
pyCOMPS

Institute for Disease Modeling

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The COmputational Modeling Platform Service (COMPS) is an online tool that provides for submitting, running, and managing computational simulations on high-performance computing clusters (HPC).

pyCOMPS is a Python package for interoperability with the COMPS REST API. It can be used as an interface for other tools such as idmtools or from standalone custom scripts.

COMPS PACKAGE

1.1 Subpackages

1.1.1 COMPS.Data package

Subpackages

COMPS.Data.WorkItems package

Submodules

COMPS.Data.WorkItems.BuilderWorkItem module

```
class COMPS.Data.WorkItems.BuilderWorkItem.BuilderWorkItem(name,          environ-
                                                             ment_name, descrip-
                                                             tion=None)

Bases: COMPS.Data.WorkItem.WorkItem
```

Submodules

COMPS.Data.AssetCollection module

```
class COMPS.Data.AssetCollection.AssetCollection
Bases: COMPS.Data.TaggableEntity.TaggableEntity, COMPS.Data.
SerializableEntity.SerializableEntity
```

Represents a collection of Assets.

Once saved, an AssetCollection is immutable, other than modifying tags. It contains various properties accessible by getters:

- id
- date_created

It also contains “child objects” (which must be specifically requested for retrieval using the QueryCriteria.select_children() method of QueryCriteria):

- tags
- assets

property id

property `date_created`

property `tags`

property `assets`

classmethod `get` (*id=None, query_criteria=None*)

Retrieve one or more AssetCollections.

Parameters

- **id** – The id (str or UUID) of the AssetCollection to retrieve
- **query_criteria** – A QueryCriteria object specifying basic property filters and tag-filters to apply to the set of AssetCollections returned, as well as which properties and child-objects to fill for the returned AssetCollections

Returns An AssetCollection or list of AssetCollections (depending on whether ‘id’ was specified) with basic properties and child-objects assigned as specified by ‘query_criteria’

refresh (*query_criteria=None*)

Update properties of an existing AssetCollection from the server.

Since AssetCollections are mostly immutable, this is usually to retrieve/update fields or child-objects that weren’t retrieved initially (e.g. assets).

Parameters **query_criteria** – A QueryCriteria object specifying which properties and child-objects to refresh on the AssetCollection

save (*return_missing_files=False, upload_files_callback=<function AssetCollection.<lambda>>*)

Save a single AssetCollection. An id is automatically assigned upon successful save.

When the AssetCollection contains a large number or large total size of new assets that need to be uploaded, this may be done in multiple “chunks”. This allows saving of arbitrarily-large AssetCollections while avoiding potential timeouts due to long processing time on the server.

Parameters

- **return_missing_files** – A boolean that determines the behavior when the AssetCollection being saved contains an AssetCollectionFile to be saved by md5 checksum (i.e. without uploading the data) that is not yet in COMPS. If true, when there are such files, return an array of UUIDs representing the md5 checksums of the missing files. If false, raise an error when there are any such files.
- **upload_files_callback** – Callback to call whenever a batch of assets completes uploading. Default behavior is to print a single ‘.’ to the console. If the callback supplied takes 1 argument, the number of assets saved so far will be passed when it is called.

add_asset (*assetcollectionfile, file_path=None, data=None, upload_callback=<function AssetCollection.<lambda>>*)

Add an AssetCollectionFile to an AssetCollection.

The contents of the file to add can be specified either by providing a path to the file or by providing the actual data as a byte-array. Alternately, if the file/data is already in COMPS, you can skip uploading it again and just provide an AssetCollectionFile that contains the md5 checksum of the data.

If the asset exceeds `AssetManager.large_asset_upload_threshold` bytes in size, the asset will be uploaded immediately, separately from the saving of the main AssetCollection. This allows saving of arbitrarily-large assets while avoiding potential timeouts or having to start from scratch in case the upload is interrupted by network issues.

NOTE: this can only be called for not-yet-saved AssetCollections, since AssetCollections are immutable once saved, other than modifying tags.

NOTE: providing both file/data and an md5 is considered invalid, as providing the md5 implies the caller knows the file/data is already in COMPS and doesn't need to be uploaded again.

Parameters

- **assetcollectionfile** – An AssetCollectionFile containing the metadata for the file to add.
- **file_path** – The path to the file to add.
- **data** – The actual bytes of data to add.
- **upload_callback** – Callback to call whenever a large asset upload completes saving of a chunk of the asset. Default behavior is to print a single '.' to the console. If the callback supplied takes 1 argument, the number of bytes saved so far will be passed when it is called.

retrieve_as_zip()

Retrieve assets associated with this AssetCollection as a single zip-file.

Returns returns a single byte-array of a zip-file.

static static_retrieve_as_zip(ac_id)

COMPS.Data.AssetCollectionFile module

```
class COMPS.Data.AssetCollectionFile.AssetCollectionFile(file_name=None, rel-
                                                         ative_path=None,
                                                         md5_checksum=None,
                                                         tags=None)
```

Bases: *COMPS.Data.AssetFile.AssetFile, COMPS.Data.TaggableEntity. TaggableEntity, COMPS.Data.SerializableEntity.SerializableEntity*

Represents a single Asset in an AssetCollection.

