YMP Documentation

Release 0.2.2.dev266+ge35de0f.d20210510

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May 10, 2021

CONTENTS

CHAPTER

ONE

YMP - A FLEXIBLE OMICS PIPELINE

Welcome to the YMP documentation!

YMP is a tool that makes it easy to process large amounts of NGS read data. It comes "batteries included" with everything needed to preprocess your reads (QC, trimming, contaminant removal), assemble metagenomes, annotate assemblies, or assemble and quantify RNA-Seq transcripts, offering a choice of tools for each of those procecssing stages. When your needs exceed what the stock YMP processing stages provide, you can easily add your own, using YMP to drive novel tools, tools specific to your area of research, or tools you wrote yourself.

1.1 Features:

batteries included YMP comes with a large number of *Stages* implementing common read processing steps. These stages cover the most common topics, including quality control, filtering and sorting of reads, assembly of metagenomes and transcripts, read mapping, community profiling, visualisation and pathway analysis.

For a complete list, check the documentation or the source.

get started quickly Simply point YMP at a folder containing read files, at a mapping file, a list of URLs or even an SRA RunTable and YMP will configure itself. Use tab expansion to complete your desired series of stages to be applied to your data. YMP will then proceed to do your bidding, downloading raw read files and reference databases as needed, installing requisite software environments and scheduling the execution of tools either locally or on your cluster.

explore alternative workflows Not sure which assembler works best for your data, or what the effect of more stringent quality trimming would be? YMP is made for this! By keeping the output of each stage in a folder named to match the stack of applied stages, YMP can manage many variant workflows in parallel, while minimizing the amount of duplicate computation and storage.

go beyond the beaten path Built on top of Bioconda and Snakemake, YMP is easily extended with your own Snakefiles, allowing you to integrate any type of processing you desire into YMP, including your own, custom made tools. Within the YMP framework, you can also make use of the extensions to the Snakemake language provided by YMP (default values, inheritance, recursive wildcard expansion, etc.), making writing rules less error prone and repetative.

1.2 Background

Bioinformatical data processing workflows can easily get very complex, even convoluted. On the way from the raw read data to publishable results, a sizeable collection of tools needs to be applied, intermediate outputs verified, reference databases selected, and summary data produced. A host of data files must be managed, processed individually or aggregated by host or spatial transect along the way. And, of course, to arrive at a workflow that is just right for a particular study, many alternative workflow variants need to be evaluated. Which tools perform best? Which parameters are right? Does re-ordering steps make a difference? Should the data be assembled individually, grouped, or should a grand co-assembly be computed? Which reference database is most appropriate?

Answering these questions is a time consuming process, justifying the plethora of published ready made pipelines each providing a polished workflow for a typical study type or use case. The price for the convenience of such a polished pipeline is the lack of flexibility - they are not meant to be adapted or extended to match the needs of a particular study. Workflow management systems on the other hand offer great flexibility by focussing on the orchestration of user defined workflows, but typicially require significant initial effort as they come without predefined workflows.

YMP strives to walk the middle ground between these. It brings everything needed to classic metagenome and RNA-Seq workflows, yet built on the workflow management system Snakemake, it can be easily expanded by simply adding Snakemake rules files. Designed around the needs of processing primarily multi-omic NGS read data, it brings a framework for handling read file meta data, provisioning reference databases, and organizing rules into semantic stages.

CHAPTER

TWO

INSTALLING AND UPDATING YMP

2.1 Working with the Github Development Version

2.1.1 Installing from GitHub

1. Clone the repository:

```
git clone  --recurse-submodules https://github.com/epruesse/ymp.git
```

   Or, if your have github ssh keys set up:

```
git clone --recurse-submodules git@github.com:epruesse/ymp.git
```

2. Create and activate conda environment:

```
conda env create -n ymp --file environment.yaml
source activate ymp
```

3. Install YMP into conda environment:

```
pip install -e .
```

4. Verify that YMP works:

```
source activate ymp
ymp --help
```

2.1.2 Updating Development Version

Usually, all you need to do is a pull:

```
git pull
git submodule update --recursive --remote
```

If environments where updated, you may want to regenerate the local installations and clean out environments no longer used to save disk space:

```
source activate ymp
ymp env update
ymp env clean
# alternatively, you can just delete existing envs and let YMP
```

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```
# reinstall as needed:
# rm -rf ~/.ymp/conda*
conda clean -a
```

If you see errors before jobs are executed, the core requirements may have changed. To update the YMP conda environment, enter the folder where you installed YMP and run the following:

```
source activate ymp
conda env update --file environment.yaml
```

If something changed in `setup.py`, a re-install may be necessary:

```
source activate ymp
pip install -U -e .
```

CHAPTER

THREE

CONFIGURATION

YMP reads its configuration from a YAML formatted file `ymp.yml`. To run YMP, you need to first tell it which datasets you want to process and where it can find them.

Contents

3.1 Getting Started

A simple configuration looks like this:

```
projects:
  myproject:
    data: mapping.csv
```

This tells YMP to look for a file `mapping.csv` located in the same folder as your `ymp.yml` listing the datasets for the project `myproject`. By default, YMP will use the left most unique column as names for your datasets and try to guess which columns point to your input data.

The matching `mapping.csv` might look like this:

```
sample,fq1,fq2
foot,sample1_1.fq.gz,sample1_2.fq.gz
hand,sample2_1.fq,gz,sample2_2.fq.gz
```

So we have two samples, `foot` and `hand`, and the read files for those in the same directory as the configuration file. Using relative or absolute paths you can point to any place in your filesystem. You can also use SRA references like `SRR123456` or URLs pointing to remote files.

The mapping file itself may be in comma separated or tab separated format or may be an Excel file. For Excel files, you may specify the sheet to be used separated from the file name by a `%` sign. For example:

```
project:
  myproject:
    data: myproject.xlsx%sheet3
```

The matching Excel file could then have a `sheet3` with this content:

sample	fq1	fq2	srr
foot	/data/foot1.fq.gz	/data/foot2.fq.gz	
hand			SRR123456
head	http://datahost/head1.fq.gz	http://datahost/head2.fq.gz	SRR234234

For `foot`, the two gzipped FastQ files are used. The data for `hand` is retrieved from SRA and the data for `head` downloaded from `datahost`. The SRR number for `head` is ignored as the URL pair is found first.

3.2 Referencing Read Files

YMP will search your map file data for references to the read data files. It understands three types of references to your reads:

Local FastQ files: `data/some_1.fq.gz, data/some_2.fq.gz` The file names should end in `.fastq` or `.fq`, optionally followed by `.gz` if your data is compressed. You need to provide forward and reverse reads in separate columns; the left most column is assumed to refer to the forward reads.

If the filename is relative (does not start with a `/`), it is assumed to be relative to the location of `ymp.yml`.

Remote FastQ files: `http://myhost/some_1.fq.gz, http://myhost/some_2.fq.gz` If the filename starts with `http://` or `https://`, YMP will download the files automatically.

Forward and reverse reads need to be either both local or both remote.

SRA Run IDs: `SRR123456` Instead of giving names for FastQ files, you may provide SRA Run accessions, e.g. `SRR123456` (or `ERRnnn` or `DRRnnn` for runs originally submitted to EMBL or DDBJ, respectively). YMP will use `fastq-dump` to download and extract the SRA files.

Which type to use is determined for each row in your map file data individually. From left to right, the first recognized data source is used in the order they are listed above.

Configuration processing an SRA RunTable:

```
projects:
  smith17:
    data:
      - SraRunTable.txt
    id_col: Sample_Name_s
```

3.3 Project Configuration

Each project must have a `data` key defining which mapping file(s) to load. This may be a simple string referring to the file (URLs are OK as well) or a more *complex configuration*.

3.3.1 Specifying Columns

By default, YMP will choose the columns to use as data set name and to locate the read data automatically. You can override this behavior by specifying the columns explicitly:

1. Data set names: `id_col: Sample`

   The left most unique column may not always be the most informative to use as names for the datasets. In the above example, we specify the column to use explicitly with the line `id_col: Sample_Name_s` as the columns in SRA run tables are sorted alpha-numerically and the left most unique one may well contain random numeric data.

   Default: left most unique column

2. Data set read columns: `reads_cols: [fq1, fq2]`

   If your map files contain multiple references to source files, e.g. local and remote, and the order of preference used by YMP does not meet your needs you can restrict the search for suitable data references to a set of columns using the key `read_cols`.

   Default: all columns

Example

```
projects:
  smith17:
    data:
      - SraRunTable.txt
    id_col: Sample_Name_s
    read_cols: Run_s
```

3.3.2 Multiple Mapping Files per Project

To combine data sets from multiple mapping files, simply list the files under the `data` key:

```
projects:
  myproject:
    data:
      - sequencing_run_1.txt
      - sequencing_run_2.txt
```

The files should at least share one column containing unique values to use as names for the datasets.

If you need to merge meta-data spread over multiple files, you can use the `join` key:

```
project:
  myproject:
    data:
      - join:
```

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```
          - SraRunTable.txt
          - metadata.xlsx%reference_project
      - metadata.xlsx%our_samples
```

This will merge rows from `SraRunTable.txt` with rows in the `reference_project` sheet in `metadata.xls` if all columns of the same name contain the same data (natural join) and add samples from the `our_samples` sheet to the bottom of the list.

3.3.3 Complete Example

```
projects:
  myproject:
    data:
      - join:
          - SraRunTable.txt
          - metadata.xlsx%reference_project
      - metadata.xlsx%our_samples
      - mapping.csv
    id_col: Sample
    read_cols:
      - fq1
      - fq2
      - Run_s
```

CHAPTER

FOUR

COMMAND LINE

4.1 ymp

Welcome to YMP!

Please find the full manual at https://ymp.readthedocs.io

```
ymp [OPTIONS] COMMAND [ARGS]...
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

--version
Show the version and exit.

--install-completion
Install command completion for the current shell. Make sure to have psutil installed.

--profile <profile>
Profile execution time using Yappi

4.1.1 env

Manipulate conda software environments

These commands allow accessing the conda software environments managed by YMP. Use e.g.

```
>>> $(ymp env activate multiqc)
```

to enter the software environment for `multiqc`.

```
ymp env [OPTIONS] COMMAND [ARGS]...
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

activate

source activate environment

Usage: $(ymp activate env [ENVNAME])

```
ymp env activate [OPTIONS] ENVNAME
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

Arguments

ENVNAME
Required argument

clean

Remove unused conda environments

```
ymp env clean [OPTIONS] [ENVNAMES]...
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

-a, --all
Delete all environments

Arguments

ENVNAMES
Optional argument(s)

export

Export conda environments

Resolved package specifications for the selected conda environments can be exported either in YAML format suitable for use with `conda env create -f FILE` or in TXT format containing a list of URLs suitable for use with `conda create --file FILE`. Please note that the TXT format is platform specific.

If other formats are desired, use `ymp env list` to view the environments' installation path ("prefix" in conda lingo) and export the specification with the `conda` command line utlity directly.

Note:
Environments must be installed before they can be exported. This is due to limitations of the conda utilities. Use the "–create" flag to automatically install missing environments.

```
ymp env export [OPTIONS] [ENVNAMES]...
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

-d, --dest <FILE>
Destination file or directory. If a directory, file names will be derived from environment names and selected export format. Default: print to standard output.

-f, --overwrite
Overwrite existing files

-c, --create-missing
Create environments not yet installed

-s, --skip-missing
Skip environments not yet installed

-t, --filetype <filetype>
Select export format. Default: yml unless FILE ends in '.txt'

Options yml | txt

Arguments

ENVNAMES
Optional argument(s)

install

Install conda software environments

```
ymp env install [OPTIONS] [ENVNAMES]...
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

-p, --conda-prefix <conda_prefix>
Override location for conda environments

-e, --conda-env-spec <conda_env_spec>
Override conda env specs settings

-n, --dry-run
Only show what would be done

-r, --reinstall
Delete existing environment and reinstall

--no-spec
Don't use conda env spec even if present

--no-archive
Delete existing archives before install

--fresh
Create fresh install. Implies reinstall, no-spec and no-archve

Arguments

ENVNAMES
Optional argument(s)

list

List conda environments

```
ymp env list [OPTIONS] [ENVNAMES]...
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

--static, --no-static
List environments statically defined via env.yml files

--dynamic, --no-dynamic
List environments defined inline from rule files

-a, --all
List all environments, including outdated ones.

-s, --sort <sort_col>
Sort by column

Options name | hash | path | installed

-r, --reverse
Reverse sort order

Arguments

ENVNAMES
Optional argument(s)

prepare

Create envs needed to build target

```
ymp env prepare [OPTIONS] TARGET_FILES
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

-n, --dryrun
Only show what would be done

-p, --printshellcmds
Print shell commands to be executed on shell

-k, --keepgoing
Don't stop after failed job

--lock, --no-lock
Use/don't use locking to prevent clobbering of files by parallel instances of YMP running

--rerun-incomplete, --ri
Re-run jobs left incomplete in last run

-F, --forceall
Force rebuilding of all stages leading to target

-f, --force
Force rebuilding of target

--notemp
Do not remove temporary files

-t, --touch
Only touch files, faking update

--shadow-prefix <shadow_prefix>
Directory to place data for shadowed rules

-r, --reason
Print reason for executing rule

-N, --nohup
Don't die once the terminal goes away.

Arguments

TARGET_FILES
Optional argument(s)

remove

Remove conda environments

```
ymp env remove [OPTIONS] [ENVNAMES]...
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

Arguments

ENVNAMES
Optional argument(s)

run

Execute COMMAND with activated environment ENV

Usage: ymp env run <ENV> [–] <COMMAND...>

(Use the "–" if your command line contains option type parameters beginning with - or –)

```
ymp env run [OPTIONS] ENVNAME [COMMAND]...
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

Arguments

ENVNAME
Required argument

COMMAND
Optional argument(s)

update

Update conda environments

```
ymp env update [OPTIONS] [ENVNAMES]...
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

Arguments

ENVNAMES
Optional argument(s)

4.1.2 init

Initialize YMP workspace

```
ymp init [OPTIONS] COMMAND [ARGS]...
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

cluster

Set up cluster

```
ymp init cluster [OPTIONS]
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

-y, --yes
Confirm every prompt

demo

Copies YMP tutorial data into the current working directory

```
ymp init demo [OPTIONS]
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

project

```
ymp init project [OPTIONS] [NAME]
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

-y, --yes
Confirm every prompt

Arguments

NAME
Optional argument

4.1.3 make

Build target(s) locally

```
ymp make [OPTIONS] TARGET_FILES
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

-n, --dryrun
Only show what would be done

-p, --printshellcmds
Print shell commands to be executed on shell

-k, --keepgoing
Don't stop after failed job

--lock, --no-lock
Use/don't use locking to prevent clobbering of files by parallel instances of YMP running

--rerun-incomplete, --ri
Re-run jobs left incomplete in last run

-F, --forceall
Force rebuilding of all stages leading to target

-f, --force
Force rebuilding of target

--notemp
Do not remove temporary files

-t, --touch
Only touch files, faking update

--shadow-prefix <shadow_prefix>
Directory to place data for shadowed rules

-r, --reason
Print reason for executing rule

-N, --nohup
Don't die once the terminal goes away.

