signac Documentation

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Note: This is documentation for the **signac** *core package*, which is part of the signac framework. See here for a comprehensive introduction to the **signac** *framework*.

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CHAPTER 1

Contents

1.1 Installation

The recommended installation method for **signac** is via conda or pip. The software is tested for Python versions 2.7.x and 3.4+ and does not have any *hard* dependencies, i.e. there are no packages or libraries required to use the core **signac** functions. However, some extra features, such as the database integration require additional packages.

1.1.1 Install with conda

You can install **signac** via conda (available on the conda-forge channel), with:

```
$ conda install -c conda-forge signac
```

All additional dependencies will be installed automatically. To upgrade the package, execute:

```
$ conda update signac
```

1.1.2 Install with pip

To install the package with the package manager pip, execute

```
$ pip install signac --user
```

Note: It is highly recommended to install the package into the user space and not as superuser!

To upgrade the package, simply execute the same command with the --upgrade option.

```
$ pip install signac --user --upgrade
```

Consider installing optional dependencies:

```
$ pip install pymongo passlib bcrypt --user
```

1.1.3 Source Code Installation

Alternatively you can clone the git repository and execute the setup.py script to install the package.

```
git clone https://github.com/glotzerlab/signac.git
cd signac
python setup.py install --user
```

Consider installing optional dependencies.

1.1.4 Optional dependencies

Unless you install via conda, optional dependencies are not installed automatically. In case you want to use extra features that require external packages, you need to install these manually.

Extra features with dependencies:

MongoDB database backend required: pymongo

```
recommended: passlib, bcrypt
```

1.2 API Reference

This is the API for the **signac** (core) application.

1.2.1 Command Line Interface

Some core **signac** functions are—in addition to the Python interface—accessible directly via the \$ signac command.

For more information, please see \$ signac --help.

```
usage: signac [-h] [--debug] [--version] [-v] [-y]
              {init,project,job,statepoint,document,rm,move,clone,index,find,view,
⇒schema, shell, sync, import, export, update-cache, config}
signac aids in the management, access and analysis of large-scale
computational investigations.
positional arguments:
  {init, project, job, statepoint, document, rm, move, clone, index, find, view, schema, shell,
⇒sync,import,export,update-cache,config}
optional arguments:
                        show this help message and exit
 -h, --help
                        Show traceback on error for debugging.
  --debug
                       Display the version number and exit.
  -v, --verbosity
                      Set level of verbosity.
                        Answer all questions with yes. Useful for scripted
  -y, --yes
                        interaction.
```

1.2.2 The Project

class signac.Project(config=None)

The handle on a signac project.

Application developers should usually not need to directly instantiate this class, but use signac. $get_project()$ instead.

Attributes

Durate to the first of the second of the design of the second	Duild a lab accord in dec
<pre>Project.build_job_search_index(index[, _trust])</pre>	Build a job search index.
Project.build_job_statepoint_index([]	Build a statepoint index to identify jobs with specific
rroject.burra_job_statepoint_index([]	parameters.
Project.check([job_ids])	Check the project's workspace for corruption.
Project.clone(job[, copytree])	Clone job into this project.
Project.config	The project's configuration.
Project.create_access_module([filename,	Create the access module for indexing
master])	Create the access module for indexing
Project.create_linked_view([prefix,])	Create or update a persistent linked view of the selected
	data space.
<pre>Project.detect_schema([exclude_const,])</pre>	Detect the project's state point schema.
Project.doc	The document associated with this project.
Project.document	The document associated with this project.
Project.dump_statepoints(statepoints)	Dump the statepoints and associated job ids.
Project.export_to(target[, path, copytree])	Export all jobs to a target location, such as a directory
	or a (compressed) archive file.
Project.find_job_documents([filter])	Find all job documents in the project's workspace.
<pre>Project.find_job_ids([filter, doc_filter, index])</pre>	Find the job_ids of all jobs matching the filters.
Project.find_jobs([filter, doc_filter, index])	Find all jobs in the project's workspace.
Project.find_statepoints([filter,])	Find all statepoints in the project's workspace.
Project.fn(filename)	Prepend a filename with the project's root directory
	path.
Project.get_id()	Get the project identifier.
Project.get_statepoint(jobid[, fn])	Get the statepoint associated with a job id.
Project.groupby([key, default])	Groups jobs according to one or more statepoint param-
	eters.
Project.groupbydoc([key, default])	Groups jobs according to one or more document values.
Project.import_from([origin, schema, sync,	Import the data space located at origin into this project.
])	
Project.index([formats, depth, skip_errors,])	Generate an index of the project's workspace.
Project.isfile(filename)	True if a file with filename exists in the project's root
	directory.
Project.min_len_unique_id()	Determine the minimum length required for an id to be
	unique.
Project.num_jobs()	Return the number of initialized jobs.
Project.open_job([statepoint, id])	Get a job handle associated with a statepoint.
Project.read_statepoints([fn])	Read all statepoints from a file.
<pre>Project.repair([fn_statepoints, index, job_ids])</pre>	Attempt to repair the workspace after it got corrupted.
Project.reset_statepoint(job,	Reset the state point of job.
new_statepoint)	
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Project.root_directory()	Returns the project's root directory.	
Project.sync(other[, strategy, exclude,])	Synchronize this project with the other project.	
Project.update_cache()	Update the persistent state point cache (experimental).	
Project.update_statepoint(job, update[,	Update the statepoint of this job.	
])		
Project.workspace()	Returns the project's workspace directory.	
Project.write_statepoints([statepoints, fn,	Dump statepoints to a file.	
])		

class signac.Project(config=None)

Bases: object

The handle on a signac project.

Application developers should usually not need to directly instantiate this class, but use signac. get_project() instead.

```
FN_CACHE = '.signac_sp_cache.json.gz'
FN_DOCUMENT = 'signac_project_document.json'
FN_STATEPOINTS = 'signac_statepoints.json'
build_job_search_index (index, _trust=False)
    Build a job search index.
```

Parameters index (list) – A document index.

Returns A job search index based on the provided index.

Return type JobSearchIndex

build_job_statepoint_index (exclude_const=False, index=None)

Build a statepoint index to identify jobs with specific parameters.

This method generates pairs of state point keys and mappings of values to a set of all corresponding job ids. The pairs are ordered by the number of different values. Since state point keys may be nested, they are represented as a tuple. For example:

```
>>> for i in range(4):
        project.open_job({'a': i, 'b': {'c': i % 2}}).init()
. . .
. . .
>>> for key, value in project.build_job_statepoint_index():
       print (key)
        pprint.pprint(value)
. . .
('b', 'c')
defaultdict (<class 'set'>,
            {0: {'3a530c13bfaf57517b4e81ecab6aec7f',
                 '4e9a45a922eae6bb5d144b36d82526e4'},
             1: {'d49c6609da84251ab096654971115d0c',
                 '5c2658722218d48a5eb1e0ef7c26240b'}})
('a',)
defaultdict (<class 'set'>,
            {0: {'4e9a45a922eae6bb5d144b36d82526e4'},
             1: {'d49c6609da84251ab096654971115d0c'},
             2: {'3a530c13bfaf57517b4e81ecab6aec7f'},
             3: {'5c2658722218d48a5eb1e0ef7c26240b'}})
```

Values that are constant over the complete data space can be optionally ignored with the exclude_const argument set to True.

Parameters

- exclude_const (bool) Exclude entries that are shared by all jobs that are part of the index.
- index A document index.

Yields Pairs of state point keys and mappings of values to a set of all corresponding job ids.

check (job_ids=None)

Check the project's workspace for corruption.

Parameters job_ids – The ids of jobs to check, defaults to all jobs.

Raises JobsCorruptedError - When one or more jobs are identified as corrupted.

```
clone (job, copytree=<function copytree>)
```

Clone job into this project.

Create an identical copy of job within this project.

Parameters job (Job) – The job to copy into this project.

Returns The job instance corresponding to the copied job.

Return type Job

Raises *DestinationExistsError* – In case that a job with the same id is already initialized within this project.

config

The project's configuration.

```
create_access_module (filename=None, master=True)
```

Create the access module for indexing

This method generates the access module required to make this project's index part of a master index.

Parameters

- **filename** (*str*) The name of the access module file. Defaults to the standard name and should usually not be changed.
- master (bool) If True, add directives for the compilation of a master index when executing the module.

Returns The name of the created access module.

Return type str

```
create_linked_view (prefix=None, job_ids=None, index=None, path=None)
```

Create or update a persistent linked view of the selected data space.

Similar to $export_to()$, this function expands the data space for the selected jobs, but instead of copying data will create symbolic links to the individual job workspace directories. This is primarily uselful for browsing through the data space using a file-browser with human-interpretable directory paths.

By default, the paths of the view will be based on variable state point keys as part of the *implicit* schema of the selected jobs that we create the view for. For example, creating a linked view for a data space with schema

```
>>> print(project.detect_schema())
{
  'foo': 'int([0, 1, 2, ..., 8, 9], 10)',
}
```

by calling project.create_linked_view('my_view') will look similar to:

```
my_view/foo/0/job -> workspace/b8fcc6b8f99c56509eb65568922e88b8
my_view/foo/1/job -> workspace/b6cd26b873ae3624653c9268deff4485
...
```

It is possible to control the paths using the path argument, which behaves in the exact same manner as the equivalent argument for $export_to()$.

Note: The behavior of this function is almost equivalent to project.export_to('my_view', copytree=os.symlink) with the major difference, that view hierarchies are actually *updated*, that means no longer valid links are automatically removed.

Parameters

- **prefix** (str) The path where the linked view will be created or updated.
- job_ids If None (the default), create the view for the complete data space, otherwise only for the sub space constituted by the provided job ids.
- index A document index.
- path The path (function) used to structure the linked data space.