Once created, an AssetCollectionFile is immutable, other than modifying tags. It contains various properties accessible by getters:

- file_name
- relative_path
- md5_checksum
- length
- uri
- tags

The md5_checksum can be used as an id for the AssetCollectionFile.

property relative_path

property tags

COMPS.Data.AssetFile module

COMPS.Data.AssetFile.get_media_type_from_filename(filename)

class COMPS.Data.AssetFile.AssetFile(file_name, md5_checksum=None)

Bases: *COMPS.Data.SerializableEntity.SerializableEntity*

A base-type for all files associated with certain entity-types. This includes AssetCollectionFile (associated with an AssetCollection), SimulationFile (associated with a Simulation), and WorkItemFile (associated with a WorkItem).

This is used only for adding properties to these file-types, and shouldn't be created directly (should probably be an ABC).

property file_name

property md5_checksum

property length

property uri

retrieve()

COMPS.Data.AssetManager module

COMPS.Data.AssetManager.retrieve_asset_files(asset_files, as_zip=False)

COMPS.Data.AssetManager.retrieve_output_file_info(entity_type, entity_id, paths,
job=None)

COMPS.Data.AssetManager.retrieve_output_files_from_info(entity_type, entity_id,
metadata, job=None,
as_zip=False)

COMPS.Data.AssetManager.retrieve_partial_output_file_from_info(metadata,
startbyte, end-
byte=None,
actual-
range=None)

Retrieve part of an output file from a Simulation or WorkItem.

Parameters

- **metadata** – An OutputFileMetadata object representing the output files to retrieve; this is likely obtained by calling the retrieve_output_file_info() method on Simulation or WorkItem.
- **startbyte** – An integer representing the first byte in the request range, or if negative, the number of bytes at the end of the file to return (in which case, endbyte must be None).
- **endbyte** – An integer representing the last byte in the request range. If this value is None and startbyte is positive, this represents the end of the file.
- **actualrange** – An optional list argument which, if passed, will contain the start byte, end byte, and total file-size upon return. This is useful if requesting “the last N bytes in the file” or “from byte N to the end” in order to know the exact bytes which were returned.

Returns A byte-array of the partial output file retrieved.

COMPS.Data.AssetManager.upload_large_asset(checksum, datastream, sta-
tus_callback=None)

```

class COMPS.Data.AssetManager.EntityType(value)
    Bases: enum.Enum

    An enumeration.

    Simulations = 0

    WorkItems = 1

```

COMPS.Data.AssetType module

```

class COMPS.Data.AssetType.AssetType(value)
    Bases: enum.Enum

    Enumeration of various asset types served by the COMPS asset service.

    Linked = 0

    Output = 1

```

COMPS.Data.BaseEntity module

```

class COMPS.Data.BaseEntity.EntityType(name, article, has_state)
    Bases: tuple

    property article
        Alias for field number 1

    property has_state
        Alias for field number 2

    property name
        Alias for field number 0

COMPS.Data.BaseEntity.get_entity_type(cls)

```

COMPS.Data.CommissionableEntity module

```

class COMPS.Data.CommissionableEntity.CommissionableEntity
    Bases: object

    commission()
        Commission an entity.

        If called on a Suite/Experiment, this attempts to commission all contained Simulations currently in SimulationState.Created. If called on a Simulation, this attempts to commission that Simulation. Only applicable if it is currently in SimulationState.Created. If called on a WorkItem, this attempts to commission that WorkItem. Only applicable if it is currently in WorkItemState.Created.

    cancel()
        Cancel a running entity.

        If called on a Suite/Experiment, this attempts to cancel all contained Simulations currently in an 'active' state:
        

- SimulationState.CommissionRequested
- SimulationState.Provisioning

```

- `SimulationState.Commissioned`
- `SimulationState.Running`
- `SimulationState.Retry`

If called on a `Simulation`, this attempts to commission that `Simulation`. Only applicable if it is currently in an ‘active’ state; see above. If called on a `WorkItem`, this attempts to commission that `WorkItem`. Only applicable if it is currently in an ‘active’ state:

- `WorkItemState.CommissionRequested`
- `WorkItemState.Commissioned`
- `WorkItemState.Validating`
- `WorkItemState.Running`
- `WorkItemState.Waiting`
- `WorkItemState.ResumeRequested`
- `WorkItemState.Resumed`

delete (*expire_now=False*)

“Soft-delete” this entity.

This entity record and all associated files, etc, will be marked for deletion in COMPS. They will remain for some period of time before being permanently deleted, but will no longer be returned by the COMPS service or visible in the UI.

If called on a `Suite/Experiment`, this delete also applies to all contained `Experiments/Simulations`.

Parameters `expire_now` – If this is set to `True`, this entity will be eligible for permanent deletion immediately (though depending on deletion activity in the system, it may still be a while before it’s fully deleted).

COMPS.Data.Configuration module

```
class COMPS.Data.Configuration.Configuration(environment_name=None,          simu-  
                                             lation_input_args=None,          work-  
                                             ing_directory_root=None,  
                                             executable_path=None,  
                                             node_group_name=None,          max-  
                                             imum_number_of_retries=None,  
                                             priority=None,          min_cores=None,  
                                             max_cores=None, exclusive=None, as-  
                                             set_collection_id=None)
```

Bases: `COMPS.Data.SerializableEntity.SerializableEntity`

Configuration properties associated with a `Suite`, `Experiment`, or `Simulation`.

A `Configuration` object is an immutable object containing various properties accessible by getters:

- `environment_name`
- `simulation_input_args`
- `working_directory_root`
- `executable_path`
- `node_group_name`

- maximum_number_of_retries
- priority
- min_cores
- max_cores
- exclusive
- asset_collection_id

Properties of a Configuration associated with a Simulation will override properties of a Configuration associated with an Experiment, either of which will override properties of a Configuration associated with a Suite.

