SBpipe documentation

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Piero Dalle Pezze and Nicolas Le Novère

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CHAPTER

ONE

SOURCE CODE

Python modules

sbpipe package

Subpackages

sbpipe.pl package

Subpackages

sbpipe.pl.create package

Submodules

sbpipe.pl.create.newproj module

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

run (project_name)

Create a project directory tree.

Parameters project_name - the name of the project
Returns 0

Module contents

sbpipe.pl.pe package

Submodules

sbpipe.pl.pe.parest module

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

```
classmethod analyse_data (simulator, model, inputdir, outputdir, fileout_final_estims, 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_details** the name of the file containing the detailed statistics for the estimated parameters
- **fileout_param_estim_summary** the name of the file containing the summary for the parameter estimation
- **sim_plots_dir** the directory of the simulation plots
- best fits percent the percent to consider for the best fits
- data_point_num the number of data points
- cluster local, 1sf for Load Sharing Facility, sge for Sun Grid Engine.
- plot_2d_66cl_corr True if 2 dim plots for the parameter sets within 66% should be plotted
- plot_2d_95cl_corr True if 2 dim plots for the parameter sets within 95% should be plotted
- plot_2d_99cl_corr True if 2 dim plots for the parameter sets within 99% should be plotted
- logspace True if parameters should be plotted in log space
- scientific_notation True if axis labels should be plotted in scientific notation

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

classmethod 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.

classmethod 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)
run (config_file)
```

Module contents

sbpipe.pl.ps1 package

Submodules

sbpipe.pl.ps1.parscan1 module

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

The second pipeline step: data analysis.

- 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, 1sf 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.

classmethod 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.

classmethod 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)
run (config_file)
```

Module contents

sbpipe.pl.ps2 package

Submodules

sbpipe.pl.ps2.parscan2 module

```
class sbpipe.pl.ps2.parscan2.ParScan2 (models_folder='Models', working_folder='Results',
                                             sim_data_folder='double_param_scan_data',
                                             sim_plots_folder='double_param_scan_plots')
     Bases: sbpipe.pl.pipeline.Pipeline (page 7)
```

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

classmethod 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.

classmethod 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, 1sf 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.

classmethod generate report (model, scanned parl, scanned par2, outputdir, *sim_plots_folder*)

The third pipeline step: report generation.

- 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)
run (config_file)
```

Module contents

sbpipe.pl.sim package

Submodules

sbpipe.pl.sim.sim module

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

Parameters

- mode1 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
- cluster local, lsf for Load Sharing Facility, sge for Sun Grid Engine.
- 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.

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, 1sf 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.

classmethod 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)
run (config_file)
```

Module contents

Submodules

sbpipe.pl.pipeline module

```
 \begin{array}{c} \textbf{class} \; \texttt{sbpipe.pl.pipeline.Pipeline} \; (models\_folder='Models', \\ ing\_folder='Results', \\ sim\_plots\_folder='sim\_plots') \\ \\ \textbf{Bases: object} \end{array}
```

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

```
get models folder()
```

Return the folder containing the models.

Returns the models 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.

```
classmethod 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.

```
get_working_folder()
```

Return the folder containing the results.

Returns the working folder.

classmethod 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

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.

Module contents

sbpipe.report package

Submodules

sbpipe.report.latex_reports module

```
sbpipe.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

Parameters

- **outputdir** the output directory
- **sim_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

Generate a report for a parameter estimation task.

- outputdir the output directory
- **sim_plots_folder** the folder containing the simulated plots

- model_noext the model name
- filename_prefix the prefix for the LaTeX file

Generate a report for a single parameter scan task.

Parameters

- **outputdir** the output directory
- **sim_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

Generate a report for a double parameter scan task.

Parameters

- outputdir the output directory
- **sim_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

Generate a report for a time course task.

Parameters

- **outputdir** the output directory
- **sim_plots_folder** the folder containing the simulated plots
- model noext the model name
- filename_prefix the prefix for the LaTeX file