-j, --cores <CORES>
The number of parallel threads used for scheduling jobs

--dag
Print the Snakemake execution DAG and exit

--rulegraph
Print the Snakemake rule graph and exit

--debug-dag
Show candidates and selections made while the rule execution graph is being built

--debug
Set the Snakemake debug flag

Arguments

TARGET_FILES
Optional argument(s)

4.1.4 show

Show configuration properties

```
ymp show [OPTIONS] PROPERTY
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

-h, --help

-s, --source
Show source

Arguments

PROPERTY
Optional argument

4.1.5 stage

Manipulate YMP stages

```
ymp stage [OPTIONS] COMMAND [ARGS]...
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

list

List available stages

```
ymp stage list [OPTIONS] STAGE
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

-l, --long
Show full stage descriptions

-s, --short
Show only stage names

-c, --code
Show definition file name and line number

-t, --types
Show input/output types

Arguments

STAGE
Optional argument(s)

4.1.6 submit

Build target(s) on cluster

The parameters for cluster execution are drawn from layered profiles. YMP includes base profiles for the "torque" and "slurm" cluster engines.

```
ymp submit [OPTIONS] TARGET_FILES
```

Options

-P, --pdb
Drop into debugger on uncaught exception

-q, --quiet
Decrease log verbosity

-v, --verbose
Increase log verbosity

--log-file <log_file>
Specify a log file

-n, --dryrun
Only show what would be done

-p, --printshellcmds
Print shell commands to be executed on shell

-k, --keepgoing
Don't stop after failed job

--lock, --no-lock
Use/don't use locking to prevent clobbering of files by parallel instances of YMP running

--rerun-incomplete, --ri
Re-run jobs left incomplete in last run

-F, --forceall
Force rebuilding of all stages leading to target

-f, --force
Force rebuilding of target

--notemp
Do not remove temporary files

-t, --touch
Only touch files, faking update

--shadow-prefix <shadow_prefix>
Directory to place data for shadowed rules

-r, --reason
Print reason for executing rule

-N, --nohup
Don't die once the terminal goes away.

-P, --profile <NAME>
Select cluster config profile to use. Overrides cluster.profile setting from config.

-c, --snake-config <FILE>
Provide snakemake cluster config file

-d, --drmaa
Use DRMAA to submit jobs to cluster. Note: Make sure you have a working DRMAA library. Set DRMAA_LIBRAY_PATH if necessary.

-s, --sync
Use synchronous cluster submission, keeping the submit command running until the job has completed. Adds qsub_sync_arg to cluster command

-i, --immediate
Use immediate submission, submitting all jobs to the cluster at once.

--command <CMD>
Use CMD to submit job script to the cluster

--wrapper <CMD>
Use CMD as script submitted to the cluster. See Snakemake documentation for more information.

--max-jobs-per-second <N>
Limit the number of jobs submitted per second

-l, --latency-wait <T>
Time in seconds to wait after job completed until files are expected to have appeared in local file system view. On NFS, this time is governed by the acdirmax mount option, which defaults to 60 seconds.

-J, --cluster-cores <N>
Limit the maximum number of cores used by jobs submitted at a time

-j, --cores <N>
Number of local threads to use

--args <ARGS>
Additional arguments passed to cluster submission command. Note: Make sure the first character of the argument is not '-', prefix with ' ' as necessary.

--scriptname <NAME>
Set the name template used for submitted jobs

Arguments

TARGET_FILES
Optional argument(s)

CHAPTER

FIVE

STAGES

Listing of stages implemented in YMP

stage Import
: Imports raw read files into YMP.

```
>>> ymp make toy
>>> ymp make mpic
```

rule export_qiime_map_file

rule symlink_raw_reads
: Normalize FQ names by creating symlinks to original files

rule symlink_raw_reads_SE
: Normalize FQ names by creating symlinks to original files

stage annotate_blast
: Annotate sequences with BLAST

Searches a reference database for hits with `blastn`. Use `E` flag to specify exponent to required E-value. Use `N` or `Mega` to specify default. Use `Best` to add `-subject_besthit` flag.

This stage produces `blast7.gz` files as output.

```
>>> ymp make toy.ref_genome.index_blast.annotate_blast
```

rule blast_db_size
: Determines size of BLAST database (for splitting)

rule blast_db_size_SPLIT
: Variant of *blast_db_size* for multi-file blast indices

rule blast_db_size_V4
: Variant of *blast_db_size* for V4 blast indices

rule blastn_join_result
: Merges BLAST results

rule blastn_query
: Runs BLAST

rule blastn_query_SPLIT
: Variant of *blastn_query* for multi-file blast indices

rule blastn_query_V4
: Variant of *blastn_query* for V4 blast indices

rule blastn_split_query_fasta
Split FASTA query file into chunks for individual BLAST runs

rule blastn_split_query_fasta_hack
Workaround for a problem with snakemake checkpoints and run: statements

stage annotate_diamond
FIXME

rule diamond_blastx_fasta

rule diamond_view
Convert Diamond binary output (daa) to BLAST6 format

stage annotate_prodigal
Call genes using prodigal

```
>>> ymp make toy.ref_genome.annotate_prodigal
```

rule prodigal
Predict genes using prodigal

stage annotate_tblastn
Runs `tblastn`

rule blast7_to_gtf
Convert from Blast Format 7 to GFF/GTF format

rule tblastn_query
Runs a TBLASTN search against an assembly.

stage assemble_megahit
Assemble metagenome using MegaHit.

```
>>> ymp make toy.assemble_megahit.map_bbmap
>>> ymp make toy.group_ALL.assemble_megahit.map_bbmap
>>> ymp make toy.group_Subject.assemble_megahit.map_bbmap
```

rule megahit
Runs MegaHit.

stage assemble_spades
Assemble reads using spades

```
>>> ymp make toy.assemble_spades
>>> ymp make toy.group_ALL.assemble_spades
>>> ymp make toy.group_Subject.assemble_spades
>>> ymp make toy.assemble_spades
>>> ymp make toy.assemble_spadesMeta
>>> ymp make toy.assemble_spadesSc
>>> ymp make toy.assemble_spadesRna
>>> ymp make toy.assemble_spadesIsolate
>>> ymp make toy.assemble_spadesNC
>>> ymp make toy.assemble_spadesMetaNC
```

rule spades
Runs Spades. Supports reads.by_COLUMN.sp/complete as target for by group co-assembly.

rule spades_input_yaml
Prepares a dataset config for spades. Spades commandline is limited to at most 9 pairs of fq files, so to allow arbitrary numbers we need to use the dataset config option.

Preparing in a separate rule so that the main spades rule can use the `shell:` rule and not `run:`, which would preclude it from using conda environments.

stage assemble_trinity

rule trinity

rule trinity_stats

stage assemble_unicycler

Assemble reads using unicycler

```
>>> ymp make toy.assemble_unicycler
```

rule unicycler

Runs unicycler

stage basecov_bedtools

Creates BLAST index running `makeblastdb` on input fasta.gz files.

```
>>> ymp make toy.ref_genome.index_blast
```

rule bedtools_genomecov

stage bin_metabat2

Bin metagenome assembly into MAGs

```
>>> ymp make mock.assemble_megahit.map_bbmap.sort_bam.bin_metabat2
>>> ymp make mock.group_ALL.assemble_megahit.map_bbmap.sort_bam.group_ALL.bin_
↪metabat2
```

rule metabat2_bin

Bin metagenome with MetaBat2

rule metabat2_depth

Generates a depth file from BAM

stage check

Verify file availability

This stage provides rules for checking the file availability at a given point in the stage stack.

Mainly useful for testing and debugging.

rule check_fasta

Verify availability of FastA type reference

rule check_fastp

Verify availability of FastP type reference

stage cluster_cdhit

Clusters protein sequences using CD-HIT

```
>>> ymp make toy.ref_query.cluster_cdhit
```

rule cdhit_clstr_to_csv

rule cdhit_faa_single

Clustering predicted genes using cdhit

rule cdhit_prepare_input

Prepares input data for CD-HIT

- rewrites '*' to 'X' as stop-codon not understood by CD-HIT
- prefixes lost ID to Fasta ID

stage correct_bbmap
Correct read errors by overlapping inside tails

Applies BBMap's "bbmerge.sh ecco" mode. This will overlap the inside of read pairs and choose the base with the higher quality where the alignment contains mismatches and increase the quality score as indicated by the double observation where the alignment contains matches.

```
>>> ymp make toy.correct_bbmap
>>> ymp make mpic.correct_bbmap
```

rule bbmap_error_correction
Error correction with BBMerge overlapping

rule bbmap_error_correction_all

rule bbmap_error_correction_se
Error correction with BBMerge overlapping

stage count_diamond

rule diamond_count

stage count_stringtie

rule stringtie

rule stringtie_abundance

rule stringtie_all

rule stringtie_all_target

rule stringtie_gather_ballgown

rule stringtie_merge

stage coverage_samtools
Computes coverage from a sorted bam file using `samtools coverage`

rule samtools_coverage

stage dedup_bbmap
Remove duplicate reads

Applies BBMap's "dedupe.sh"

```
>>> ymp make toy.dedup_bbmap
>>> ymp make mpic.dedup_bbmap
```

rule bbmap_dedupe
Deduplicate reads using BBMap's dedupe.sh

rule bbmap_dedupe_all

rule bbmap_dedupe_se
Deduplicate reads using BBMap's dedupe.sh

stage dust_bbmap
Perform entropy filtering on reads using `BBMap's` bbduk.sh

The parameter `Enn` gives the entropy cutoff. Higher values filter more sequences.

```
>>> ymp make toy.dust_bbmap
>>> ymp make toy.dust_bbmapE60
```

rule bbmap_dust

stage extract_reads
Extract reads from BAM file using `samtools fastq`.

Parameters `fn`, `Fn` and `Gn` are passed through to `samtools view`. Reads are output *only* if all bits in `f` are set, *none* of the bits in `F` are set, and *any* of the bits in `G` is *unset*.

1: paired 2: proper pair (both aligned in right orientation) 4: unmapped 8: other read unmapped

Some options include:

- f2: correctly mapped (only proper pairs)
- F12: both ends mapped (but potentially "improper")
- G12: either end mapped
- F2: not correctly mapped (not proper pair, could also be unmapped)
- f12: not mapped (neither read mapped)

rule samtools_fastq

stage extract_seqs
Extract sequences from `.fasta.gz` file using `samtools faidx`

Currently requires a `.blast7` file as input.

Use parameter `Nomatch` to instead keep unmatched sequences.

rule samtools_faidx

rule samtools_select_blast

stage filter_bmtagger
Filter(-out) contaminant reads using BMTagger

```
>>> ymp make toy.ref_phiX.index_bmtagger.remove_bmtagger
>>> ymp make toy.ref_phiX.index_bmtagger.remove_bmtagger.assemble_megahit
>>> ymp make toy.ref_phiX.index_bmtagger.filter_bmtagger
>>> ymp make mpic.ref_phiX.index_bmtagger.remove_bmtagger
```

rule bmtagger_filter
Filter reads using reference

rule bmtagger_filter_all

rule bmtagger_filter_out
Filter-out reads using reference

rule bmtagger_filter_revread
Filter reads using reference

rule bmtagger_find
Match paired end reads against reference

rule bmtagger_find_se
Match single end reads against reference

rule bmtagger_remove_all

stage format_bbmap
Process sequences with BBMap's format.sh

Parameter Ln filters sequences at a minimum length.

```
>>> ymp make toy.assemble_spades.format_bbmapL200
```

rule bbmap_reformat

stage humann2
Compute functional profiles using HUMAnN2

rule humann2
Runs HUMAnN2 with separately processed Metaphlan2 output.

Note: HUMAnN2 has no special support for paired end reads. As per manual, we just feed it the concatenated forward and reverse reads.

---

rule humann2_all

rule humann2_join_tables
Joins HUMAnN2 per sample output tables

rule humann2_renorm_table
Renormalizes humann2 output tables

stage index_bbmap
Creates BBMap index

```
>>> ymp make toy.ref_genome.index_bbmap
```

rule bbmap_makedb
Precomputes BBMap index

stage index_blast

rule blast_makedb
Build Blast index

stage index_bmtagger

rule bmtagger_bitmask

rule bmtagger_index

stage index_bowtie2

```
>>> ymp make toy.ref_genome.index_bowtie2
```

rule bowtie2_index

stage index_diamond

rule diamond_makedb
Build Diamond index file

stage map_bbmap
Map reads using BBMap

```
>>> ymp make toy.assemble_megahit.map_bbmap
>>> ymp make toy.ref_genome.map_bbmap
>>> ymp make mpic.ref_ssu.map_bbmap
```

rule bbmap_map
Map read from each (co-)assembly read file to the assembly

rule bbmap_map_SE
Map read from each (co-)assembly read file to the assembly

stage map_bowtie2
Map reads using Bowtie2

```
>>> ymp make toy.ref_genome.index_bowtie2.map_bowtie2
>>> ymp make toy.ref_genome.index_bowtie2.map_bowtie2VF
>>> ymp make toy.ref_genome.index_bowtie2.map_bowtie2F
>>> ymp make toy.ref_genome.index_bowtie2.map_bowtie2S
>>> ymp make toy.ref_genome.index_bowtie2.map_bowtie2VS
>>> ymp make toy.ref_genome.index_bowtie2.map_bowtie2X800
>>> ymp make toy.ref_genome.index_bowtie2.map_bowtie2I5
>>> ymp make toy.ref_genome.index_bowtie2.map_bowtie2L
>>> ymp make toy.assemble_megahit.index_bowtie2.map_bowtie2
>>> ymp make toy.group_Subject.assemble_megahit.index_bowtie2.map_bowtie2
>>> ymp make mpic.ref_ssu.index_bowtie2.map_bowtie2
```

rule bowtie2_map

rule bowtie2_map_SE

stage map_diamond

rule diamond_blastx_fastq

rule diamond_blastx_fastq2

rule diamond_view_2
Convert Diamond binary output (daa) to BLAST6 format

stage map_hisat2
Map reads using Hisat2

rule hisat2_map
For hisat we always assume a pre-build index as providing SNPs and haplotypes etc is beyond this pipelines scope.

stage map_star
Map RNA-Seq reads with STAR

rule star_map

stage markdup_sambamba

rule sambamba_markdup

stage metaphlan2
Assess metagenome community composition using Metaphlan 2

rule metaphlan2
Computes community profile from mapped reads and Metaphlan's custom reference database.

rule metaphlan2_map
Align reads to Metaphlan's custom reference database.

rule metaphlan2_merge
Merges Metaphlan community profiles.

stage polish_pilon
Polish genomes with Pilon

Requires fasta.gz and sorted.bam files as input.

rule pilon_polish

stage primermatch_bbmap
Filters reads by matching reference primer using BBMap's "bbduk.sh".