No properties are required at any given level in the Suite/Experiment/Simulation hierarchy, but in order to create and run a simulation, at least the environment_name and executable_name must be specified somewhere in the hierarchy.

property environment_name

property simulation_input_args

property working_directory_root

property executable_path

property node_group_name

property maximum_number_of_retries

property priority

property min_cores

property max_cores

property exclusive

property asset_collection_id

COMPS.Data.Experiment module

class COMPS.Data.Experiment.**Experiment** (*name, suite_id=None, description=None, configuration=None*)

Bases: *COMPS.Data.TaggableEntity.TaggableEntity, COMPS.Data.CommissionableEntity.CommissionableEntity, COMPS.Data.SerializableEntity.SerializableEntity*

Represents a grouping of Simulations.

Contains various basic properties accessible by getters (and, in some cases, +setters):

- id
- +suite_id
- +name
- +description
- owner
- date_created
- last_modified

Also contains “child objects” (which must be specifically requested for retrieval using the `QueryCriteria.select_children()` method of `QueryCriteria`):

- tags
- configuration

property id

property suite_id

property name

property description

property owner

property date_created

property last_modified

property tags

property configuration

classmethod `get` (*id=None, query_criteria=None*)

Retrieve one or more Experiments.

Parameters

- **id** – The id (str or UUID) of the Experiment to retrieve
- **query_criteria** – A `QueryCriteria` object specifying basic property filters and tag-filters to apply to the set of Experiments returned, as well as which properties and child-objects to fill for the returned Experiments

Returns An Experiment or list of Experiments (depending on whether ‘id’ was specified) with basic properties and child-objects assigned as specified by ‘query_criteria’

refresh (*query_criteria=None*)

Update properties of an existing Experiment from the server.

Parameters **query_criteria** – A `QueryCriteria` object specifying which properties and child-objects to refresh on the Experiment

get_simulations (*query_criteria=None*)

Retrieve Simulations contained in this Experiment.

Parameters **query_criteria** – A `QueryCriteria` object specifying basic property filters and tag-filters to apply to the set of Simulations returned, as well as which properties and child-objects to fill for the returned Simulations

Returns A list of Simulations with basic properties and child-objects assigned as specified by ‘query_criteria’

save ()

Save a single Experiment. If it’s a new Experiment, an id is automatically assigned.

COMPS.Data.HpcJob module**class** COMPS.Data.HpcJob.HpcJobBases: *COMPS.Data.SerializableEntity.SerializableEntity*

Represents a single HPC Job.

Contains various properties accessible by getters:

- job_id
- job_state
- priority
- working_directory
- output_directory_size
- submit_time
- start_time
- end_time
- error_message
- configuration

HpcJobs are created by the COMPS Job Service, so they're read-only, used for tracking HPC Jobs.

Note: Tasks are not currently used in the COMPS system, so task properties are only there for future use.

property job_id**property** job_state**property** priority**property** working_directory**property** output_directory_size**property** submit_time**property** start_time**property** end_time**property** error_message**property** configuration**class** COMPS.Data.HpcJob.HpcState (*value*)Bases: *enum.Enum*

An enumeration representing the state of the job, as tracked by the HPC cluster.

NotSet = 0**Configuring** = 1**Submitted** = 2**Validating** = 4**ExternalValidation** = 8**Queued** = 16

```
Running = 32
Finishing = 64
Finished = 128
Failed = 256
Canceled = 512
Canceling = 1024
```

COMPS.Data.OutputFileMetadata module

```
class COMPS.Data.OutputFileMetadata.OutputFileMetadata
    Bases: COMPS.Data.SerializableEntity.SerializableEntity
    Metadata associated with output files served by the COMPS asset service.
    property length
    property friendly_name
    property path_from_root
    property url
    property mime_type
```

COMPS.Data.Priority module

```
class COMPS.Data.Priority.Priority(value)
    Bases: enum.Enum
    An enumeration representing the Priority to run at.
    Lowest = 0
    BelowNormal = 1
    Normal = 2
    AboveNormal = 3
    Highest = 4
```

COMPS.Data.QueryCriteria module

```
class COMPS.Data.QueryCriteria.QueryCriteria
    Bases: object
    A helper class to control query return-sets by filtering on basic properties and tags, as well as controlling which
    properties and child-objects to fill for returned objects.
    property fields
    property children
    property filters
    property tag_filters
```


property xparams**select** (*fields*)

Set which basic properties to fill for returned objects.

Parameters **fields** – A list of basic properties to fill; e.g. ['id','description'].

Returns A reference to this object so calls can be chained.

select_children (*children*)

Set which child objects to fill for returned objects.

Parameters **children** – A list of child objects to fill; e.g. ['tags','hpc_jobs'].

Returns A reference to this object so calls can be chained.

where (*filters*)

Set filter criteria for basic properties.

For string filter values, '~' is used for the “like”-operator (i.e. string-contains). For numeric filter values, standard arithmetic operators are allowed.

Parameters **filters** – A list of basic property filter-criteria; e.g. ['name~Test','state=Failed'].

Returns A reference to this object so calls can be chained.

where_tag (*tag_filters*)

Set filter criteria for tags.

For string filter values, '~' is used for the “like”-operator (i.e. string-contains). For numeric filter values, standard arithmetic operators are allowed.

Parameters **tag_filters** – A list of tag filter-criteria; e.g. ['Replicate=3','DiseaseType~Malaria'].

Returns A reference to this object so calls can be chained.

orderby (*orderby_field*)

Set which basic property to sort returned results-set by.