Returns A dict that maps the source directory paths, to the linked directory paths.

detect_schema (*exclude_const=False*, *subset=None*, *index=None*)

Detect the project's state point schema.

Parameters

- **exclude_const** (bool) Exclude all state point keys that are shared by all jobs within this project.
- **subset** A sequence of jobs or job ids specifying a subset over which the state point schema should be detected.
- index A document index.

Returns The detected project schema.

Return type signac.contrib.schema.ProjectSchema

doc

The document associated with this project.

Alias for document.

Returns The project document handle.

Return type JSONDict

document

The document associated with this project.

Returns The project document handle.

Return type JSONDict

dump_statepoints (statepoints)

Dump the statepoints and associated job ids.

Equivalent to:

```
{project.open_job(sp).get_id(): sp for sp in statepoints}
```

Parameters statepoints (iterable) - A list of statepoints.

Returns A mapping, where the key is the job id and the value is the statepoint.

Return type dict

```
export_to (target, path=None, copytree=None)
```

Export all jobs to a target location, such as a directory or a (compressed) archive file.

Use this function in combination with find_jobs() to export only a select number of jobs, for example:

```
project.find_jobs({'foo': 0}).export_to('foo_0.tar')
```

The path argument enables users to control how exactly the exported data space is to be expanded. By default, the path-function will be based on the *implicit* schema of the exported jobs. For example, exporting jobs that all differ by a state point key *foo* with project.export_to('data/'), the exported directory structure could look like this:

```
data/foo/0
data/foo/1
...
```

That would be equivalent to specifying path=lambda job: os.path.join('foo', job. sp.foo).

Instead of a function, we can also provide a string, where fields for state point keys are automatically formatted. For example, the following two path arguments are equivalent: "foo/{foo}" and "foo/{job.sp.foo}".

Any attribute of job can be used as a field here, so job.doc.bar, job._id, and job.ws can also be used as path fields.

A special $\{\{auto\}\}\$ field allows us to expand the path automatically with state point keys that have not been specified explicitly. So, for example, one can provide $path="foo/\{foo\}/\{\{auto\}\}\}"$ to specify that the path shall begin with $foo/\{foo\}/$, but is then automatically expanded with all other state point key-value pairs. How key-value pairs are concatenated can be controlled via the format-specifier, so for example, $path="\{\{auto:_\}\}"$ will generate a structure such as

```
data/foo_0
data/foo_1
...
```

Finally, providing path=False is equivalent to path="{job._id}".

See also:

Previously exported or non-signac data spaces can be imported with import_from().

Parameters

- **target** A path to a directory to export to. The target can not already exist. Besides directories, possible targets are tar-files (*.tar*), gzipped tar-files (*.tar.gz*), zip-files (*.zip*), bzip2-compressed files (*.bz2*), and xz-compressed files (*.xz*).
- path The path (function) used to structure the exported data space. This argument must either be a callable which returns a path (str) as a function of *job*, a string where fields are replaced using the job-state point dictionary, or *False*, which means that we just use the job-id as path. Defaults to the equivalent of {{auto}}.
- **copytree** The function used for the actualy copying of directory tree structures. Defaults to shutil.copytree(). Can only be used when the target is a directory.

Returns A dict that maps the source directory paths, to the target directory paths.

find_job_documents(filter=None)

Find all job documents in the project's workspace.

This method iterates through all jobs or all jobs matching the filter and yields each job's document as a dict. Each dict additionally contains a field 'statepoint', with the job's statepoint and a field '_id', which is the job's id.

Parameters filter (*mapping*) – If not None, only find job documents matching filter.

Yields Instances of dict.

Raises KeyError – If the job document already contains the fields '_id' or 'statepoint'.

find_job_ids (filter=None, doc_filter=None, index=None)

Find the job_ids of all jobs matching the filters.

The optional filter arguments must be a Mapping of key-value pairs and JSON serializable.

Note: Providing a pre-calculated index may vastly increase the performance of this function.

Parameters

- **filter** (Mapping) A mapping of key-value pairs that all indexed job statepoints are compared against.
- doc_filter A mapping of key-value pairs that all indexed job documents are compared against.
- index A document index.

Yields The ids of all indexed jobs matching both filters.

Raises

- **TypeError** If the filters are not JSON serializable.
- ValueError If the filters are invalid.
- RuntimeError If the filters are not supported by the index.

find_jobs (filter=None, doc_filter=None, index=None)

Find all jobs in the project's workspace.

The optional filter arguments must be a Mapping of key-value pairs and JSON serializable.

Note: Providing a pre-calculated index may vastly increase the performance of this function.

Parameters

- filter (Mapping) A mapping of key-value pairs that all indexed job statepoints are compared against.
- doc_filter A mapping of key-value pairs that all indexed job documents are compared against.

Yields Instances of Job

Raises

- **TypeError** If the filters are not JSON serializable.
- ValueError If the filters are invalid.
- **RuntimeError** If the filters are not supported by the index.

find_statepoints (*filter=None*, *doc_filter=None*, *index=None*, *skip_errors=False*) Find all statepoints in the project's workspace.

Parameters

- **filter** (*mapping*) If not None, only yield statepoints matching the filter.
- **skip_errors** (bool) Show, but otherwise ignore errors while iterating over the workspace. Use this argument to repair a corrupted workspace.

Yields statepoints as dict

fn (filename)

Prepend a filename with the project's root directory path.

Parameters filename (str) – The filename of the file.

Returns The joined path of project root directory and filename.

get_id()

Get the project identifier.

Returns The project id.

Return type str

Raises LookupError – If no project id could be determined.

classmethod get_project(root=None)

Find a project configuration and return the associated project.

Parameters root (*str*) – The project root directory. If no root directory is given, the next project found within or above the current working directory is returned.

Returns The project handle.

Raises LookupError – If no project configuration can be found.

get_statepoint (jobid, fn=None)

Get the statepoint associated with a job id.

The state point is retrieved from the internal cache, from the workspace or from a state points file.

Parameters

- **jobid** (str) A job id to get the statepoint for.
- **fn** (*str*) The filename of the file containing the statepoints, defaults to FN STATEPOINTS.

Returns The state point corresponding to jobid.

Return type dict

Raises

- **KeyError** If the state point associated with jobid could not be found.
- JobsCorruptedError If the state point manifest file corresponding to jobid is inaccessible or corrupted.

groupby (key=None, default=None)

Groups jobs according to one or more statepoint parameters. This method can be called on any JobsCursor such as the one returned by find_jobs() or by iterating over a project. Examples:

```
# Group jobs by statepoint parameter 'a'.
for key, group in project.groupby('a'):
    print(key, list(group))

# Find jobs where job.sp['a'] is 1 and group them
# by job.sp['b'] and job.sp['c'].
for key, group in project.find_jobs({'a': 1}).groupby(('b', 'c')):
    print(key, list(group))

# Group by job.sp['d'] and job.document['count'] using a lambda.
for key, group in project.groupby(
    lambda job: (job.sp['d'], job.document['count'])
):
    print(key, list(group))
```

If key is None, jobs are grouped by identity (by id), placing one job into each group.

Parameters

- **key** (str, iterable, or function) The statepoint grouping parameter(s) passed as a string, iterable of strings, or a function that will be passed one argument, the job.
- **default** A default value to be used when a given state point key is not present (must be sortable).

groupbydoc (key=None, default=None)

Groups jobs according to one or more document values. This method can be called on any JobsCursor such as the one returned by find_jobs() or by iterating over a project. Examples:

```
# Group jobs by document value 'a'.
for key, group in project.groupbydoc('a'):
    print(key, list(group))

# Find jobs where job.sp['a'] is 1 and group them
# by job.document['b'] and job.document['c'].
for key, group in project.find_jobs({'a': 1}).groupbydoc(('b', 'c')):
    print(key, list(group))

# Group by whether 'd' is a field in the job.document using a lambda.
for key, group in project.groupbydoc(lambda doc: 'd' in doc):
    print(key, list(group))
```

If key is None, jobs are grouped by identity (by id), placing one job into each group.

Parameters

- **key** (str, iterable, or function) The statepoint grouping parameter(s) passed as a string, iterable of strings, or a function that will be passed one argument, Job.document.
- default A default value to be used when a given state point key is not present (must be sortable).

import_from (origin=None, schema=None, sync=None, copytree=None)
Import the data space located at origin into this project.

This function will walk through the data space located at origin and will try to identify data space paths that can be imported as a job workspace into this project.

The schema argument expects a function that takes a path argument and returns a state point dictionary. A default function is used when no argument is provided. The default schema function will simply look for state point manifest files—usually named signac_statepoint.json—and then import all data located within that path into the job workspace corresponding to the state point specified in the manifest file.

Alternatively the schema argument may be a string, that is converted into a schema function, for example: Providing $foo/\{foo:int\}$ as schema argument means that all directories under foo/ will be imported and their names will be interpeted as the value for foo within the state point.

Tip: Use copytree=os.rename or copytree=shutil.move to move dataspaces on import instead of copying them.

Warning: Imports can fail due to conflicts. Moving data instead of copying may therefore lead to inconsistent states and users are advised to apply caution.

See also:

Export the project data space with export_to().

Parameters

- **origin** The path to the data space origin, which is to be imported. This may be a path to a directory, a zip-file, or a tarball archive.
- **schema** An optional schema function, which is either a string or a function that accepts a path as its first and only argument and returns the corresponding state point as dict.
- **copytree** Specify which exact function to use for the actual copytree operation. Defaults to shutil.copytree().

Returns A dict that maps the source directory paths, to the target directory paths.

index (formats=None, depth=0, skip_errors=False, include_job_document=True) Generate an index of the project's workspace.

