
SBpipe documentation

Release 4.10.0

Piero Dalle Pezze and Nicolas Le Novère

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USER MANUAL

1.1 Metadata

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Contacts: Dr Piero Dalle Pezze (piero.dallepezze AT gmail.com) and Dr Nicolas Le Novère (lenov AT babraham.ac.uk)

Affiliation: The Babraham Institute, Cambridge, CB22 3AT, UK

Mailing list: sbpipe AT googlegroups.com

Forum: <https://groups.google.com/forum/#!forum/sbpipe>

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1.2 Introduction

The rapid growth of the number of mathematical models in Systems Biology fostered the development of many tools to simulate and analyse them. The reliability and precision of these tasks often depend on multiple repetitions and they can be optimised if executed as pipelines. In addition, new formal analyses can be performed on these repeat sequences, revealing important insights about the accuracy of model predictions. SBpipe allows users to automatically repeat the tasks of model simulation and parameter estimation, and extract robustness information from these repeat sequences in a solid and consistent manner, facilitating model development and analysis.

1.3 Installation

1.3.1 Requirements

In order to use SBpipe, the following packages must be installed:

- Python 2.7+ or 3.4+ - <https://www.python.org/>
- R 3.3.0+ - <https://cran.r-project.org/>

SBpipe can work with the simulators:

- COPASI 4.19+ - <http://copasi.org/> (for model simulation, parameter scan, and parameter estimation)
- Python (directly or as a wrapper to call models coded in any programming language)

If LaTeX/PDF reports are also desired, the following package must also be installed:

- LaTeX 2013+

1.3.2 Installation on GNU/Linux

1.3.2.1 Install COPASI

As of 2016, COPASI is not available as a package in GNU/Linux distributions. Users must add the path to COPASI binary files manually editing the GNU/Linux `$HOME/.bashrc` file as follows:

```
# Path to CopasiSE (update this accordingly)
export PATH=$PATH:/path/to/CopasiSE/
```

The correct installation of CopasiSE can be tested with:

```
# Reload the .bashrc file
source $HOME/.bashrc

CopasiSE -h
> COPASI 4.19 (Build 140)
```

1.3.2.2 Install LaTeX

Users are recommended to install LaTeX/texlive using the package manager of their GNU/Linux distribution. On GNU/Linux Ubuntu machines the following package is required:

```
texlive-latex-base
```

The correct installation of LaTeX can be tested with:

```
pdflatex -v
> pdfTeX 3.14159265-2.6-1.40.16 (TeX Live 2015/Debian)
> kpathsea version 6.2.1
> Copyright 2015 Peter Breitenlohner (eTeX)/Han The Thanh (pdfTeX).
```

1.3.2.3 Install SBpipe via Miniconda3

Users need to download and install Miniconda3 (<https://conda.io/miniconda.html>).

1st Method

This method creates a new environment and installs SBpipe dependencies in this environment. SBpipe is installed locally, enabling an easy access to the package documentation and test suite.

```
# download SBpipe
wget https://github.com/pdp10/sbpipe/tarball/master
# or clone it from GitHub
git clone https://github.com/pdp10/sbpipe.git

# move to sbpipe folder
cd path/to/sbpipe

# install the dependencies within an isolated Miniconda3 environment
conda env create --name sbpipe --file environment.yaml

# activate the environment.
# For recent versions of conda, replace `source` with `conda`.
source activate sbpipe
```

To run sbpipe from any shell, users need to add 'sbpipe/scripts' to their PATH environment variable by adding the following lines to their `$HOME/.bashrc` file:


```
# SBPIPE (update accordingly)
export PATH=$PATH:/path/to/sbpipe/scripts
```

The `.bashrc` file should be reloaded to apply the previous edits:

```
# Reload the .bashrc file
source $HOME/.bashrc
```

2nd Method

This method installs SBpipe as a conda package in a dedicated conda environment:

```
# create a new environment `sbpipe`
conda create -n sbpipe

# activate the environment.
# For recent versions of conda, replace `source` with `conda`.
source activate sbpipe

# install sbpipe and its dependencies (including sbpiper)
conda install sbpipe -c pdpl0 -c conda-forge -c fbergmann -c defaults
```

1.3.2.4 Install SBpipe manually

For this type of installation, SBpipe must be downloaded from the website or cloned using git.

```
# download SBpipe
wget https://github.com/pdpl0/sbpipe/tarball/master
# or clone it from GitHub
git clone https://github.com/pdpl0/sbpipe.git
```

Users need to make sure that the package `python-pip` and `r-base` are installed. The correct installation of Python and R can be tested by running the commands:

```
python -V
> Python 3.6.4
pip -V
> pip 9.0.1 from /home/ariel/.local/lib/python3.6/site-packages (python 3.6)

R --version
> R version 3.4.1 (2017-06-30) -- "Single Candle"
> Copyright (C) 2017 The R Foundation for Statistical Computing
> Platform: x86_64-pc-linux-gnu (64-bit)
```

The next step is the installation of SBpipe dependencies. To install Python dependencies on GNU/Linux, run:

```
cd path/to/sbpipe
./install_pydeps.py
```

To install SBpipe R dependencies on GNU/Linux, run:

```
cd path/to/sbpipe
R
>>> # Inside R environment, answer 'y' to install packages locally
>>> source('install_rdeps.r')
```

Finally, to run sbpipe from any shell, users need to add `'sbpipe/scripts'` to their `PATH` environment variable by adding the following lines to their `$HOME/.bashrc` file:

```
# SBPIPE (update this accordingly)
export PATH=$PATH:/path/to/sbpipe/scripts
```

The `.bashrc` file should be reloaded to apply the previous edits:

```
# Reload the .bashrc file
source $HOME/.bashrc
```

NOTES:

1. If R package dependencies must be compiled, it is worth checking that the following additional packages are installed in your machine: `build-essential`, `liblapack-dev`, `libblas-dev`, `libcairo-dev`, `libssl-dev`, `libcurl4-openssl-dev`, and `gfortran`. These can be installed using the package manager coming with your distribution. Other packages might be needed, depending on R dependencies. After installing these packages, `install_rdeps.R` must be executed again.
2. If Python bindings for COPASI are installed, SBpipe automatically checks whether the COPASI model can be loaded and executed, before generating the data. As of January 2018, this code is released for Python 2.7 and Python 3.6 on the COPASI website and Anaconda Cloud. The installation of SBpipe via Miniconda3 automatically installs this dependency.

1.3.3 Installation on Windows

1.3.3.1 Install MINGW

We advise users to install Git for Windows <https://git-for-windows.github.io/> as a simple Shell (MINGW) running on Windows. Leave the default setting during installation.

1.3.3.2 Installation of COPASI

Windows users need to install the Windows versions of COPASI from the COPASI website. Once Git for Windows is started, a Shell-like window appears and enables users to run commands. A `.bashrc` file must be created and configured:

```
touch .bashrc
wordpad .bashrc
```

A Wordpad window should be visible, loading the file `.bashrc`. The following lines must be copied into this file:

```
#!/bin/bash/

# COPASI (update this accordingly. Use \ to escape spaces)
export PATH=/path/to/copasi/bin/:$PATH
```

1.3.3.3 Installation of LaTeX

Windows users need to install LaTeX MikTeX <https://miktex.org/>.

1.3.3.4 Install SBpipe via Miniconda3

See GNU/Linux.

1.3.3.5 Install SBpipe manually

Start Git for Windows and clone SBpipe from GitHub using the command:

```
git clone https://github.com/pdp10/sbpipe.git
```

We now need to set up the path to SBpipe:

```
wordpad .bashrc
```

The following lines must be appended to this file:

```
# SBPIPE
export PATH=$PATH:~/sbpipe/scripts
```

Save the file and close wordpad. Now you should reload the .bashrc file to apply the previous changes:

```
# Reload the .bashrc file
source $HOME/.bashrc
```

Python and R dependencies should be installed as explained in the corresponding section for GNU/Linux section.

1.3.4 Test SBpipe

The correct installation of SBpipe and its dependencies can be verified by running the following commands. For the correct execution of all tests, LaTeX must be installed.

```
# SBpipe version:
sbpipe -V
> sbpipe 4.6.0
```

```
# run model simulation using COPASI (see results in tests/copasi_models):
cd path/to/sbpipe/tests
nosetests test_copasi_sim.py --nocapture --verbose
```

```
# run all tests:
nosetests test_suite.py --nocapture --verbose
```

```
# generate the manuscript figures (see results in tests/insulin_receptor):
nosetests test_suite_manuscript.py --nocapture --verbose
```

1.4 How to use SBpipe

SBpipe pipelines can be executed natively or via Snakemake, a dedicated and more advanced tool for running computational pipelines.

1.4.1 Run SBpipe natively

SBpipe is executed via the command *sbpipe*. The syntax for this command and its complete list of options can be retrieved by running *sbpipe -h*. The first step is to create a new project. This can be done with the command:

```
sbpipe --create-project project_name
```

This generates the following structure:

```
project_name/  
| - Models/  
| - Results/  
| - (store configuration files here)
```

Mathematical models must be stored in the Models/ folder. COPASI data sets used by a model should also be stored in Models. To run SBpipe, users need to create a configuration file for each pipeline they intend to run (see next section). These configuration files should be placed in the root project folder. In Results/ users will eventually find all the results generated by SBpipe.

Each pipeline is invoked using a specific option (type `sbpipe -h` for the complete command set):

```
# runs model simulation.  
sbpipe -s config_file.yaml  
  
# runs parameter estimation.  
sbpipe -e config_file.yaml  
  
# runs single parameter scan.  
sbpipe -p config_file.yaml  
  
# runs double parameter scan  
sbpipe -d config_file.yaml
```

1.4.1.1 Pipeline configuration files

Pipelines are configured using files (here called configuration files). These files are YAML files. In SBpipe each pipeline executes four tasks: data generation, data analysis, report generation, and tarball generation. These tasks can be activated in each configuration files using the options:

- `generate_data`: True
- `analyse_data`: True
- `generate_report`: True
- `generate_tarball`: False

The `generate_data` task runs a simulator accordingly to the options in the configuration file. Hence, this task collects and organises the reports generated from the simulator. The `analyse_data` task processes the reports to generate plots and compute statistics. The `generate_report` task generates a LaTeX report containing the computed plots and invokes the utility `pdflatex` to produce a PDF file. Finally, `generate_tarball` creates a `tar.gz` file of the results. By default, this is not executed. This modularisation allows users to analyse the same data without having to re-generate it, or to skip the report generation if not wanted.

Pipelines for parameter estimation or stochastic model simulation can be computationally intensive. SBpipe allows users to generate simulated data in parallel using the following options in the pipeline configuration file:

- `cluster`: "local"
- `local_cpus`: 7
- `runs`: 250

The `cluster` option defines whether the simulator should be executed locally (`local`: Python multiprocessing), or in a computer cluster (`sge`: Sun Grid Engine (SGE), `lsf`: Load Sharing Facility (LSF)). If `local` is selected, the `local_cpus` option determines the maximum number of CPUs to be allocated for local simulations. The `runs` option specifies the number of simulations (or parameter estimations for the pipeline `param_estim`) to be run.

Assuming that the configuration files are placed in the root directory of a certain project (e.g. `project_name/`), examples are given as follow:

Example 1: configuration file for the pipeline *simulation*

```

# True if data should be generated, False otherwise
generate_data: True
# True if data should be analysed, False otherwise
analyse_data: True
# True if a report should be generated, False otherwise
generate_report: True
# True if a zipped tarball should be generated, False otherwise
generate_tarball: False
# The relative path to the project directory
project_dir: "."
# The name of the configurator (e.g. Copasi, Python)
simulator: "Copasi"
# The model name
model: "insulin_receptor_stoch.cps"
# The cluster type. local if the model is run locally,
# sge/lsf if run on cluster.
cluster: "local"
# The number of CPU if local is used, ignored otherwise
local_cpus: 7
# The number of simulations to perform.
# n>: 1 for stochastic simulations.
runs: 40
# An experimental data set (or blank) to add to the
# simulated plots as additional layer
exp_dataset: "insulin_receptor_dataset.csv"
# True if the experimental data set should be plotted.
plot_exp_dataset: True
# The alpha level used for plotting the experimental dataset
exp_dataset_alpha: 1.0
# The label for the x axis.
xaxis_label: "Time [min]"
# The label for the y axis.
yaxis_label: "Level [a.u.]"