```
>>> ymp make mpic.ref_primers.primermatch_bbmap
```

rule bbduk_primer
Splits reads based on primer matching into "primermatch" and "primerfail".

rule bbduk_primer_all

rule bbduk_primer_se
Splits reads based on primer matching into "primermatch" and "primerfail".

stage profile_centrifuge
Classify reads using centrifuge

rule centrifuge

stage qc_fastqc
Quality screen reads using FastQC

```
>>> ymp make toy.qc_fastqc
```

rule qc_fastqc
Run FastQC on read files

stage qc_multiqc
Aggregate QC reports using MultiQC

rule multiqc_fastqc
Assemble report on all FQ files in a directory

stage qc_quast
Estimate assemly quality using Quast

rule metaquast_all_at_once
Run quast on all assemblies in the previous stage at once.

rule metaquast_by_sample
Run quast on each assembly

rule metaquast_multiq_summary
Aggregate Quast per assembly reports

stage quant_rsem
Quantify transcripts using RSEM

rule rsem_all

rule rsem_all_for_target

rule rsem_quant

stage references
This is a "virtual" stage. It does not process read data, but comprises rules used for reference provisioning.

rule human_db_download
Download HUMAnN2 reference databases

rule prepare_reference
Provisions files in `<reference_dir>/<reference_name>`

- Creates symlinks to downloaded references
- Compresses references provided uncompressed upstream
- Connects files requested by stages with downloaded files and unpacked archives

rule unpack_archive
Template rule for unpacking references provisioned upstream as archive.

rule unpack_ref_GRCh38_eaa4c10f
Unpacks ref_GRCh38 archive:

URL: ftp://ftp.ccb.jhu.edu/pub/infphilo/hisat2/data/grch38_snp_tran.tar.gz

Files:

- ALL.1.ht2
- ALL.2.ht2
- ALL.3.ht2
- ALL.4.ht2
- ALL.5.ht2
- ALL.6.ht2
- ALL.7.ht2
- ALL.8.ht2

rule unpack_ref_centrifuge_0d910a96
Unpacks ref_centrifuge archive:

URL: ftp://ftp.ccb.jhu.edu/pub/infphilo/centrifuge/data/p+h+v.tar.gz

Files:

- p+h+v.1.cf
- p+h+v.2.cf
- p+h+v.3.cf

rule unpack_ref_centrifuge_1ee7c028
Unpacks ref_centrifuge archive:

URL: ftp://ftp.ccb.jhu.edu/pub/infphilo/centrifuge/data/nt.tar.gz

Files:

- nt.1.cf
- nt.2.cf
- nt.3.cf

rule unpack_ref_centrifuge_43ba6165
Unpacks ref_centrifuge archive:

URL: ftp://ftp.ccb.jhu.edu/pub/infphilo/centrifuge/data/p_compressed.tar.gz

Files:

- p_compressed.1.cf
- p_compressed.2.cf
- p_compressed.3.cf

rule unpack_ref_centrifuge_a9964521
Unpacks ref_centrifuge archive:

URL: ftp://ftp.ccb.jhu.edu/pub/infphilo/centrifuge/data/p_compressed+h+v.tar.gz

Files:

- p_compressed+h+v.1.cf
- p_compressed+h+v.2.cf
- p_compressed+h+v.3.cf

rule unpack_ref_greengenes_305aa905
Unpacks ref_greengenes archive:

URL: ftp://greengenes.microbio.me/greengenes_release/gg_13_5/gg_13_8_otus.tar.gz

Files:

- rep_set/99_otus.fasta
- rep_set/97_otus.fasta
- rep_set/94_otus.fasta

rule unpack_ref_metaphlan2_a6545140
Unpacks ref_metaphlan2 archive:

URL: https://depot.galaxyproject.org/software/metaphlan2/metaphlan2_2.6.0_src_all.tar.gz

Files:

- db_v20/mpa_v20_m200.1.bt2
- db_v20/mpa_v20_m200.2.bt2
- db_v20/mpa_v20_m200.3.bt2
- db_v20/mpa_v20_m200.4.bt2
- db_v20/mpa_v20_m200.rev.1.bt2
- db_v20/mpa_v20_m200.rev.2.bt2
- db_v20/mpa_v20_m200.pkl

rule unpack_ref_mothur_SEED_39c9f686
Unpacks ref_mothur_SEED archive:

URL: https://www.mothur.org/w/images/a/a4/Silva.seed_v128.tgz

Files:

- silva.seed_v128.tax
- silva.seed_v128.align

stage remove_bbmap
Filter reads by reference

This stage aligns the reads with a given reference using BBMap in fast mode. Matching reads are collected in the stage *filter_bbmap* and remaining reads are collectec in the stage *remove_bbmap*.

```
>>> ymp make toy.ref_phiX.index_bbmap.remove_bbmap
>>> ymp make toy.ref_phiX.index_bbmap.filter_bbmap
>>> ymp make mpic.ref_phiX.index_bbmap.remove_bbmap
```

rule bbmap_split

rule bbmap_split_all

rule bbmap_split_all_remove

rule bbmap_split_se

stage sort_bam

rule sambamba_sort

stage split_library
Demultiplexes amplicon sequencing files

This rule is treated specially. If a configured project specifies a `barcode_col`, reads from the file (or files) are used in combination with

rule fastq_multix

rule split_library_compress_sample

stage trim_bbmap
Trim adapters and low quality bases from reads

Applies BBMap's "bbduk.sh".

Parameters: A: append to enable adapter trimming Q20: append to select phred score cutoff (default 20) L20: append to select minimum read length (default 20)

```
>>> ymp make toy.trim_bbmap
>>> ymp make toy.trim_bbmapA
>>> ymp make toy.trim_bbmapAQ10L10
>>> ymp make mpic.trim_bbmap
```

rule bbmap_trim
Trimming and Adapter Removal using BBTools BBDuk

rule bbmap_trim_all

rule bbmap_trim_se
Trimming and Adapter Removal using BBTools BBDuk

stage trim_sickle
Perform read trimming using Sickle

```
>>> ymp make toy.trim_sickle
>>> ymp make toy.trim_sickleQ10L10
>>> ymp make mpic.trim_sickleL20
```

rule sicke_all

rule sickle

rule sickle_se

stage trim_trimmomatic
Adapter trim reads using trimmomatic

```
>>> ymp make toy.trim_trimmomaticT32
>>> ymp make mpic.trim_trimmomatic
```

rule trimmomatic_adapter
Trimming with Trimmomatic

rule trimmomatic_adapter_all

rule trimmomatic_adapter_se
Trimming with Trimmomatic

rule download_file_ftp
Downloads remote file using *wget*

rule download_file_http
Downloads remote file using internal downloader

rule mkdir
Auto-create directories listed in ymp config.

Use these as input: >>> input: tmpdir = ancient(ymp.get_config().dir.tmp) Or as param: >>> param: tmpdir = "/home/docs/checkouts/readthedocs.org/user_builds/ymp/checkouts/latest/doc/tmp"

rule prefetch
Downloads SRA files into NCBI SRA folder (ncbi/public/sra).

rule fastq_dump
Extracts FQ from SRA files

rule cdhit_fna_single
Clustering predicted genes (nuc) using cdhit-est

rule normalize_16S
Normalize 16S by copy number using picrust, must be run with closed reference OTU table

rule predict_metagenome
Predict metagenome using picrust

rule categorize_by_function
Categorize PICRUSt KOs into pathways

rule rsem_index
Build Genome Index for RSEM

rule star_index
Build Genome Index for Star

CHAPTER

SIX

API

6.1 ymp package

ymp.**get_config**()
Access the current YMP configuration object.

This object might change once during normal execution: it is deleted before passing control to Snakemake. During unit test execution the object is deleted between all tests.

Return type *ConfigMgr*

ymp.**print_rule = 0**
Set to 1 to show the YMP expansion process as it is applied to the next Snakemake rule definition.

```
>>> ymp.print_rule = 1
>>> rule broken:
>>>   ...
```

```
>>> ymp make broken -vvv
```

ymp.**snakemake_versions = ['6.0.5', '6.1.0', '6.1.1', '6.2.1']**
List of versions this version of YMP has been verified to work with

6.1.1 Subpackages

ymp.cli package

ymp.cli.**install_completion**(*ctx*, *attr*, *value*)
Installs click_completion tab expansion into users shell

ymp.cli.**install_profiler**(*ctx*, *attr*, *value*)

Submodules

ymp.cli.env module

ymp.cli.env.**get_env**(*envname*)
Get single environment matching glob pattern

Parameters **envname** – environment glob pattern

ymp.cli.env.**get_envs**(*patterns=None*)
Get environments matching glob pattern

Parameters **envnames** – list of strings to match

ymp.cli.init module

Implements subcommands for `ymp init`

ymp.cli.init.**have_command**(*cmd*)

ymp.cli.make module

Implements subcommands for `ymp make` and `ymp submit`

class ymp.cli.make.**TargetParam**
Bases: `click.types.ParamType`

Handles tab expansion for build targets

classmethod complete(*ctx*, *incomplete*)
Try to complete incomplete command

This is executed on tab or tab-tab from the shell

Parameters

- **ctx** – click context object
- **incomplete** – last word in command line up until cursor

Returns list of words incomplete can be completed to

ymp.cli.make.**debug**(*msg*, **args*, ***kwargs*)

ymp.cli.make.**snake_params**(*func*)
Default parameters for subcommands launching Snakemake

ymp.cli.make.**start_snakemake**(*kwargs*)
Execute Snakemake with given parameters and targets

Fixes paths of kwargs['targets'] to be relative to YMP root.

ymp.cli.shared_options module

class ymp.cli.shared_options.**Group**(*name=None*, *commands=None*, ***attrs*)
Bases: click.core.Group

command(**args*, ***kwargs*)
A shortcut decorator for declaring and attaching a command to the group. This takes the same arguments as *command()* but immediately registers the created command with this instance by calling into add_command().

class ymp.cli.shared_options.**Log**
Bases: object

Set up Logging

classmethod logfile_option(*ctx*, *param*, *val*)

mod_level(*n*)

classmethod quiet_option(*ctx*, *param*, *val*)

static set_logfile(*filename*)

classmethod verbose_option(*ctx*, *param*, *val*)

class ymp.cli.shared_options.**LogFormatter**
Bases: coloredlogs.ColoredFormatter

Initialize a ColoredFormatter object.

Parameters

- **fmt** – A log format string (defaults to DEFAULT_LOG_FORMAT).
- **datefmt** – A date/time format string (defaults to None, but see the documentation of BasicFormatter.formatTime()).
- **style** – One of the characters %, { or $ (defaults to DEFAULT_FORMAT_STYLE)
- **level_styles** – A dictionary with custom level styles (defaults to DEFAULT_LEVEL_STYLES).
- **field_styles** – A dictionary with custom field styles (defaults to DEFAULT_FIELD_STYLES).

Raises Refer to check_style().

This initializer uses colorize_format() to inject ANSI escape sequences in the log format string before it is passed to the initializer of the base class.

format(*record*)
Apply level-specific styling to log records.

Parameters **record** – A LogRecord object.

Returns The result of logging.Formatter.format().

This method injects ANSI escape sequences that are specific to the level of each log record (because such logic cannot be expressed in the syntax of a log format string). It works by making a copy of the log record, changing the msg field inside the copy and passing the copy into the format() method of the base class.

snakemake_level_styles = {'criirical': {'color': 'red'}, 'debug': {'color': 'blue'}

class ymp.cli.shared_options.**TqdmHandler**(*stream=None*)
Bases: logging.StreamHandler

Tqdm aware logging StreamHandler

Passes all log writes through tqdm to allow progress bars and log messages to coexist without clobbering terminal

Initialize the handler.

If stream is not specified, sys.stderr is used.

emit(*record*)
Emit a record.

If a formatter is specified, it is used to format the record. The record is then written to the stream with a trailing newline. If exception information is present, it is formatted using traceback.print_exception and appended to the stream. If the stream has an 'encoding' attribute, it is used to determine how to do the output to the stream.

ymp.cli.shared_options.**command**(**args*, ***kwargs*)

ymp.cli.shared_options.**enable_debug**(*_ctx*, *param*, *val*)

ymp.cli.shared_options.**group**(**args*, ***kwargs*)

ymp.cli.shared_options.**log_options**(*f*)

ymp.cli.shared_options.**nohup**(*ctx*, *param*, *val*)
Make YMP continue after the shell dies.

- redirects stdout and stderr into pipes and sub process that won't die if it can't write to either anymore
- closes stdin

ymp.cli.show module

Implements subcommands for `ymp show`

class ymp.cli.show.**ConfigPropertyParam**
Bases: `click.types.ParamType`

Handles tab expansion for `ymp show` arguments

complete(*_ctx*, *incomplete*)
Try to complete incomplete command

This is executed on tab or tab-tab from the shell

Parameters

- **ctx** – click context object
- **incomplete** – last word in command line up until cursor

Returns list of words incomplete can be completed to

convert(*value*, *param*, *ctx*)
Convert value of param given context

Parameters

- **value** – string passed on command line
- **param** – click parameter object
- **ctx** – click context object

property properties
Find properties offered by ConfigMgr

ymp.cli.show.**show_help**(*ctx*, *_param=None*, *value=True*)
Display click command help

ymp.cli.stage module

ymp.cli.stage.**wrap**(*header*, *data*)

ymp.stage package

YMP processes data in stages, each of which is contained in its own directory.