This generator function indexes every file in the project's workspace until the specified *depth*. The job document if it exists, is always indexed, other files need to be specified with the formats argument.

```
for doc in project.index({r'.*\.txt', 'TextFile'}):
    print(doc)
```

Parameters

- **formats** (dict) The format definitions as mapping.
- **depth** (*int*) Specifies the crawling depth. A value of 0 (default) means no limit.

- **skip_errors** (bool) Skip all errors which occur during indexing. This is useful when trying to repair a broken workspace.
- include_job_document (bool) Include the contents of job documents.

Yields index documents

classmethod init_project (name, root=None, workspace=None, make_dir=True)
Initialize a project with the given name.

It is safe to call this function multiple times with the same arguments. However, a RuntimeError is raised in case where an existing project configuration would conflict with the provided initialization parameters.

Parameters

- name (str) The name of the project to initialize.
- root (str) The root directory for the project. Defaults to the current working directory.
- workspace (str) The workspace directory for the project. Defaults to \$project_root/workspace.
- make_dir (bool) Create the project root directory, if it does not exist yet.

Returns The project handle of the initialized project.

Return type Project

Raises RuntimeError – If the project root path already contains a conflicting project configuration.

isfile(filename)

True if a file with filename exists in the project's root directory.

Parameters filename (str) – The filename of the file.

Returns True if a file with filename exists in the project's root directory.

Return type bool

min_len_unique_id()

Determine the minimum length required for an id to be unique.

num_jobs()

Return the number of initialized jobs.

open_job (statepoint=None, id=None)

Get a job handle associated with a statepoint.

This method returns the job instance associated with the given statepoint or job id. Opening a job by a valid statepoint never fails. Opening a job by id, requires a lookup of the statepoint from the job id, which may fail if the job was not previously initialized.

Parameters

- **statepoint** (*mapping*) The job's unique set of parameters.
- **id** (*str*) The job id.

Returns The job instance.

Return type Job

Raises

• **KeyError** – If the attempt to open the job by id fails.

• LookupError – If the attempt to open the job by an abbreviated id returns more than one match.

read_statepoints (fn=None)

Read all statepoints from a file.

Parameters fn (str) – The filename of the file containing the statepoints, defaults to FN_STATEPOINTS.

See also dump statepoints () and write statepoints ().

```
repair (fn_statepoints=None, index=None, job_ids=None)
```

Attempt to repair the workspace after it got corrupted.

This method will attempt to repair lost or corrupted job state point manifest files using a state points file or a document index or both.

Parameters

- **fn_statepoints** (*str*) The filename of the file containing the statepoints, defaults to FN_STATEPOINTS.
- index A document index
- job_ids An iterable of job ids that should get repaired. Defaults to all jobs.

Raises JobsCorruptedError - When one or more corrupted job could not be repaired.

```
reset_statepoint (job, new_statepoint)
```

Reset the state point of job.

Danger: Use this function with caution! Resetting a job's state point, may sometimes be necessary, but can possibly lead to incoherent data spaces.

Parameters

- job (Job) The job, that should be reset to a new state point.
- new_statepoint (mapping) The job's new state point.

Raises

- DestinationExistsError If a job associated with the new state point is already initialized.
- OSError If the move failed due to an unknown system related error.

root_directory()

Returns the project's root directory.

```
sync (other, strategy=None, exclude=None, doc_sync=None, selection=None, **kwargs) Synchronize this project with the other project.
```

Try to clone all jobs from the other project to this project. If a job is already part of this project, try to synchronize the job using the optionally specified strategies.

Parameters

- other (Project) The other project to synchronize this project with.
- **strategy** A file synchronization strategy.

- exclude Files with names matching the given pattern will be excluded from the synchronization.
- **doc_sync** The function applied for synchronizing documents.
- **selection** Only sync the given jobs.
- **kwargs** This method accepts the same keyword arguments as the <code>sync_projects()</code> function.

Raises

- **DocumentSyncConflict** If there are conflicting keys within the project or job documents that cannot be resolved with the given strategy or if there is no strategy provided.
- FileSyncConflict If there are differing files that cannot be resolved with the given strategy or if no strategy is provided.
- SyncSchemaConflict In case that the check_schema argument is True and the detected state point schema of this and the other project differ.

temporary project (name=None, dir=None)

Context manager for the initialization of a temporary project.

The temporary project is by default created within the root project's workspace to ensure that they share the same file system. This is an example for how this method can be used for the import and synchronization of external data spaces.

```
with project.temporary_project() as tmp_project:
    tmp_project.import_from('/data')
    project.sync(tmp_project)
```

Parameters

- name An optional name for the temporary project. Defaults to a unique random string.
- dir Optionally specify where the temporary project root directory is to be created.
 Defaults to the project's workspace directory.

Returns An instance of *Project*.

update_cache()

Update the persistent state point cache (experimental).

This function updates a persistent state point cache, which is stored in the project root directory. Most data space operations, including iteration and filtering or selection are expected to be significantly faster after calling this function, especially for large data spaces.

update statepoint(job, update, overwrite=False)

Update the statepoint of this job.

Warning: While appending to a job's state point is generally safe, modifying existing parameters may lead to data inconsistency. Use the overwrite argument with caution!

Parameters

- job (Job) The job, whose statepoint shall be updated.
- update (mapping) A mapping used for the statepoint update.

• **overwrite** – Set to true, to ignore whether this update overwrites parameters, which are currently part of the job's state point. Use with caution!

Raises

- **KeyError** If the update contains keys, which are already part of the job's state point and overwrite is False.
- DestinationExistsError If a job associated with the new state point is already initialized.
- OSError If the move failed due to an unknown system related error.

workspace()

Returns the project's workspace directory.

The workspace defaults to *project_root/workspace*. Configure this directory with the 'workspace_dir' attribute. If the specified directory is a relative path, the absolute path is relative from the project's root directory.

Note: The configuration will respect environment variables, such as \$HOME.

write_statepoints (statepoints=None, fn=None, indent=2)

Dump statepoints to a file.

If the file already contains statepoints, all new statepoints will be appended, while the old ones are preserved.

Parameters

- **statepoints** (*iterable*) A list of statepoints, defaults to all statepoints which are defined in the workspace.
- fn (str) The filename of the file containing the statepoints, defaults to FN_STATEPOINTS.
- **indent** (*int*) Specify the indentation of the json file.

See also dump_statepoints().

1.2.3 The Job class

class signac.contrib.job.Job(project, statepoint, _id=None)

The job instance is a handle to the data of a unique statepoint.

Application developers should usually not need to directly instantiate this class, but use <code>open_job()</code> instead.

Attributes

Job.clear()	Remove all job data, but not the job itself.
Job.close()	Close the job and switch to the previous working direc-
	tory.
Job.doc	Alias for document.
Job.document	The document associated with this job.

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Table 2 – continued from previous page	Table 2 –	continued	from	previous	page
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Job.fn(filename)	Prepend a filename with the job's workspace directory
	path.
Job.get_id()	The unique identifier for the job's statepoint.
Job.init([force])	Initialize the job's workspace directory.
Job.isfile(filename)	Return True if file exists in the job's workspace.
Job.move(project)	Move this job to project.
Job.open()	Enter the job's workspace directory.
Job.remove()	Remove the job's workspace including the job docu-
	ment.
Job.reset()	Remove all job data, but not the job itself.
Job.reset_statepoint(new_statepoint)	Reset the state point of this job.
Job.sp	Alias for statepoint.
Job.statepoint	Access the job's state point as attribute dictionary.
Job.sync(other[, strategy, exclude, doc_sync])	Perform a one-way synchronization of this job with the
	other job.
<pre>Job.update_statepoint(update[, overwrite])</pre>	Update the statepoint of this job.
Job.workspace()	Each job is associated with a unique workspace direc-
	tory.
Job.ws	Alias for workspace.

class signac.contrib.job.Job(project, statepoint, _id=None)

Bases: object

The job instance is a handle to the data of a unique statepoint.

Application developers should usually not need to directly instantiate this class, but use <code>open_job()</code> instead.

```
FN_DOCUMENT = 'signac_job_document.json'
FN_MANIFEST = 'signac_statepoint.json'
```

clear()

Remove all job data, but not the job itself.

This function will do nothing if the job was not previously initialized.

close()

Close the job and switch to the previous working directory.

doc

Alias for document.

document

The document associated with this job.

Returns The job document handle.

Return type JSONDict

fn (filename)

Prepend a filename with the job's workspace directory path.

Parameters filename (str) – The filename of the file.

Returns The full workspace path of the file.

get_id()

The unique identifier for the job's statepoint.

Returns The job id.

Return type str

```
init (force=False)
```

Initialize the job's workspace directory.

This function will do nothing if the directory and the job manifest already exist.

Parameters force (bool) – Overwrite any existing state point's manifest files, e.g., to repair them when they got corrupted.

isfile (filename)

Return True if file exists in the job's workspace.

Parameters filename (str) – The filename of the file.

Returns True if file with filename exists in workspace.

Return type bool

move (project)

Move this job to project.

This function will attempt to move this instance of job from its original project to a different project.

Parameters project (Project) – The project to move this job to.

Raises DestinationExistsError - If the job is already initialized in project.

open()

Enter the job's workspace directory.

You can use the Job class as context manager:

```
with project.open_job(my_statepoint) as job:
    # manipulate your job data
```

Opening the context will switch into the job's workspace, leaving it will switch back to the previous working directory.

remove()

Remove the job's workspace including the job document.

This function will do nothing if the workspace directory does not exist.

reset()

Remove all job data, but not the job itself.

This function will initialize the job if it was not previously initialized.

```
reset_statepoint (new_statepoint)
```

Reset the state point of this job.

Danger: Use this function with caution! Resetting a job's state point, may sometimes be necessary, but can possibly lead to incoherent data spaces.

Parameters new_statepoint (mapping) - The job's new state point.