```

Example 2: configuration file for the pipeline *single parameter scan*

```

# True if data should be generated, False otherwise
generate_data: True
# True if data should be analysed, False otherwise
analyse_data: True
# True if a report should be generated, False otherwise
generate_report: True
# True if a zipped tarball should be generated, False otherwise
generate_tarball: False
# The relative path to the project directory
project_dir: "."
# The name of the configurator (e.g. Copasi, Python)
simulator: "Copasi"
# The model name
model: "insulin_receptor_inhib_scan_IR_beta.cps"
# The variable to scan (as set in Copasi Parameter Scan Task)
scanned_par: "IR_beta"
# The cluster type. local if the model is run locally,
# sge/lsf if run on cluster.
cluster: "local"
# The number of CPU if local is used, ignored otherwise
local_cpus: 7
# The number of simulations to perform per run.
# n>: 1 for stochastic simulations.
runs: 1
# The number of intervals in the simulation
simulate_intervals: 100

```

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```

# True if the variable is only reduced (knock down), False otherwise.
ps1_knock_down_only: True
# True if the scanning represents percent levels.
ps1_percent_levels: True
# The minimum level (as set in Copasi Parameter Scan Task)
min_level: 0
# The maximum level (as set in Copasi Parameter Scan Task)
max_level: 100
# The number of scans (as set in Copasi Parameter Scan Task)
levels_number: 10
# True if plot lines are the same between scans
# (e.g. full lines, same colour)
homogeneous_lines: False
# The label for the x axis.
xaxis_label: "Time [min]"
# The label for the y axis.
yaxis_label: "Level [a.u.]"

```

Example 3: configuration file for the pipeline *double parameter scan*

```

# True if data should be generated, False otherwise
generate_data: True
# True if data should be analysed, False otherwise
analyse_data: True
# True if a report should be generated, False otherwise
generate_report: True
# True if a zipped tarball should be generated, False otherwise
generate_tarball: False
# The relative path to the project directory
project_dir: "."
# The name of the configurator (e.g. Copasi, Python)
simulator: "Copasi"
# The model name
model: "insulin_receptor_inhib_dbl_scan_InsulinPercent__IRbetaPercent.cps"
# The 1st variable to scan (as set in Copasi Parameter Scan Task)
scanned_par1: "InsulinPercent"
# The 2nd variable to scan (as set in Copasi Parameter Scan Task)
scanned_par2: "IRbetaPercent"
# The cluster type. local if the model is run locally,
# sge/lsf if run on cluster.
cluster: "local"
# The number of CPU if local is used, ignored otherwise
local_cpus: 7
# The number of simulations to perform.
# n>: 1 for stochastic simulations.
runs: 1
# The simulation length (as set in Copasi Time Course Task)
sim_length: 10

```

Example 4: configuration file for the pipeline *parameter estimation*

```

# True if data should be generated, False otherwise
generate_data: True
# True if data should be analysed, False otherwise
analyse_data: True
# True if a report should be generated, False otherwise
generate_report: True
# True if a zipped tarball should be generated, False otherwise
generate_tarball: False
# The relative path to the project directory
project_dir: "."

```

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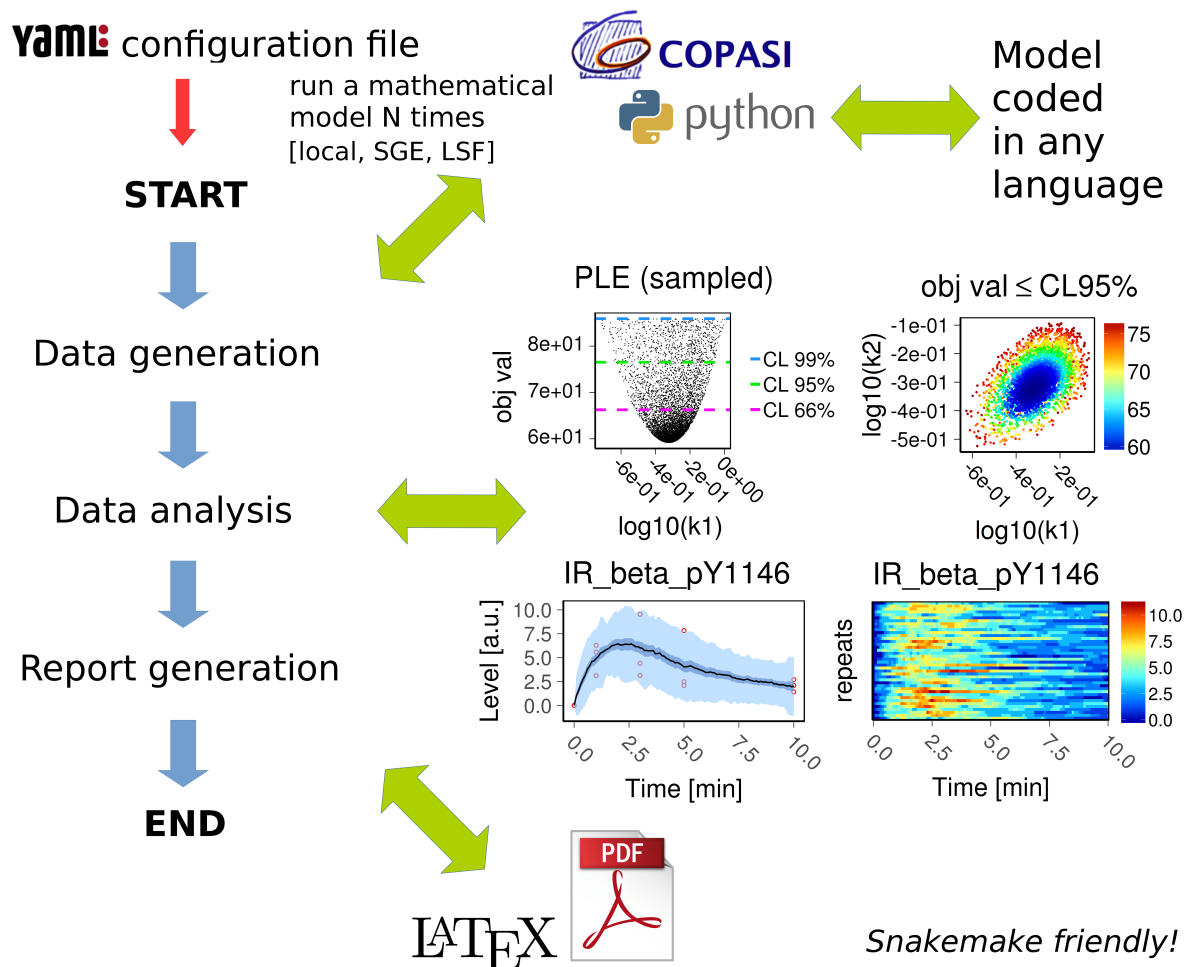
```

# The name of the configurator (e.g. Copasi, Python)
simulator: "Copasi"
# The model name
model: "insulin_receptor_param_estim.cps"
# The cluster type. local if the model is run locally,
# sge/lsf if run on cluster.
cluster: "local"
# The number of CPU if local is used, ignored otherwise
local_cpus: 7
# The parameter estimation round which is used to distinguish
# phases of parameter estimations when parameters cannot be
# estimated at the same time
round: 1
# The number of parameter estimations
# (the length of the fit sequence)
runs: 250
# The threshold percentage of the best fits to consider
best_fits_percent: 75
# The number of available data points
data_point_num: 33
# True if 2D all fits plots for 66% confidence levels
# should be plotted. This can be computationally expensive.
plot_2d_66cl_corr: True
# True if 2D all fits plots for 95% confidence levels
# should be plotted. This can be computationally expensive.
plot_2d_95cl_corr: True
# True if 2D all fits plots for 99% confidence levels
# should be plotted. This can be computationally expensive.
plot_2d_99cl_corr: True
# True if parameter values should be plotted in log space.
logspace: True
# True if plot axis labels should be plotted in scientific notation.
scientific_notation: True

```

Additional examples of configuration files can be found in:

```
sbpipe/tests/insulin_receptor/
```



1.4.2 Run SBpipe via Snakemake

SBpipe pipelines can also be executed using [Snakemake](https://snakemake.readthedocs.io) (<https://snakemake.readthedocs.io>). Snakemake offers an infrastructure for running computational pipelines using declarative rules.

Snakemake can be installed manually via package manager or using the conda command:

```
# Install snakemake (note: it requires python 3+ to run)
conda install -c bioconda snakemake
```

SBpipe pipelines for parameter estimation, single/double parameter scan, and model simulation are also implemented as snakemake files (which contain the set of rules for each pipeline). These are:

- sbpipe_pe.snake
- sbpipe_ps1.snake
- sbpipe_ps2.snake
- sbpipe_sim.snake

and are stored on the root folder of SBpipe. The advantage of using snakemake as pipeline infrastructure is that it offers an extended command sets compared to the one provided with the standard sbpipe. For details, run

```
snakemake -h
```

Snakemake also offers a strong support for dependency management at coding level and reentrancy at execution level. The former is defined as a way to precisely define the dependency order of functions. The latter is the

capacity of a program to continue from the last interrupted task. Benefitting of dependency declaration and execution reentrancy can be beneficial for running SBpipe on clusters or on the cloud.

Under the current implementation of SBpipe snakefile, the configuration files described above require the additional field:

```
# The name of the report variables
report_variables: ['IR_beta_pY1146']
```

which contain the names of the variables exported by the simulator. For the parameter estimation pipeline, `report_variables` will contain the names of the estimated parameters.

For the parameter estimation pipeline, the following option must also be added:

```
# An experimental data set (or blank) to add to the
# simulated plots as additional layer
exp_dataset: "insulin_receptor_dataset.csv"
```

A complete example of configuration file for the parameter estimation pipeline is the following:

```
simulator: "Copasi"
model: "insulin_receptor_param_estim.cps"
round: 1
runs: 4
best_fits_percent: 75
data_point_num: 33
plot_2d_66cl_corr: True
plot_2d_95cl_corr: True
plot_2d_99cl_corr: True
logspace: True
scientific_notation: True
report_variables: ['k1', 'k2', 'k3']
exp_dataset: "insulin_receptor_dataset.csv"
```

NOTE: As it can be noticed, a configuration files for SBpipe using snakemake requires less options than the corresponding configuration file using SBpipe directly. This because Snakemake files is more automated than SBpipe. Nevertheless, the removal of those additional options is not necessary for running the configuration file using Snakemake.

Examples of configuration files for running SBpipe using Snakemake are in `tests/snakemake`.

Examples of commands running SBpipe pipelines using Snakemake are:

```
# run model simulation
snakemake -s path/to/sbpipe/sbpipe_sim.snake --configfile SBPIPE_CONFIG_FILE.yaml -
↳-cores 7

# run model parameter estimation using 40 jobs on an SGE cluster.
# snakemake waits for output files for 100 s.
snakemake -s path/to/sbpipe/sbpipe_pe.snake --configfile SBPIPE_CONFIG_FILE.yaml --
↳latency-wait 100 -j 40 --cluster "qsub -cwd -V -S /bin/sh"

# run model parameter parameter scan using 5 jobs
snakemake -s path/to/sbpipe/sbpipe_ps1.snake --configfile SBPIPE_CONFIG_FILE.yaml -
↳j 5 --cluster "bsub"

# run model parameter parameter scan using 5 jobs
snakemake -s path/to/sbpipe/sbpipe_ps2.snake --configfile SBPIPE_CONFIG_FILE.yaml -
↳j 1 --cluster "qsub"
```

If the grid engine supports DRMAA, it can be convenient to use Snakemake with the option `--drmaa`.

```
# See the DRMAA Python bindings for a preliminary documentation: https://pypi.python.org/pypi/drmaa
# The following is an example of configuration for DRMAA for the grid engine_
# installed at the Babraham Institute
# (Cambridge, UK).

# load Python 3
module load python3/3.5.1
alias python=python3
# install python drmaa locally
easy_install-3.5 --user drmaa