```
with Stage("trim_bbmap") as S:
  S.doc("Trim reads with BBMap")
  rule bbmap_trim:
    output: "{:this:}/{sample}{:pairnames:}.fq.gz"
    input:  "{:prev:}/{sample}{:pairnames:}.fq.gz"
    ...
```

Submodules

ymp.stage.base module

Base classes for all Stage types

class ymp.stage.base.**Activateable**(**args*, ***kwargs*)
Bases: object

Mixin for Stages that can be filled with rules from Snakefiles.

add_rule(*rule*, *workflow*)

Return type None

check_active_stage(*name*)

Return type None

static get_active()

Return type *BaseStage*

register_inout(*name*, *target*, *item*)
Determine stage input/output file type from prev/this filename

Detects patterns like "PREFIX{: NAME :}/INFIX{TARGET}.EXT". Also checks if there is an active stage.

Parameters

- **name** (str) – The NAME
- **target** (Set) – Set to which to add the type
- **item** (str) – The filename

Return type None

Returns Normalized output pattern

rules: List[snakemake.rules.Rule]
Rules in this stage

static set_active(*stage*)

Return type None

class ymp.stage.base.**BaseStage**(*name*)
Bases: object

Base class for stage types

altname
Alternative name

can_provide(*inputs*)
Determines which of `inputs` this stage can provide.

Returns a dictionary with the keys a subset of `inputs` and the values identifying redirections. An empty string indicates that no redirection is to take place. Otherwise, the string is the suffix to be appended to the prior *StageStack*.

Return type Dict[str, str]

doc(*doc*)
Add documentation to Stage

Parameters **doc** (str) – Docstring passed to Sphinx

Return type None

docstring: Optional[str]
The docstring describing this stage. Visible via `ymp stage list` and in the generated sphinx documentation.

get_all_targets(*stack*, *output_types=None*)
Targets to build to complete this stage given `stack`.

Typically, this is the StageStack's path appended with the stamp name.

Return type List[str]

get_group(*stack*, *default_groups*)
Determine output grouping for stage

Parameters

- **stack** (StageStack) – The stack for which output grouping is requested.
- **default_groups** (List[str]) – Grouping determined from stage inputs
- **override_groups** – Override grouping from GroupBy stage or None.

Return type List[str]

get_ids(*stack*, *groups*, *match_groups=None*, *match_value=None*)
Determine the target ID names for a set of active groupings

Called from `{:target:}` and `{:targets:}`. For `{:targets:}`, `groups` is the set of active groupings for the stage stack. For `{:target:}`, it's the same set for the source of the file type, the current grouping and the current target.

Parameters

- **groups** (List[str]) – Set of columns the values of which should form IDs

- **match_value** (Optional[str]) – Limit output to rows with this value
- **match_groups** (Optional[List[str]]) – ... in these groups

Return type List[str]

get_inputs()
Returns the set of inputs required by this stage

This function must return a copy, to ensure internal data is not modified.

Return type Set[str]

get_outputs(*path*)
Returns a dictionary of outputs

Return type Dict[str, str]

get_path(*stack*)
On disk location for this stage given stack.

Called by *StageStack* to determine the real path for virtual stages (which must override this function).

Return type str

has_checkpoint()

Return type bool

match(*name*)
Check if the name can refer to this stage

As component of a *StageStack*, a stage may be identified by alternative names and may also be parametrized by suffix modifiers. Stage types supporting this behavior must override this function.

Return type bool

modify_next_group(*_stack*)

name
The name of the stage is a string uniquely identifying it among all stages.

property outputs
Returns the set of outputs this stage is able to generate.

May return either a set or a dict with the dictionary values representing redirections in the case of virtual stages such as *Pipeline* or *Reference*.

Return type Union[Set[str], Dict[str, str]]

class ymp.stage.base.**ConfigStage**(*name*, *cfg*)
Bases: *ymp.stage.base.BaseStage*

Base for stages created via configuration

These Stages derive from the yml.yml and not from a rules file.

cfg
The configuration object defining this Stage.

property defined_in
List of files defining this stage

Used to invalidate caches.

docstring: Optional[str]
The docstring describing this stage. Visible via `ymp stage list` and in the generated sphinx documentation.

filename
Semi-colon separated list of file names defining this Stage.

lineno
Line number within the first file at which this Stage is defined.

ymp.stage.expander module

class ymp.stage.expander.**StageExpander**
Bases: *ymp.snakemake.ColonExpander*

- Registers rules with stages when they are created

class Formatter(*expander*)
Bases: *ymp.snakemake.FormatExpander.Formatter*, *ymp.string.PartialFormatter*

get_value(*key*, *args*, *kwargs*)

get_value_(*key*, *args*, *kwargs*)

regroup = re.compile('(?<!{){\\s*([^{}\\s]+)\\s*}(?!})')

expand_ruleinfo(*rule*, *item*, *expand_args*, *rec*)

expand_str(*rule*, *item*, *expand_args*, *rec*, *cb*)

expands_field(*field*)
Checks if this expander should expand a Rule field type

Parameters **field** – the field to check

Returns True if *field* should be expanded.

ymp.stage.groupby module

Implements forward grouping

Grouping allows processing multiple input datasets at once, such as in a co-assembly. It is initiated by adding the virtual stage "group_<COL>" directly before the stage that should be grouping its output. "<COL>" may be a project data column, in which case all data for which column COL shares a value will be combined, or "ALL", which combines all samples. The output filename prefix will be either the column value or "ALL".

```
>>> ymp make mock.group_sample.assemble_megahit
>>> ymp make mock.group_ALL.assemble_megahit
```

Subsequent stages will use the most finegrained grouping required by their input data.

FIXME: How to avoid re-specifying groupby?

class ymp.stage.groupby.**GroupBy**(*name*)
Bases: *ymp.stage.base.BaseStage*

Virtual stage for grouping

PREFIX = 'group_'

docstring: Optional[str]
The docstring describing this stage. Visible via `ymp stage list` and in the generated sphinx documentation.

get_group(*stack*, *default_groups*)
Determine output grouping for stage

Parameters

- **stack** (StageStack) – The stack for which output grouping is requested.
- **default_groups** (List[str]) – Grouping determined from stage inputs
- **override_groups** – Override grouping from GroupBy stage or None.

Return type List[str]

match(*name*)
Check if the `name` can refer to this stage

As component of a *StageStack*, a stage may be identified by alternative names and may also be parametrized by suffix modifiers. Stage types supporting this behavior must override this function.

Return type bool

modify_next_group(*stack*)

Return type List[str]

ymp.stage.params module

class ymp.stage.params.**Param**(*stage*, *key*, *name*, *value=None*, *default=None*)
Bases: abc.ABC

Stage Parameter (base class)

property constraint

format(*groupdict*)

classmethod make(*stage*, *typ*, *key*, *name*, *value*, *default*)

Return type *Param*

parse(*wildcards*, *nodefault=False*)

pattern(*show_constraint=True*)
String to add to filenames passed to Snakemake

I.e. a pattern of the form `{wildcard,constraint}`

regex: str = NotImplemented

type_name: str = NotImplemented
Name of type, must be overwritten by children

types: Dict[str, Type[*ymp.stage.params.Param*]] = {'choice': <class 'ymp.stage.params
Type/Class mapping for param types

property wildcard

class ymp.stage.params.**ParamChoice**(**args*, ***kwargs*)
Bases: *ymp.stage.params.Param*

Stage Choice Parameter

type_name: str = 'choice'
Name of type, must be overwritten by children

class ymp.stage.params.**ParamFlag**(**args*, ***kwargs*)
Bases: *ymp.stage.params.Param*

Stage Flag Parameter

format(*groupdict*)

parse(*wildcards*)
Returns function that will extract parameter value from wildcards

type_name: str = 'flag'
Name of type, must be overwritten by children

class ymp.stage.params.**ParamInt**(**args*, ***kwargs*)
Bases: *ymp.stage.params.Param*

Stage Int Parameter

type_name: str = 'int'
Name of type, must be overwritten by children

class ymp.stage.params.**ParamRef**(*stage*, *key*, *name*, *value=None*, *default=None*)
Bases: *ymp.stage.params.Param*

Reference Choice Parameter

property regex

type_name: str = 'ref'
Name of type, must be overwritten by children

class ymp.stage.params.**Parametrizable**(**args*, ***kwargs*)
Bases: *ymp.stage.base.BaseStage*

add_param(*key*, *typ*, *name*, *value=None*, *default=None*)
Add parameter to stage

Example

```
>>> with Stage("test") as S
>>>    S.add_param("N", "int", "nval", default=50)
>>>    rule:
>>>       shell: "echo {param.nval}"
```

This would add a stage "test", optionally callable as "testN123", printing "50" or in the case of "testN123" printing "123".

Parameters

- **char** – The character to use in the Stage name
- **typ** – The type of the parameter (int, flag)
- **param** – Name of parameter in params
- **value** – value `{param.xyz}` should be set to if param given
- **default** – default value for `{{param.xyz}}` if no param given

Return type `bool`

docstring: Optional[str]
The docstring describing this stage. Visible via `ymp stage list` and in the generated sphinx documentation.

format(*groupdict*)

match(*name*)
Check if the `name` can refer to this stage

As component of a *StageStack*, a stage may be identified by alternative names and may also be parametrized by suffix modifiers. Stage types supporting this behavior must override this function.

Return type bool

property params

parse(*name*)

Return type Dict[str, str]

property regex

ymp.stage.pipeline module

Pipelines Module

Contains classes for pre-configured pipelines comprising multiple stages.

class ymp.stage.pipeline.**Pipeline**(*name*, *cfg*)
Bases: *ymp.stage.params.Parametrizable*, *ymp.stage.base.ConfigStage*

A virtual stage aggregating a sequence of stages, i.e. a pipeline or sub-workflow.

Pipelines are configured via `ymp.yml`.

Example

pipelines:

my_pipeline: hide: false params:

Unexpected indentation.

length: key: L type: int default: 20

Block quote ends without a blank line; unexpected unindent.

stages:

- **stage_1{length}:** hide: true
- stage_2
- stage_3

can_provide(*inputs*)
Determines which of `inputs` this stage can provide.

The result dictionary values will point to the "real" output.

Return type Dict[str, str]

docstring: Optional[str]
The docstring describing this stage. Visible via `ymp stage list` and in the generated sphinx documentation.

get_all_targets(*stack*)
Targets to build to complete this stage given `stack`.

Typically, this is the StageStack's path appended with the stamp name.

get_group(*stack*, *default_groups*)
Determine output grouping for stage

Parameters

- **stack** (*StageStack*) – The stack for which output grouping is requested.
- **default_groups** (List[str]) – Grouping determined from stage inputs
- **override_groups** – Override grouping from GroupBy stage or None.

Return type List[str]

get_ids(*stack*, *groups*, *mygroups=None*, *target=None*)
Determine the target ID names for a set of active groupings

Called from `{:target:}` and `{:targets:}`. For `{:targets:}`, `groups` is the set of active groupings for the stage stack. For `{:target:}`, it's the same set for the source of the file type, the current grouping and the current target.

Parameters

- **groups** – Set of columns the values of which should form IDs
- **match_value** – Limit output to rows with this value
- **match_groups** – ... in these groups

get_path(*stack*, *typ=None*)
On disk location for this stage given `stack`.

Called by *StageStack* to determine the real path for virtual stages (which must override this function).

hide_outputs
If true, outputs of stages are hidden by default

property outputs
The outputs of a pipeline are the sum of the outputs of each component stage. Outputs of stages further down the pipeline override those generated earlier.

Return type Dict[str, str]

property params

pipeline
Path fragment describing this pipeline

stages
Dictionary of stages with configuration options for each

ymp.stage.project module

This module defines "Project", a Stage type defined by a project matrix file giving units and meta data for input files.

class ymp.stage.project.**PandasTableBuilder**
Bases: object

Builds the data table describing each sample in a project

This class implements loading and combining tabular data files as specified by the YAML configuration.

Format:

- string items are files
- lists of files are concatenated top to bottom
- dicts must have one "command" value:
  - 'join' contains a two-item list the two items are joined 'naturally' on shared headers
  - 'table' contains a list of one-item dicts dicts have form `key:value[,value...]` a in-place table is created from the keys list-of-dict is necessary as dicts are unordered
  - 'paste' contains a list of tables pasted left to right tables pasted must be of equal length or length 1
- if a value is a valid path relative to the csv/tsv/xls file's location, it is expanded to a path relative to CWD

Example