Raises

• **DestinationExistsError** – If a job associated with the new state point is already initialized.

• OSError – If the move failed due to an unknown system related error.

sp

Alias for statepoint.

statepoint

Access the job's state point as attribute dictionary.

sync (other, strategy=None, exclude=None, doc_sync=None, **kwargs)

Perform a one-way synchronization of this job with the other job.

By default, this method will synchronize all files and document data with the other job to this job until a synchronization conflict occurs. There are two different kinds of synchronization conflicts:

- 1. The two jobs have files with the same, but different content.
- 2. The two jobs have documents that share keys, but those keys are associated with different values.

A file conflict can be resolved by providing a 'FileSync' *strategy* or by *excluding* files from the synchronization. An unresolvable conflict is indicated with the raise of a *FileSyncConflict* exception.

A document synchronization conflict can be resolved by providing a doc_sync function that takes the source and the destination document as first and second argument.

Parameters

- **other** (.*Job*) The other job to synchronize from.
- **strategy** A synchronization strategy for file conflicts. If no strategy is provided, a *SyncConflict* exception will be raised upon conflict.
- **exclude** (*str*) An filename exclude pattern. All files matching this pattern will be excluded from synchronization.
- doc_sync A synchronization strategy for document keys. If this argument is None, by default no keys will be synchronized upon conflict.
- **dry_run** If True, do not actually perform the synchronization.
- **kwargs** Extra keyword arguments will be forward to the *sync_jobs()* function which actually excutes the synchronization operation.

Raises FileSyncConflict - In case that a file synchronization results in a conflict.

update statepoint(update, overwrite=False)

Update the statepoint of this job.

Warning: While appending to a job's state point is generally safe, modifying existing parameters may lead to data inconsistency. Use the overwrite argument with caution!

Parameters

- update (mapping) A mapping used for the statepoint update.
- **overwrite** Set to true, to ignore whether this update overwrites parameters, which are currently part of the job's state point. Use with caution!

Raises

• **KeyError** – If the update contains keys, which are already part of the job's state point and overwrite is False.

- DestinationExistsError If a job associated with the new state point is already initialized.
- OSError If the move failed due to an unknown system related error.

```
workspace()
```

Each job is associated with a unique workspace directory.

Returns The path to the job's workspace directory.

Return type str

ws

Alias for workspace.

1.2.4 The Collection

A collection of documents.

The Collection class manages a collection of documents in memory or in a file on disk. A document is defined as a dictionary mapping of key-value pairs.

An instance of collection may be used to manage and search documents. For example, given a collection with member data, where each document contains a *name* entry and an *age* entry, we can find the name of all members that are at age 32 like this:

To iterate over all documents in the collection, use:

```
for doc in collection:
    print(doc)
```

By default a collection object will reside in memory. However, it is possible to manage a collection associated to a file on disk. To open a collection which is associated with a file on disk, use the <code>Collection.open()</code> class method:

```
with Collection.open('collection.txt') as collection:
   for doc in collection.find({'age': 32}):
        print(doc)
```

The collection file is by default opened in a+ mode, which means it can be read from and written to and will be created if it does not exist yet.

Parameters

• docs – Initialize the collection with these documents.

• primary_key – The name of the key which serves as the primary index of the collection. Selecting documents by primary key has time complexity of O(N) in the worst case and O(1) on average. All documents must have a primary key value. The default primary key is _id.

clear()

Remove all documents from the collection.

close()

Close this collection instance.

In case that the collection is associated with a file-object, all changes are flushed to the file and the file is closed.

It is not possible to re-open the same collection instance after closing it.

delete_many (filter)

Delete all documents that match the filter.

```
delete_one (filter)
```

Delete one document that matches the filter.

```
dump (file=<_io.TextIOWrapper name='<stdout>' mode='w' encoding='UTF-8'>)
```

Dump the collection in JSON-encoding to file.

The file argument defaults to *sys.stdout*, which means the encoded blob will be printed to screen in case that no file argument is provided.

For example, to dump to a file on disk, one could write:

```
with open('my_collection.txt', 'w') as file:
    collection.dump(file)
```

Parameters file – The file to write the encoded blob to.

find (filter=None, limit=0)

Find all documents matching filter, but not more than limit.

This function searches the collection for all documents that match the given filter and returns a result vector. For example:

```
for doc in collection.find(my_filter):
    print(doc)
```

Nested values should be searched using the . operator, for example:

```
docs = collection.find({'nested.value': 42})
```

```
will return documents with a nested structure: { 'nested': {'value': 42}}.
```

The result of find() can be stored and iterated over multiple times. In addition, the result vector can be queried for its size:

```
docs = collection.find(my_filter)

print(len(docs))  # the number of documents matching

for doc in docs:  # iterate over the result vector
    pass
```

Arithmetic Operators

- *\$eq*: equal
- \$neq: not equal
- \$gt: greater than
- \$gte: greater or equal than
- \$lt: less than
- *\$lte*: less or equal than

```
project.find({"a": {"$lt": 5})
```

Matches all docs with a less than 5.

Logical Operators

That includes \$and and \$or; both expect a list of expressions.

```
project.find({"$or": [{"a": 4}, {"b": {"$gt": 3}}]})
```

Matches all docs, where *a* is 4 or *b* is greater than 3.

Exists operator

Determines whether a specific key exists, or not, e.g.:

```
project.find({"a": {"$exists": True}})
```

Array operator

To determine whether specific elements are in (\$in), or not in (\$nin) an array, e.g.:

```
project.find({"a": {"$in": [0, 1, 2]}})
```

Matches all docs, where a is either 0, 1, or 2. Usage of \$nin is equivalent.

Regular expression operator

Allows the "on-the-fly" evaluation of regular expressoions, e.g.:

```
project.find({"protocol": {"$regex": "foo"}})
```

Will match all docs with a protocol that contains the term 'foo'.

\$type operator

Matches when a value is of specific type, e.g.:

```
project.find({"protocol": {"$type": str}})
```

Finds all docs, where the value of protocol is of type str. Other types that can be checked are: *int*, *float*, *bool*, *list*, and *null*.

\$where operator

Matches an arbitrary python expression, e.g.:

```
project.find({"foo": {"$where": "lambda x: x.startswith('bar')"}}

→)
```

Matches all docs, where the value for foo starts with the word 'bar'.

Parameters

- **filter** (*Mapping*) All documents must match the given filter.
- limit (int) Do not return more than limit number of documents. A limit value of 0 (the default) means no limit.

Returns A result object that iterates over all matching documents.

Raises ValueError – In case that the filter argument is invalid.

find_one (filter=None)

Return one document that matches the filter or None.

```
doc = collection.find_one(my_filter)
if doc is None:
    print("No result found for filter", my_filter)
else:
    print("Doc matching filter:", my_filter, doc)
```

Parameters filter – The returned document must match the given filter.

Raises ValueError – In case that the filter argument is invalid.

Returns A matching document or None.

flush()

Write all changes to the associated file.

If the collection instance is associated with a file-object, calling the flush() method will write all changes to this file.

This method is also called when the collection is explicitly or implicitly closed.

ids

Return an iterator over the primary key in the collection.

```
index (key, build=False)
```

Get (and optionally build) the index for a given key.

An index allows to access documents by a specific key with minimal time complexity, e.g.:

```
age_index = member_collection.index('age')
for _id in age_index[32]:
    print(member_collection[_id]['name'])
```

This means we can access documents by the 'age' key in O(1) time on average in addition to the primary key. Using the find() method will automatically build all required indexes for the particular search.

Once an index has been built, it will be internally managed by the class and updated with subsequent changes. An index returned by this method is always current with the latest state of the collection.

Parameters

- **key** (str) The primary key of the requested index.
- build If True, build a non-existing index if necessary, otherwise raise KeyError.

Raises KeyError – In case that build is False and the index has not been built yet.

insert one(doc)

Insert one document into the collection

If the document does not have a value for the collection's primary key yet, it will be assigned one.

```
_id = collection.insert_one(doc)
assert _id in collection
```

Note: The document will be directly updated in case that it has no primary key and must therefore be mutable!

Parameters doc – The document to be inserted.

Returns The _id of the inserted documented.

main()

Start a command line interface for this Collection.

Use this function to interact with this instance of Collection on the command line. For example, executing the following script:

```
# find.py
with Collection.open('my_collection.txt') as c:
    c.main()
```

will enable us to search for documents on the command line like this:

```
$ python find.py '{"age": 32}'
{"name": "John", "age": 32}
{"name": "Kevin", "age": 32}
```

classmethod open (filename, mode='a+')

Open a collection associated with a file on disk.

Using this factory method will return a collection that is associated with a collection file on disk. For example:

```
with Collection.open('collection.txt') as collection:
    for doc in collection:
        print(doc)
```

will read all documents from the *collection.txt* file or create the file if it does not exist yet.

Modifications to the file will be written to the file when the flush() method is called or the collection is explicitly closed by calling the Collection.close() method or implicitly by leaving the with-clause:

```
with Collection.open('collection.txt') as collection:
    collection.update(my_docs)
# All changes to the collection have been written to collection.txt.
```

The open-modes work as expected, so for example to open a collection file in read-only mode, use Collection.open('collection.txt', 'r').

primary_key

The name of the collection's primary key (default='_id').

```
replace_one (filter, replacement, upsert=False)
```

Replace one document that matches the given filter.

The first document matching the filter will be replaced by the given replacement document. If the *upsert* argument is True, the replacement will be inserted in case that no document matches the filter.

Parameters

- **filter** A document that should be replaced must match this filter.
- replacement The replacement document.
- **upsert** If True, insert the replacement document in the case that no document matches the filter.

Raises ValueError – In case that the filter argument is invalid.

Returns The _id of the replaced (or upserted) documented.

```
update (docs)
```

Update the collection with these documents.