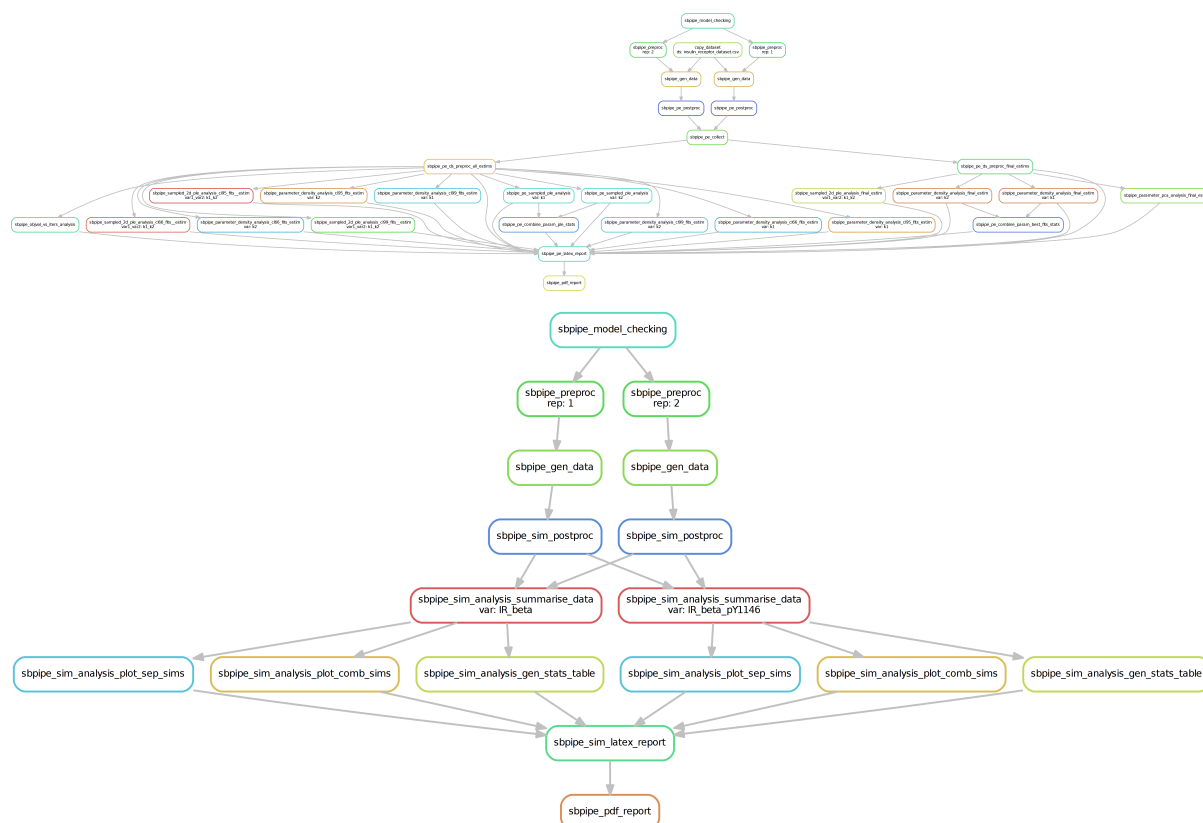
# Update accordingly and add the following line to your ~/.bashrc file:
export SGE_ROOT=/opt/gridengine
export SGE_CELL=default
export DRMAA_LIBRARY_PATH=/opt/gridengine/lib/lx26-amd64/libdrmaa.so.1.0
```

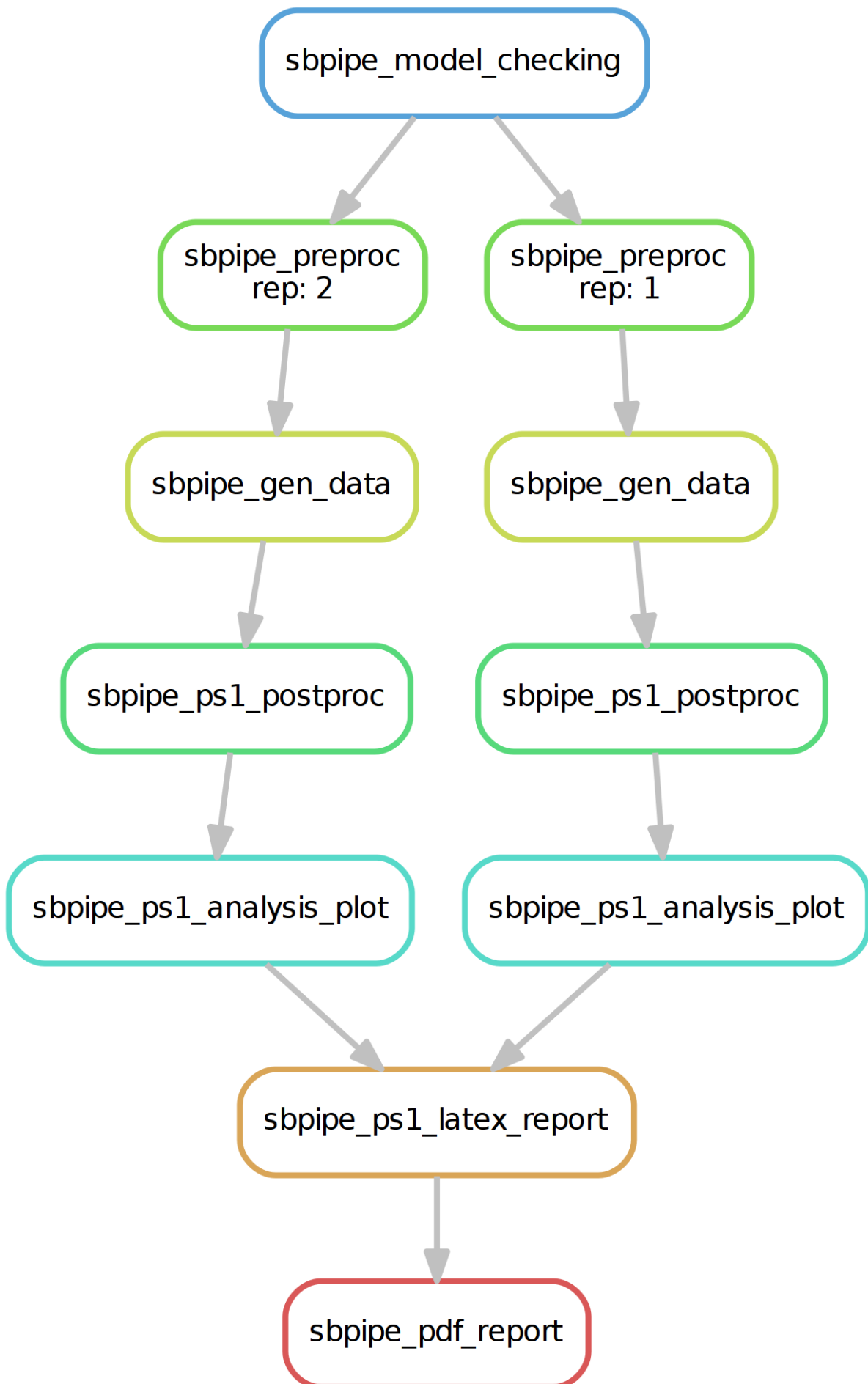
Snakemake can now be executed using drmaa as follows:

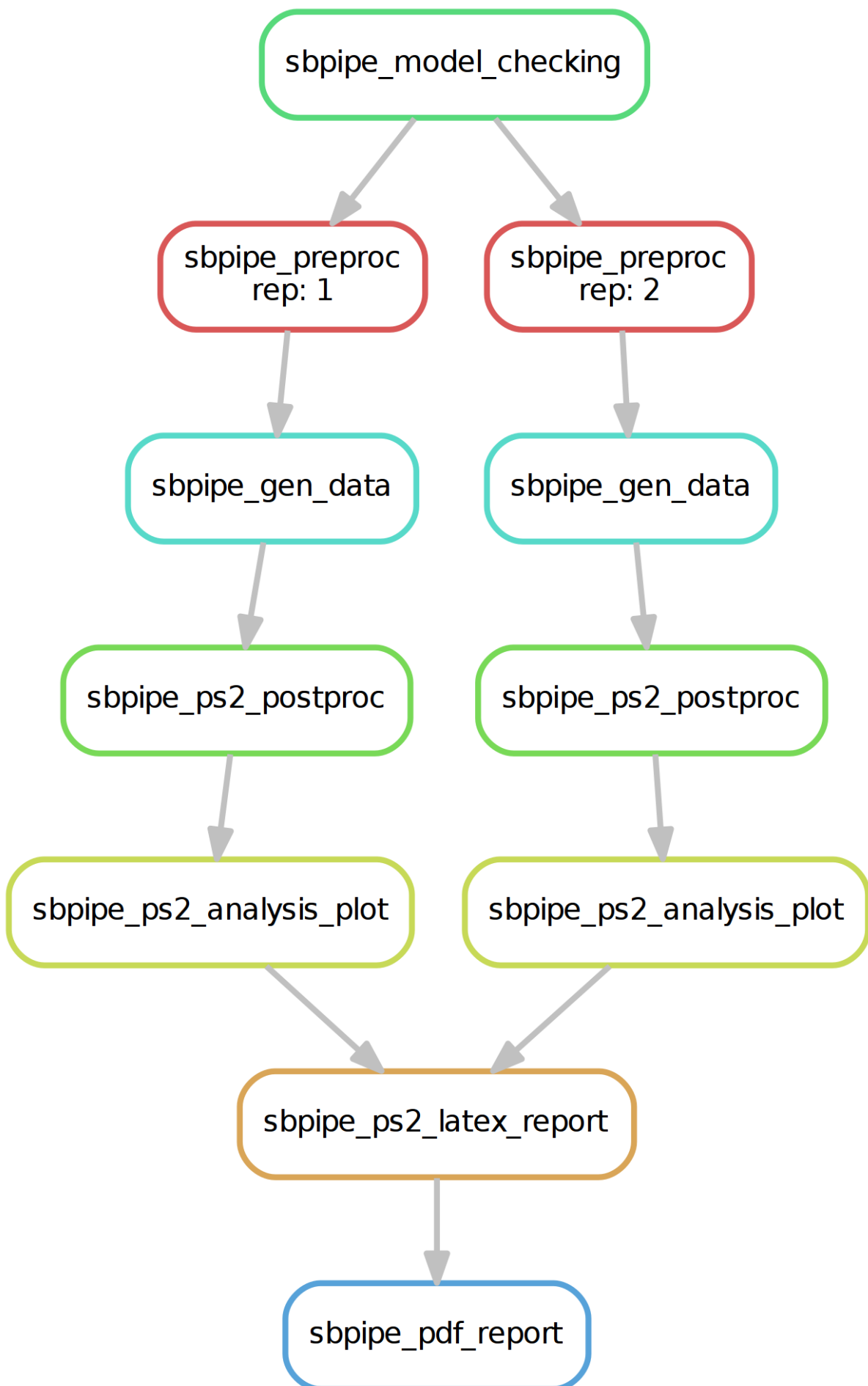
```
snakemake -s ../../sbpipe_sim.snake --configfile ir_model_stoch_simul.yaml -j 200 -
--latency-wait 100 --drmaa " -cwd -V -S /bin/sh"
```

See `snakemake -h` for a complete list of commands.

The implementation of SBpipe pipelines for Snakemake is more scalable and allows for additional controls and resilience.







1.4.3 Configuration for the mathematical models

SBpipe can run COPASI models or models coded in any programming language using a Python wrapper to invoke them.

1.4.3.1 COPASI models

A COPASI model must be configured as follow using the command `CopasiUI`:

pipeline: simulation

- Tick the flag *executable* in the Time Course Task.
- Select a report template for the Time Course Task.
- Save the report in the same folder with the same name as the model but replacing the extension `.cps` with `.csv` (extensions `.txt`, `.tsv`, or `.dat` are also accepted by SBpipe).

pipelines: single or double parameter scan

- Tick the flag *executable* in the Parameter Scan Task.
- Select a report template for the Parameter Scan Task.
- Save the report in the same folder with the same name as the model but replacing the extension `.cps` with `.csv` (extensions `.txt`, `.tsv`, or `.dat` are also accepted by SBpipe)

pipeline: parameter estimation

- Tick the flag *executable* in the Parameter Estimation Task.
- Select the report template for the Parameter Estimation Task.
- Save the report in the same folder with the same name as the model but replacing the extension `.cps` with `.csv` (extensions `.txt`, `.tsv`, or `.dat` are also accepted by SBpipe)

For tasks such as parameter estimation using COPASI, it is recommended to move the data set into the folder `Models/` so that the COPASI model file and its associated experimental data files are stored in the same folder.

1.4.3.2 Python wrapper executing models coded in any language

Users can use Python as a wrapper to execute models (programs) coded in any programming language. The model must be functional and a Python wrapper should be able to run it via the command `python`. The program must receive the report file name as input argument (see examples in `sbpipe/tests/`). If the program generates a model simulation, a report file must be generated including the column `Time`. Report fields must be separated by TAB, and row names must be discarded. If the program runs a parameter estimation, a report file must be generated including the objective value as first column column, and the estimated parameters as following columns. Rows are the evaluated functions. Report fields must be separated by TAB, and row names must be discarded.

The following example illustrates how SBpipe can simulate a model called `sde_periodic_drift.r` and coded in R, using a Python wrapper called `sde_periodic_drift.py`. Both the Python wrapper and R model are stored in the folder `Models/`. The idea is that the configuration file tells SBpipe to run the Python wrapper which receives the report file name as input argument and forwards it to the R model. After executing, the results are stored in this report, enabling SBpipe to analyse the results. The full example is stored in: `sbpipe/tests/r_models/`.