```
- top.csv
- join:
  - excel.xslx%left.csv
  - right.tsv
- table:
  - sample: s1,s2,s3
  - fq1: s1.1.fq, s2.1.fq, s3.1.fq
  - fq2: s1.2.fq, s2.2.fq, s3.2.fq
```

load_data(*cfg*, *key*)

class ymp.stage.project.**Project**(*name*, *cfg*)
Bases: *ymp.stage.base.ConfigStage*

Contains configuration for a source dataset to be processed

KEY_BCCOL = 'barcode_col'

KEY_DATA = 'data'

KEY_IDCOL = 'id_col'

KEY_READCOLS = 'read_cols'

RE_FILE = re.compile('^(?!http://).*(?:fq|fastq)(?:|\\.gz)$')

RE_REMOTE = re.compile('^(?:https?|ftp|sftp)://(?:.*)')

RE_SRR = re.compile('^[SED]RR[0-9]+$')

choose_fq_columns()
Configures the columns referencing the fastq sources

choose_id_column()
Configures column to use as index on runs

If explicitly configured via KEY_IDCOL, verifies that the column exists and that it is unique. Otherwise chooses the leftmost unique column in the data.

property data
Pandas dataframe of runs

Lazy loading property, first call may take a while.

do_get_ids(*_stack*, *groups*, *match_groups=None*, *match_values=None*)

docstring: Optional[str]
The docstring describing this stage. Visible via `ymp stage list` and in the generated sphinx documentation.

encode_barcode_path(*barcode_file*, *run*, *pair*)

property fq_names
Names of all FastQ files

property fwd_fq_names
Names of forward FastQ files (se and pe)

property fwd_pe_fq_names
Names of forward FastQ files part of pair

get_all_targets(*stack*, *output_types=None*)
Targets to build to complete this stage given `stack`.

Typically, this is the StageStack's path appended with the stamp name.

Return type List[str]

get_fq_names(*only_fwd=False*, *only_rev=False*, *only_pe=False*, *only_se=False*)
Get pipeline names of fq files

get_group(*stack*, *default_groups*)
Determine output grouping for stage

Parameters

- **stack** (StageStack) – The stack for which output grouping is requested.
- **default_groups** (List[str]) – Grouping determined from stage inputs
- **override_groups** – Override grouping from GroupBy stage or None.

Return type List[str]

get_ids(*stack*, *groups*, *match_groups=None*, *match_values=None*)
Determine the target ID names for a set of active groupings

Called from `{:target:}` and `{:targets:}`. For `{:targets:}`, `groups` is the set of active groupings for the stage stack. For `{:target:}`, it's the same set for the source of the file type, the current grouping and the current target.

Parameters

- **groups** – Set of columns the values of which should form IDs
- **match_value** – Limit output to rows with this value
- **match_groups** – ... in these groups

property idcol

iter_samples(*variables=None*)

minimize_variables(*groups*)
Removes redundant groupings

property outputs
Returns the set of outputs this stage is able to generate.

May return either a `set` or a `dict` with the dictionary values representing redirections in the case of virtual stages such as *`Pipeline`* or *`Reference`*.

Return type `Union`[`Set`[`str`], `Dict`[`str`, `str`]]

property pe_fq_names
Names of paired end FastQ files

property project_name

raw_reads_source_path(*args*, *kwargs*)

property rev_pe_fq_names
Names of reverse FastQ files part of pair

property runs
Pandas dataframe index of runs

Lazy loading property, first call may take a while.

property se_fq_names
Names of single end FastQ files

property source_cfg

source_path(*target*, *pair*, *nosplit=False*)
Get path for FQ file for `run` and `pair`

unsplit_path(*barcode_id*, *pairname*)

property variables

class ymp.stage.project.**SQLiteProjectData**(*cfg*, *key*, *name='data'*)
Bases: `object`

columns()

property db_url

dump()

duplicate_rows(*column*)

fetch(*cols*, *idcols=None*, *values=None*)

Return type `List`[`List`[`str`]]

groupby_dedup(*cols*)

identifying_columns()

property nrows

query(**args*)

rows(*col*)

string_columns()

ymp.stage.reference module

class ymp.stage.reference.**Archive**(*name*, *dirname*, *tar*, *url*, *strip*, *files*)
Bases: object

dirname = None

files = None

get_files()

hash = None

make_unpack_rule(*baserule*)

name = None

strip_components = None

tar = None

class ymp.stage.reference.**Reference**(*name*, *cfg*)
Bases: *ymp.stage.base.Activateable*, *ymp.stage.base.ConfigStage*

Represents (remote) reference file/database configuration

add_resource(*rsc*)

files: Dict[str, str]
Files provided by the reference. Keys are the file names within ymp ("target.extension"), symlinked into dir.ref/ref_name/ and values are the path to the reference file from workspace root.

get_all_targets(*stack*)
Targets to build to complete this stage given `stack`.

Typically, this is the StageStack's path appended with the stamp name.

Return type List[str]

get_file(*filename*)

get_group(*stack*, *default_groups*)
Determine output grouping for stage

Parameters

- **stack** (StageStack) – The stack for which output grouping is requested.
- **default_groups** (List[str]) – Grouping determined from stage inputs
- **override_groups** – Override grouping from GroupBy stage or None.

Return type List[str]

get_ids(*stack*, *groups*, *match_groups=None*, *match_value=None*)
Determine the target ID names for a set of active groupings

Called from `{:target:}` and `{:targets:}`. For `{:targets:}`, `groups` is the set of active groupings for the stage stack. For `{:target:}`, it's the same set for the source of the file type, the current grouping and the current target.

Parameters

- **groups** (List[str]) – Set of columns the values of which should form IDs
- **match_value** (Optional[str]) – Limit output to rows with this value
- **match_groups** (Optional[List[str]]) – ... in these groups

Return type List[str]

get_path(*_stack*)
On disk location for this stage given stack.

Called by *StageStack* to determine the real path for virtual stages (which must override this function).

make_unpack_rules(*baserule*)

property outputs
Returns the set of outputs this stage is able to generate.

May return either a set or a dict with the dictionary values representing redirections in the case of virtual stages such as *Pipeline* or *Reference*.

Return type Union[Set[str], Dict[str, str]]

prev(*args=None*, *kwargs=None*)

rules: List[snakemake.rules.Rule]
Rules in this stage

this(*args=None*, *kwargs=None*)

ymp.stage.stack module

Implements the StageStack

class ymp.stage.stack.**StageStack**(*path*)
Bases: object

The "head" of a processing chain - a stack of stages

all_targets()

complete(*incomplete*)

debug = False
Set to true to enable additional Stack debug logging

property defined_in

get_ids(*select_cols*, *where_cols=None*, *where_vals=None*)

group: List[str]
Grouping in effect for this StageStack. And empty list groups into one pseudo target, 'ALL'.

classmethod instance(*path*)
Cached access to StageStack

Parameters

- **path** – Stage path
- **stage** – Stage object at head of stack

name
Name of stack, aka is its full path

property path
On disk location of files provided by this stack

prev(*_args=None*, *kwargs=None*)
Directory of previous stage

Return type *StageStack*

prev_stage
Stage below top stage or None if first in stack

prevs
Mapping of each input type required by the stage of this stack to the prefix stack providing it.

project
Project on which stack operates This is needed for grouping variables currently.

resolve_prevs()

show_info()

stage
Top Stage

stage_name
Top Stage Name

stage_names
Names of stages on stack

stages
Stages on stack

target(*args*, *kwargs*)
Determines the IDs for a given input data type and output ID (replaces "{:target:}").

property targets
Determines the IDs to be built by this Stage Stack (replaces "{:targets:}").

used_stacks = {}

ymp.stage.stack.**find_stage**(*name*)

ymp.stage.stack.**norm_wildcards**(*pattern*)

ymp.stage.stage module

Implements the "Stage"

At it's most basic, a "Stage" is a set of Snakemake rules that share an output folder.

class ymp.stage.stage.**Stage**(*name*, *altname=None*, *env=None*, *doc=None*)
Bases: *ymp.snakemake.WorkflowObject*, *ymp.stage.params.Parametrizable*, *ymp.stage.base.Activateable*, *ymp.stage.base.BaseStage*

Creates a new stage

While entered using `with`, several stage specific variables are expanded within rules:

- `{:this:}` – The current stage directory
- `{:that:}` – The alternate output stage directory
- `{:prev:}` – The previous stage's directory

Parameters

- **name** (*str*) – Name of this stage

- **altname** (Optional[str]) – Alternate name of this stage (used for stages with multiple output variants, e.g. filter_x and remove_x.
- **doc** (Optional[str]) – See *doc()*
- **env** (Optional[str]) – See *env()*

altname: **str**
Alternative stage name (deprecated)

bin(*_args=None*, *kwargs=None*)
Dynamic ID for splitting stages

checkpoints: **Dict[str, Set[str]]**
Checkpoints in this stage

env(*name*)
Add package specifications to Stage environment

Note: This sets the environment for all rules within the stage, which leads to errors with Snakemake rule types not supporting conda environments

---

Parameters **name** (str) – Environment name or filename

```
>>> Env("blast", packages="blast =2.7*")
>>> with Stage("test") as S:
>>>     S.env("blast")
>>>     rule testing:
>>>         ...
```

```
>>> with Stage("test", env="blast") as S:
>>>     rule testing:
>>>         ...
```

```
>>> with Stage("test") as S:
>>>     rule testing:
>>>         conda: "blast"
>>>         ...
```

Return type None

get_all_targets(*stack*)
Targets to build to complete this stage given `stack`.

Typically, this is the StageStack's path appended with the stamp name.

get_checkpoint_ids(*stack*, *mygroup*, *target*)

get_group(*stack*, *default_groups*)
Determine output grouping for stage

Parameters

- **stack** – The stack for which output grouping is requested.
- **default_groups** (List[str]) – Grouping determined from stage inputs
- **override_groups** – Override grouping from GroupBy stage or None.

Return type List[str]

get_ids(*stack*, *groups*, *mygroups=None*, *target=None*)
Determine the target ID names for a set of active groupings

Called from {:target:} and {:targets:}. For {:targets:}, groups is the set of active groupings for the stage stack. For {:target:}, it's the same set for the source of the file type, the current grouping and the current target.

Parameters

- **groups** – Set of columns the values of which should form IDs
- **match_value** – Limit output to rows with this value
- **match_groups** – ... in these groups

get_inputs()
Returns the set of inputs required by this stage

This function must return a copy, to ensure internal data is not modified.

has_checkpoint()

Return type bool

match(*name*)
Check if the name can refer to this stage

As component of a *StageStack*, a stage may be identified by alternative names and may also be parametrized by suffix modifiers. Stage types supporting this behavior must override this function.

property outputs
Returns the set of outputs this stage is able to generate.

May return either a set or a dict with the dictionary values representing redirections in the case of virtual stages such as *Pipeline* or *Reference*.

Return type Set[str]

prev(*_args*, *kwargs*)
Gathers {:prev:} calls from rules

Here, input requirements for each stage are collected.

Return type None

require(***kwargs*)
Override inferred stage inputs

In theory, this should not be needed. But it's simpler for now.

requires
Contains override stage inputs

satisfy_inputs(*other_stage*, *inputs*)

Return type Dict[str, str]

that(*_args=None*, *kwargs=None*)
Alternate directory of current stage

Used for splitting stages

this(*args=None*, *kwargs=None*)
Replaces {:this:} in rules

Also gathers output capabilities of each stage.

wc2path(*wc*)

6.1.2 Submodules

6.1.3 ymp.blast module

Parsers for blast output formats 6 (CSV) and 7 (CSV with comments between queries).

class ymp.blast.**BlastBase**
Bases: object

Base class for BLAST readers and writers

FIELD_MAP = {'% identity': 'pident', 'alignment length': 'length', 'bit score': 'bi
Map between field short and long names

FIELD_REV_MAP = {'bitscore': 'bit score', 'evalue': 'evalue', 'gapopen': 'gap opens
Reversed map from short to long name

FIELD_TYPE = {'bitscore': <class 'float'>, 'evalue': <class 'float'>, 'gapopen': <c
Map defining types of fields

tupleofint()

class ymp.blast.**BlastParser**
Bases: *ymp.blast.BlastBase*

Base class for BLAST readers

get_fields()

class ymp.blast.**BlastWriter**
Bases: *ymp.blast.BlastBase*

Base class for BLAST writers

write_hit(*hit*)

class ymp.blast.**Fmt6Parser**(*fileobj*)
Bases: *ymp.blast.BlastParser*

Parser for BLAST format 6 (CSV)

Hit
alias of ymp.blast.BlastHit

field_types = [None, None, <class 'float'>, <class 'int'>, <class 'int'>, <class 'int'

fields = ['qseqid', 'sseqid', 'pident', 'length', 'mismatch', 'gapopen', 'qstart', 'qe
Default field types

get_fields()

class ymp.blast.**Fmt7Parser**(*fileobj*)
Bases: *ymp.blast.BlastParser*

Parses BLAST results in format '7' (CSV with comments)

PAT_DATABASE = '# Database: '

PAT_FIELDS = '# Fields: '

PAT_HITSFOUND = ' hits found'

PAT_QUERY = '# Query: '

get_fields()
Returns list of available field names

Format 7 specifies which columns it contains in comment lines, allowing this parser to be agnostic of the selection of columns made when running BLAST.

Return type List[str]

Returns List of field names (e.g. ['sacc', 'qacc', 'evalue'])

isfirsthit()
Returns True if the current hit is the first hit for the current query

Return type bool

class ymp.blast.**Fmt7Writer**(*fileobj*)
Bases: *ymp.blast.BlastWriter*

write_header()
Writes BLAST7 format header

write_hit(*hit*)

write_hitset()

ymp.blast.**reader**(*fileobj*, *t=7*)
Creates a reader for files in BLAST format

```
>>> with open(blast_file) as infile:
>>>     reader = blast.reader(infile)
>>>     for hit in reader:
>>>         print(hit)
```

Parameters

- **fileobj** – iterable yielding lines in blast format
- **t** (int) – number of blast format type

Return type *BlastParser*

ymp.blast.**writer**(*fileobj*, *t=7*)
Creates a writer for files in BLAST format

```
>>> with open(blast_file) as outfile:
>>>     writer = blast.writer(outfile)
>>>     for hit in hits:
>>>         writer.write_hit(hit)
```

Return type *BlastWriter*

6.1.4 ymp.blast2gff module

6.1.5 ymp.cluster module

Module handling talking to cluster management systems

```
>>> python -m ymp.cluster slurm status <jobid>
```

class ymp.cluster.**ClusterMS**
Bases: object

class ymp.cluster.**Lsf**
Bases: *ymp.cluster.ClusterMS*

Talking to LSF

states = {'DONE': 'success', 'EXIT': 'failed', 'PEND': 'running', 'POST_DONE': 'succes

static status(*jobid*)

static submit(*args*)

class ymp.cluster.**Slurm**
Bases: *ymp.cluster.ClusterMS*

Talking to Slurm

states = {'BOOT_FAIL': 'failed', 'CANCELLED': 'failed', 'COMPLETED': 'success', 'COMPL

static status(*jobid*)
Print status of job @param jobid to stdout (as needed by snakemake)

Anectotal benchmarking shows 200ms per invocation, half used by Python startup and half by calling sacct. Using `scontrol show job` instead of `sacct -pbs` is faster by 80ms, but finished jobs are purged after unknown time window.

ymp.cluster.**error**(**args*, ***kwargs*)

6.1.6 ymp.common module

Collection of shared utility classes and methods

class ymp.common.**AttrDict**
Bases: dict

AttrDict adds accessing stored keys as attributes to dict

class ymp.common.**Cache**(*root*)
Bases: object

close()

commit()

get_cache(*name*, *clean=False*, **args*, ***kwargs*)

load(*cache*, *key*)

load_all(*cache*)

store(*cache*, *key*, *obj*)

class ymp.common.**CacheDict**(*cache*, *name*, **args*, *loadfunc=None*, *itemloadfunc=None*, *itemdata=None*, ***kwargs*)

Bases: *ymp.common.AttrDict*

get(*key*, *default=None*)
Return the value for key if key is in the dictionary, else default.

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

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

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

class ymp.common.**MkdirDict**

Bases: *ymp.common.AttrDict*

Creates directories as they are requested

class ymp.common.**NoCache**(*root*)

Bases: object

close()

commit()

get_cache(*name*, *clean=False*, **args*, ***kwargs*)

load(*_cache*, *_key*)

load_all(*_cache*)

store(*cache*, *key*, *obj*)

ymp.common.**ensure_list**(*obj*)
Wrap obj in a list as needed

ymp.common.**flatten**(*item*)
Flatten lists without turning strings into letters

ymp.common.**format_number**(*num*, *unit=''*)

Return type int

ymp.common.**format_time**(*seconds*, *unit=None*)
Prints time in SLURM format

Return type str

ymp.common.**is_container**(*obj*)
Check if object is container, considering strings not containers

ymp.common.**parse_number**(*s=''*)
Basic 1k 1m 1g 1t parsing.

- assumes base 2
- returns "byte" value
- accepts "1kib", "1kb" or "1k"

ymp.common.**parse_time**(*timestr*)
Parses time in "SLURM" format

<minutes> <minutes>:<seconds> <hours>:<minutes>:<seconds> <days>-<hours> <days>-<hours>:<minutes> <days>-<hours>:<minutes>:<seconds>

Return type int

6.1.7 ymp.config module

class ymp.config.**ConfigExpander**(*config_mgr*)
Bases: *ymp.snakemake.ColonExpander*

class Formatter(*expander*)
Bases: *ymp.snakemake.FormatExpander.Formatter*, *ymp.string.PartialFormatter*

get_value(*field_name*, *args*, *kwargs*)

expands_field(*field*)
Checks if this expander should expand a Rule field type

Parameters **field** – the field to check

Returns True if *field* should be expanded.

class ymp.config.**ConfigMgr**(*root*, *conffiles*)
Bases: object

Manages workflow configuration

This is a singleton object of which only one instance should be around at a given time. It is available in the rules files as `icfg` and via *ymp.get_config()* elsewhere.

ConfigMgr loads and maintains the workflow configuration as given in the `ymp.yml` files located in the workflow root directory, the user config folder (`~/.ymp`) and the installation `etc` folder.

CONF_DEFAULT_FNAME = '/home/docs/checkouts/readthedocs.org/user_builds/ymp/checkouts/l

CONF_FNAME = 'ymp.yml'

CONF_USER_FNAME = '/home/docs/.ymp/ymp.yml'

KEY_LIMITS = 'resource_limits'

KEY_PIPELINES = 'pipelines'

KEY_PROJECTS = 'projects'

KEY_REFERENCES = 'references'

RULE_MAIN_FNAME = '/home/docs/checkouts/readthedocs.org/user_builds/ymp/checkouts/late

property absdir
Dictionary of absolute paths of named YMP directories

classmethod activate()

property cluster
The YMP cluster configuration.

property conda

property dir
Dictionary of relative paths of named YMP directories

The directory paths are relative to the YMP root workdir.

property ensuredir
Dictionary of absolute paths of named YMP directories

Directories will be created on the fly as they are requested.

expand(*item*, ***kwargs*)

classmethod find_config()
Locates ymp config files and ymp root

The root ymp work dir is determined as the first (parent) directory containing a file named `ConfigMgr.CONF_FNAME` (default `ymp.yml`).

The stack of config files comprises 1. the default config `ConfigMgr.CONF_DEFAULT_FNAME` (`etc/defaults.yml` in the ymp package directory), 2. the user config `ConfigMgr.CONF_USER_FNAME` (`~/.ymp/ymp.yml`) and 3. the `yml.yml` in the ymp root.

Returns Root working directory conffiles: list of active configuration files

Return type root

classmethod instance()
Returns the active Ymp ConfigMgr instance

property pairnames

property pipeline
Configure pipelines

property platform
Name of current platform (macos or linux)

property ref
Configure references

property rules

property shell
The shell used by YMP

Change by adding e.g. `shell: /path/to/shell` to `ymp.yml`.

property snakefiles
Snakefiles used under this config in parsing order

classmethod unload()

property workflow

class ymp.config.**OverrideExpander**(*cfgmgr*)
Bases: *ymp.snakemake.BaseExpander*

Override rule parameters, resources and threads using config values

Example

Set the `wordsize` parameter in the *bmtagger_bitmask* rule to 12:

Listing 1: ymp.yml