Any existing documents with the same primary key will be replaced.

Parameters docs – A sequence of documents to be upserted into the collection.

1.2.5 Top-level functions

The signac framework aids in the management of large and heterogeneous data spaces.

It provides a simple and robust data model to create a well-defined indexable storage layout for data and metadata. This makes it easier to operate on large data spaces, streamlines post-processing and analysis and makes data collectively accessible.

```
signac.TemporaryProject(name=None, **kwargs)
```

Context manager for the generation of a temporary project.

This is a factory function that creates a Project within a temporary directory and must be used as context manager, for example like this:

```
with TemporaryProject() as tmp_project:
    tmp_project.import_from('/data')
```

Parameters

- name An optional name for the temporary project. Defaults to a unique random string.
- kwargs Optional key-word arguments that are forwarded to the TemporaryDirectory class constructor, which is used to create a temporary root directory.

Returns An instance of *Project*.

```
signac.get project(root=None)
```

Find a project configuration and return the associated project.

Parameters root (str) – The project root directory. If no root directory is given, the next project found within or above the current working directory is returned.

Returns The project handle.

Return type Project

Raises LookupError – If no project configuration can be found.

```
signac.init_project (name, root=None, workspace=None, make_dir=True)
Initialize a project with the given name.
```

It is safe to call this function multiple times with the same arguments. However, a RuntimeError is raised in case where an existing project configuration would conflict with the provided initialization parameters.

Parameters

- name (str) The name of the project to initialize.
- root (str) The root directory for the project. Defaults to the current working directory.
- workspace (str) The workspace directory for the project. Defaults to \$project_root/workspace.
- make_dir (bool) Create the project root directory, if it does not exist yet.

Returns The project handle of the initialized project.

Return type Project

Raises RuntimeError – If the project root path already contains a conflicting project configuration.

signac.get_database(name, hostname=None, config=None)

Get a database handle.

The database handle is an instance of Database, which provides access to the document collections within one database.

```
db = signac.db.get_database('MyDatabase')
docs = db.my_collection.find()
```

Please note, that a collection which did not exist at the point of access, will automatically be created.

Parameters

- name (str) The name of the database to get.
- hostname (str) The name of the configured host. Defaults to the first configured host, or the host specified by *default host*.
- **config** (common.config.Config) The config object to retrieve the host configuration from. Defaults to the global configuration.

Returns The database handle.

Return type pymongo.database.Database

See also:

https://api.mongodb.org/python/current/api/pymongo/database.html

signac.**fetch** (doc_or_id , mode='r', mirrors=None, $num_tries=3$, timeout=60, $ignore_local=False$)

Fetch the file associated with this document or file id.

This function retrieves a file associated with the provided index document or file id and behaves like the built-in open () function, e.g.:

```
for doc in index:
    with signac.fetch(doc) as file:
        do_something_with(file)
```

Parameters

- doc_or_id A file_id or a document with a file_id value.
- mode Mode to use for opening files.
- mirrors An optional set of mirrors to fetch the file from.

- num_tries (int) The number of automatic retry attempts in case of mirror connection errors.
- **timeout** (*int*) The time in seconds to wait before an automatic retry attempt.

Returns The file associated with the document or file id.

Return type A file-like object

signac.export_one (doc, index, mirrors=None, num_tries=3, timeout=60) Export one document to index and an optionally associated file to mirrors.

Parameters

- doc A document with a file_id entry.
- docs The index collection to export to.
- mirrors An optional set of mirrors to export files to.
- num_tries (int) The number of automatic retry attempts in case of mirror connection errors.
- **timeout** (*int*) The time in seconds to wait before an automatic retry attempt.

Returns The id and file id after successful export.

signac.export (*docs*, *index*, *mirrors=None*, *update=False*, *num_tries=3*, *timeout=60*, **kwargs) Export docs to index and optionally associated files to mirrors.

The behavior of this function is equivalent to:

```
for doc in docs:
    export_one(doc, index, mirrors, num_tries)
```

If the *update* argument is set to True, the export algorithm will automatically identify stale index documents, that means documents that refer to files or state points that have been removed and are no longer part of the data space. Any document which shares the *root*, but not the *_id* field with any of the updated documents is considered stale and removed. Using *update* in combination with an empty docs sequence will raise *ExportError*, since it is not possible to identify stale documents in that case.

Note: This function will automatically delegate to specialized implementations for special index types. For example, if the index argument is a MongoDB document collection, the index documents will be exported via <code>export_pymongo()</code>.

Parameters

- docs The index documents to export.
- **index** The collection to export the index to.
- mirrors An optional set of mirrors to export files to.
- **update** (bool) If True, remove stale index documents, that means documents that refer to files or state points that no longer exist.
- num_tries (int) The number of automatic retry attempts in case of mirror connection errors.
- **timeout** (*int*) The time in seconds to wait before an automatic retry attempt.
- **kwargs** Optional keyword arguments to pass to delegate implementations.

Raises *ExportError* – When using the update argument in combination with an empty docs sequence.

signac.export_to_mirror(doc, mirror, num_tries=3, timeout=60)

Export a file associated with doc to mirror.

Parameters

- doc A document with a file_id entry.
- mirror A file-system object to export the file to.
- num_tries (int) The number of automatic retry attempts in case of mirror connection errors.
- **timeout** (*int*) The time in seconds to wait before an automatic retry attempt.

Returns The file id after successful export.

signac.export_pymongo (docs, index, mirrors=None, update=False, num_tries=3, timeout=60, chunk-size=100)

Optimized export () function for pymongo index collections.

The behavior of this function is roughly equivalent to:

```
for doc in docs:
    export_one(doc, index, mirrors, num_tries)
```

Note: All index documents must be JSON-serializable to be able to be exported to a MongoDB collection.

Parameters

- docs The index documents to export.
- index (pymongo.collection.Collection) The database collection to export the index to.
- num_tries (int) The number of automatic retry attempts in case of mirror connection errors.
- timeout (int) The time in seconds to wait before an automatic retry attempt.
- **chunksize** (*int*) The buffer size for export operations.

```
signac.index_files (root='.', formats=None, depth=0)
```

Generate a file index.

This generator function yields file index documents, where each index document corresponds to one file.

To index all files in the current working directory, simply execute:

```
for doc in signac.index_files():
    print(doc)
```

A file associated with a file index document can be fetched via the fetch () function:

```
for doc in signac.index_files():
    with signac.fetch(doc) as file:
        print(file.read())
```

This is especially useful if the file index is part of a collection (Collection) which can be searched for specific entries.

To limit the file index to files with a specific filename formats, provide a regular expression as the formats argument. To index all files that have file ending .txt, execute:

```
for doc in signac.index_files(formats='.*\.txt'):
    print(doc)
```

We can specify specific formats by providing a dictionary as formats argument, where the key is the filename pattern and the value is an arbitrary formats string, e.g.:

Parameters

- **root** (*str*) The directory to index, defaults to the current working directory.
- **formats** Limit the index to files that match the given regular expression and optionally associate formats with given patterns.
- **depth** (*int*) Limit the search to the specified directory depth.

Yields The file index documents as dicts.

```
signac.index (root='.', tags=None, depth=0, **kwargs)
Generate a master index.
```

A master index is compiled from other indexes by searching for modules named signac_access.py and compiling all indexes which are yielded from a function get_indexes(root) defined within that module as well as the indexes generated by crawlers yielded from a function get_crawlers(root) defined within that module.

This is a minimal example for a signac access.py file:

```
import signac

def get_indexes(root):
    yield signac.index_files(root, r'.*\.txt')
```

Internally, this function constructs an instance of MasterCrawler and all extra key-word arguments will be forwarded to the constructor of said master crawler.

Parameters

- **root** (*str*) Look for access modules under this directory path.
- tags If tags are provided, do not execute slave crawlers that don't match the same tags.
- **depth** (*int*) Limit the search to the specified directory depth.
- **kwargs** These keyword-arguments are forwarded to the internal MasterCrawler instance.

Yields The master index documents as instances of dict.

```
signac.buffered (buffer_size=33554432, force_write=False)
Enter a global buffer mode for all JSONDict instances.
```

All future write operations are written to the buffer, read operations are performed from the buffer whenever

possible.

All write operations are deferred until the flush_all() function is called, the buffer overflows, or upon exiting the buffer mode.

This context may be entered multiple times, however the buffer size can only be set *once*. Any subsequent specifications of the buffer size are ignored.

Parameters buffer_size (int) – Specify the maximum size of the read/write buffer. Defaults to DEFAULT_BUFFER_SIZE. A negative number indicates to not restrict the buffer size.

```
signac.is buffered()
```

Return true if in buffered read/write mode.

```
signac.flush()
```

Execute all deferred JSONDict write operations.

```
signac.get_buffer_size()
```

Returns the current maximum size of the read/write buffer.

```
signac.get_buffer_load()
```

Returns the current actual size of the read/write buffer.

1.2.6 Submodules

signac.cite module

Functions to support citing this software.

```
signac.cite.bibtex(file=None)
```

Generate bibtex entries for signac.

The bibtex entries will be printed to screen unless a filename or a file-like object are provided, in which case they will be written to the corresponding file.

Note: A full reference should also include the version of this software. Please refer to the documentation on how to cite a specific version.

Parameters file – A str or file-like object. Defaults to sys.stdout.

```
signac.cite.reference(file=None)
```

Generate formatted reference entries for signac.

The references will be printed to screen unless a filename or a file-like object are provided, in which case they will be written to the corresponding file.

Note: A full reference should also include the version of this software. Please refer to the documentation on how to cite a specific version.

Parameters file – A str or file-like object. Defaults to sys.stdout.

signac.sync module

Synchronization of jobs and projects.