Parameters **orderby_field** – A string containing the basic property name to sort by. By default, ascending-sort is assumed, but descending-sort can be specified by appending a space and 'desc' to this argument; e.g. 'date_created desc'.

Returns A reference to this object so calls can be chained.

offset (*offset_num*)

Set the offset within the results-set to start returning results from.

Parameters **offset_num** – An int to specify offset within the results-set.

Returns A reference to this object so calls can be chained.

count (*count_num*)

Set the maximum number of results to return in the results-set.

Parameters **count_num** – An int to specify maximum number of results to return.

Returns A reference to this object so calls can be chained.

add_extra_params (*xp_dict*)

Set any parameters that aren't otherwise explicitly supported. This allows taking advantage of future potential changes to COMPS even if pyCOMPS support is not yet implemented or using an older version of pyCOMPS.

Parameters `xp_dict` – A dictionary of additional parameters and values to pass to the COMPS API.

Returns A reference to this object so calls can be chained.

`to_param_dict (ent_type)`

COMPS.Data.SerializableEntity module

`COMPS.Data.SerializableEntity.convert_if_string(o, fn)`

`COMPS.Data.SerializableEntity.json_entity(ignore_props=None)`

`COMPS.Data.SerializableEntity.json_entity_internal(cls)`

`COMPS.Data.SerializableEntity.json_property(rename_str=None)`

```
class COMPS.Data.SerializableEntity.json_property_internal (fget=None,
                                                            fset=None,
                                                            fdel=None,
                                                            doc=None)
```

Bases: `property`

`COMPS.Data.SerializableEntity.parse_ISO8601_date(date_str)`

`COMPS.Data.SerializableEntity.parse_namedtuple_from_dict(d)`

class `COMPS.Data.SerializableEntity.SerializableEntity`

Bases: `object`

classmethod `py2rest(obj)`

classmethod `rest2py(obj)`

static `convertToDict(obj, use_property_map=True, include_nulls=False, include_hidden_props=False)`

COMPS.Data.Simulation module

class `COMPS.Data.Simulation.Simulation(name, experiment_id=None, description=None, configuration=None)`

Bases: `COMPS.Data.TaggableEntity.TaggableEntity`, `COMPS.Data.CommissionableEntity.CommissionableEntity`, `COMPS.Data.SerializableEntity.SerializableEntity`

Represents a single simulation run.

Contains various basic properties accessible by getters (and, in some cases, +setters):

- `id`
- `+experiment_id`
- `+name`
- `+description`
- `owner`
- `date_created`
- `last_modified`

- state
- error_message

Also contains “child objects” (which must be specifically requested for retrieval using the `QueryCriteria.select_children()` method of `QueryCriteria`):

- tags
- configuration
- files
- hpc_jobs

property id

property experiment_id

property name

property description

property owner

property date_created

property last_modified

property state

property error_message

property tags

property configuration

property files

property hpc_jobs

classmethod get (*id=None, query_criteria=None*)

Retrieve one or more Simulations.

Parameters

- **id** – The id (str or UUID) of the Simulation to retrieve
- **query_criteria** – A `QueryCriteria` object specifying basic property filters and tag-filters to apply to the set of Simulations returned, as well as which properties and child-objects to fill for the returned Simulations

Returns A Simulation or list of Simulations (depending on whether ‘id’ was specified) with basic properties and child-objects assigned as specified by ‘query_criteria’

refresh (*query_criteria=None*)

Update properties of an existing Simulation from the server.

Parameters **query_criteria** – A `QueryCriteria` object specifying which properties and child-objects to refresh on the Simulation

save (*return_missing_files=False, save_semaphore=None*)

Save a single Simulation. If it’s a new Simulation, an id is automatically assigned.

Parameters **return_missing_files** – A boolean that determines the behavior when the Simulation being saved contains a `SimulationFile` to be saved by md5 checksum (i.e. without uploading the data) that is not yet in COMPS. If true, when there are such files, return an array

of UUIDs representing the md5 checksums of the missing files. If false, raise an error when there are any such files.

classmethod `get_save_semaphore()`

static `save_all(save_batch_callback=<function Simulation.<lambda>>, re-
turn_missing_files=False, save_semaphore=None)`

Batch-save all unsaved Simulations.

Simulations are saved in batches of at most ‘__max_sim_batch_count’ and with a maximum request size of ‘__max_sim_batch_request_size_kb’.

Parameters

- **save_batch_callback** – Callback to call whenever a request to save a batch of Simulations completes. Default behavior is to print a single ‘.’ to the console. If the callback supplied takes 1 argument, the number of Simulations saved so far will be passed when it is called.
- **return_missing_files** – A boolean that determines the behavior when any of the Simulations being saved contains a SimulationFile to be saved by md5 checksum (i.e. without uploading the data) that is not yet in COMPS. If true, when there are such files, return an array of UUIDs representing the md5 checksums of the missing files. If false, raise an error when there are any such files.

add_file (*simulationfile*, *file_path=None*, *data=None*, *upload_callback=<function Simulation.<lambda>>*)

Add a SimulationFile to a Simulation.

The contents of the file to add can be specified either by providing a path to the file or by providing the actual data as a byte-array. Alternately, if the file/data is already in COMPS, you can skip uploading it again and just provide a SimulationFile that contains the md5 checksum of the data.

If the file exceeds `AssetManager.large_asset_upload_threshold` bytes in size, the file will be uploaded immediately, separately from the saving of the main Simulation. This allows saving of arbitrarily-large files while avoiding potential timeouts or having to start from scratch in case the upload is interrupted by network issues.