```
overrides:
  rules:
    bmtagger_bitmask:
      params:
        wordsize: 12
      resources:
        memory: 15G
      threads: 12
```

expand(*rule*, *ruleinfo*, ***kwargs*)
Expands RuleInfo object and children recursively.

Will call :meth:format (via :meth:format_annotated) on `str` items encountered in the tree and wrap encountered functions to be called once the wildcards object is available.

Set `ymp.print_rule = 1` before a `rule:` statement in snakefiles to enable debug logging of recursion.

Parameters

- **rule** – The :class:snakemake.rules.Rule object to be populated with the data from the RuleInfo object passed from *item*
- **item** – The item to be expanded. Initially a :class:snakemake.workflow.RuleInfo object into which is recursively decendet. May ultimately be `None`, `str`, `function`, `int`, `float`, `dict`, `list` or `tuple`.
- **expand_args** – Parameters passed on late expansion (when the `dag` tries to instantiate the *`rule`* into a `job`.
- **rec** – Recursion level

types = {'params': typing.Mapping, 'resources': typing.Mapping, 'threads': <class '

class ymp.config.**ResourceLimitsExpander**(*cfg*)
Bases: *`ymp.snakemake.BaseExpander`*

Allows adjusting resources to local compute environment

Each config item defines processing for an item in `resources:` or the special resource``threads``. Each item may have a `default` value filled in for rules not defining the resource, `min` and `max` defining the lower and uppeer bounds, and a `scale` value applied to the `default` to adjust resources up or down globally. Values in time or "human readable" format mabe parsed specially by passing the `format` values `time` or `number`, respectively. These values will also be reformatted, with the optional paramter `unit` defining the output format (k/g/m/t for numbers and minutes/seconds for time). Additional resource values may be generated from configured onces using the `from` keyword (e.g. to provide both `mem_mb` and `mem_gb` from a generic `mem` value.

static adjust_value(*value*, *default*, *scale*, *minimum*, *maximum*)
Applies default, scale, minimum and maximum to a numeric value)

Return type `Optional`[`int`]

expand(*rule*, *ruleinfo*, ***kwargs*)
Expands RuleInfo object and children recursively.

Will call :meth:format (via :meth:format_annotated) on `str` items encountered in the tree and wrap encountered functions to be called once the wildcards object is available.

Set `ymp.print_rule = 1` before a `rule:` statement in snakefiles to enable debug logging of recursion.

Parameters

- **rule** – The :class:snakemake.rules.Rule object to be populated with the data from the RuleInfo object passed from *item*
- **item** – The item to be expanded. Initially a :class:snakemake.workflow.RuleInfo object into which is recursively decendet. May ultimately be `None`, `str`, `function`, `int`, `float`, `dict`, `list` or `tuple`.
- **expand_args** – Parameters passed on late expansion (when the `dag` tries to instantiate the *`rule`* into a `job`.

- **rec** – Recursion level

Return type None

expands_field(*field*)
Checks if this expander should expand a Rule field type

Parameters **field** (str) – the field to check

Return type bool

Returns True if *field* should be expanded.

formatters = {'number': <function format_number>, 'time': <function format_time>}

parse_config(*cfg*)
Parses limits config

parsers = {'number': <function parse_number>, 'time': <function parse_time>}

6.1.8 ymp.dna module

ymp.dna.**nuc2aa**(*seq*)

ymp.dna.**nuc2num**(*seq*)

6.1.9 ymp.download module

class ymp.download.**DownloadThread**
Bases: object

get(*url*, *dest*, *md5*)

main()

terminate()

class ymp.download.**FileDownloader**(*block_size=4096*, *timeout=300*, *parallel=4*, *loglevel=30*, *alturls=None*, *retry=3*)
Bases: object

Manages download of a set of URLs

Downloads happen concurrently using asyncronous network IO.

Parameters

- **block_size** (int) – Byte size of chunks to download
- **timeout** (int) – Aiohttp cumulative timeout
- **parallel** (int) – Number of files to download in parallel
- **loglevel** (int) – Log level for messages send to logging (Errors are send with loglevel+10)
- **alturls** – List of regexps modifying URLs
- **retry** (int) – Number of times to retry download

error(*msg*, **args*, ***kwargs*)
Send error to logger

Message is sent with a log level 10 higher than the default for this object.

Return type None

get(*urls*, *dest*, *md5s=None*)
Download a list of URLs

Parameters

- **urls** (Union[str, List[str]]) – List of URLs
- **dest** (str) – Destination folder
- **md5s** (Optional[List[str]]) – List of MD5 sums to check

Return type None

log(*msg*, **args*, *modlvl=0*, ***kwargs*)
Send message to logger

Honors loglevel set for the FileDownloader object.

Parameters

- **msg** (str) – The log message
- **modlvl** (int) – Added to default logging level for object

Return type None

static make_bar_format(*desc_width=20*, *count_width=0*, *rate=False*, *eta=False*, *have_total=True*)
Construct bar_format for tqdm

Parameters

- **desc_width** (int) – minimum space allocated for description
- **count_width** (int) – min space for counts
- **rate** (bool) – show rate to right of progress bar
- **eta** (bool) – show eta to right of progress bar
- **have_total** (bool) – whether a total exists (required to add percentage)

Return type str

6.1.10 ymp.env module

This module manages the conda environments.

class ymp.env.**CondaPathExpander**(*config*, **args*, ***kwargs*)
Bases: *ymp.snakemake.BaseExpander*

Applies search path for conda environment specifications

File names supplied via `rule: conda: "some.yml"` are replaced with absolute paths if they are found in any searched directory. Each `search_paths` entry is appended to the directory containing the top level Snakefile and the directory checked for the filename. Thereafter, the stack of including Snakefiles is traversed backwards. If no file is found, the original name is returned.

expands_field(*field*)
Checks if this expander should expand a Rule field type

Parameters **field** – the field to check

Returns True if *field* should be expanded.

format (*conda_env*, **args*, ***kwargs*)
Format *item* using **args* and ***kwargs*

class ymp.env.**Env**(*env_file=None*, *workflow=None*, *env_dir=None*, *container_img=None*, *cleanup=None*, *name=None*, *packages=None*, *base='none'*, *channels=None*)
Bases: *ymp.snakemake.WorkflowObject*, snakemake.deployment.conda.Env

Represents YMP conda environment

Snakemake expects the conda environments in a per-workflow directory configured by `conda_prefix`. YMP sets this value by default to `~/.ymp/conda`, which has a greater chance of being on the same file system as the conda cache, allowing for hard linking of environment files.

Within the folder `conda_prefix`, each environment is created in a folder named by the hash of the environment definition file's contents and the `conda_prefix` path. This class inherits from `snakemake.deployment.conda.Env` to ensure that the hash we use is identical to the one Snakemake will use during workflow execution.

The class provides additional features for updating environments, creating environments dynamically and executing commands within those environments.

Note: This is not called from within the execution. Snakemake instanciates its own Env object purely based on the filename.

Creates an inline defined conda environment

Parameters

- **name** (Optional[str]) – Name of conda environment (and basename of file)
- **packages** (Union[list, str, None]) – package(s) to be installed into environment. Version constraints can be specified in each package string separated from the package name by whitespace. E.g. `"blast =2.6*"`
- **channels** (Union[list, str, None]) – channel(s) to be selected for the environment
- **base** (str) – Select a set of default channels and packages to be added to the newly created environment. Sets are defined in conda.defaults in `yml.yml`

create (*dryrun=False*, *reinstall=False*, *nospec=False*, *noarchive=False*)
Ensure the conda environment has been created

Inherits from snakemake.deployment.conda.Env.create

Behavior of super class

- Resolve remote file
- If containerized, check environment path exists and return if true
- Check for interrupted env create, delete if so
- Return if environment exists
- Install from archive if env_archive exists
- Install using self.frontent if not_careful

Handling pre-computed environment specs In addition to freezing environments by maintaining a copy of the package binaries, we allow maintaining a copy of the package binary URLs, from which the archive folder is populated on demand. We just download those to self.archive and pass on.

export (*stream*, *typ='yml'*)
Freeze environment

static get_installed_env_hashes()

property installed

run(*command*)
Execute command in environment

Returns exit code of command run.

set_prefix(*prefix*)

update()
Update conda environment

6.1.11 ymp.exceptions module

Exceptions raised by YMP

exception ymp.exceptions.**YmpConfigError**(*obj*, *msg*, *key=None*)
Bases: *ymp.exceptions.YmpLocateableError*

Indicates an error in the ymp.yml config files

Parameters

- **obj** (object) – Subtree of config causing error
- **msg** (str) – The message to display
- **key** (Optional[object]) – Key indicating part of obj causing error
- **exc** – Upstream exception causing error

get_fileline()
Retrieve filename and linenumber from object associated with exception

Returns Tuple of filename and linenumber

exception ymp.exceptions.**YmpException**
Bases: Exception

Base class of all YMP Exceptions

exception ymp.exceptions.**YmpLocateableError**(*obj*, *msg*, *show_includes=True*)
Bases: *ymp.exceptions.YmpPrettyException*

Errors that have a file location to be shown

Parameters

- **obj** (object) – The object causing the exception. Must have lineno and filename as these will be shown as part of the error message on the command line.
- **msg** (str) – The message to display
- **show_includes** (bool) – Whether or not the "stack" of includes should be printed.

get_fileline()
Retrieve filename and linenumber from object associated with exception

Return type Tuple[str, int]

Returns Tuple of filename and linenumber

show(*file=None*)

Return type None

exception ymp.exceptions.**YmpPrettyException**(*message*)
Bases: *ymp.exceptions.YmpException*, click.exceptions.ClickException, snakemake.exceptions.WorkflowError

Exception that does not lead to stack trace on CLI

Inheriting from ClickException makes `click` print only the `self.msg` value of the exception, rather than allowing Python to print a full stack trace.

This is useful for exceptions indicating usage or configuration errors. We use this, instead of `click.UsageError` and friends so that the exceptions can be caught and handled explicitly where needed.

Note that click will call the `show` method on this object to print the exception. The default implementation from click will just prefix the `msg` with `Error:`.

FIXME: This does not work if the exception is raised from within the snakemake workflow as snakemake.snakemake catches and reformats exceptions.

rule = None

snakefile = None

exception ymp.exceptions.**YmpRuleError**(*obj*, *msg*, *show_includes=True*)
Bases: *ymp.exceptions.YmpLocateableError*

Indicates an error in the rules files

This could e.g. be a Stage or Environment defined twice.

exception ymp.exceptions.**YmpStageError**(*msg*)
Bases: *ymp.exceptions.YmpPrettyException*

Indicates an error in the requested stage stack

show(*file=None*)

Return type None

exception ymp.exceptions.**YmpSystemError**(*message*)
Bases: *ymp.exceptions.YmpPrettyException*

Indicates problem running YMP with available system software

exception ymp.exceptions.**YmpUsageError**(*message*)
Bases: *ymp.exceptions.YmpPrettyException*

General usage error

exception ymp.exceptions.**YmpWorkflowError**(*message*)
Bases: *ymp.exceptions.YmpPrettyException*

Indicates an error during workflow execution

E.g. failures to expand dynamic variables

6.1.12 ymp.gff module

Implements simple reader and writer for GFF (general feature format) files.

Unfinished

- only supports one version, GFF 3.2.3.
- no escaping

class ymp.gff.**Attributes**(*ID*, *Name*, *Alias*, *Parent*, *Target*, *Gap*, *Derives_From*, *Note*, *Dbxref*, *Ontology_term*, *Is_circular*)

Bases: tuple

Create new instance of Attributes(ID, Name, Alias, Parent, Target, Gap, Derives_From, Note, Dbxref, Ontology_term, Is_circular)

Alias
Alias for field number 2

Dbxref
Alias for field number 8

Derives_From
Alias for field number 6

Gap
Alias for field number 5

ID
Alias for field number 0

Is_circular
Alias for field number 10

Name
Alias for field number 1

Note
Alias for field number 7

Ontology_term
Alias for field number 9

Parent
Alias for field number 3

Target
Alias for field number 4

class ymp.gff.**Feature**(*seqid*, *source*, *type*, *start*, *end*, *score*, *strand*, *phase*, *attributes*)

Bases: tuple

Create new instance of Feature(seqid, source, type, start, end, score, strand, phase, attributes)

attributes
Alias for field number 8

end
Alias for field number 4

phase
Alias for field number 7

score
Alias for field number 5

seqid
Alias for field number 0

source
Alias for field number 1

start
Alias for field number 3

strand
Alias for field number 6

type
Alias for field number 2

class ymp.gff.**reader**(*fileobj*)
Bases: object

class ymp.gff.**writer**(*fileobj*)
Bases: object

write(*feature*)

6.1.13 ymp.helpers module

This module contains helper functions.

Not all of these are currently in use

class ymp.helpers.**OrderedDictMaker**
Bases: object

odict creates OrderedDict objects in a dict-literal like syntax