```
# Configuration file invoking the Python wrapper `sde_periodic_drift.py`
# Note that simulator must be set to "Python"
generate_data: True
analyse_data: True
generate_report: True
project_dir: "."
simulator: "Python"
model: "sde_periodic_drift.py"
```

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```
cluster: "local"
local_cpus: 7
runs: 14
exp_dataset: ""
plot_exp_dataset: False
exp_dataset_alpha: 1.0
xaxis_label: "Time"
yaxis_label: "#"
```

```
# Python wrapper: `sde_periodic_drift.py`.

import os
import sys
import subprocess
import shlex

# This is a Python wrapper used to run an R model.
# The R model receives the report_filename as input
# and must add the results to it.

# Retrieve the report file name
report_filename = "sde_periodic_drift.csv"
if len(sys.argv) > 1:
    report_filename = sys.argv[1]

command = 'Rscript --vanilla ' + \
    os.path.join(os.path.dirname(__file__), 'sde_periodic_drift.r') + \
    ' ' + report_filename

# Block until command is finished
subprocess.call(shlex.split(command))
```

```
# R model `sde_periodic_drift.r`

# Model from https://cran.r-project.org/web/packages/sde/sde.pdf

# import sde package
# sde and its dependencies must be installed.
if(!require(sde)){
  install.packages('sde')
  library(sde)
}

# Retrieve the report file name (necessary for stochastic simulations)
args <- commandArgs(trailingOnly=TRUE)
report_filename = "sde_periodic_drift.csv"
if(length(args) > 0) {
  report_filename <- args[1]
}

# Model definition
# -----
# set.seed()
d <- expression(sin(x))
d.x <- expression(cos(x))
A <- function(x) 1-cos(x)

X0 <- 0
delta <- 1/20
```

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```
N <- 500
time <- seq(X0, N*delta, by=delta)

# EA = exact method
periodic_drift <- sde.sim(method="EA", delta=delta, X0=X0, N=N, drift=d, drift.x=d.
  ↪x, A=A)

out <- data.frame(time, periodic_drift)
# -----

# Write the output. The output file must be the model name with csv or txt_
  ↪extension.
# Fields must be separated by TAB, and row names must be discarded.
write.table(out, file=report_filename, sep="\t", row.names=FALSE)
```

1.5 How to report bugs or request new features

SBpipe is a relatively young project and there is a chance that some error occurs. The following mailing list should be used for general questions:

```
sbpipe AT googlegroups.com
```

All the topics discussed in this mailing list are also available at the website:

<https://groups.google.com/forum/#!forum/sbpipe>

To help us better identify and reproduce your problem, some technical information is needed. This detail data can be found in SBpipe log files which are stored in `${HOME}/.sbpipe/logs/`. When using the mailing list above, it would be worth providing this extra information.

Issues and feature requests can also be notified using the github issue tracking system for SBpipe at the web page:

<https://github.com/pdp10/sbpipe/issues>.

DEVELOPER MANUAL

Mailing list: sbpipe AT googlegroups.com

Forum: <https://groups.google.com/forum/#!forum/sbpipe>

2.1 Introduction

This guide is meant for developers.

2.2 Package structure

This section presents the structure of the SBpipe package. The root of the project contains general management scripts for installing Python and R dependencies (`install_pydeps.py` and `install_rdeps.r`), and installing SBpipe (`setup.py`). Additionally, the logging configuration file (`logging_config.ini`) is also at this level.

In order to automatically compile and run the test suite, Travis-CI is used and configured accordingly (`.travis.yml`).

The project is structured as follows:

```
sbpipe:
| - docs/
| - sbpipe/
|   | - pl
|   | - report
|   | - simul
|   | - tasks
|   | - utils
| - scripts/
| - tests/
```

These folders will be discussed in the next sections. In SBpipe, Python is the project main language, whereas R is used for computing statistics and for generating plots. This choice allows users to run these scripts independently of SBpipe if needed using an R environment like Rstudio. This can be convenient if further data analysis is needed or plots need to be annotated or edited. The R code for SBpipe is distributed as a separate R package and installed as a dependency using the provided script (`install_rdeps.r`) or conda. The source code for this package can be found here: <https://github.com/pdp10/sbpiper> and on CRAN <https://cran.r-project.org/package=sbpiper>.

2.2.1 docs

The folder `docs/` contains the documentation for this project. The user and developer manuals in markdown format are contained in `docs/source`. In order to generate the complete documentation for SBpipe, the following packages must be installed:

- `python-sphinx`
- `pandoc`

- texlive-fonts-recommended
- texlive-latex-extra

By default the documentation is generated in html and LaTeX/PDF. Instruction for generating or cleaning SBpipe documentation are provided below.

To generate the source code documentation:

```
cd path/to/sbpipe/docs
./gen_doc.sh
```

To clean the documentation:

```
cd path/to/sbpipe/docs
./cleanup_doc.sh
```

The complete source code documentation for this project is stored in docs/build/html (html format) and docs/build/latex (LaTeX/PDF format). A shortcut to the documentation in html format is available at the page docs/index.html.

2.2.2 sbpipe

This folder contains the source code of the project SBpipe. At this level a file called `__main__.py` enables users to run SBpipe programmatically as a Python module via the command:

```
python sbpipe
```

Alternatively sbpipe can programmatically be imported within a Python environment as shown below:

```
cd path/to/sbpipe
python
>>> # Python environment
>>> from sbpipe.main import sbpipe
>>> sbpipe(simulate="my_model.yaml")
```

The following subsections describe sbpipe subpackages.

2.2.2.1 pl

The subpackage `sbpipe.pl` contains the class `Pipeline` in the file `pipeline.py`. This class represents a generic pipeline which is extended by SBpipe pipelines. These are organised in the following subpackages:

- `create`: creates a new project
- `ps1`: scan a model parameter, generate plots and report;
- `ps2`: scan two model parameters, generate plots and report;
- `pe`: generate a parameter fit sequence, tables of statistics, plots and report;
- `sim`: generate deterministic or stochastic model simulations, plots and report.

All these pipelines can be invoked directly via the script `sbpipe/scripts/sbpipe`. Each SBpipe pipeline extends the class `Pipeline` and therefore must implement the following methods:

```
# executes a pipeline
def run(self, config_file)

# process the dictionary of the configuration file loaded by Pipeline.load()
def parse(self, config_dict)
```

- The method `run()` can invoke `Pipeline.load()` to load the YAML `config_file` as a dictionary. Once the configuration is loaded and the parameters are imported, `run()` executes the pipeline.
- The method `parse()` parses the dictionary and collects the values.

2.2.2.2 report

The subpackage `sbpipe.report` contains Python modules for generating LaTeX/PDF reports.

2.2.2.3 simul

The subpackage `sbpipe.simul` contains the class `Simul` in the file `simul.py`. This is a generic simulator interface used by the pipelines in SBpipe. This mechanism uncouples pipelines from specific simulators which can therefore be configured in each pipeline configuration file. As of 2016, the following simulators are available in SBpipe:

- Copasi, package `sbpipe.simul.copasi`, which implements all the methods of the class `Simul`;
- Python, package `sbpipe.simul.python`.

Pipelines can dynamically load a simulator via the class method `Pipeline.get_simul_obj(simulator)`. This method instantiates an object of subtype `Simul` by refracting the simulator name as parameter. A simulator class (e.g. `Copasi`) must have the same name of their package (e.g. `copasi`) but start with an upper case letter. A simulator class must be contained in a file with the same name of their package (e.g. `copasi`). Therefore, for each simulator package, exactly one simulator class can be instantiated. Simulators can be configured in the configuration file using the field `simulator`.

2.2.2.4 tasks

The subpackage `sbpipe.tasks` contains the Python scripts to invoke the single SBpipe tasks. These are invoked by the rules in the SBpipe snakemake files. These snakemake files are:

- `sbpipe_pe.snake`
- `sbpipe_ps1.snake`
- `sbpipe_ps2.snake`
- `sbpipe_sim.snake`

and are stored on the root folder of SBpipe.

2.2.2.5 utils

The subpackage `sbpipe.utils` contains a collection of Python utility modules which are used by `sbpipe`. Here are also contained the functions for running commands in parallel.

2.2.3 scripts

The folder `scripts` contains the scripts: `cleanup_sbpipe` and `sbpipe`. `sbpipe` is the main script and is used to run the pipelines. `cleanup_sbpipe.py` is used for cleaning the package including the test results.

2.2.4 tests

The package `tests` contains the script `test_suite.py` which executes all `sbpipe` tests. It should be used for testing the correct installation of SBpipe dependencies as well as reference for configuring a project before running any pipeline. Projects inside the folder `sbpipe/tests/` have the SBpipe project structure:

- Models: (e.g. `models`, COPASI models, Python models, data sets directly used by Copasi models);

- Results: (e.g. pipelines results, etc).

Examples of configuration files (*.yaml) using COPASI can be found in `sbpipe/tests/insulin_receptor/`.

To run tests for Python models, the Python packages `numpy`, `scipy`, and `pandas` must be installed. In principle, users may define their Python models using arbitrary packages.

As of 2016, the repository for SBpipe source code is `github.com`. This is configured to run Travis-CI every time a `git push` into the repository is performed. The exact details of execution of Travis-CI can be found in Travis-CI configuration file `sbpipe/.travis.yml`. Importantly, Travis-CI runs all SBpipe tests using `nosetests`.

2.3 Development model

This project follows the Feature-Branching model. Briefly, there are two main branches: `master` and `develop`. The former contains the history of stable releases, the latter contains the history of development. The `master` branch contains checkout points for production hotfixes or merge points for `release-x.x.x` branches. The `develop` branch is used for feature-bugfix integration and checkout point in development. Nobody should directly develop in here.

2.3.1 Conventions

To manage the project in a more consistent way, here is a list of conventions to follow:

- Each new feature is developed in a separate branch forked from `develop`. This new branch is called *featureNUMBER*, where *NUMBER* is the number of the GitHub Issue discussing that feature. The first line of each commit message for this branch should contain the string *Issue #NUMBER* at the beginning. Doing so, the commit is automatically recorded by the Issue Tracking System for that specific Issue. Note that the sharp (#) symbol is required.
- The same for each new bugfix, but in this case the branch name is called *bugfixNUMBER*.
- The same for each new hotfix, but in this case the branch name is called *hotfixNUMBER* and is forked from *master*.

2.3.2 Work flow

The procedure for checking out a new feature from the `develop` branch is:

```
git checkout -b feature10 develop
```

This creates the `feature10` branch off `develop`. This `feature10` is discussed in *Issue #10* in GitHub. When you are ready to commit your work, run:

```
git commit -am "Issue #10, summary of the changes. Detailed
description of the changes, if any."
git push origin feature10      # sometimes and at the end.
```

As of June 2016, the branches `master` and `develop` are protected and a status check using Travis-CI must be performed before merging or pushing into these branches. This automatically forces a merge without fast-forward. In order to merge **any** new feature, bugfix or simple edits into `master` or `develop`, a developer **must** checkout a new branch and, once committed and pushed, **merge** it to `master` or `develop` using a pull request. To merge `feature10` to `develop`, the pull request output will look like this in GitHub Pull Requests:

```
base:develop  compare:feature10  Able to merge. These branches can be
automatically merged.
```

A small discussion about feature10 should also be included to allow other users to understand the feature.

Finally delete the branch:

```
git branch -d feature10      # delete the branch feature10 (locally)
```

2.3.3 New releases

The script `release.sh` at the root of the package allows to release a new version of SBpipe or update the last github tag. This script also creates and uploads a new SBpipe package for Anaconda Cloud.

The following two sections describe how to release a new version for SBpipe, manually.

2.3.3.1 How to release a new tag

When the `develop` branch includes all the desired feature for a release, it is time to checkout this branch in a new one called `release-x.x.x`. It is at this stage that a version is established.

```
# record the release add a tag:
git tag -a v1.3 -m "SBpipe v1.3"

# transfer the tag to the remote server:
git push origin v1.3    # Note: this goes to a separate 'branch'

# see all the releases:
git show
```

2.3.3.2 How to release a new SBpipe conda package (Anaconda Cloud)

This is a short guide for building SBpipe as a conda package. Miniconda must be installed. In order to proceed, the package `conda-build` must be installed:

```
conda install conda-build

# DON'T FORGET TO SET THIS so that your built package is not uploaded automatically
conda config --set anaconda_upload no
```

The recipe for SBpipe is already prepared (file: `meta.yaml`). To create the conda package for SBpipe:

```
cd path/to/sbpipe
conda-build conda_recipe/meta.yaml -c pdp10 -c conda-forge -c fbergmann -c defaults
```

To test this package locally:

```
# install
conda install sbpipe --use-local

# uninstall
conda remove sbpipe
```

To upload the package to Anaconda Cloud repository:

```
anaconda upload ~/miniconda/conda-bld/noarch/sbpipe-x.x.x-py_y.tar.bz2
```

2.4 Miscellaneous of useful commands

2.4.1 Git

Startup

```
# clone master
git clone https://github.com/pdp10/sbpipe.git
# get develop branch
git checkout -b develop origin/develop
# to update all the branches with remote
git fetch --all
```

Update

```
# ONLY use --rebase for private branches. Never use it for shared
# branches otherwise it breaks the history. --rebase moves your
# commits ahead. For shared branches, you should use
# `git fetch && git merge --no-ff`
git pull [--rebase] origin BRANCH
```

Managing tags

```
# Update an existing tag to include the last commits
# Assuming that you are in the branch associated to the tag to update:
git tag -f -a tagName
# push your new commit:
git push
# force push your moved tag:
git push -f --tags

# rename a tag
git tag new old
git tag -d old
git push origin :refs/tags/old
git push --tags
# make sure that the other users remove the deleted tag. Tell them(co-workers) to
↳ run the following command:
git pull --prune --tags

# removing a tag remotely and locally
git push --delete origin tagName
git tag -d tagName
```

File system

```
git rm [--cache] filename
git add filename
```

Information

```
git status
git log [--stat]
git branch      # list the branches
```

Maintenance

```
git fsck      # check errors
git gc        # clean up
```

Rename a branch locally and remotely

```
git branch -m old_branch new_branch      # Rename branch locally
git push origin :old_branch              # Delete the old branch
git push --set-upstream origin new_branch # Push the new branch, set local_
↪branch to track the new remote
```

Reset

```
git reset --hard HEAD    # to undo all the local uncommitted changes
```

Syncing a fork (assuming upstreams are set)