```
sbpipe.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

Module contents

sbpipe.simul package

Subpackages

sbpipe.simul.copasi package

Submodules

sbpipe.simul.copasi.copasi module

```
class sbpipe.simul.copasi.copasi.Copasi
    Bases: sbpipe.simul.simul.Simul (page 11)

Copasi simulator.

pe (model, inputdir, cluster, local_cpus, runs, outputdir, sim_data_dir, 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)

replace_str_in_report (report)

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

Module contents

sbpipe.simul.python package

Submodules

sbpipe.simul.python.python module

```
class sbpipe.simul.python.python.Python
    Bases: sbpipe.simul.pl_simul.PLSimul(page 10)
    Python Simulator.
```

Module contents

Submodules

sbpipe.simul.pl_simul module

```
class sbpipe.simul.pl_simul.PLSimul (lang, lang_err_msg, options)
    Bases: sbpipe.simul.simul.Simul (page 11)

A generic simulator for models coded in a programming language.

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.

pe (model, inputdir, cluster, local_cpus, runs, outputdir, sim_data_dir, 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)
replace_str_in_report (report)
```

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

sbpipe.simul.simul module

```
class sbpipe.simul.simul.Simul
```

Bases: object

Generic simulator.

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

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

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, 1sf 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)

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, 1sf 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)
- ${\tt ps1_postproc} \ (model, \ scanned_par, \ simulate_intervals, \ single_param_scan_intervals, \ output-dir)$

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

 Double paramter 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)
- 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

replace_str_in_report (report)

Replaces strings in a report file.

Parameters report – a report file with its absolute path

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, 1sf 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)

Module contents

sbpipe.utils package

Submodules

sbpipe.utils.io module

```
sbpipe.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.

```
sbpipe.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

sbpipe.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

```
sbpipe.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

sbpipe.utils.io.replace_str_in_file (filename_out, old_string, new_string)

Replace a string with another in filename_out

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

sbpipe.utils.io.replace_str_in_report(report)

Replace nasty strings in COPASI report file.

Parameters report - the report

sbpipe.utils.io.write_mat_on_file(path, filename_out, data)

Write the matrix results stored in data to filename_out

Parameters

- path the path to filename_out
- filename_out the output file
- data the data to store in a file

sbpipe.utils.parcomp module

sbpipe.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)

sbpipe.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

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
- local_cpus the number of cpus to use at most
- output_msg print the output messages on screen (available for cluster='local' only)

Returns True if the computation succeeded.

sbpipe.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 contining the standard error files

Returns True

sbpipe.utils.parcomp.run_cmd(cmd)

Run a command using Python subprocess.

Parameters cmd – The string of the command to run

sbpipe.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

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 to execute
- 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)

Returns True

sbpipe.utils.parcomp.run_jobs_lsf(cmd, cmd_iter_substr, out_dir, err_dir, runs=1)
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 to execute

Returns True if the computation succeeded.

sbpipe.utils.parcomp.run_jobs_sge (cmd, cmd_iter_substr, out_dir, err_dir, runs=1)
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 to execute

Returns True if the computation succeeded.

```
sbpipe.utils.rand module
sbpipe.utils.rand.get_rand_alphanum_str(length)
     Return a random alphanumeric string
         Parameters length – the length of the string
         Returns the generated string
sbpipe.utils.rand.get_rand_num_str(length)
     Return a random numeric string
         Parameters length – the length of the string
         Returns the generated string
sbpipe.utils.re utils module
sbpipe.utils.re_utils.escape_special_chars(text)
```

command with escaped special characters

```
sbpipe.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

Module contents

Submodules

```
sbpipe.__main__ module
```

sbpipe.main module

```
sbpipe.main.main(argv=None)
     SBpipe main function.
```

Returns 0 if OK, 1 if trouble

```
sbpipe.main.read_file_header(filename)
```

Read the first line of a file

Parameters filename – the file name to read

Returns the first line

```
sbpipe.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.

- **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 argu-
- 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 (WARNING+)
- **verbose** True if verbose (DEBUG+)

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

sbpipe.main.sbpipe_logo()

Return sbpipe logo.

Returns sbpipe logo

```
sbpipe.main.set_basic_logger(level='INFO')
```

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

```
sbpipe.main.set_color_logger(level='INFO')
```

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

```
sbpipe.main.set_console_logger(new_level='NOTSET', current_level='INFO', no-
color=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 shouls be used

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

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

sbpipe.sbpipe_config module

```
sbpipe.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.

sbpipe.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

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