Jobs may be synchronized by copying all data from the source job to the destination job. This means all files are copied and the documents are synchronized. Conflicts, that means both jobs contain conflicting data, may be resolved with a user defined strategy.

The synchronization of projects is in essence the synchronization of all jobs which are in the destination project with the ones in the source project and the sync synchronization of the project document. If a specific job does not exist yet at the destination it is simply cloned, otherwise it is synchronized.

A sync strategy is a function (or functor) that takes the source job, the destination job, and the name of the file generating the conflict as arguments and returns the decision whether to overwrite the file as Boolean. There are some default strategies defined within this module as part of the FileSync class. These are the default strategies:

- 1. always Always overwrite on conflict.
- 2. never Never overwrite on conflict.
- 3. time Overwrite when the modification time of the source file is newer.
- 4. Ask Ask the user interactively about each conflicting filename.

For example, to synchronize two projects resolving conflicts by modification time, use:

```
dest_project.sync(source_project, strategy=sync.FileSync.time)
```

Unlike files, which are always either overwritten as a whole or not, documents can be synchronized more fine-grained with a *sync function*. Such a function (or functor) takes the source and the destination document as arguments and performs the synchronization. The user is encouraged to implement their own sync functions, but there are a few default functions implemented as part of the *DocSync* class:

- 1. NO_SYNC Do not perform any synchronization.
- 2. COPY Apply the same strategy used to resolve file conflicts.
- 3. update Equivalent to dst.update(src).
- 4. ByKey Synchronize the source document key by key, more information below.

This is how we could synchronize two jobs, where the documents are synchronized with a simple update function:

```
dst_job.sync(src_job, doc_sync=sync.DocSync.update)
```

The <code>DocSync.ByKey</code> functor attempts to synchronize the destination document with the source document without overwriting any data. That means this function behaves similar to update() for a non-intersecting set of keys, but in addition will preserve nested mappings without overwriting values. In addition, any key conflict, that means keys that are present in both documents, but have differing data, will lead to the raise of a <code>DocumentSyncConflict</code> exception. The user may expelitly decide to overwrite certain keys by providing a "key-strategy", which is a function that takes the conflicting key as argument, and returns the decision whether to overwrite that specific key as Boolean. For example, to sync two jobs, where conflicting keys should only be overwritten if they contain the term 'foo', we could execute:

```
dst_job.sync(src_job, doc_sync=sync.DocSync.ByKey(lambda key: 'foo' in key))
```

This means that all documents are synchronized 'key-by-key' and only conflicting keys that contain the word "foo" will be overwritten, any other conflicts would lead to the raise of a <code>DocumentSyncConflict</code> exception. A key-strategy may also be a regular expression, so the synchronization above could also be achieved with:

```
dst_job.sync(src_job, doc_sync=sync.DocSync.ByKey('foo'))
```

class signac.sync.FileSync

Bases: object

Collection of file synchronization strategies.

```
class Ask
          Bases: object
          Ask whether a file should be overwritten interactively.
     static always (src, dst, fn)
          Always overwrite files on conflict.
     classmethod keys()
     static never(src, dst, fn)
          Never overwrite files on conflict.
     static update(src, dst, fn)
          Overwrite a file if the source file was modified last (based on timestamp).
class signac.sync.DocSync
     Bases: object
     Collection of document synchronization functions.
     class ByKey (key_strategy=None)
          Bases: object
          Synchronize documents key by key.
     COPY = 'copy'
     NO SYNC = False
     static update(src, dst)
          Perform a simple update.
signac.sync.sync_jobs (src, dst, strategy=None, exclude=None, doc_sync=None, recursive=False, fol-
                             low_symlinks=True, preserve_permissions=False, preserve_times=False, pre-
```

By default, this method will synchronize all files and document data of dst job with the src job until a synchronization conflict occurs. There are two different kinds of synchronization conflicts:

serve owner=False, preserve group=False, deep=False, dry run=False)

- 1. The two jobs have files with the same name, but different content.
- 2. The two jobs have documents that share keys, but those keys are mapped to different values.

A file conflict can be resolved by providing a 'FileSync' *strategy* or by *excluding* files from the synchronization. An unresolvable conflict is indicated with the raise of a *FileSyncConflict* exception.

A document synchronization conflict can be resolved by providing a doc_sync function that takes the source and the destination document as first and second argument.

Parameters

Synchronize the src job with the dst job.

- $src(\sim .Job)$ The src job, data will be copied from this job's workspace.
- **dst** (~. *Job*) The dst job, data will be copied to this job's workspace.
- **strategy** A synchronization strategy for file conflicts. If no strategy is provided, a *errors*. SyncConflict exception will be raised upon conflict.
- **exclude** (*str*) A filename exclusion pattern. All files matching this pattern will be excluded from the synchronization process.
- doc_sync A synchronization strategy for document keys. The default is to use a safe key-by-key strategy that will not overwrite any values on conflict, but instead raises a <code>DocumentSyncConflict</code> exception.

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- recursive (bool) Recursively synchronize sub-directories encountered within the job workspace directories.
- follow_symlinks (bool) Follow and copy the target of symbolic links.
- preserve_permissions (bool) Preserve file permissions
- **preserve_times** (bool) Preserve file modification times
- preserve_owner (bool) Preserve file owner
- preserve_group (bool) Preserve file group ownership
- dry_run If True, do not actually perform any synchronization operations.

```
signac.sync.sync_projects (source, destination, strategy=None, exclude=None, doc_sync=None, selection=None, check_schema=True, recursive=False, follow_symlinks=True, preserve_permissions=False, preserve_times=False, preserve_owner=False, preserve_group=False, deep=False, dry_run=False, parallel=False, collect_stats=False)
```

Synchronize the destination project with the source project.

Try to clone all jobs from the source to the destination. If the destination job already exist, try to synchronize the job using the optionally specified strategy.

Parameters

- **source** (*Project*) The project presenting the source for synchronization.
- **destination** (*Project*) The project that is modified for synchronization.
- **strategy** A file synchronization strategy.
- exclude Files with names matching the given pattern will be excluded from the synchronization.
- doc_sync The function applied for synchronizing documents.
- **selection** Only synchronize the given selection of jobs.
- **check_schema** (bool) If True, only synchronize if this and the other project have a matching state point schema. See also: detect_schema().
- **recursive** (bool) Recursively synchronize sub-directories encountered within the job workspace directories.
- **follow_symlinks** (bool) Follow and copy the target of symbolic links.
- preserve_permissions (bool) Preserve file permissions
- preserve_times (bool) Preserve file modification times
- preserve_owner (bool) Preserve file owner
- **preserve_group** (bool) Preserve file group ownership
- **dry_run** (bool) If True, do not actually perform the synchronization operation, just log what would happen theoretically. Useful to test synchronization strategies without the risk of data loss.

Raises

- DocumentSyncConflict If there are conflicting keys within the project or job documents that cannot be resolved with the given strategy or if there is no strategy provided.
- FileSyncConflict If there are differing files that cannot be resolved with the given strategy or if no strategy is provided.

• **SchemaSyncConflict** – In case that the check_schema argument is True and the detected state point schema of this and the other project differ.

signac.warnings module

exception signac.warnings.SignacDeprecationWarning

Bases: UserWarning

Indicates the deprecation of a signac feature, API or behavior.

This class indicates a user-relevant deprecation and is therefore a UserWarning, not a DeprecationWarning which is hidden by default.

signac.errors module

exception signac.errors.Error

Bases: Exception

exception signac.errors.BufferException

Bases: signac.core.errors.Error

An exception occured in buffered mode.

exception signac.errors.BufferedFileError(files)

Bases: signac.core.jsondict.BufferException

Raised when an error occured while flushing one or more buffered files.

files

A dictionary of files that caused issues during the flush operation, mapped to a possible reason for the issue or None in case that it cannot be determined.

exception signac.errors.ConfigError

Bases: signac.core.errors.Error, RuntimeError

exception signac.errors.AuthenticationError

Bases: signac.core.errors.Error, RuntimeError

exception signac.errors.ExportError

 $Bases: \verb|signac.core.errors.Error|, \verb|RuntimeError|$

exception signac.errors.FileNotFoundError

Bases: signac.core.errors.Error, FileNotFoundError

exception signac.errors.FetchError

Bases: signac.common.errors.FileNotFoundError

exception signac.errors.DestinationExistsError(destination)

Bases: signac.core.errors.Error, RuntimeError

The destination for a move or copy operation already exists.

exception signac.errors.JobsCorruptedError(job_ids)

Bases: signac.core.errors.Error, RuntimeError

The state point manifest file of one or more jobs cannot be opened or is corrupted.

exception signac.errors.SyncConflict

Bases: signac.core.errors.Error, RuntimeError

Raised when a synchronization operation fails.

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```
exception signac.errors.FileSyncConflict(filename)
```

Bases: signac.errors.SyncConflict

Raised when a synchronization operation fails due to a file conflict.

```
exception signac.errors.DocumentSyncConflict(keys)
```

Bases: signac.errors.SyncConflict

Raised when a synchronization operation fails due to a document conflict.