```
git fetch upstream
git checkout develop
git merge upstream/develop
```


SPHINX AUTOAPI INDEX

This page is the top-level of your generated API documentation. Below is a list of all items that are documented here.

3.1 sbpipe_config

3.1.1 Module Contents

`sbpipe_config.which(cmd_name)`

Utility equivalent to *which* in GNU/Linux OS.

Parameters `cmd_name` – a command name

Returns return the command name with absolute path if this exists, or None

`sbpipe_config.isPyPackageInstalled(package)`

Utility checking whether a Python package is installed.

Parameters `package` – a Python package name

Returns True if it is installed, false otherwise.

3.2 main

3.2.1 Module Contents

`class main.NullHandler`

`emit(record)`

`main.sbpipe_logo()`

Return sbpipe logo.

Returns sbpipe logo

`main.read_file_header(filename)`

Read the first line of a file

Parameters `filename` – the file name to read

Returns the first line

`main.set_basic_logger(level="INFO")`

Set a basic StreamHandler logger. :param level: the level for this console logger

`main.set_color_logger(level="INFO")`

Replace the current logging.StreamHandler with colorlog.StreamHandler. :param level: the level for this console logger

`main.set_console_logger (new_level="NOTSET", current_level="INFO", nocolor=False)`

Set the console logger to a new level if this is different from NOTSET

Parameters

- **new_level** – the new level to set for the console logger
- **current_level** – the current level to set for the console logger
- **nocolor** – True if no colors should be used

`main.set_logger (level="NOTSET", nocolor=False)`

Set the logger :param level: the level for the console logger :param nocolor: True if no colors should be used

`main.sbpipe (create_project="", simulate="", parameter_scan1="", parameter_scan2="", parameter_estimation="", logo=False, license=False, nocolor=False, log_level="", quiet=False, verbose=False)`

SBpipe function.

Parameters

- **create_project** – create a project with the name as argument
- **simulate** – model simulation using a configuration file as argument
- **parameter_scan1** – model one parameter scan using a configuration file as argument
- **parameter_scan2** – model two parameters scan using a configuration file as argument
- **parameter_estimation** – model parameter estimation using a configuration file as argument
- **logo** – True to print the logo
- **license** – True to print the license
- **nocolor** – True to print logging messages without colors
- **log_level** – Set the logging level
- **quiet** – True if quiet (CRITICAL+)
- **verbose** – True if verbose (DEBUG+)

Returns 0 if OK, 1 if trouble (e.g. a pipeline did not execute correctly).

`main.main (argv=None)`

SBpipe main function.

Returns 0 if OK, 1 if trouble

3.3 `__main__`

3.3.1 Module Contents

`__main__.main (argv=None)`

3.4 simul

3.4.1 Subpackages

3.4.1.1 simul.copasi

Submodules

`simul.copasi.copasi`

Module Contents

class `simul.copasi.copasi.Copasi`

Copasi simulator.

`__init__()`

`model_checking(model_filename, fileout, task_name="")`

Check whether the Copasi model can be loaded and executed correctly.

Parameters

- **model_filename** – the COPASI filename
- **fileout** – the file containing the model checking results
- **task_name** – the task to check

Returns boolean indicating whether the model could be loaded and executed successfully

`sim(model, inputdir, outputdir, cluster="local", local_cpus=1, runs=1, output_msg=False)`

`ps1(model, scanned_par, simulate_intervals, single_param_scan_intervals, inputdir, outputdir, cluster="local", local_cpus=1, runs=1, output_msg=False)`

`ps2(model, sim_length, inputdir, outputdir, cluster="local", local_cpus=1, runs=1, output_msg=False)`

`pe(model, inputdir, cluster, local_cpus, runs, outputdir, sim_data_dir, output_msg=False)`

`_run_par_comput(inputdir, model, outputdir, cluster="local", local_cpus=1, runs=1, output_msg=False)`

`_get_params_list(filein)`

Return the list of parameter names from filein

Parameters **filein** – a Copasi parameter estimation report file

Returns the list of parameter names

`_write_best_fits(files, path_out, filename_out)`

Write the final estimates to filename_out

Parameters

- **files** – the list of Copasi parameter estimation reports
- **path_out** – the path to store the file combining the final (best) estimates (filename_out)
- **filename_out** – the file containing the final (best) estimates

`_write_all_fits(files, path_out, filename_out)`

Write all the estimates to filename_out

Parameters

- **files** – the list of Copasi parameter estimation reports

- **path_out** – the path to store the file combining all the estimates
- **filename_out** – the file containing all the estimates

`simul.copasi.model_checking`

Module Contents

`simul.copasi.model_checking.copasi_model_checking` (*model_filename*, *fileout*,
task_name="")

Perform a basic model checking for a COPASI model file.

Parameters

- **model_filename** – the filename to a COPASI file
- **fileout** – the file containing the model checking results
- **task_name** – the task to check

Returns a boolean indicating whether the model could be loaded successfully

`simul.copasi.model_checking.severity2string` (*severity*)

Return a string representing the severity of the error message :param severity: an integer representing severity :return: a string of the error message

`simul.copasi.model_checking.check_model_loading` (*model_filename*, *data_model*)

Check whether the COPASI model can be loaded

Parameters

- **model_filename** – the filename to a COPASI file
- **data_model** – the COPASI data model structure

Returns a boolean indicating whether the model could be loaded successfully

`simul.copasi.model_checking.check_task_selection` (*model_filename*, *task_name*,
data_model)

Check whether the COPASI model task can be executed

Parameters

- **model_filename** – the filename to a COPASI file
- **task_name** – the task to check
- **data_model** – the COPASI data model structure.

Returns a boolean indicating whether the model task can be executed correctly

`simul.copasi.model_checking.check_task_report` (*model_filename*, *task_name*,
data_model, *task*)

Check whether the COPASI model task can be executed

Parameters

- **model_filename** – the filename to a COPASI file
- **task_name** – the task to check
- **data_model** – the COPASI data model structure
- **task** – the COPASI task data structure

Returns a boolean indicating whether the model task can be executed correctly

3.4.1.2 simul.python

Submodules

`simul.python.python`

Module Contents

```
class simul.python.python.Python
    Python Simulator.
    __init__()
```

3.4.2 Submodules

3.4.2.1 simul.pl_simul

Module Contents

```
class simul.pl_simul.PLSimul (lang, lang_err_msg, options)
    A generic simulator for models coded in a programming language.
    __init__ (lang, lang_err_msg, options)
        A constructor for a simulator of models coded in a programming language :param lang: the program-
        ming language name (e.g. python, Rscript, java, octave, ..) :param lang_err_msg: the message to print
        if lang is not found. :param options: the options to use when invoking the command (e.g. "-jar" for
        java, "-vanilla" for Rscript, "" for python, "" for octave).

    get_lang()
        Return the programming language name :return: the name

    get_lang_err_msg()
        Return the error if the programming language is not found :return: the error message

    get_lang_options()
        Return the options for the programming language command :return: the options. Return None, if no
        options are used.

    sim (model, inputdir, outputdir, cluster="local", local_cpus=1, runs=1, output_msg=False)

    ps1 (model, scanned_par, simulate_intervals, single_param_scan_intervals, inputdir, outputdir,
        cluster="local", local_cpus=1, runs=1, output_msg=False)

    ps2 (model, sim_length, inputdir, outputdir, cluster="local", local_cpus=1, runs=1, out-
        put_msg=False)

    pe (model, inputdir, cluster, local_cpus, runs, outputdir, sim_data_dir, output_msg=False)

    _run_par_comput (model, inputdir, outputdir, cluster="local", local_cpus=1, runs=1, out-
        put_msg=False)