```
>>>  my_ordered_dict = odict[
>>>    'key': 'value'
>>>  ]
```

Implementation: odict uses the python slice syntax which is similar to dict literals. The [] operator is implemented by overriding __getitem__. Slices passed to the operator as `object[start1:stop1:step1, start2:...]`, are passed to the implementation as a list of objects with start, stop and step members. odict simply creates an OrderedDictionary by iterating over that list.

ymp.helpers.**update_dict**(*dst*, *src*)
Recursively update dictionary `dst` with `src`

- Treats a `list` as atomic, replacing it with new list.
- Dictionaries are overwritten by item
- None is replaced by empty dict if necessary

6.1.14 ymp.map2otu module

class ymp.map2otu.**MapfileParser**(*minid=0*)
Bases: object

read(*mapfiles*)

write(*outfile*)

class ymp.map2otu.**emirge_info**(*line*)
Bases: object

ymp.map2otu.**main**()

6.1.15 ymp.nuc2aa module

ymp.nuc2aa.**fasta_dna2aa**(*inf*, *outf*)

ymp.nuc2aa.**nuc2aa**(*seq*)

ymp.nuc2aa.**nuc2num**(*seq*)

6.1.16 ymp.snakemake module

Extends Snakemake Features

class ymp.snakemake.**BaseExpander**
Bases: object

Base class for Snakemake expansion modules.

Subclasses should override the :meth:expand method if they need to work on the entire RuleInfo object or the :meth:format and :meth:expands_field methods if they intend to modify specific fields.

expand(*rule*, *item*, *expand_args=None*, *rec=- 1*, *cb=False*)
Expands RuleInfo object and children recursively.

Will call :meth:format (via :meth:format_annotated) on `str` items encountered in the tree and wrap encountered functions to be called once the wildcards object is available.

Set `ymp.print_rule = 1` before a `rule:` statement in snakefiles to enable debug logging of recursion.

Parameters

- **rule** – The :class:snakemake.rules.Rule object to be populated with the data from the RuleInfo object passed from *item*
- **item** – The item to be expanded. Initially a :class:snakemake.workflow.RuleInfo object into which is recursively decendet. May ultimately be `None`, `str`, `function`, `int`, `float`, `dict`, `list` or `tuple`.
- **expand_args** – Parameters passed on late expansion (when the `dag` tries to instantiate the *`rule`* into a `job`.
- **rec** – Recursion level

expand_dict(*rule*, *item*, *expand_args*, *rec*)

expand_func(*rule*, *item*, *expand_args*, *rec*, *debug*)

expand_list(*rule*, *item*, *expand_args*, *rec*, *cb*)

expand_ruleinfo(*rule*, *item*, *expand_args*, *rec*)

expand_str(*rule*, *item*, *expand_args*, *rec*, *cb*)

expand_tuple(*rule*, *item*, *expand_args*, *rec*, *cb*)

expands_field(*field*)
Checks if this expander should expand a Rule field type

Parameters **field** – the field to check

Returns True if *field* should be expanded.

format(*item*, **args*, ***kwargs*)
Format *item* using **args* and ***kwargs*

format_annotated(*item*, *expand_args*)
Wrapper for :meth:format preserving *AnnotatedString* flags

Calls :meth:format to format *item* into a new string and copies flags from original item.

This is used by :meth:expand

link_workflow(*workflow*)
Called when the Expander is associated with a workflow

May be called multiple times if a new workflow object is created.

exception ymp.snakemake.**CircularReferenceException**(*deps*, *rule*)
Bases: *ymp.exceptions.YmpRuleError*

Exception raised if parameters in rule contain a circular reference

class ymp.snakemake.**ColonExpander**
Bases: *ymp.snakemake.FormatExpander*

Expander using `{:xyz:}` formatted variables.

regex = re.compile('\n \\{:\n (?=(\n \\s*\n (?P<name>(?:.(?!\\s*\\:\\}))*.)\n \\s*\n)

spec = '{{:{}:}}'

class ymp.snakemake.**DefaultExpander**(***kwargs*)
Bases: *ymp.snakemake.InheritanceExpander*

Adds default values to rules

The implementation simply makes all rules inherit from a defaults rule.

Creates DefaultExpander

Each parameter passed is considered a RuleInfo default value. Where applicable, Snakemake's argtuples `([], {})` must be passed.

get_super(*rule*, *ruleinfo*)
Find rule parent

Parameters

- **rule** (`Rule`) – Rule object being built
- **ruleinfo** (`RuleInfo`) – RuleInfo object describing rule being built

Returns name of parent rule and RuleInfo describing parent rule or (None, None).

Return type 2-Tuple

exception ymp.snakemake.**ExpandLateException**
Bases: Exception

class ymp.snakemake.**ExpandableWorkflow**(**args*, ***kwargs*)
Bases: snakemake.workflow.Workflow

Adds hook for additional rule expansion methods to Snakemake

Constructor for ExpandableWorkflow overlay attributes

This may be called on an already initialized Workflow object.

classmethod activate()
Installs the ExpandableWorkflow

Replaces the Workflow object in the snakemake.workflow module with an instance of this class and initializes default expanders (the snakemake syntax).

add_rule(*name=None*, *lineno=None*, *snakefile=None*, *checkpoint=False*, *allow_overwrite=False*)
Add a rule.

Parameters

- **name** – name of the rule
- **lineno** – line number within the snakefile where the rule was defined
- **snakefile** – name of file in which rule was defined

classmethod clear()

classmethod ensure_global_workflow()

get_rule(*name=None*)
Get rule by name. If name is none, the last created rule is returned.

Parameters **name** – the name of the rule

global_workflow = <ymp.snakemake.ExpandableWorkflow object>

classmethod load_workflow(*snakefile='/home/docs/checkouts/readthedocs.org/user_builds/ymp/checkouts/latest/src/ym*

classmethod register_expanders(**expanders*)
Register an object the expand() function of which will be called on each RuleInfo object before it is passed on to snakemake.

rule(*name=None*, *lineno=None*, *snakefile=None*, *checkpoint=None*)
Intercepts "rule:" Here we have the entire ruleinfo object

class ymp.snakemake.**FormatExpander**
Bases: *ymp.snakemake.BaseExpander*

Expander using a custom formatter object.

class Formatter(*expander*)
Bases: *ymp.string.ProductFormatter*

parse(*format_string*)

format(**args*, ***kwargs*)
Format *item* using **args* and ***kwargs*

get_names(*pattern*)

regex = re.compile('\n \\{\n (?=(\n (?P<name>[^{}]+)\n))\\1\n \\}\n ', re.VERBOSE)

spec = '{{{}}}'

exception ymp.snakemake.**InheritanceException**(*msg*, *rule*, *parent*, *include=None*, *lineno=None*, *snakefile=None*)

Bases: snakemake.exceptions.RuleException

Exception raised for errors during rule inheritance

Creates a new instance of RuleException.

Arguments message – the exception message include – iterable of other exceptions to be included lineno – the line the exception originates snakefile – the file the exception originates

class ymp.snakemake.**InheritanceExpander**

Bases: *ymp.snakemake.BaseExpander*

Adds class-like inheritance to Snakemake rules

To avoid redundancy between closely related rules, e.g. rules for single ended and paired end data, YMP allows Snakemake rules to inherit from another rule.

Example

Derived rules are always created with an implicit `ruleorder` statement, making Snakemake prefer the parent rule if either parent or child rule could be used to generate the requested output file(s).

Derived rules initially contain the same attributes as the parent rule. Each attribute assigned to the child rule overrides the matching attribute in the parent. Where attributes may contain named and unnamed values, specifying a named value overrides only the value of that name while specifying an unnamed value overrides all unnamed values in the parent attribute.

KEYWORD = 'ymp: extends'

Comment keyword enabling inheritance

expand(*rule*, *ruleinfo*)

Expands RuleInfo object and children recursively.

Will call :meth:format (via :meth:format_annotated) on `str` items encountered in the tree and wrap encountered functions to be called once the wildcards object is available.

Set `ymp.print_rule = 1` before a `rule:` statement in snakefiles to enable debug logging of recursion.

Parameters

- **rule** – The :class:snakemake.rules.Rule object to be populated with the data from the RuleInfo object passed from *item*
- **item** – The item to be expanded. Initially a :class:snakemake.workflow.RuleInfo object into which is recursively decendet. May ultimately be `None`, `str`, `function`, `int`, `float`, `dict`, `list` or `tuple`.
- **expand_args** – Parameters passed on late expansion (when the `dag` tries to instantiate the *rule* into a `job`.
- **rec** – Recursion level

get_code_line(*rule*)

Returns the source line defining *rule*

Return type `str`

get_super(*rule*, *ruleinfo*)

Find rule parent

Parameters

- **rule** (Rule) – Rule object being built
- **ruleinfo** (RuleInfo) – RuleInfo object describing rule being built

Returns name of parent rule and RuleInfo describing parent rule or (None, None).

Return type 2-Tuple

class ymp.snakemake.**NamedList**(*fromtuple=None*, ***kwargs*)

Bases: snakemake.io.Namedlist

Extended version of Snakemake's Namedlist

- Fixes array assignment operator: Writing a field via `[]` operator updates the value accessed via `.` operator.
- Adds `fromtuple` to constructor: Builds from Snakemake's typial `(args, kwargs)` tuples as present in ruleinfo structures.
- Adds *update_tuple* method: Updates values in `(args,kwargs)` tuples as present in `ruleinfo` structures.

get_names(**args*, ***kwargs*)

Export `get_names` as public func

update_tuple(*totuple*)

Update values in `(args, kwargs)` tuple.

The tuple must be the same as used in the constructor and must not have been modified.

class ymp.snakemake.**RecursiveExpander**

Bases: *ymp.snakemake.BaseExpander*

Recursively expands `{xyz}` wildcards in Snakemake rules.

expand(*rule*, *ruleinfo*)

Recursively expand wildcards within `RuleInfo` object

expands_field(*field*)

Returns true for all fields but `shell:`, `message:` and `wildcard_constraints`.

We don't want to mess with the regular expressions in the fields in `wildcard_constraints:`, and there is little use in expanding `message:` or `shell:` as these already have all wildcards applied just before job execution (by `format_wildcards()`).

exception ymp.snakemake.**RemoveValue**

Bases: Exception

Return to remove a value from the list

class ymp.snakemake.**SnakemakeExpander**

Bases: *ymp.snakemake.BaseExpander*

Expand wildcards in strings returned from functions.

Snakemake does not do this by default, leaving wildcard expansion to the functions provided themselves. Since we never want `{input}` to be in a string returned as a file, we expand those always.

expands_field(*field*)

Checks if this expander should expand a Rule field type

Parameters **field** – the field to check

Returns True if *field* should be expanded.

format(*item*, **args*, ***kwargs*)
Format *item* using **args* and ***kwargs*

class ymp.snakemake.**WorkflowObject**(**args*, ***kwargs*)
Bases: object

Base for extension classes defined from snakefiles

This currently encompasses *ymp.env.Env* and *ymp.stage.stage.Stage*.

This mixin sets the properties `filename` and `lineno` according to the definition source in the rules file. It also maintains a registry within the Snakemake workflow object and provides an accessor method to this registry.

property defined_in

filename
Name of file in which object was defined

Type str

classmethod get_registry(*clean=False*)
Return all objects of this class registered with current workflow

lineno
Line number of object definition

Type int

classmethod new_registry()

register()
Add self to registry

ymp.snakemake.**check_snakemake**()

Return type bool

ymp.snakemake.**get_workflow**()
Get active workflow, loading one if necessary

ymp.snakemake.**load_workflow**(*snakefile*)
Load new workflow

ymp.snakemake.**make_rule**(*name=None*, *lineno=None*, *snakefile=None*, ***kwargs*)

ymp.snakemake.**networkx**()

ymp.snakemake.**print_ruleinfo**(*rule*, *ruleinfo*, *func=<bound method Logger.debug of <Logger ymp.snakemake (WARNING)>>*)
Logs contents of Rule and RuleInfo objects.

Parameters

- **rule** (Rule) – Rule object to be printed
- **ruleinfo** (RuleInfo) – Matching RuleInfo object to be printed
- **func** – Function used for printing (default is log.error)

ymp.snakemake.**ruleinfo_fields = {'benchmark': {'apply_wildcards': True, 'format': 'strin**
describes attributes of `snakemake.workflow.RuleInfo`

6.1.17 ymp.snakemakelexer module

ymp.snakemakelexer

class ymp.snakemakelexer.**SnakemakeLexer**(**args*, ***kwds*)
Bases: pygments.lexers.python.PythonLexer

name = 'Snakemake'
Name of the lexer

tokens = {'globalkeyword': [(<pygments.lexer.words object>, Token.Keyword)], 'root':
Dict of {'state': [(regex, tokentype, new_state), ...], ...}

The initial state is 'root'. new_state can be omitted to signify no state transition. If it is a string, the state is pushed on the stack and changed. If it is a tuple of strings, all states are pushed on the stack and the current state will be the topmost. It can also be combined('state1', 'state2', ...) to signify a new, anonymous state combined from the rules of two or more existing ones. Furthermore, it can be '#pop' to signify going back one step in the state stack, or '#push' to push the current state on the stack again.

The tuple can also be replaced with include('state'), in which case the rules from the state named by the string are included in the current one.

6.1.18 ymp.sphinxext module

This module contains a Sphinx extension for documenting YMP stages and Snakemake rules.

The *SnakemakeDomain* (name **sm**) provides the following directives:

.. **sm:rule::** name
Describes a Snakemake rule

.. **sm:stage::** name
Describes a *YMP Stage*

Both directives accept an optional source parameter. If given, a link to the source code of the stage or rule definition will be added. The format of the string passed is filename:line. Referenced Snakefiles will be highlighted with pygments and added to the documentation when building HTML.

The extension also provides an autodoc-like directive:

.. **autosnake::** filename
Generates documentation from Snakefile filename.

class ymp.sphinxext.**AutoSnakefileDirective**(*name*, *arguments*, *options*, *content*, *lineno*, *content_offset*, *block_text*, *state*, *state_machine*)
Bases: docutils.parsers.rst.Directive

Implements RSt directive .. autosnake:: filename

The directive extracts docstrings from rules in snakefile and auto-generates documentation.

has_content = False
This rule does not accept content

Type bool

load_workflow(*file_path*)
Load the Snakefile

Return type *ExpandableWorkflow*

parse_doc(*doc*, *source*, *idt=0*)
Convert doc string to StringList

Parameters

- **doc** (str) – Documentation text
- **source** (str) – Source filename
- **idt** (int) – Result indentation in characters (default 0)

Return type StringList

Returns StringList of re-indented documentation wrapped in newlines

parse_rule(*rule_name*, *idt=0*)
Convert Rule to StringList

Parameters

- **rule** – Rule object
- **idt** (int) – Result indentation in characters (default 0)

Retuns: StringList containing formatted Rule documentation

Return type StringList

parse_stage(*stage*, *idt=0*)

Return type StringList

required_arguments = 1
This rule needs one argument (the filename)

Type int

run()
Entry point

tpl_rule = '.. sm:rule:: {name}'
Template for generated Rule RSt

Type str

tpl_source = ' :source: {filename}:{lineno}'
Template option source

Type str

tpl_stage = '.. sm:stage:: {name}'
Template for generated Stage RSt

Type str

ymp.sphinxext.**BASEPATH = '/home/docs/checkouts/readthedocs.org/user_builds/ymp/checkouts/la**
Path in which YMP package is located

Type str

class ymp.sphinxext.**CondaDomain**(*env*)
Bases: sphinx.domains.Domain

name = 'conda'
should be short, but unique

Type domain name

object_types: Dict[str, ObjType] = {'package': <sphinx.domains.ObjType object>}
type (usually directive) name -> ObjType instance

roles: Dict[str, Union[RoleFunction, XRefRole]] = {'package': <sphinx.roles.XRefRole
role name -> role callable

class ymp.sphinxext.**DomainTocTreeCollector**
Bases: sphinx.environment.collectors.EnvironmentCollector

Add Sphinx Domain entries to the TOC

clear_doc(*app*, *env*, *docname*)
Clear data from environment

If we have cached data in environment for document `docname`, we should clear it here.

Return type None

get_ref(*node*)

Return type Optional[Node]

locate_in_toc(*app*, *node*)

Return type Optional[Node]

make_heading(*node*)

Return type List[Node]

merge_other(*app*, *env*, *docnames*, *other*)
Merge with results from parallel processes

Called if Sphinx is processing documents in parallel. We should merge this from `other` into `env` for all `docnames`.

Return type None

process_doc(*app*, *doctree*)
Process `doctree`

This is called by `read-doctree`, so after the doctree has been loaded. The signal is processed in registered first order, so we are called after built-in extensions, such as the `sphinx.environment.collectors.toctree` extension building the TOC.

Return type None

select_doc_nodes(*doctree*)
Select the nodes for which entries in the TOC are desired

This is a separate method so that it might be overriden by subclasses wanting to add other types of nodes to the TOC.

Return type List[Node]

select_toc_location(*app*, *node*)
Select location in TOC where `node` should be referenced

Return type Node

toc_insert(*docname*, *tocnode*, *node*, *heading*)

Return type None

class ymp.sphinxext.**SnakemakeDomain**(*env*)

Bases: sphinx.domains.Domain

Snakemake language domain

clear_doc(*docname*)

Delete objects derived from file docname

data_version = 0

data version, bump this when the format of self.data changes

directives: Dict[str, Any] = {'rule': <class 'ymp.sphinxext.SnakemakeRule'>, 'stage'

directive name -> directive class

get_objects()

Return an iterable of "object descriptions".

Object descriptions are tuples with six items:

name Fully qualified name.

dispname Name to display when searching/linking.

type Object type, a key in self.object_types.

docname The document where it is to be found.

anchor The anchor name for the object.

priority How "important" the object is (determines placement in search results). One of:

1 Default priority (placed before full-text matches).

0 Object is important (placed before default-priority objects).

2 Object is unimportant (placed after full-text matches).

-1 Object should not show up in search at all.

initial_data: Dict = {'objects': {}}

data value for a fresh environment

label = 'Snakemake'

longer, more descriptive (used in messages)

Type domain label

name = 'sm'

should be short, but unique

Type domain name

object_types: Dict[str, ObjType] = {'rule': <sphinx.domains.ObjType object>, 'stage'

type (usually directive) name -> ObjType instance

resolve_xref(*env*, *fromdocname*, *builder*, *typ*, *target*, *node*, *contnode*)

Resolve the pending_xref *node* with the given *typ* and *target*.

This method should return a new node, to replace the xref node, containing the *contnode* which is the markup content of the cross-reference.

If no resolution can be found, None can be returned; the xref node will then given to the **:event:`missing-reference`** event, and if that yields no resolution, replaced by *contnode*.

Unknown interpreted text role "event".

The method can also raise `sphinx.environment.NoUri` to suppress the **:event:`missing-reference`** event being emitted.

Unknown interpreted text role "event".

roles: Dict[str, Union[RoleFunction, XRefRole]] = {'rule': <sphinx.roles.XRefRole ob
role name -> role callable

class ymp.sphinxext.**SnakemakeRule**(*name*, *arguments*, *options*, *content*, *lineno*, *content_offset*, *block_text*, *state*, *state_machine*)
Bases: `sphinx.util.docutils.SphinxDirective`, `Generic[sphinx.directives.T]`

Directive `sm:rule::` describing a Snakemake rule

typename = 'rule'

class ymp.sphinxext.**YmpObjectDescription**(*name*, *arguments*, *options*, *content*, *lineno*, *content_offset*, *block_text*, *state*, *state_machine*)
Bases: `sphinx.util.docutils.SphinxDirective`, `Generic[sphinx.directives.T]`

Base class for RSt directives in SnakemakeDomain

Since this inherhits from Sphinx' ObjectDescription, content generated by the directive will always be inside an addnodes.desc.

Parameters **source** – Specify source position as `file:line` to create link

add_source_link(*signode*)
Add link to source code to *signode*

Return type `None`

add_target_and_index(*name*, *sig*, *signode*)
Add cross-reference IDs and entries to `self.indexnode`

Return type `None`

get_index_text(*typename*, *name*)
Formats object for entry into index

Return type `str`

handle_signature(*sig*, *signode*)
Parse rule signature *sig* into RST nodes and append them to *signode*.

The retun value identifies the object and is passed to *add_target_and_index()* unchanged

Parameters

- **sig** (`str`) – Signature string (i.e. string passed after directive)
- **signode** (`desc`) – Node created for object signature

Return type `str`

Returns Normalized signature (white space removed)

option_spec: Dict[str, DirectiveOption] = {'source': <function unchanged>}
Mapping of option names to validator functions.

typename = '[object name]'

class ymp.sphinxext.**YmpStage**(*name*, *arguments*, *options*, *content*, *lineno*, *content_offset*, *block_text*, *state*, *state_machine*)
Bases: `sphinx.util.docutils.SphinxDirective`, `Generic[sphinx.directives.T]`

Directive `sm:stage::` describing an YMP stage

typename = 'stage'

ymp.sphinxext.**collect_pages**(*app*)
Add Snakefiles to documentation (in HTML mode)

ymp.sphinxext.**relpath**(*path*)
Make absolute path relative to BASEPATH

Parameters **path** (str) – absolute path

Return type str

Returns path relative to BASEPATH

ymp.sphinxext.**setup**(*app*)
Register the extension with Sphinx

6.1.19 ymp.string module

exception ymp.string.**FormattingError**(*message*, *fieldname*)
Bases: AttributeError

class ymp.string.**GetNameFormatter**
Bases: string.Formatter

get_names(*pattern*)

class ymp.string.**OverrideJoinFormatter**
Bases: string.Formatter

Formatter with overridable join method

The default formatter joins all arguments with `"".join(args)`. This class overrides `_vformat()` with identical code, changing only that line to one that can be overridden by a derived class.

join(*args*)
Joins the expanded pieces of the template string to form the output.

This function is equivalent to `''.join(args)`. By overriding it, alternative methods can be implemented, e.g. to create a list of strings, each corresponding to a the cross product of the expanded variables.

Return type Union[List[str], str]

class ymp.string.**PartialFormatter**
Bases: string.Formatter

Formats what it can and leaves the remainder untouched

get_field(*field_name*, *args*, *kwargs*)

class ymp.string.**ProductFormatter**
Bases: *ymp.string.OverrideJoinFormatter*

String Formatter that creates a list of strings each expanded using one point in the cartesian product of all replacement values.

If none of the arguments evaluate to lists, the result is a string, otherwise it is a list.