```
exception signac.errors.SchemaSyncConflict(schema_src, schema_dst)
```

Bases: signac.errors.SyncConflict

Raised when a synchronization operation fails due to schema differences.

1.3 Changelog

The **signac** package follows semantic versioning.

1.3.1 Version 0.9

Highlights

- Adds persistent state point index caching, which speeds up all functions that require indexing, for example the \$ signac find command.
- Adds the \$ signac sync tool for synchronization of multiple signac projects.
- Adds the \$ signac schema function for the automatic detection of the implicit schema of a signac project.
- Adds the \$near operator to match numbers with up to a specific precision.
- Adds functions for the import and export of data spaces.
- Add functions for the management of data on the project level, as opposed to the job level.

[0.9.5] - 2019-01-31

Fixed

- Ensure that the next() function can be called for a JobsIterator, e.g., project.find().
- Pickling issue that occurs when a _SyncedDict (job.statepoint, job.document, etc.) contains a list.
- Issue with the readline module that would cause signac shell to fail on Windows operating systems.

[0.9.4] - 2018-10-24

- Adds the \$ signac import command and the Project.import_from() method for the import of data spaces into a project workspace, such as a directory, a tarball, or a zip-file.
- Adds the \$ signac export command and the Project.export_to() method for the export of project workspaces to an external location, such as a directory, a tarball, or a zip-file.

- Adds functionality for the rapid initialization of temporary projects with the signac. TemporaryProject context manager.
- Adds the signac.Project.temporary_project() context manager which creates a temporary project within the root project workspace.
- Add signac to the default namespace when invoking signac shell.
- Add option to specify a custom view path for the signac view/Project.create_linked_view() function.
- Iterables of documents used to construct a Collection no longer require an _id field.

Changed

• The default path for linked views has been adjusted to match the one used for data exports.

Fixed

- Fix issue where differently typed integer values stored within a Collection under the same key would not be indexed correctly. This issue affected the correct function of the *\$type* operator for aforementioned cases and would lead to incorrect types in the Project schema detection algorithm for integer values.
- Fix issue where jobs that are migrated (state point change), but are not initialized, were not properly updated.
- Fix issue where changes to lists as part of synchronized dictionary, for example a state point or document would not be saved.
- Fix non-deterministic issue occuring on network file systems when trying to open jobs where the user has no write access to the job workspace directory.

[0.9.3] - 2018-06-14

Added

- Add *\$near* operator to express queries for numerical values that match up to a certain precision.
- Add the \$ signac shell sub command to directly launch a Python interpreter within a project directory.

Fixed

• Fix issue where a job instance would not be properly updated after more than one state point reset.

[0.9.2] - 2017-12-18

Added

- Add provisional feature (persistent state point caching); calling the Project.update_cache() method will generate and store a persistent state point cache in the project root directory, which will increase the speed of many project iteration, search, and selection operations.
- Add Project.check() method which checks for workspace corruption, but does not make any attempt to repair it.

• The Project.repair() method will attempt to repair jobs, that have been corrupted by manually renaming the job's workspace directory.

Changed

- Enable the write concern flag for the job.document.
- Allow to omit the specification of an authentication mechanism in the MongoDB host configuration.

Fixed

- Fix critical issue in the JSONDict implementation that would previously overwrite the underlying file when attempting to store values that are not JSON serializable.
- Fix issue where the Project.export () function would ignore the update argument when the index to export to would be a MongoDB collection.

[0.9.1] - 2017-11-07

Fixed

• Fix critical issue in the SyncedAttrDict implementation that would previously overwrite the underlying file if the first operation was a __setitem__() operation.

[0.9.0] - 2017-10-28

Added

- Introduction of \$ signac sync, Project.sync(), and Job.sync() for the simplified and fine-grained synchronization of multiple project data spaces.
- Introduction of \$ signac schema and Project.detect_schema() for the automatic detection of the implicit and semi-structured state point schema of a project data space.
- Simplified aggregation of jobs over projects and Project.find_jobs() results with the Project. groupby() function.
- Support for project-centralized data with the Project.document attribute and the Project.fn() method for the wrapping of filenames within the project root directory.
- Added the Job.clear() and the Job.reset() methods to clear or reset a job's workspace data.

Changed

- Both Job.statepoint and Job.document now use the same underlying data structure and provide the exact same API (copy with () and access of keys as attributes).
- The Collection class uses an internal counter instead of UUIDs for the generation of primary keys (resulting in improved performance).
- Major performance improvements (faster Collection, improved caching)
- Overhaul of the reference documentation.

1.3.2 Version 0.8

Highlights

- Adds boolean and arithmetic operators to search queries.
- Major revision of the indexing system.
- Adds \$ signac document command line function.
- Add the signac. Collection class for the management of persistent document collections.

[0.8.7] - 2017-10-05

Fixed

- Fix an issue where the creation of linked views was non-deterministic in some cases.
- Fix an issue where the creation of linked views would fail when the project contains job with state points that have lists as values.

[0.8.6] - 2017-08-25

Fixed

• Fix Collection append truncation issue (see issue #66).

[0.8.5] - 2017-06-07

Changed

• The signac ids in the signac find –show view are no longer enclosed by quotation marks.

Fixed

- Fix compatibility issue that broke the signac find -view and all -pretty commands on Python 2.7.
- Fix issue where view directories would be incomplete in combination with heterogeneous state point schemas.

[0.8.4] - 2017-05-19

Added

- All search queries on project and collection objects support various operators including: \$and, \$or, \$gt, \$gte, \$lt, \$lte, \$eq, \$ne, \$exists, \$regex, \$where, \$in, \$nin, and \$type.
- The \$ signac find command supports a simple filter syntax, where key value pairs can be provided as individual arguments.
- The \$ signac find command is extended by a -show option, to display the state point and the document contents directly. The contents are truncated to an adjustable depth to reduce output noise.

- The \$ signac view command has an additional filter option to select a sub data space directly without needing to pipe job ids.
- The new \$ signac document command can be used to display a job's document directly.

Changed

• Minor performance improvements.

[0.8.3] - 2017-05-10

Changed

• Raise ExportError when updating with an empty index.

Fixed

- Fix command line logic issue with \$signac config host.
- Fix bug, where Collection.replace_one () would ignore the upsert argument under specific conditions.

[0.8.2] - 2017-04-19

Fixed

• Fixes a TypeError which occurred under specific conditions when calling Collection.find() with nested filter arguments.

[0.8.1] - 2017-04-17

Fixed

• Fixes wide-spread typo (indeces -> indexes).

[0.8.0] - 2017-04-16

Overall major simplification of the generation of indexes and the management and searching of index collections without external database.

- Introduction of the Collection class for the management of document collections, such as indexes in memory and on disk.
- Generation of file indexes directly via the signac.index_files() function.
- Generation of master indexes directly via the signac.index() function and the \$ signac index command.

- The API of signac_access.py files has been simplified, including the possibility to use a blank file for a minimal configuration.
- Use the \$ signac project --access command to create a minimal access module in addition to Project.create_access_module().
- The update of existing index collections has been simplified by using the export () function with the *update=True* argument, which means that stale documents (the associated file or state point no longer exists) are automatically identified and removed.
- Added the Job.ws attribute, as short-cut for Job.workspace().
- The Job.sp interface has a get () function which can be used to specify a default value in case that the requested key is not part of the state point.

Changed (breaking API)

- The \$ signac index command generates a master index instead of a project index. To generate a project index from the command line use \$ signac project --index instead.
- The SignacProjectCrawler class expects the project's root directory as first argument, not the workspace directory.
- The get_crawlers() function defined within a signac_access.py access module is expected to yield crawler instances directly, not a mapping of crawler ids and instances.
- The simplification of the signac_access.py module API is reflected in a reduction of arguments to the Project.create_access_module() method.

Changed (non-breaking)

- The RegexFileCrawler, SignacProjectCrawler and MasterCrawler classes were moved into the root namespace.
- If a MasterCrawler object is instantiated with the raise_on_error argument set to True, any errors encountered during crawling are raised instead of ignored and skipped; this simplifies the debugging of erroneous access modules.
- Improved error message for invalid configuration files.
- Better error messages for invalid \$ signac find queries.
- Check a host configuration on the command line via \$ signac host --test.
- A MongoDB database host configuration defaults to none when no authentication method is explicitly specified.
- Using the ——debug option in combination with \$ signac index will show the traceback of errors encountered during indexing instead of ignoring them.
- Instances of Job are hashable, making it possible to use them as dict keys for instance.
- \bullet The representation of Job instances via ${\tt repr}$ () can actually serves as copy constructor command.
- The project interface implementation performs all non-trivial search operations on an internally management index collection, which improves performance and simplifies the code base.

Deprecated

• The DocumentSearchEngine class has been deprecated, its functionality is now provided by the Collection class.

Fixed

 An issue related to exporting documents to MongoDB collections via pymongo in combination with Python 2.7 has been fixed.

1.3.3 Version 0.7

Highlights

- Add support for Python 3.6, PyPy and PyPy3.
- Make any instance of Project behave like an iterable (for job in project).
- Introduction of the Job.sp attribute to access state point variables.
- Revision of the linked view function, which now allows the update of previous views.
- Support for searching by job document keys on the command line.
- Add functions for moving and cloning jobs.
- Add functions for changing a job's state point.
- Enable opening of jobs by abbreviated id.

[0.7.1] - 2017-01-09

Added

• When the python-rapidjson package is installed, it will be used for JSON encoding/decoding (experimental).

Changed

- All job move-related methods raise DestinationExistsError in case of destination conflicts.
- Optimized \$ signac find command.

Fixed

42

- Fixed bug in \$ signac statepoint.
- Suppress 'broken pipe error' message when using \$ signac find for example in combination with \$ head.

[0.7.0] - 2017-01-04

Added

- Add support for Python version 3.6.
- Add support for PyPy and PyPy3.
- Simplified iteration over project data spaces.
- An existing linked view can be updated by executing the view command again.
- Add attribute interface for the access and modification of job state points: Job.sp.