    replace_str_in_report (report)
```

3.4.2.2 simul.simul

Module Contents

```
class simul.simul.Simul
    Generic simulator.
```

`__init__()`

Default constructor.

sim (*model*, *inputdir*, *outputdir*, *cluster*="local", *local_cpus*=1, *runs*=1, *output_msg*=False)

Time course simulator.

Parameters

- **model** – the model to process
- **inputdir** – the directory containing the model
- **outputdir** – the directory containing the output files
- **cluster** – local, lsf for Load Sharing Facility, sge for Sun Grid Engine.
- **local_cpus** – the number of CPU.
- **runs** – the number of model simulation
- **output_msg** – print the output messages on screen (available for cluster='local' only)

ps1 (*model*, *scanned_par*, *simulate_intervals*, *single_param_scan_intervals*, *inputdir*, *outputdir*, *cluster*="local", *local_cpus*=1, *runs*=1, *output_msg*=False)

Single parameter scan.

Parameters

- **model** – the model to process
- **scanned_par** – the scanned parameter
- **simulate_intervals** – the time step of each simulation
- **single_param_scan_intervals** – the number of scans to perform
- **inputdir** – the directory containing the model
- **outputdir** – the directory to store the results
- **cluster** – local, lsf for Load Sharing Facility, sge for Sun Grid Engine.
- **local_cpus** – the number of CPU used.
- **runs** – the number of model simulation
- **output_msg** – print the output messages on screen (available for cluster='local' only)

ps2 (*model*, *sim_length*, *inputdir*, *outputdir*, *cluster*="local", *local_cpus*=1, *runs*=1, *output_msg*=False)

Double parameter scan.

Parameters

- **model** – the model to process
- **sim_length** – the length of the simulation
- **inputdir** – the directory containing the model
- **outputdir** – the directory to store the results
- **cluster** – local, lsf for Load Sharing Facility, sge for Sun Grid Engine.
- **local_cpus** – the number of CPU.
- **runs** – the number of model simulation
- **output_msg** – print the output messages on screen (available for cluster='local' only)

pe (*model, inputdir, cluster, local_cpus, runs, outputdir, sim_data_dir, output_msg=False*)
parameter estimation.

Parameters

- **model** – the model to process
- **inputdir** – the directory containing the model
- **cluster** – local, lsf for load sharing facility, sge for sun grid engine
- **local_cpus** – the number of cpu
- **runs** – the number of fits to perform
- **outputdir** – the directory to store the results
- **sim_data_dir** – the directory containing the simulation data sets
- **output_msg** – print the output messages on screen (available for cluster='local' only)

get_sim_columns (*path_in="."*)

Return the columns to analyse (sim task)

Parameters **path_in** – the path to the input files

get_best_fits (*path_in=".", path_out=".", filename_out="final_estimates.csv"*)

Collect the final parameter estimates. Results are stored in filename_out.

Parameters

- **path_in** – the path to the input files
- **path_out** – the path to the output files
- **filename_out** – a global file containing the best fits from independent parameter estimations.

Returns the number of retrieved files

get_all_fits (*path_in=".", path_out=".", filename_out="all_estimates.csv"*)

Collect all the parameter estimates. Results are stored in filename_out.

Parameters

- **path_in** – the path to the input files
- **path_out** – the path to the output files
- **filename_out** – a global file containing all fits from independent parameter estimations.

Returns the number of retrieved files

_run_par_comput (*model, inputdir, outputdir, cluster="local", local_cpus=1, runs=1, output_msg=False*)

Run generic parallel computation.

Parameters

- **model** – the model to process
- **inputdir** – the directory containing the model
- **outputdir** – the directory to store the results
- **cluster** – local, lsf for load sharing facility, sge for sun grid engine
- **local_cpus** – the number of cpus
- **runs** – the number of runs to perform

- **output_msg** – print the output messages on screen (available for cluster='local' only)

Returns (groupid, group_model)

_get_model_group (*model*)

Return the model without extension concatenated with the groupid string :param model: the model name :return: the concatenated string

_move_reports (*inputdir, outputdir, model, groupid*)

Move the report files

Parameters

- **inputdir** – the directory containing the model
- **outputdir** – the directory containing the output files
- **model** – the model to process
- **groupid** – a string identifier in the file name characterising the batch of simulated models.

replace_str_in_report (*report*)

Replaces strings in a report file.

Parameters **report** – a report file with its absolute path

_get_input_files (*path*)

Retrieve the input files in a path.

Parameters **path** – the path containing the input files to retrieve

Returns the list of input files

_get_params_list (*filein*)

Return the list of parameter names from filein

Parameters **filein** – a report file

Returns the list of parameter names

_write_params (*col_names, path_out, filename_out*)

Write the list of parameter names to filename_out

Parameters

- **col_names** – the list of parameter names
- **path_out** – the path to store filename_out
- **filename_out** – the output file to store the parameter names

_write_best_fits (*files, path_out, filename_out*)

Write the final estimates to filename_out

Parameters

- **files** – the list of parameter estimation reports
- **path_out** – the path to store the file combining the final (best) estimates (filename_out)
- **filename_out** – the file containing the final (best) estimates

_write_all_fits (*files, path_out, filename_out*)

Write all the estimates to filename_out

Parameters

- **files** – the list of parameter estimation reports
- **path_out** – the path to store the file combining all the estimates

- **filename_out** – the file containing all the estimates

_ps1_header_init (*report, scanned_par*)

Header report initialisation for single parameter scan pipeline.

Parameters

- **report** – a report
- **scanned_par** – the scanned parameter

:return a list containing the header or an empty list if no header was created.

ps1_postproc (*model, scanned_par, simulate_intervals, single_param_scan_intervals, output-dir*)

Perform post processing organisation to single parameter scan report files.

Parameters

- **model** – the model to process
- **scanned_par** – the scanned parameter
- **simulate_intervals** – the time step of each simulation
- **single_param_scan_intervals** – the number of scans to perform
- **outputdir** – the directory to store the results

ps2_postproc (*model, sim_length, outputdir*)

Perform post processing organisation to double parameter scan report files.

Parameters

- **model** – the model to process
- **sim_length** – the length of the simulation
- **outputdir** – the directory to store the results

3.5 tasks

3.5.1 Submodules

3.5.1.1 tasks.generate_data

Module Contents

`tasks.generate_data.run_copasi_model` (*infile*)

Run a Copasi model

Parameters **infile** – the input file

`tasks.generate_data.run_generic_model` (*infile*)

Run a generic model

Parameters **infile** – the input file

`tasks.generate_data.generate_data` (*infile, copasi=False*)

Replicate a copasi model and adds an id.

Parameters

- **infile** – the input file
- **copasi** – True if the model is a Copasi model

`tasks.generate_data.main` (*argv=None*)

3.5.1.2 `tasks.model_checking`

Module Contents

`tasks.model_checking.model_checking` (*infile, fileout, task_name*)

Check the consistency for the COPASI file.

Parameters

- **infile** – the input file
- **fileout** – the output file
- **task_name** – the name of the task (Copasi models)

Returns False if model checking can be executed and fails or if the COPASI simulator is not found.

`tasks.model_checking.main` (*argv=None*)

3.5.1.3 `tasks.pe_collect`

Module Contents

`tasks.pe_collect.pe_collect` (*inputdir, outputdir, fileout_final_estims, fileout_all_estims, copasi=True*)

Collect the results so that they can be processed. :param inputdir: the input folder containing the data :param outputdir: the output folder to stored the collected results :param fileout_final_estims: the name of the file containing the best estimations :param fileout_all_estims: the name of the file containing all the estimations :param copasi: True if COPASI was used to generate the data.

`tasks.pe_collect.main` (*argv=None*)

3.5.1.4 `tasks.pe_combine_param_best_fits_stats`

Module Contents

`tasks.pe_combine_param_best_fits_stats.pe_combine_param_best_fits_stats` (*plots_dir, fileout_param_estim_best_fits_details*)

Combine the statistics for the parameter estimation details

Parameters

- **plots_dir** – the directory to save the generated plots
- **fileout_param_estim_best_fits_details** – the name of the file containing the detailed statistics for the estimated parameters

`tasks.pe_combine_param_best_fits_stats.main` (*argv=None*)

3.5.1.5 `tasks.pe_combine_param_ple_stats`

Module Contents

`tasks.pe_combine_param_ple_stats.pe_combine_param_ple_stats` (*plots_dir, fileout_param_estim_details*)

Combine the statistics for the parameter estimation details

Parameters

- **plots_dir** – the directory to save the generated plots

- **fileout_param_estim_details** – the name of the file containing the detailed statistics for the estimated parameters

`tasks.pe_combine_param_ple_stats.main(argv=None)`

3.5.1.6 tasks.pe_ds_preproc

Module Contents

`tasks.pe_ds_preproc.pe_ds_preproc(filename, param_names, logspace=True, all_fits=False, data_point_num=0, fileout_param_estim_summary="param_estim_summary.csv")`

Parameter estimation pre-processing. It renames the data set columns, and applies a log10 transformation if logspace is TRUE. If all.fits is true, it also computes the confidence levels.

Parameters

- **filename** – the dataset filename containing the fits sequence
- **param_names** – the list of estimated parameter names
- **logspace** – true if the data set should be log10-transformed.
- **all_fits** – true if filename contains all fits, false otherwise
- **data_point_num** – the number of data points used for parameterise the model. Ignored if all.fits is false
- **fileout_param_estim_summary** – the name of the file containing the summary for the parameter estimation. Ignored if all.fits is false

`tasks.pe_ds_preproc.main(argv=None)`

3.5.1.7 tasks.pe_objval_vs_iters_analysis

Module Contents

`tasks.pe_objval_vs_iters_analysis.pe_objval_vs_iters_analysis(model_name, filename, plots_dir)`

Analysis of the Objective values vs Iterations.

Parameters

- **model_name** – the model name without extension
- **filename** – the filename containing the fits sequence
- **plots_dir** – the directory for storing the plots

`tasks.pe_objval_vs_iters_analysis.main(argv=None)`

3.5.1.8 `tasks.pe_parameter_density_analysis`

Module Contents

`tasks.pe_parameter_density_analysis.pe_parameter_density_analysis` (*model_name*,
file-
name,
param-
eter,
plots_dir,
thres="BestFits",
best_fits_percent=100,
file-
out_param_estim_summary="",
logspace=True,
scien-
tific_notation=True)

Parameter density analysis.

Parameters

- **model_name** – the model name without extension
- **filename** – the filename containing the fits sequence
- **parameter** – the name of the parameter to plot the density
- **plots_dir** – the directory for storing the plots
- **thres** – the threshold used to filter the dataset. Values: “BestFits”, “CL66”, “CL95”, “CL99”, “All”.
- **best_fits_percent** – the percent of best fits to analyse. Only used if `thres="BestFits"`.
- **fileout_param_estim_summary** – the name of the file containing the summary for the parameter estimation. Only used if `thres!="BestFits"`.
- **logspace** – true if the parameters should be plotted in logspace
- **scientific_notation** – true if the axis labels should be plotted in scientific notation

`tasks.pe_parameter_density_analysis.main` (*argv=None*)

3.5.1.9 `tasks.pe_parameter_pca_analysis`

Module Contents

`tasks.pe_parameter_pca_analysis.pe_parameter_pca_analysis` (*model_name*, *file-*
name, *plots_dir*,
best_fits_percent=100)

PCA for the best fits of the estimated parameters.

Parameters

- **model_name** – the model name without extension
- **filename** – the filename containing the fits sequence
- **plots_dir** – the directory for storing the plots
- **best_fits_percent** – the percent of best fits to analyse. Only used if `thres="BestFits"`.

`tasks.pe_parameter_pca_analysis.main` (*argv=None*)

3.5.1.10 `tasks.pe_postproc`

Module Contents

`tasks.pe_postproc.generic_postproc` (*infile*, *outfile*, *copasi=True*)

Perform post processing file editing for the *pe* pipeline

Parameters

- **infile** – the model to process
- **outfile** – the directory to store the results
- **copasi** – True if the model is a Copasi model

`tasks.pe_postproc.pe_postproc` (*infile*, *outfile*, *copasi=True*)

Perform post processing file editing for the *pe* pipeline

Parameters

- **infile** – the model to process
- **outfile** – the directory to store the results
- **copasi** – True if the model is a Copasi model

`tasks.pe_postproc.main` (*argv=None*)

3.5.1.11 `tasks.pe_sampled_2d_ple_analysis`

Module Contents

`tasks.pe_sampled_2d_ple_analysis.pe_sampled_2d_ple_analysis` (*model_name*,
filename, *parameter1*, *parameter2*, *plots_dir*,
thres="BestFits", *best_fits_percent*=100,
file-
out_param_estim_summary="",
logspace=True,
scientific-
notation=True)

2D profile likelihood estimation analysis.

Parameters

- **model_name** – the model name without extension
- **filename** – the filename containing the fits sequence
- **parameter1** – the name of the first parameter
- **parameter2** – the name of the second parameter
- **plots_dir** – the directory for storing the plots
- **thres** – the threshold used to filter the dataset. Values: "BestFits", "CL66", "CL95", "CL99", "All".
- **best_fits_percent** – the percent of best fits to analyse. Only used if *thres*="BestFits".
- **fileout_param_estim_summary** – the name of the file containing the summary for the parameter estimation. Only used if *thres*!="BestFits".
- **logspace** – true if the parameters should be plotted in logspace

- **scientific_notation** – true if the axis labels should be plotted in scientific notation

```
tasks.pe_sampled_2d_ple_analysis.main(argv=None)
```

3.5.1.12 tasks.pe_sampled_ple_analysis

Module Contents

```
tasks.pe_sampled_ple_analysis.pe_sampled_ple_analysis(model_name, filename,
parameter, plots_dir, fileout_param_estim_summary,
logspace=True, scientific_notation=True)
```

Run the profile likelihood estimation analysis.

Parameters

- **model_name** – the model name without extension
- **filename** – the filename containing the fits sequence
- **parameter** – the parameter to compute the PLE analysis
- **plots_dir** – the directory to save the generated plots
- **fileout_param_estim_summary** – the name of the file containing the summary for the parameter estimation
- **logspace** – true if parameters should be plotted in logspace
- **scientific_notation** – true if the axis labels should be plotted in scientific notation

```
tasks.pe_sampled_ple_analysis.main(argv=None)
```

3.5.1.13 tasks.preproc

Module Contents

```
tasks.preproc.generic_preproc(infile, outfile)
```

Copy the model file

Parameters

- **infile** – the input file
- **outfile** – the output file

```
tasks.preproc.copasi_preproc(infile, outfile)
```

Replicate a copasi model and adds an id.

Parameters

- **infile** – the input file
- **outfile** – the output file

```
tasks.preproc.preproc(infile, outfile, copasi=False)
```

Replicate a copasi model and adds an id.

Parameters

- **infile** – the input file
- **outfile** – the output file

- **copasi** – True if the model is a Copasi model

`tasks.preproc.main (argv=None)`

3.5.1.14 `tasks.ps1_analyse_plot`

Module Contents

`tasks.ps1_analyse_plot.ps1_analyse_plot (model_name, inhibition_only, inputdir, outputdir, repeat, percent_levels, min_level, max_level, levels_number, xaxis_label, yaxis_label)`

Plot model single parameter scan time courses (Python wrapper).

Parameters

- **model_name** – the model name without extension
- **inhibition_only** – true if the scanning only decreases the variable amount (inhibition only)
- **inputdir** – the input directory containing the simulated data
- **outputdir** – the output directory that will contain the simulated plots
- **repeat** – the simulation number
- **percent_levels** – true if scanning levels are in percent
- **min_level** – the minimum level
- **max_level** – the maximum level
- **levels_number** – the number of levels
- **homogeneous_lines** – true if lines should be plotted homogeneously
- **xaxis_label** – the label for the x axis (e.g. Time [min])
- **yaxis_label** – the label for the y axis (e.g. Level [a.u.])

`tasks.ps1_analyse_plot.main (argv=None)`

3.5.1.15 `tasks.ps1_analyse_plot_homogen`

Module Contents

`tasks.ps1_analyse_plot_homogen.ps1_analyse_plot_homogen (model_name, inputdir, outputdir, repeat, xaxis_label, yaxis_label)`

Plot model single parameter scan time courses using homogeneous lines (Python wrapper).

Parameters

- **model_name** – the model name without extension
- **inputdir** – the input directory containing the simulated data
- **outputdir** – the output directory that will contain the simulated plots
- **repeat** – the simulation number
- **xaxis_label** – the label for the x axis (e.g. Time [min])
- **yaxis_label** – the label for the y axis (e.g. Level [a.u.])

`tasks.ps1_analyse_plot_homogen.main (argv=None)`

3.5.1.16 `tasks.ps1_postproc`

Module Contents

`tasks.ps1_postproc.ps1_header_init` (*report, scanned_par*)

Header report initialisation for single parameter scan pipeline.

Parameters

- **report** – a report
- **scanned_par** – the scanned parameter

:return a list containing the header or an empty list if no header was created.

`tasks.ps1_postproc.generic_postproc` (*infile, outfile, scanned_par, simulate_intervals, single_param_scan_intervals, copasi=True*)

Perform post processing organisation to single parameter scan report files.

Parameters

- **infile** – the model to process
- **outfile** – the directory to store the results
- **scanned_par** – the scanned parameter
- **simulate_intervals** – the time step of each simulation
- **single_param_scan_intervals** – the number of scans to perform
- **copasi** – True if the model is a Copasi model

`tasks.ps1_postproc.ps1_postproc` (*infile, outfile, scanned_par, simulate_intervals, single_param_scan_intervals, copasi=True*)

Perform post processing organisation to single parameter scan report files.

Parameters

- **infile** – the model to process
- **outfile** – the directory to store the results
- **scanned_par** – the scanned parameter
- **simulate_intervals** – the time step of each simulation
- **single_param_scan_intervals** – the number of scans to perform
- **copasi** – True if the model is a Copasi model

`tasks.ps1_postproc.main` (*argv=None*)

3.5.1.17 `tasks.ps2_analyse_plot`

Module Contents

`tasks.ps2_analyse_plot.ps2_analyse_plot` (*model, scanned_par1, scanned_par2, inputdir, outputdir, id*)

Plot model double parameter scan time courses (Python wrapper).

Parameters

- **model** – the model name without extension
- **scanned_par1** – the 1st scanned parameter
- **scanned_par2** – the 2nd scanned parameter
- **inputdir** – the input directory

- **outputdir** – the output directory
- **run** – the simulation number

`tasks.ps2_analyse_plot.main (argv=None)`

3.5.1.18 tasks.ps2_postproc

Module Contents

`tasks.ps2_postproc.generic_postproc (infile, outfile, sim_length, copasi=True)`

Perform post processing organisation to double parameter scan report files.

Parameters

- **infile** – the model to process
- **outfile** – the directory to store the results
- **sim_length** – the length of the simulation
- **copasi** – True if the model is a Copasi model

`tasks.ps2_postproc.ps2_postproc (infile, outfile, sim_length, copasi=True)`

Perform post processing organisation to double parameter scan report files.

Parameters

- **infile** – the model to process
- **outfile** – the directory to store the results
- **sim_length** – the length of the simulation
- **copasi** – True if the model is a Copasi model

`tasks.ps2_postproc.main (argv=None)`

3.5.1.19 tasks.sim_analyse_gen_stats_table

Module Contents

`tasks.sim_analyse_gen_stats_table.sim_analyse_gen_stats_table (inputfile, outfile, variable)`

Plot model simulation time courses (Python wrapper).

Parameters

- **inputfile** – the file containing the repeats
- **outputfile** – the output file containing the statistics
- **variable** – the model variable to analyse

`tasks.sim_analyse_gen_stats_table.main (argv=None)`

3.5.1.20 `tasks.sim_analyse_plot_comb_sims`

Module Contents