```
>>> ProductFormatter().format("{A} and {B}", A=[1,2], B=[3,4])
"1 and 3"
"1 and 4"
"2 and 3"
"2 and 4"
```

format_field(*value*, *format_spec*)

join(*args*)
Joins the expanded pieces of the template string to form the output.

This function is equivalent to `''.join(args)`. By overriding it, alternative methods can be implemented, e.g. to create a list of strings, each corresponding to a the cross product of the expanded variables.

Return type Union[List[str], str]

class ymp.string.**QuotedElementFormatter**(**args*, ***kwargs*)
Bases: snakemake.utils.SequenceFormatter

class ymp.string.**RegexFormatter**(*regex*)
Bases: string.Formatter

String Formatter accepting a regular expression defining the format of the expanded tags.

get_names(*format_string*)
Get set of field names in format_string)

Return type Set[str]

parse(*format_string*)
Parse format_string into tuples. Tuples contain literal_text: text to copy field_name: follwed by field name format_spec: conversion:

ymp.string.**make_formatter**(*product=None*, *regex=None*, *partial=None*, *quoted=None*)

Return type Formatter

6.1.20 ymp.util module

ymp.util.**R**(*code=''*, ***kwargs*)
Execute R code

This function executes the R code given as a string. Additional arguments are injected into the R environment. The value of the last R statement is returned.

The function requires rpy2 to be installed.

Parameters

- **code** (*str*) – R code to be executed
- ****kwargs** (*dict*) – variables to inject into R globalenv

Yields value of last R statement

```
>>> R("1*1", input=input)
```

ymp.util.**Rmd**(*rmd*, *out*, ***kwargs*)

ymp.util.**activate_R**()

ymp.util.**check_input**(*names*, *minlines=0*, *minbytes=0*)

Return type Callable

ymp.util.**ensure_list**(*arg*)

ymp.util.**fasta_names**(*fasta_file*)

ymp.util.**file_not_empty**(*fn*, *minsize=1*)
Checks is a file is not empty, accounting for gz mininum size 20

ymp.util.**filter_input**(*name*, *also=None*, *join=None*, *minsize=None*)

Return type Callable

ymp.util.**filter_out_empty**(**args*)
Removes empty sets of files from input file lists.

Takes a variable number of file lists of equal length and removes indices where any of the files is empty. Strings are converted to lists of length 1.

Returns a generator tuple.

Example: r1, r2 = filter_out_empty(input.r1, input.r2)

ymp.util.**glob_wildcards**(*pattern*, *files=None*)
Glob the values of the wildcards by matching the given pattern to the filesystem. Returns a named tuple with a list of values for each wildcard.

ymp.util.**is_fq**(*path*)

ymp.util.**make_local_path**(*icfg*, *url*)

ymp.util.**read_propfiles**(*files*)

6.1.21 ymp.yaml module

class ymp.yaml.**AttrItemAccessMixin**
Bases: object

Mixin class mapping dot to bracket access

Added to classes implementing __getitem__, __setitem__ and __delitem__, this mixin will allow acessing items using dot notation. I.e. "object.xyz" is translated to "object[xyz]".

class ymp.yaml.**Entry**(*filename*, *yaml*, *index*)
Bases: object

exception ymp.yaml.**LayeredConfAccessError**(*obj*, *msg*, *key=None*, *stack=None*)
Bases: *ymp.yaml.LayeredConfError*, KeyError, IndexError

Can't access

exception ymp.yaml.**LayeredConfError**(*obj*, *msg*, *key=None*, *stack=None*)
Bases: *ymp.exceptions.YmpConfigError*

Error in LayeredConf

get_fileline()
Retrieve filename and linenumber from object associated with exception

Returns Tuple of filename and linenumber

class ymp.yaml.**LayeredConfProxy**(*maps*, *root=None*, *parent=None*, *key=None*)
Bases: *ymp.yaml.MultiMapProxy*

Layered configuration

save(*outstream=None*, *layer=0*)

exception ymp.yaml.**LayeredConfWriteError**(*obj*, *msg*, *key=None*, *stack=None*)
Bases: *ymp.yaml.LayeredConfError*

Can't write

exception ymp.yaml.**MixedTypeError**(*obj*, *msg*, *key=None*, *stack=None*)
Bases: *ymp.yaml.LayeredConfError*

Mixed types in proxy collection

class ymp.yaml.**MultiMapProxy**(*maps*, *root=None*, *parent=None*, *key=None*)
Bases: *ymp.yaml.MultiProxy*, *ymp.yaml.AttrItemAccessMixin*, collections.abc.Mapping

Mapping Proxy for layered containers

get(*k*[, *d*]) → D[k] if k in D, else d. d defaults to None.

get_paths(*absolute=False*)

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

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

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

class ymp.yaml.**MultiMapProxyItemsView**(*mapping*)
Bases: *ymp.yaml.MultiMapProxyMappingView*, collections.abc.ItemsView

ItemsView for MultiMapProxy

class ymp.yaml.**MultiMapProxyKeysView**(*mapping*)
Bases: *ymp.yaml.MultiMapProxyMappingView*, collections.abc.KeysView

KeysView for MultiMapProxy

class ymp.yaml.**MultiMapProxyMappingView**(*mapping*)
Bases: collections.abc.MappingView

MappingView for MultiMapProxy

class ymp.yaml.**MultiMapProxyValuesView**(*mapping*)
Bases: *ymp.yaml.MultiMapProxyMappingView*, collections.abc.ValuesView

ValuesView for MultiMapProxy

class ymp.yaml.**MultiProxy**(*maps*, *root=None*, *parent=None*, *key=None*)
Bases: object

Base class for layered container structure

add_layer(*name*, *container*)

get_fileline(*key=None*)

get_files()

get_linenos()

get_path(*key=None*, *absolute=False*)

remove_layer(*name*)

to_yaml(*show_source=False*)

class ymp.yaml.**MultiSeqProxy**(*maps*, *root=None*, *parent=None*, *key=None*)
Bases: *ymp.yaml.MultiProxy*, *ymp.yaml.AttrItemAccessMixin*, collections.abc.Sequence

Sequence Proxy for layered containers

extend(*item*)

get_paths(*absolute=False*)

class ymp.yaml.**WorkdirTag**(*path*)
Bases: object

classmethod from_yaml(*_constructor*, *node*)

classmethod to_yaml(*representer*, *instance*)

yaml_tag = '!workdir'

ymp.yaml.**load**(*files*, *root=None*)
Load configuration files

Creates a *LayeredConfProxy* configuration object from a set of YAML files.

Files listed later will override parts of earlier included files

ymp.yaml.**resolve_installed_package**(*fname*, *stack*)

CHAPTER

SEVEN

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PYTHON MODULE INDEX

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