- Add function for moving and copying of jobs between projects.
- All project related iterators support the len-operator.
- Enable iteration over all jobs with: for job in project:.
- Make len (project) an alias for project.num_jobs().
- Add in-operator to determine whether a job is initialized within a project.
- Add Job. sp attribute to access and modify a job's state point.
- The Project.open_job() method accepts abbreviated job ids.
- Add Project.min_len_unique_id() method to determine the minimum length of job ids to be unique within the project's data space.
- Add Job.move () method to move jobs between projects.
- Add Project.clone() method to copy jobs between projects.
- Add \$ signac move and \$ signac clone command line functions.
- Add Job.reset_statepoint() method to reset a job's state point.
- Add Job.update_statepoint() method to update a job's state point.
- Add a Job.FN_DOCUMENT constant which defines the default filename of the job document file
- The \$ signac find command accepts a -d/--doc-filter option to filter by job document contents.
- Add the Project.create_linked_view() method as replacement for the previously deprecated Project.create view() method.

Changed

- Linked views use relative paths.
- The Guide documentation chapter has been renamed to Reference and generally overhauled.
- The Quick Reference documentation chapter has been extended.

Fixed

- Fix error when using an instance of Job after calling Job. remove ().
- A project created in one the standard config directories (such as the home directory) does not take prevalence over project configurations in or above the current working directory.

Removed

- The signac-gui component has been removed.
- The Project.create_linked_view() force argument is removed.
- The Project.find_variable_parameters () method has been removed

1.3.4 Version 0.6

Highlights

- General revision of the indexing and export system.
- General consolidation including the removal of the *conversion framework*.

[0.6.2] - 2017-12-15

Added

- Add instructions on how to acknowledge **signac** in publications to documentation.
- Add cite module for the auto-generation of formatted references and BibTeX entries.

Removed

• Remove SSL authentication support.

[0.6.1] - 2017-11-26

Changed

- The Project.create_view() method triggers a DeprecationWarning instead of a PendingDeprecationWarning.
- The Project.find_variable_parameters() method triggers a DeprecationWarning instead of a PendingDeprecationWarning.

Fixed

- Make package more robust against PySide import errors.
- Fix Project.__repr__ method.
- Fix critical bug in fs.GridFS class, which rendered it unusuable.
- Fix issue in indexing. fetch () previously resulting in local paths being ignored.
- Fix error signac.__all__ namespace directive.

[0.6.0] - 2016-11-18

Added

- Add the export_to_mirror() function for mirroring files.
- Introduction of the signac.fs namespace to simplify the configuration of mirror filesystems.
- Add *errors* module to root namespace. Many exceptions raised inherit from the base exception types defined within that module, making it easier to catch signac related errors.
- Add the export_one () function for the export of a single index document; simplifies the implementation of custom export functions.
- Opening an instance of Job with the open_job() method multiple times and entering a job context recursively is now well-defined behavior: Opening a job now adds the current working directory onto a stack, closing it switches into the directory on top of the stack.
- The return type of Project.open_job() can be configured to make it easier to specialize projects with custom job types.

Changed

- The MasterCrawler logic has been simplified; their primary function is the compilation of index documents from slave crawlers, all export logic, including data mirroring is now provided by the signac.export() function.
- Each index document is now uniquely coupled with only one file or data object, which is why signac. fetch() replaces signac.fetch_one() and the latter one has been deprecated and is currently an alias of the former one.
- The signac.fetch() function always returns a file-like object, regardless of format definition.
- The format argument in the crawler define () function is now optional and has now very well defined behavior for str types. It is encouraged to define a format with a str constant rather than a file-like object type.
- The TextFile file-like object class definition in the formats module has been replaced with a constant of type str.
- The signac.export() function automatically delegates to specialized implementations such as export_pymongo() and is more robust against errors, such as broken connections.
- The export_pymongo() function makes multiple automatic restart attempts when encountering errors.
- Documentation: The tutorial is now based on signac-examples jupyter notebooks.
- The contrib.crawler module has been renamed to contrib.indexing to better reflect the semantic context.
- The signac.export () function now implements the logic for data linking and mirroring.
- Provide default argument for '-indent' option for \$ signac statepoint command.
- Log, but do not reraise exceptions during MasterCrawler execution, making the compilation of master indexes more robust against errors.
- The object representation of Job and Project instances is simplified.
- The warning verbosity has been reduced when importing modules with optional dependencies.

Removed

- All modules related to the stale *conversion framework* feature have been removed resulting in a removal of the optional networkx dependency.
- Multiple modules related to the *conversion framework* feature have been removed, including: contrib. formats_network, contrib.conversion, and contrib.adapters.

Fixed

• Opening instances of Job with the Job.open() method multiple times, equivalently entering the job context recursively, does not cause an error anymore, but instead the behavior is well-defined.

1.3.5 Version 0.5

[0.5.0] - 2016-08-31

Added

- New function: signac.init_project() simplifies project initialization within Python
- Added optional root argument to signac.get_project() to simplify getting a project handle outside of the current working directory
- Added optional argument to signac.get_project(), to allow fetching of projects outside of the current working directory.
- Added two class factory methods to *Project*: get_project() and init_project().

Changed

• The performance of project indexing and crawling has been improved.

1.3.6 Version 0.4

[0.4.0] - 2016-08-05

- The performance of find operations can be greatly improved by using pre-generated job indexes.
- New top-level commands: \$ signac find, \$ signac index, \$ signac statepoint, and \$ signac view.
- New method: Project.create_linked_view()
- New method: Project.build_job_statepoint_index()
- New method: Project.build_job_search_index()
- The Project.find_jobs() method allows to filter by job document.

Changed

- The SignacProjectCrawler indexes all jobs, not only those with non-empty job documents.
- The signac.fetch_one() function returns None if no associated object can be fetched.
- The tutorial is restructured into multiple parts.
- Instructions for installation are separated from the guide.

Removed

- Remove previously deprecated crawl keyword argument in index export functions.
- Remove previously deprecated function common.config.write_config().

1.3.7 Version 0.3

[0.3.0] - 2016-06-23

Added

• Add contributing agreement and guidelines.

Changed

• Change license from MIT to BSD 3-clause license.

1.3.8 Version 0.2

[0.2.9] - 2016-06-06

Added

- Addition of the signac config command line API.
- Password updates are encrypted with borypt when passlib is installed.
- The user is prompted to enter missing credentials (username/password) in case that they are not stored in the configuration.
- The \$ signac confg tool provides the --update-pw argument, which allows users to update their own password.
- Added MIT license, in addition, all source code files contain a short licensing header.

Changed

- Improved documentation on how to configure signac.
- The OSI classifiers are updated, including an upgrade of the development status to '4 beta'.

Fixed

 Nested job state points can no longer get corrupted. This bug occurred when trying to operate on nested state point mappings.

Deprecated

• Deprecated pymongo versions 2.x are no longer supported.

[0.2.8] - 2016-04-18

Added

- Project is now in the root namespace.
- Add index () method to Project.
- Add create_access_module() method to Project.
- Add find_variable_parameters() method to Project.
- Add fn () method to Job, which prepends the job's workspace path to a filename.
- The documentation contains a comprehensive tutorial

Changed

- The crawl () function yields only the index documents and not a tuple of (_id, doc).
- export () and export_pymongo() expect the index documents as first argument, not a crawler instance. The old API is still supported, but will trigger a DeprecationWarning.

[0.2.7] - 2016-02-29

Added

• Add job.isfile() method

Changed

• Optimize project.find_statepoints() and project.repair() functions.

[0.2.6] - 2016-02-20

- Add job.reset_statepoint() and job.update_statepoint()
- Add job.remove() function

Changed

- Sanitize filter argument in all project.find_*() methods.
- The job.statepoint() function accurately represents saved statepoints, e.g. tuples are represented as lists, as there is no difference between tuples and lists in JSON.
- signac-gui does not block on database operations.
- signac-gui allows reload of databases and collections of connected hosts.

Fixed

- RegexFileCrawler define() class function only acts upon the actual specialization and not globally on all RegexFileCrawler classes.
- signac-gui does not crash when replica sets are configured.

[0.2.5] - 2016-02-10

Added

- Added signac.get_project(), signac.get_database(), signac.fetch() and signac.fetch_one() to top-level namespace.
- Added basic shell commands, see \$ signac --help.
- Allow opening of jobs by id: project.open_job(id='abc123...').
- Mirror data while crawling.
- Use extra sources for fetch () and fetch_one ().
- Add file system handler: LocalFS, handler for local file system.
- Add file system handler: GridFS, handler for MongoDB GridFS file system.
- Crawler tags, to control which crawlers are used for a specific index.
- Allow explicit job workspace creation with job.init().
- Forwarding of pymongo host configuration via **signac** configuration.

Changed

- Major reorganization of the documentation, split into: Overview, Guide, Quick Reference and API.
- Documentation: Add notes for system administrators about advanced indexing.
- Warn about outdated pymongo versions.
- Set *zip_safe* flag to true in *setup.py*.
- Remove dependency on six module, by adding it to the common subpackage.

Deprecated

Fixed

- Fixed hard import of pymongo bug (issue #24).
- · Crawler issues with malformed documents.

[0.2.4] - 2016-01-11

Added

- Implement Project.repair() function for projects with corrupted workspaces.
- Allow environment variables in workspace path definition.
- Check and fix config permission errors.

Changed

• Increase robustness of job manifest file creation.

Fixed

• Fix project crawler deep directory issue (hotfix).

[0.2.3] - 2015-12-09

Fixed

• Fix a few bugs related to project views.

[0.2.2] - 2015-11-30

Fixed

• Fix SignacProjectCrawler super() bug.

[0.2.1] - 2015-11-29

- Add support for Python 2.7
- Add signac-gui (early alpha)
- · Allow specification of relative and default workspace paths
- Add the ability to create project views
- Add Project.find_*() functions to search the workspace

• Add function to write and read state point hash tables

[0.2.0] - 2015-11-05

- Major consolidation of the package.
- Remove all hard dependencies, but six.

1.4 Support and Development

To get help using the **signac** package, either send an email to signac-support@umich.edu or join the signac gitter chatroom.

The **signac** package is hosted on GitHub and licensed under the open-source BSD 3-Clause license. Please use the repository's issue tracker to report bugs or request new features.

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