```
tasks.sim_analyse_plot_comb_sims.sim_analyse_plot_comb_sims(inputdir,  out-  
                                                                putdir,  model,  
                                                                exp_dataset,  
                                                                plot_exp_dataset,  
                                                                exp_dataset_alpha,  
                                                                xaxis_label,  
                                                                yaxis_label,  
                                                                variable)
```

Plot model simulation time courses (Python wrapper).

Parameters

- **inputdir** – the directory containing the data to analyse
- **outputdir** – the output directory containing the results
- **model** – the model name
- **exp_dataset** – the full path of the experimental data set
- **plot_exp_dataset** – True if the experimental data set should also be plotted
- **exp_dataset_alpha** – the alpha level for the data set
- **xaxis_label** – the label for the x axis (e.g. Time [min])
- **yaxis_label** – the label for the y axis (e.g. Level [a.u.])
- **variable** – the model variable to analyse

```
tasks.sim_analyse_plot_comb_sims.main(argv=None)
```

3.5.1.21 `tasks.sim_analyse_plot_sep_sims`

Module Contents

```
tasks.sim_analyse_plot_sep_sims.sim_analyse_plot_sep_sims(inputdir, outputdir,  
                                                            model, exp_dataset,  
                                                            plot_exp_dataset,  
                                                            exp_dataset_alpha,  
                                                            xaxis_label,  
                                                            yaxis_label,  vari-  
                                                            able)
```

Plot model simulation time courses (Python wrapper).

Parameters

- **inputdir** – the directory containing the data to analyse
- **outputdir** – the output directory containing the results
- **model** – the model name
- **exp_dataset** – the full path of the experimental data set
- **plot_exp_dataset** – True if the experimental data set should also be plotted
- **exp_dataset_alpha** – the alpha level for the data set
- **xaxis_label** – the label for the x axis (e.g. Time [min])
- **yaxis_label** – the label for the y axis (e.g. Level [a.u.])
- **variable** – the model variable to analyse

```
tasks.sim_analyse_plot_sep_sims.main(argv=None)
```

3.5.1.22 tasks.sim_analyse_summarise_data

Module Contents

```
tasks.sim_analyse_summarise_data.sim_analyse_summarise_data(inputdir,  
                                                             model,      out-  
                                                             putfile_repeats,  
                                                             variable)
```

Plot model simulation time courses (Python wrapper).

Parameters

- **inputdir** – the directory containing the data to analyse
- **model** – the model name
- **outputfile_repeats** – the output file containing the model simulation repeats
- **variable** – the model variable to analyse

```
tasks.sim_analyse_summarise_data.main(argv=None)
```

3.5.1.23 tasks.sim_postproc

Module Contents

```
tasks.sim_postproc.generic_postproc(infile, outfile, copasi=True)
```

Perform post processing file editing for the *simulate* pipeline

Parameters

- **infile** – the model to process
- **outfile** – the directory to store the results
- **copasi** – True if the model is a Copasi model

```
tasks.sim_postproc.sim_postproc(infile, outfile, copasi=True)
```

Perform post processing file editing for the *simulate* pipeline

Parameters

- **infile** – the model to process
- **outfile** – the directory to store the results
- **copasi** – True if the model is a Copasi model

```
tasks.sim_postproc.main(argv=None)
```

3.6 pl

3.6.1 Subpackages

3.6.1.1 pl.create

Submodules

`pl.create.newproj`

Module Contents

class `pl.create.newproj.NewProj` (*models_folder="Models", working_folder="Results"*)
This module initialises the folder tree for a new project.

Parameters

- **models_folder** – the folder containing the models
- **working_folder** – the folder to store the results

__init__ (*models_folder="Models", working_folder="Results"*)
Constructor.

run (*project_name*)
Create a project directory tree.

Parameters **project_name** – the name of the project

Returns 0

3.6.1.2 pl.pe

Submodules

`pl.pe.parest`

Module Contents

class `pl.pe.parest.ParEst` (*models_folder="Models", working_folder="Results",
sim_data_folder="param_estim_data",
sim_plots_folder="param_estim_plots"*)

This module provides the user with a complete pipeline of scripts for running model parameter estimations

__init__ (*models_folder="Models", working_folder="Results",
sim_data_folder="param_estim_data", sim_plots_folder="param_estim_plots"*)

run (*config_file*)

generate_data (*simulator, model, inputdir, cluster, local_cpus, runs, outputdir, sim_data_dir*)
The first pipeline step: data generation.

Parameters

- **simulator** – the name of the simulator (e.g. Copasi)
- **model** – the model to process
- **inputdir** – the directory containing the model
- **cluster** – local, lsf for load sharing facility, sge for sun grid engine
- **local_cpus** – the number of cpu

- **runs** – the number of fits to perform
- **outputdir** – the directory to store the results
- **sim_data_dir** – the directory containing the simulation data sets

Returns True if the task was completed successfully, False otherwise.

analyse_data (*simulator, model, inputdir, outputdir, fileout_final_estims, fileout_all_estims, fileout_param_estim_best_fits_details, fileout_param_estim_details, fileout_param_estim_summary, sim_plots_dir, best_fits_percent, data_point_num, cluster="local", plot_2d_66cl_corr=False, plot_2d_95cl_corr=False, plot_2d_99cl_corr=False, logspace=True, scientific_notation=True*)

The second pipeline step: data analysis.

Parameters

- **simulator** – the name of the simulator (e.g. Copasi)
- **model** – the model name
- **inputdir** – the directory containing the simulation data
- **outputdir** – the directory to store the results
- **fileout_final_estims** – the name of the file containing final parameter sets with the objective value
- **fileout_all_estims** – the name of the file containing all the parameter sets with the objective value
- **fileout_param_estim_best_fits_details** – the name of the file containing the detailed statistics for the

estimated parameters from the best fits analysis :param fileout_param_estim_details: the name of the file containing the detailed statistics for the estimated parameters from the PLE analysis :param fileout_param_estim_summary: the name of the file containing the summary for the parameter estimation :param sim_plots_dir: the directory of the simulation plots :param best_fits_percent: the percent to consider for the best fits :param data_point_num: the number of data points :param cluster: local, lsf for Load Sharing Facility, sge for Sun Grid Engine. :param plot_2d_66cl_corr: True if 2 dim plots for the parameter sets within 66% should be plotted :param plot_2d_95cl_corr: True if 2 dim plots for the parameter sets within 95% should be plotted :param plot_2d_99cl_corr: True if 2 dim plots for the parameter sets within 99% should be plotted :param logspace: True if parameters should be plotted in log space :param scientific_notation: True if axis labels should be plotted in scientific notation :return: True if the task was completed successfully, False otherwise.

generate_report (*model, outputdir, sim_plots_folder*)

The third pipeline step: report generation.

Parameters

- **model** – the model name
- **outputdir** – the directory to store the report
- **sim_plots_folder** – the folder containing the plots

Returns True if the task was completed successfully, False otherwise.

parse (*my_dict*)

3.6.1.3 pl.ps1

Submodules

pl.ps1.parscan1

Module Contents

```
class pl.ps1.parscan1.ParScan1 (models_folder="Models", working_folder="Results",  
                                sim_data_folder="single_param_scan_data",  
                                sim_plots_folder="single_param_scan_plots")
```

This module provides the user with a complete pipeline of scripts for computing single parameter scans.

```
__init__ (models_folder="Models", working_folder="Results",  
          sim_data_folder="single_param_scan_data", sim_plots_folder="single_param_scan_plots")
```

```
run (config_file)
```

```
generate_data (simulator, model, scanned_par, cluster, local_cpus, runs, simulate_intervals,  
                single_param_scan_intervals, inputdir, outputdir)
```

The first pipeline step: data generation.

Parameters

- **simulator** – the name of the simulator (e.g. Copasi)
- **model** – the model to process
- **scanned_par** – the scanned parameter
- **cluster** – local, lsf for Load Sharing Facility, sge for Sun Grid Engine.
- **local_cpus** – the number of CPU.
- **runs** – the number of model simulation
- **simulate_intervals** – the time step of each simulation
- **single_param_scan_intervals** – the number of scans to perform
- **inputdir** – the directory containing the model
- **outputdir** – the directory to store the results

Returns True if the task was completed successfully, False otherwise.

```
analyse_data (model, knock_down_only, outputdir, sim_data_folder, sim_plots_folder, runs,  
               local_cpus, percent_levels, min_level, max_level, levels_number, homoge-  
               neous_lines, cluster="local", xaxis_label="", yaxis_label="")
```

The second pipeline step: data analysis.

Parameters

- **model** – the model name
- **knock_down_only** – True for knock down simulation, false if also scanning over expression.
- **outputdir** – the directory containing the results
- **sim_data_folder** – the folder containing the simulated data sets
- **sim_plots_folder** – the folder containing the generated plots
- **runs** – the number of simulations
- **local_cpus** – the number of cpus
- **percent_levels** – True if the levels are percents.
- **min_level** – the minimum level

- **max_level** – the maximum level
- **levels_number** – the number of levels
- **homogeneous_lines** – True if generated line style should be homogeneous
- **cluster** – local, lsf for Load Sharing Facility, sge for Sun Grid Engine.
- **xaxis_label** – the name of the x axis (e.g. Time [min])
- **yaxis_label** – the name of the y axis (e.g. Level [a.u.])

Returns True if the task was completed successfully, False otherwise.

generate_report (*model, scanned_par, outputdir, sim_plots_folder*)
The third pipeline step: report generation.

Parameters

- **model** – the model name
- **scanned_par** – the scanned parameter
- **outputdir** – the directory containing the report
- **sim_plots_folder** – the folder containing the plots

Returns True if the task was completed successfully, False otherwise.

parse (*my_dict*)

3.6.1.4 pl.ps2

Submodules

pl.ps2.parscan2

Module Contents

```
class pl.ps2.parscan2.ParScan2 (models_folder="Models",          working_folder="Results",
                                sim_data_folder="double_param_scan_data",
                                sim_plots_folder="double_param_scan_plots")
```

This module provides the user with a complete pipeline of scripts for computing double parameter scans.