NOTE: providing both file/data and an md5 is considered invalid, as providing the md5 implies the caller knows the file/data is already in COMPS and doesn’t need to be uploaded again.

Parameters

- **simulationfile** – A SimulationFile containing the metadata for the file to add.
- **file_path** – The path to the file to add.
- **data** – The actual bytes of data to add.
- **upload_callback** – Callback to call whenever a large file upload completes saving of a chunk of the file. Default behavior is to print a single ‘.’ to the console. If the callback supplied takes 1 argument, the number of bytes saved so far will be passed when it is called.

retrieve_output_files (*paths*, *job=None*, *as_zip=False*)

Retrieve output files associated with this Simulation.

This essentially combines the functionality of `retrieve_output_file_info()` and `retrieve_output_files_from_info()`, and can be used if user doesn’t care about specific metadata related to the files being retrieved.

Parameters

- **paths** – Partial paths (relative to the working directory) of the output files to retrieve. If ‘as_zip’ is true, this can be None/empty or not specified, and all output files will be included in the zip returned.
- **job** – The HpcJob associated with the given Simulation to retrieve assets for. If not specified, will default to the last HpcJob chronologically.
- **as_zip** – A boolean controlling whether the output files are returned individually or as a single zip-file (useful for attaching to an e-mail, etc).

Returns If ‘as_zip’ is true, returns a single byte-array of a zip-file; otherwise, returns a list of byte-arrays of the output files retrieved, in the same order as the ‘paths’ parameter.

retrieve_output_file_info (*paths, job=None*)

Retrieve OutputFileMetadata about output files associated with this Simulation.

Parameters

- **paths** – Partial paths (relative to the working directory) of the output files to retrieve. If None/empty or not specified, will default to return all output files.
- **job** – The HpcJob associated with the given Simulation to retrieve output files for. If not specified, will default to the last HpcJob chronologically.

Returns A list of OutputFileMetadata objects for the output files to retrieve, in the same order as the ‘paths’ parameter.

retrieve_output_files_from_info (*metadata, job=None, as_zip=False*)

Actually retrieve the output files associated with this Simulation.

Parameters

- **metadata** – A list of OutputFileMetadata objects representing the output files to retrieve associated with this Simulation.
- **job** – The HpcJob associated with the given Simulation to retrieve output files for. This should match the ‘job’ provided to the retrieve_output_file_info() call. If not specified, will default to the last HpcJob chronologically.
- **as_zip** – A boolean controlling whether the output files are returned individually or as a single zip-file (useful for attaching to an e-mail, etc).

Returns If ‘as_zip’ is true, returns a single byte-array of a zip-file; otherwise, returns a list of byte-arrays of the output files retrieved, in the same order as the ‘paths’ parameter.

static static_retrieve_output_files (*sim_id, paths, job=None, as_zip=False*)

class COMPS.Data.Simulation.SimulationState (*value*)

Bases: enum.Enum

An enumeration representing the current state of a Simulation

Created = 0

CommissionRequested = 1

Provisioning = 2

Commissioned = 3

Running = 4

Retry = 5

Succeeded = 6

```
Failed = 7
CancelRequested = 8
Canceled = 9
```

COMPS.Data.SimulationFile module

```
class COMPS.Data.SimulationFile.SimulationFile(file_name, file_type, description="",
                                                md5_checksum=None)
    Bases: COMPS.Data.AssetFile.AssetFile, COMPS.Data.SerializableEntity.
           SerializableEntity
```

Represents metadata for a Simulation file.

Contains various basic properties accessible by getters:

- file_name
- file_type
- description
- md5_checksum
- length
- uri

‘file_name’, ‘file_type’ and (optionally) ‘description’ must be set on creation.

```
property file_type
property description
```

COMPS.Data.Suite module

```
class COMPS.Data.Suite.Suite(name, description=None, configuration=None)
    Bases: COMPS.Data.TagableEntity.TagableEntity, COMPS.Data.
           CommissionableEntity.CommissionableEntity, COMPS.Data.SerializableEntity.
           SerializableEntity
```

Represents a grouping of Experiments.

Contains various basic properties accessible by getters (and, in some cases, +setters):

- id
- +name
- +description
- owner
- date_created
- last_modified

Also contains “child objects” (which must be specifically requested for retrieval using the `QueryCriteria.select_children()` method of `QueryCriteria`):

- tags
- configuration

```

property id
property name
property description
property owner
property date_created
property last_modified
property tags
property configuration
classmethod get (id=None, query_criteria=None)
    Retrieve one or more Suites.

```

Parameters

- **id** – The id (str or UUID) of the Suite to retrieve
- **query_criteria** – A QueryCriteria object specifying basic property filters and tag-filters to apply to the set of Suites returned, as well as which properties and child-objects to fill for the returned Suites

Returns A Suite or list of Suites (depending on whether ‘id’ was specified) with basic properties and child-objects assigned as specified by ‘query_criteria’

```

refresh (query_criteria=None)
    Update properties of an existing Suite from the server.

```

Parameters **query_criteria** – A QueryCriteria object specifying which properties and child-objects to refresh on the Suite

```

get_experiments (query_criteria=None)
    Retrieve Experiments contained in this Suite.

```

Parameters **query_criteria** – A QueryCriteria object specifying basic property filters and tag-filters to apply to the set of Experiments returned, as well as which properties and child-objects to fill for the returned Experiments

Returns A list of Experiments with basic properties and child-objects assigned as specified by ‘query_criteria’

```

save ()
    Save a single Suite. If it’s a new Suite, an id is automatically assigned.

