remove this comment and replace it with your own documentation. Describe what your analysis does and how a user can use it. Note, a user will call the function execute(...) which takes care of storing parameters, collecting execution data etc., so that you only need to implement your analysis, the rest is taken care of by analysis_base.

Keyword Arguments:

Parameters **mydata** – ...

Returns This function may return any developer-defined data. Note, all output that should be recorded must be put into the data list.

groups = None
EDIT_ME

Add a list of names of input parameters for your analysis using the self.add_add_parameter.

For parameters that define n-dimension arrays you should specify the dtypes['ndarray'] as dtype. This will allow discovery of dependencies and proper function with the analysis drivers. Other available dtypes include standard built-ins, e.g, int, float etc. See self.get_default_dtypes() for details.

It is also recommended to organize parameters into groups using the default set of groups, e.g., groups['input'], groups['settings'], groups['stop'].

classmethod v_qmz(*analysis_object*, *qslice_viewer_option=0*, *qspectrum_viewer_option=0*)
Get the mz axes for the analysis

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **qslice_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qslice URL pattern.

- **qspectrum_viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them for the qspectrum URL pattern.

Returns

The following four arrays are returned by the analysis:

- mz_spectra : Array with the static mz values for the spectra.
- label_spectra : Lable for the spectral mz axis
- mz_slice : Array of the static mz values for the slices or None if identical to the mz_spectra.
- label_slice : Lable for the slice mz axis or None if identical to label_spectra.

classmethod v_qslice(*analysis_object*, *z*, *viewer_option=0*)

Get 3D analysis dataset for which z-slices should be extracted for presentation in the OMSI viewer

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **z** – Selection string indicting which z values should be selected.
- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns numpy array with the data to be displayed in the image slice viewer. Slicing will be performed typically like [:,:,zmin:zmax].

classmethod v_qslice_viewer_options(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qslice. The default implementation tries to take care of handling the spectra retrieval for all the depencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

Parameters **analysis_object** – The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decision based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

Returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qslice requests (i.e., v_qslice(...) is not available).

classmethod v_qspectrum(*analysis_object*, *x*, *y*, *viewer_option=0*)

Get from which 3D analysis spectra in x/y should be extracted for presentation in the OMSI viewer

Developer Note: h5py currently supports only a single index list. If the user provides an index-list for both x and y, then we need to construct the proper merged list and load the data manually, or if the data is small enough, one can load the full data into a numpy array which supports mulitple lists in the selection.

Parameters

- **analysis_object** – The omsi_file_analysis object for which slicing should be performed
- **x** – x selection string
- **y** – y selection string

- **viewer_option** – If multiple default viewer behaviors are available for a given analysis then this option is used to switch between them.

Returns

The following two elemnts are expected to be returned by this function :

1. 1D, 2D or 3D numpy array of the requested spectra. NOTE: The mass (m/z) axis must be the last axis. For index selection x=1,y=1 a 1D array is usually expected. For indexList selections x=[0]&y=[1] usually a 2D array is expected. For ragne selections x=0:1&y=1:2 we one usually expects a 3D array.
2. None in case that the spectra axis returned by v_qmz are valid for the returned spectrum. Otherwise, return a 1D numpy array with the m/z values for the spectrum (i.e., if custom m/z values are needed for interpretation of the returned spectrum).This may be needed, e.g., in cases where a per-spectrum peak analysis is performed and the peaks for each spectrum appear at different m/z values.

classmethod v_qspectrum_viewer_options(*analysis_object*)

Get a list of strings describing the different default viewer options for the analysis for qspectrum. The default implementation tries to take care of handling the spectra retrieval for all the dependencies but can naturally not decide how the qspectrum should be handled by a derived class. However, this implementation is often called at the end of custom implementations to also allow access to data from other dependencies.

param analysis_object The omsi_file_analysis object for which slicing should be performed. For most cases this is not needed here as the support for slice operations is usually a static decission based on the class type, however, in some cases additional checks may be needed (e.g., ensure that the required data is available).

returns List of strings indicating the different available viewer options. The list should be empty if the analysis does not support qspectrum requests (i.e., v_qspectrum(...) is not available).

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Symbols

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