```
__init__ (models_folder="Models",          working_folder="Results",
           sim_data_folder="double_param_scan_data", sim_plots_folder="double_param_scan_plots")
```

```
run (config_file)
```

```
generate_data (simulator, model, sim_length, inputdir, outputdir, cluster, local_cpus, runs)
```

The first pipeline step: data generation.

Parameters

- **simulator** – the name of the simulator (e.g. Copasi)
- **model** – the model to process
- **sim_length** – the length of the simulation
- **inputdir** – the directory containing the model
- **outputdir** – the directory to store the results
- **cluster** – local, lsf for Load Sharing Facility, sge for Sun Grid Engine.
- **local_cpus** – the number of CPU.
- **runs** – the number of model simulation

Returns True if the task was completed successfully, False otherwise.

analyse_data (*model, scanned_par1, scanned_par2, inputdir, outputdir, cluster="local", local_cpus=1, runs=1*)

The second pipeline step: data analysis.

Parameters

- **model** – the model name
- **scanned_par1** – the first scanned parameter
- **scanned_par2** – the second scanned parameter
- **inputdir** – the directory containing the simulated data sets to process
- **outputdir** – the directory to store the performed analysis
- **cluster** – local, lsf for Load Sharing Facility, sge for Sun Grid Engine.
- **local_cpus** – the number of CPU.
- **runs** – the number of model simulation

Returns True if the task was completed successfully, False otherwise.

generate_report (*model, scanned_par1, scanned_par2, outputdir, sim_plots_folder*)

The third pipeline step: report generation.

Parameters

- **model** – the model name
- **scanned_par1** – the first scanned parameter
- **scanned_par2** – the second scanned parameter
- **outputdir** – the directory containing the report
- **sim_plots_folder** – the folder containing the plots.

Returns True if the task was completed successfully, False otherwise.

parse (*my_dict*)

3.6.1.5 pl.sim

Submodules

pl.sim.sim

Module Contents

```
class pl.sim.sim.Sim(models_folder="Models",                                working_folder="Results",  
                    sim_data_folder="simulate_data", sim_plots_folder="simulate_plots")
```

This module provides the user with a complete pipeline of scripts for running model simulations

```
__init__(models_folder="Models",                                working_folder="Results",  
         sim_data_folder="simulate_data", sim_plots_folder="simulate_plots")
```

```
run (config_file)
```

```
generate_data (simulator, model, inputdir, outputdir, cluster="local", local_cpus=2, runs=1)
```

The first pipeline step: data generation.

Parameters

- **simulator** – the name of the simulator (e.g. Copasi)
- **model** – the model to process

- **inputdir** – the directory containing the model
- **outputdir** – the directory containing the output files
- **cluster** – local, lsf for Load Sharing Facility, sge for Sun Grid Engine.
- **local_cpus** – the number of CPUs.
- **runs** – the number of model simulation

Returns True if the task was completed successfully, False otherwise.

analyse_data (*simulator, model, inputdir, outputdir, sim_plots_dir, exp_dataset, plot_exp_dataset, exp_dataset_alpha=1.0, cluster="local", local_cpus=2, xaxis_label="", yaxis_label=""*)

The second pipeline step: data analysis.

Parameters

- **simulator** – the name of the simulator (e.g. Copasi)
- **model** – the model name
- **inputdir** – the directory containing the data to analyse
- **outputdir** – the output directory containing the results
- **sim_plots_dir** – the directory to save the plots
- **exp_dataset** – the full path of the experimental data set
- **plot_exp_dataset** – True if the experimental data set should also be plotted
- **exp_dataset_alpha** – the alpha level for the data set
- **cluster** – local, lsf for Load Sharing Facility, sge for Sun Grid Engine.
- **local_cpus** – the number of CPUs.
- **xaxis_label** – the label for the x axis (e.g. Time [min])
- **yaxis_label** – the label for the y axis (e.g. Level [a.u.])

Returns True if the task was completed successfully, False otherwise.

generate_report (*model, outputdir, sim_plots_folder*)

The third pipeline step: report generation.

Parameters

- **model** – the model name
- **outputdir** – the output directory to store the report
- **sim_plots_folder** – the folder containing the plots

Returns True if the task was completed successfully, False otherwise.

parse (*my_dict*)

3.6.2 Submodules

3.6.2.1 pl.pipeline

Module Contents

class pl.pipeline.**Pipeline** (*models_folder="Models", working_folder="Results", sim_data_folder="sim_data", sim_plots_folder="sim_plots"*)

Generic pipeline.

Parameters

- **models_folder** – the folder containing the models
- **working_folder** – the folder to store the results
- **sim_data_folder** – the folder to store the simulation data
- **sim_plots_folder** – the folder to store the graphic results

__init__ (*models_folder="Models", working_folder="Results", sim_data_folder="sim_data", sim_plots_folder="sim_plots"*)

run (*config_file*)

Run the pipeline.

Parameters **config_file** – a configuration file for this pipeline.

Returns True if the pipeline was executed correctly, False otherwise.

get_models_folder ()

Return the folder containing the models.

Returns the models folder.

get_working_folder ()

Return the folder containing the results.

Returns the working folder.

get_sim_data_folder ()

Return the folder containing the in-silico generated data sets.

Returns the folder of the simulated data sets.

get_sim_plots_folder ()

Return the folder containing the in-silico generated plots.

Returns the folder of the simulated plots.

generate_tarball (*output_folder*)

Create a gz tarball.

Parameters

- **working_dir** – the working directory
- **output_folder** – the name of the folder to store the tar.gz file

Returns True if the generation of the tarball succeeded.

get_simul_obj (*simulator*)

Return the simulator object if this exists. Otherwise throws an exception. The simulator name starts with an upper case letter. Each simulator is in a package within *sbpipe.simulator*.

Parameters **simulator** – the simulator name

Returns the simulator object.

load (*config*)

Safely load a YAML configuration file and return its structure as a dictionary object.

Parameters **config** – a YAML configuration file

Returns the dictionary structure of the configuration file

Raise `yaml.YAMLError` if the config cannot be loaded.

parse (*config_dict*)

Read a dictionary structure containing the pipeline configuration. This method is abstract.

Returns a tuple containing the configuration

3.7 utils

3.7.1 Submodules

3.7.1.1 utils.io

Module Contents

`utils.io.refresh` (*path, file_pattern*)

Clean and create the folder if this does not exist.

Parameters

- **path** – the path containing the files to remove
- **file_pattern** – the string pattern of the files to remove

`utils.io.get_pattern_pos` (*pattern, filename*)

Return the line number (as string) of the first occurrence of a pattern in filename

Parameters

- **pattern** – the pattern of the string to find
- **filename** – the file name containing the pattern to search

Returns the line number containing the pattern or “-1” if the pattern was not found

`utils.io.files_with_pattern_recur` (*folder, pattern*)

Return all files with a certain pattern in folder+subdirectories

Parameters

- **folder** – the folder to search for
- **pattern** – the string to search for

Returns the files containing the pattern.

`utils.io.write_mat_on_file` (*fileout, data*)

Write the matrix results stored in data to filename_out

Parameters

- **fileout** – the output file
- **data** – the data to store in a file

`utils.io.replace_str_in_file` (*filename_out, old_string, new_string*)

Replace a string with another in filename_out

Parameters

- **filename_out** – the output file
- **old_string** – the old string that should be replaced
- **new_string** – the new string replacing old_string

`utils.io.replace_str_in_report` (*report*)

Replace nasty strings in COPASI report file.

Parameters **report** – the report

`utils.io.remove_file_silently` (*filename*)

Remove a filename silently, without reporting warnings or error messages. This is not really needed by Linux, but Windows sometimes fails to remove the file even if this exists.

Parameters **filename** – the file to remove

3.7.1.2 `utils.parcomp`

Module Contents

`utils.parcomp.run_cmd(cmd)`

Run a command using Python subprocess.

Parameters `cmd` – The string of the command to run

`utils.parcomp.run_cmd_block(cmd)`

Run a command using Python subprocess. Block the call until the command has finished.

Parameters `cmd` – A tuple containing the string of the command to run

`utils.parcomp.parcomp(cmd, cmd_iter_substr, output_dir, cluster="local", runs=1, local_cpus=1, output_msg=False, colnames=list)`

Generic function to run a command in parallel

Parameters

- `cmd` – the command string to run in parallel
- `cmd_iter_substr` – the substring of the iteration number. This will be replaced in a number automatically
- `output_dir` – the output directory
- `cluster` – the cluster type among local (Python multiprocessing), sge, or lsf
- `runs` – the number of runs. Ignored if `colnames` is not empty
- `local_cpus` – the number of cpus to use at most
- `output_msg` – print the output messages on screen (available for `cluster='local'` only)
- `colnames` – the name of the columns to process

Returns True if the computation succeeded.

`utils.parcomp.progress_bar(it, total)`

A minimal CLI progress bar.

Parameters

- `it` – current iteration starting from 1
- `total` – total iterations

`utils.parcomp.progress_bar2(it, total)`

A CLI progress bar.

Parameters

- `it` – current iteration starting from 1
- `total` – total iterations

`utils.parcomp.call_proc(params)`

Run a command using Python subprocess.

Parameters `params` – A tuple containing (the string of the command to run, the command id)

`utils.parcomp.run_jobs_local(cmd, cmd_iter_substr, runs=1, local_cpus=1, output_msg=False, colnames=list)`

Run jobs using python multiprocessing locally.

Parameters

- `cmd` – the full command to run as a job
- `cmd_iter_substr` – the substring in command to be replaced with a number
- `runs` – the number of runs. Ignored if `colnames` is not empty

- **local_cpus** – The number of available cpus. If `local_cpus <= 0`, only one core will be used.
- **output_msg** – print the output messages on screen (available for `cluster_type='local'` only)
- **colnames** – the name of the columns to process

Returns True

`utils.parcomp.run_jobs_sge(cmd, cmd_iter_substr, out_dir, err_dir, runs=1, colnames=list)`
Run jobs using a Sun Grid Engine (SGE) cluster.

Parameters

- **cmd** – the full command to run as a job
- **cmd_iter_substr** – the substring in command to be replaced with a number
- **out_dir** – the directory containing the standard output from qsub
- **err_dir** – the directory containing the standard error from qsub
- **runs** – the number of runs. Ignored if `colnames` is not empty
- **colnames** – the name of the columns to process

Returns True if the computation succeeded.

`utils.parcomp.run_jobs_lsf(cmd, cmd_iter_substr, out_dir, err_dir, runs=1, colnames=list)`
Run jobs using a Load Sharing Facility (LSF) cluster.

Parameters

- **cmd** – the full command to run as a job
- **cmd_iter_substr** – the substring in command to be replaced with a number
- **out_dir** – the directory containing the standard output from bsub
- **err_dir** – the directory containing the standard error from bsub
- **runs** – the number of runs. Ignored if `colnames` is not empty
- **colnames** – the name of the columns to process

Returns True if the computation succeeded.

`utils.parcomp.quick_debug(cmd, out_dir, err_dir)`

Look up for *error* and *warning* in the standard output and error files. A simple debugging function checking the generated log files. We don't stop the computation because it happens that these messages are more *warnings* than real errors.

Parameters

- **cmd** – the executed command
- **out_dir** – the directory containing the standard output files
- **err_dir** – the directory containing the standard error files

Returns True

`utils.parcomp.is_output_file_clean(filename, stream_type="standard output")`
Check whether a file contains the string 'error' or 'warning'. If so a message is printed.

Parameters

- **filename** – a file
- **stream_type** – 'stderr' for standard error, 'stdout' for standard output.

Returns True

3.7.1.3 `utils.rand`

Module Contents

`utils.rand.get_rand_alphanum_str` (*length*)

Return a random alphanumeric string

Parameters `length` – the length of the string

Returns the generated string

`utils.rand.get_rand_num_str` (*length*)

Return a random numeric string

Parameters `length` – the length of the string

Returns the generated string

3.7.1.4 `utils.re_utils`

Module Contents

`utils.re_utils.nat_sort_key` (*str*)

The key to sort a list of strings alphanumerically (e.g. “file10” is correctly placed after “file2”)

Parameters `str` – the string to sort alphanumerically in a list of strings

Returns the key to sort strings alphanumerically

`utils.re_utils.escape_special_chars` (*text*)

Escape `^,% ,,{,}` from text :param text: the command to escape special characters inside :return: the command with escaped special characters

3.8 report

3.8.1 Submodules

3.8.1.1 `report.latex_reports`

Module Contents

`report.latex_reports.get_latex_header` (*pdftitle="SBpipe report", title="SBpipe report", abstract="Generic report."*)

Initialize a Latex header with a title and an abstract.

Parameters

- **pdftitle** – the pdftitle for the LaTeX header
- **title** – the title for the LaTeX header
- **abstract** – the abstract for the LaTeX header

Returns the LaTeX header

`report.latex_reports.latex_report_ps1` (*outputdir, plots_folder, filename_prefix, model_noext, scanned_par*)

Generate a report for a single parameter scan task.

Parameters

- **outputdir** – the output directory

- **plots_folder** – the folder containing the simulated plots
- **filename_prefix** – the prefix for the LaTeX file
- **model_noext** – the model name
- **scanned_par** – the scanned parameter

```
report.latex_reports.latex_report_ps2(outputdir, plots_folder, filename_prefix,
                                     model_noext, scanned_par1, scanned_par2)
```

Generate a report for a double parameter scan task.

Parameters

- **outputdir** – the output directory
- **plots_folder** – the folder containing the simulated plots
- **filename_prefix** – the prefix for the LaTeX file
- **model_noext** – the model name
- **scanned_par1** – the 1st scanned parameter
- **scanned_par2** – the 2nd scanned parameter

```
report.latex_reports.latex_report_sim(outputdir, plots_folder, model_noext, file-
                                     name_prefix)
```

Generate a report for a time course task.

Parameters

- **outputdir** – the output directory
- **plots_folder** – the folder containing the simulated plots
- **model_noext** – the model name
- **filename_prefix** – the prefix for the LaTeX file

```
report.latex_reports.latex_report_pe(outputdir, plots_folder, model_noext, file-
                                     name_prefix)
```

Generate a report for a parameter estimation task.

Parameters

- **outputdir** – the output directory
- **plots_folder** – the folder containing the simulated plots
- **model_noext** – the model name
- **filename_prefix** – the prefix for the LaTeX file

```
report.latex_reports.latex_report(outputdir, plots_folder, model_noext, filename_prefix,
                                  caption=False)
```

Generate a generic report.

Parameters

- **outputdir** – the output directory
- **plots_folder** – the folder containing the simulated plots
- **model_noext** – the model name
- **filename_prefix** – the prefix for the LaTeX file
- **caption** – True if figure captions (=figure file name) should be added

```
report.latex_reports.pdf_report(outputdir, filename)
```

Generate a PDF report from LaTeX report using pdflatex.

Parameters

- **outputdir** – the output directory
- **filename** – the LaTeX file name

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