```

COMPS.Data.TaggableEntity module

```

class COMPS.Data.TaggableEntity.TaggableEntity
    Bases: object

```

```

set_tags (tags)
    Set the tag key/value pairs associated with this entity.

```

If the entity has any existing tags, they will be replaced by the tags specified. If this is a new entity, tags will not be updated until the entity is saved, otherwise tags are updated immediately.

Parameters **tags** – A dictionary containing the key/value tag-string pairs to set.

merge_tags (*tags*)

Merge the given tag key/value pairs with existing tags for this entity.

Any tag keys that already have an existing tag with that key specified for the entity will have their values replaced by the value specified. Any tag keys that don't already exist for the entity will be added with their specified value.

Parameters **tags** – A dictionary containing the key/value tag-string pairs to merge.

delete_tags (*tags*)

Delete the given tag keys for this entity.

Parameters **tags** – A dictionary containing the key tag-strings to delete (Note: values are ignored).

class COMPS.Data.TaggableEntity.TagOperationMode (*value*)

Bases: enum.Enum

An enumeration.

Merge = 1

Replace = 2

Delete = 3

COMPS.Data.WorkItem module

class COMPS.Data.WorkItem.WorkItem (*name, worker, environment_name, description=None, as-set_collection_id=None, priority=None*)

Bases: *COMPS.Data.TaggableEntity.TaggableEntity, COMPS.Data.CommissionableEntity.CommissionableEntity, COMPS.Data.SerializableEntity.SerializableEntity*

Represents a single work-item.

Contains various basic properties accessible by getters (and, in some cases, +setters):

- id
- +name
- +description
- owner
- date_created
- last_modified
- state
- error_message
- worker
- environment_name
- host_name
- worker_instance_id
- priority
- working_directory

- `working_directory_size`
- `asset_collection_id`

Also contains “child objects” (which must be specifically requested for retrieval using the `QueryCriteria.select_children()` method of `QueryCriteria`):

- `tags`
- `files`
- `plugins`

property id

property name

property worker

property environment_name

property description

property owner

property date_created

property last_modified

property state

property error_message

property host_name

property worker_instance_id

property priority

property working_directory

property working_directory_size

property asset_collection_id

property tags

property files

property plugins

classmethod `get` (*id=None, query_criteria=None*)

Retrieve one or more WorkItems.

Parameters

- **id** – The id (str or UUID) of the WorkItem to retrieve
- **query_criteria** – A `QueryCriteria` object specifying basic property filters and tag-filters to apply to the set of WorkItems returned, as well as which properties and child-objects to fill for the returned WorkItems

Returns A WorkItem or list of WorkItems (depending on whether ‘id’ was specified) with basic properties and child-objects assigned as specified by ‘query_criteria’

refresh (*query_criteria=None*)

Update properties of an existing WorkItem from the server.

Parameters `query_criteria` – A QueryCriteria object specifying which properties and child-objects to refresh on the WorkItem

get_related_work_items (*relation_type=None*)

Get a list of WorkItems related to this WorkItem

Parameters `relation_type` – A RelationType object specifying which related WorkItems to filter to. If none is specified, all related WorkItems are returned.

get_related_suites (*relation_type=None*)

Get a list of Suites related to this WorkItem

Parameters `relation_type` – A RelationType object specifying which related Suites to filter to. If none is specified, all related Suites are returned.

get_related_experiments (*relation_type=None*)

Get a list of Experiments related to this WorkItem

Parameters `relation_type` – A RelationType object specifying which related Experiments to filter to. If none is specified, all related Experiments are returned.

get_related_simulations (*relation_type=None*)

Get a list of Simulations related to this WorkItem

Parameters `relation_type` – A RelationType object specifying which related Simulations to filter to. If none is specified, all related Simulations are returned.

get_related_asset_collections (*relation_type=None*)

Get a list of AssetCollections related to this WorkItem

Parameters `relation_type` – A RelationType object specifying which related AssetCollections to filter to. If none is specified, all related AssetCollections are returned.

add_related_work_item (*related_id, relation_type*)

Add a relationship between this WorkItem and a related WorkItem

Parameters

- **related_id** – The id (str or UUID) of the related WorkItem
- **relation_type** – The RelationType that describes how this WorkItem is related to the related WorkItem

add_related_suite (*related_id, relation_type*)

Add a relationship between this WorkItem and a related Suite

Parameters

- **related_id** – The id (str or UUID) of the related Suite
- **relation_type** – The RelationType that describes how this WorkItem is related to the related Suite

add_related_experiment (*related_id, relation_type*)

Add a relationship between this WorkItem and a related Experiment

Parameters

- **related_id** – The id (str or UUID) of the related Experiment
- **relation_type** – The RelationType that describes how this WorkItem is related to the related Experiment

add_related_simulation (*related_id, relation_type*)

Add a relationship between this WorkItem and a related Simulation

Parameters

- **related_id** – The id (str or UUID) of the related Simulation
- **relation_type** – The RelationType that describes how this WorkItem is related to the related Simulation

add_related_asset_collection (*related_id, relation_type*)

Add a relationship between this WorkItem and a related AssetCollection

Parameters

- **related_id** – The id (str or UUID) of the related AssetCollection
- **relation_type** – The RelationType that describes how this WorkItem is related to the related AssetCollection

save (*return_missing_files=False, save_semaphore=None*)

Save a single WorkItem. If it's a new WorkItem, an id is automatically assigned.

Parameters return_missing_files – A boolean that determines the behavior when the WorkItem being saved contains a WorkItemFile to be saved by md5 checksum (i.e. without uploading the data) that is not yet in COMPS. If true, when there are such files, return an array of UUIDs representing the md5 checksums of the missing files. If false, raise an error when there are any such files.

classmethod get_save_semaphore ()

static save_all (*save_batch_callback=<function WorkItem.<lambda>>, return_missing_files=False, save_semaphore=None*) *re-*

Batch-save all unsaved WorkItems.

WorkItems are saved in batches of at most '`__max_wi_batch_count`' and with a maximum request size of '`__max_wi_batch_request_size_kb`'.

Parameters

- **save_batch_callback** – Callback to call whenever a request to save a batch of WorkItems completes. Default behavior is to print a single '.' to the console. If the callback supplied takes 1 argument, the number of WorkItems saved so far will be passed when it is called.
- **return_missing_files** – A boolean that determines the behavior when any of the WorkItems being saved contains a WorkItemFile to be saved by md5 checksum (i.e. without uploading the data) that is not yet in COMPS. If true, when there are such files, return an array of UUIDs representing the md5 checksums of the missing files. If false, raise an error when there are any such files.

add_work_order (*file_path=None, data=None*)

Add the WorkOrder for a WorkItem.

The contents of the WorkOrder file to add can be specified either by providing a path to the file or by providing the actual data as a string.

Parameters

- **file_path** – The path to the work-order file to add.
- **data** – The actual bytes of work-order data to add.

add_file (*workitemfile, file_path=None, data=None, upload_callback=<function WorkItem.<lambda>>>*)

Add a WorkItemFile to a WorkItem.

The contents of the file to add can be specified either by providing a path to the file or by providing the actual data as a byte-array. Alternately, if the file/data is already in COMPS, you can skip uploading it again and just provide a `WorkItemFile` that contains the md5 checksum of the data.

If the file exceeds `AssetManager.large_asset_upload_threshold` bytes in size, the file will be uploaded immediately, separately from the saving of the main `WorkItem`. This allows saving of arbitrarily-large files while avoiding potential timeouts or having to start from scratch in case the upload is interrupted by network issues.

NOTE: providing both file/data and an md5 is considered invalid, as providing the md5 implies the caller knows the file/data is already in COMPS and doesn't need to be uploaded again.

Parameters

- **workitemfile** – A `WorkItemFile` containing the metadata for the file to add.
- **file_path** – The path to the file to add.
- **data** – The actual bytes of data to add.
- **upload_callback** – Callback to call whenever a large file upload completes saving of a chunk of the file. Default behavior is to print a single '.' to the console. If the callback supplied takes 1 argument, the number of bytes saved so far will be passed when it is called.

retrieve_output_files (*paths, as_zip=False*)

Retrieve output files associated with this `WorkItem`.

This essentially combines the functionality of `retrieve_output_file_info()` and `retrieve_output_files_from_info()`, and can be used if user doesn't care about specific metadata related to the files being retrieved.

Parameters

- **paths** – Partial paths (relative to the working directory) of the output files to retrieve. If 'as_zip' is true, this can be None/empty or not specified, and all output files will be included in the zip returned.
- **as_zip** – A boolean controlling whether the output files are returned individually or as a single zip-file (useful for attaching to an e-mail, etc).

Returns If 'as_zip' is true, returns a single byte-array of a zip-file; otherwise, returns a list of byte-arrays of the output files retrieved, in the same order as the 'paths' parameter.

retrieve_output_file_info (*paths*)

Retrieve `OutputFileMetadata` about output files associated with this `WorkItem`.

Parameters **paths** – Partial paths (relative to the working directory) of the output files to retrieve. If None/empty or not specified, will default to return all output files.

Returns A list of `OutputFileMetadata` objects for the output files to retrieve, in the same order as the 'paths' parameter.

retrieve_output_files_from_info (*metadata, as_zip=False*)

Actually retrieve the output files associated with this `WorkItem`.

Parameters

- **metadata** – A list of `OutputFileMetadata` objects representing the output files to retrieve associated with this `WorkItem`.
- **as_zip** – A boolean controlling whether the output files are returned individually or as a single zip-file (useful for attaching to an e-mail, etc).

Returns If 'as_zip' is true, returns a single byte-array of a zip-file; otherwise, returns a list of byte-arrays of the output files retrieved, in the same order as the 'paths' parameter.

static static_retrieve_output_files (*workitem_id, paths, as_zip=False*)

class COMPS.Data.WorkItem.WorkerOrPluginKey (*name, version*)

Bases: tuple

property name

Alias for field number 0

property version

Alias for field number 1

class COMPS.Data.WorkItem.WorkItemState (*value*)

Bases: enum.Enum

An enumeration representing the current state of a WorkItem

Created = 0

CommissionRequested = 5

Commissioned = 10

Validating = 30

Running = 40

Waiting = 50

ResumeRequested = 60

CancelRequested = 80

Canceled = 90

Resumed = 100

Canceling = 120

Succeeded = 130

Failed = 140

class COMPS.Data.WorkItem.RelationType (*value*)

Bases: enum.Enum

An enumeration representing the type of relationship for related entities

DependsOn = 0

Created = 1

COMPS.Data.WorkItemFile module

class COMPS.Data.WorkItemFile.WorkItemFile (*file_name, file_type, description="", md5_checksum=None*)

Bases: *COMPS.Data.AssetFile.AssetFile, COMPS.Data.SerializableEntity.SerializableEntity*

Represents metadata for a WorkItem file.

Contains various basic properties accessible by getters:

- *file_name*

- file_type
- description
- md5_checksum
- length
- uri

'file_name', 'file_type' and (optionally) 'description' must be set on creation.

property file_type

property description

1.2 Submodules

1.2.1 COMPS.AuthManager module

```
class COMPS.AuthManager.AuthManager(hoststring, verify_certs=False, credential_prompt=None)
```

Bases: object

Manage authentication to COMPS.

property username

property hoststring

property groups

property environments

has_auth_token()

get_auth_token()

clear_auth_token()

static **get_environment_macros**(*environment_name*)

Retrieve the environment macros for a COMPS environment.

This may be a somewhat temporary requirement until the Asset Service handles file dependencies more completely (allows uploads, etc).

Parameters *environment_name* – the COMPS environment to retrieve macros for

Returns a dictionary of environment macro key/value pairs

static **get_group_name_for_environment**(*environment_name*)

Retrieve the Group associated with a particular COMPS environment.

Parameters *environment_name* – the COMPS environment to retrieve the Group for

Returns a string of the Group name

1.2.2 COMPS.Client module

class COMPS.Client.Client

Bases: object

Client object for managing access to COMPS

classmethod auth_manager()

Retrieve the AuthManager.

Must be logged in first in, otherwise this raises a RuntimeError.

Returns the AuthManager instance

classmethod login(*hoststring*, *credential_prompt=None*)

Log in to the COMPS service.

The specified COMPS hoststring allows a couple points of flexibility:

- Secure vs. Unsecure - Specifying the protocol as http or https allows the user to control whether the SSL transport is used for requests. By default, https is used.
- Port - Specifying a particular port allows the user to control the port to communicate over for requests. By default, the standard port for the chosen protocol is used (i.e. 80 for http, 443 for https).

For example, the following are all valid formats:

- comps.idmod.org - uses secure https protocol over port 443.
- <http://internal.idmod.org> - uses unsecure http protocol over port 80.
- localhost:54321 - uses secure https protocol over port 54321.

Calling login() when already logged into a different host is invalid and will raise a RuntimeError. When already logged into the same host, nothing is done and the function returns immediately.

Parameters

- **hoststring** – the COMPS host to connect to
- **credential_prompt** – a CredentialPrompt object that controls how the user will supply their login credentials. By default, pyCOMPS will try to open a graphical prompt (TKCredentialPrompt) and fall back to console (ConsoleCredentialPrompt) if that fails.

classmethod logout(*hoststring=None*)

Log out of the COMPS service.

If logged in, this clears any cached credentials and nulls the AuthManager instance. Otherwise, you may pass a hoststring parameter to clear cached credentials for a particular COMPS host.

Parameters **hoststring** – the COMPS host to clear credentials for

classmethod post(*path*, *include_comps_auth_token=True*, *http_err_handle_exceptions=None*, ***kwargs*)

classmethod put(*path*, *include_comps_auth_token=True*, *http_err_handle_exceptions=None*, ***kwargs*)

classmethod get(*path*, *include_comps_auth_token=True*, *http_err_handle_exceptions=None*, ***kwargs*)

classmethod delete(*path*, *include_comps_auth_token=True*, *http_err_handle_exceptions=None*, ***kwargs*)

classmethod request(*method*, *path*, *include_comps_auth_token=True*, *http_err_handle_exceptions=None*, ***kwargs*)

```
classmethod raise_err_from_resp (resp)
```

1.2.3 COMPS.CredentialPrompt module

```
class COMPS.CredentialPrompt.CredentialPrompt
```

Bases: object

Abstract definition for our credential prompts.

```
abstract prompt ()
```

The prompt method will ask a user for COMPS username and password. It should return a duct containing the username and password keys and values :return:

```
class COMPS.CredentialPrompt.ConsoleCredentialPrompt
```

Bases: *COMPS.CredentialPrompt.CredentialPrompt*

A simple console based credential prompt

```
prompt ()
```

The prompt method will ask a user for COMPS username and password. It should return a duct containing the username and password keys and values :return:

```
class COMPS.CredentialPrompt.TKCredentialPrompt
```

Bases: *COMPS.CredentialPrompt.CredentialPrompt*

A TK based credential prompt

```
prompt ()
```

The prompt method will ask a user for COMPS username and password. It should return a duct containing the username and password keys and values :return:

```
COMPS.CredentialPrompt.get_credential_prompt ()
```

Determines the appropriate CredentialPrompt. If TK is available, we use that, otherwise we fallback to Console based login.

Returns CredentialPrompt factory

GLOSSARY

The following terms are used to describe processes, concepts, and the files, features, and functionality related to using COMPS.

asset collection Collection of user created input files, such as demographics, temperature, weather, and overlay files. These files are stored in COMPS and can be available for use by other users.

dashboard The COMPS dashboard provides an overview of computing cluster usage, including current and queued jobs. Resource management is simple due to the job-priority system used by the platform.

experiments Logical grouping of simulations. This allows for managing numerous simulations as a single unit or grouping.

multi-chart COMPS provides powerful charting functionality to visualize the output channels for simulations. A chart can include output for a single simulation or for multiple simulations. Viewing multiple simulations in a single chart (multi-chart) provides a fast, flexible way to filter simulations to view only data of interest.

suites Logical grouping of experiments. This allows for managing multiple experiments as a single unit or grouping.

work item Work item is used to build experiments and suites. It builds a set of simulations or groups of simulations, such as creating parameter sweeps. Work item defines how many simulations run at the start of the experiment to determine if the configuration settings are functional.

work order JSON formatted file used for the creation of a work item, in combination with a configuration file, and (optional) campaign and additional files.

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