autosubmit Documentation

Release 3.1

Domingo Manubens - Javier Vegas

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CHAPTER

ONE

INTRODUCTION

1.1 What is Autosubmit?

Autosubmit is a python-based tool to create, manage and monitor experiments by using Computing Clusters, HPC's and Supercomputers remotely via ssh. It has support for experiments running in more than one HPC and for different workflow configurations.

Autosubmit is currently used at IC3 to run EC-Earth and NEMO models and at Barcelona Supercomputing Centre (BSC) to run NMMB air quality model.

Autosubmit has been used to manage models running at supercomputers in IC3, BSC, ECMWF, EPCC, PDC and OLCF.

Autosubmit 3.0 version is now available via PyPi package under the terms of GNU General Public License.

1.2 Why is Autosubmit needed?

Autosubmit is the only existing tool that satisfies the following requirements from the weather and climate community:

- Automatisation: Job submission to machines and dependencies between jobs are managed by Autosubmit. No user intervention is needed.
- *Data provenance*: Assigns unique identifiers for each experiment and stores information about model version, experiment configuration and computing facilities used in the whole process.
- Failure tolerance: Automatic retrials and ability to rerun chunks in case of corrupted or missing data.
- Resource management: Autosubmit manages supercomputer particularities, allowing users to run their experiments in the available machine without having to adapt the code. Autosubmit also allows to submit tasks from the same experiment to different platforms.

1.3 How does Autosubmit work?

You can find help about how to use autosubmit and a list of available commands, just executing:

```
autosubmit -h
```

Execute autosubmit <command> -h for detailed help for each command:

```
autosubmit expid -h
```

1.3.1 Experiment creation

To create a new experiment, run the command:

```
autosubmit expid -H HPCname -d Description
```

HPCname is the name of the main HPC platform for the experiment: it will be the default platform for the tasks. *Description* is a brief experiment description.

This command assigns a unique four character identifier (xxxx, names starting from a letter, the other three characters) to the experiment and creates a new folder in experiments repository with structure shown in Figure 1.1.

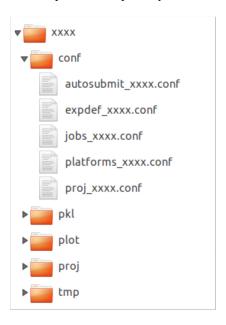


Figure 1.1: Example of an experiment directory tree.

1.3.2 Experiment configuration

To configure the experiment, edit expdef_xxxx.conf, jobs_xxxx.conf and platforms_xxxx.conf in the conf folder of the experiment (see contents in Figure 1.2).

After that, you are expected to run the command:

```
autosubmit create xxxx
```

This command creates the experiment project in the proj folder. The experiment project contains the scripts specified in jobs_xxxx.conf and a copy of model source code and data specified in expdef_xxxx.conf.

1.3.3 Experiment run

To run the experiment, just execute the command:

```
autosubmit run xxxx
```

Autosubmit will start submitting jobs to the relevant platforms (both HPC and supporting computers) by using the scripts specified in jobs_xxxx.conf. Autosubmit will substitute variables present on scripts where handlers ap-

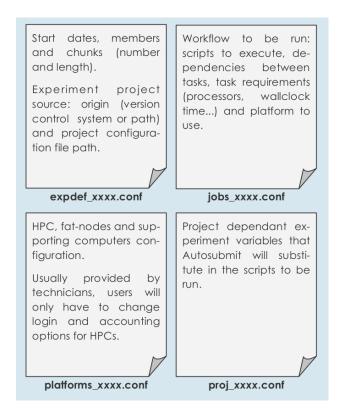


Figure 1.2: Configuration files content

pear in %variable_name% format. Autosubmit provides variables for current chunk, start date, member, computer configuration and more, and also will replace variables form proj_xxxx.conf.

To monitor the status of the experiment, the command:

autosubmit monitor xxxx

is available. This will plot the workflow of the experiment and the current status.

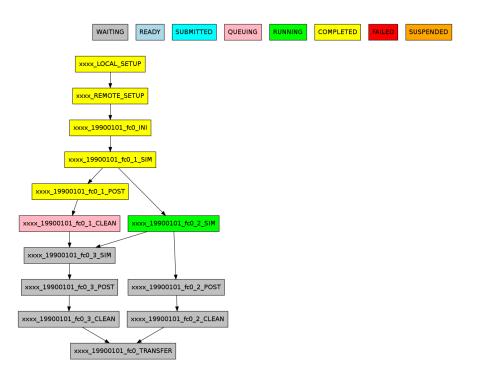


Figure 1.3: Example of monitoring plot for EC-Earth run with Autosubmit for 1 start date, 1 member and 3 chunks.

CHAPTER

TWO

TUTORIAL

2.1 Quick start guide

2.1.1 First Step: Experiment creation

To create a new experiment, run the command:

```
autosubmit expid -H HPCname -d Description
```

HPCname is the name of the main HPC platform for the experiment: it will be the default platform for the tasks. *Description* is a brief experiment description.

This command assigns a unique four character identifier (xxxx, names starting from a letter, the other three characters) to the experiment and creates a new folder in experiments repository.

Examples:

```
autosubmit expid --HPC ithaca --description "experiment is about..."
```

Caution: The *HPCname*, e.g. ithaca, must be defined in the platforms configuration. See next section *Second Step: Experiment configuration*.

```
autosubmit expid --copy a000 --HPC ithaca -d "experiment is about..."
```

Warning: You can only copy experiments created with Autosubmit 3.0 or above.

2.1.2 Second Step: Experiment configuration

To configure the experiment, edit expdef_cxxx.conf, jobs_cxxx.conf and platforms_cxxx.conf in the conf folder of the experiment.

expdef_cxxx.conf contains:

- Start dates, members and chunks (number and length).
- Experiment project source: origin (version control system or path)
- Project configuration file path.

jobs_cxxx.conf contains the workflow to be run:

- · Scripts to execute.
- Dependencies between tasks.

- Task requirements (processors, wallclock time...).
- Platform to use.

platforms_cxxx.conf contains:

• HPC, fat-nodes and supporting computers configuration.

Note: platforms_cxxx.conf is usually provided by technicians, users will only have to change login and accounting options for HPCs.

You may want to configure Autosubmit parameters for the experiment. Just edit autosubmit_cxxx.conf.

autosubmit_cxxx.conf contains:

- Maximum number of jobs to be waiting in the HPC queue.
- Maximum number of jobs to be running at the same time at the HPC.
- Time (seconds) between connections to the HPC queue scheduler to poll already submitted jobs status.
- Number of retrials if a job fails.

Examples:

vi <experiments_directory>/cxxx/conf/expdef_cxxx.conf

```
[DEFAULT]
```

```
# Experiment identifier
# No need to change
EXPID = cxxx
# HPC name.
# No need to change
HPCARCH = ithaca
```

```
[experiment]
# Supply the list of start dates. Available formats: YYYYMMDD YYYYMMDDhh YYYYMMDDhhmm
# Also you can use an abreviated sintax for multiple dates with common parts:
# 200001[01 15] <=> 20000101 20000115
# DATELIST = 19600101 19650101 19700101
# DATELIST = 1960[0101 0201 0301]
DATELIST = 19900101
# Supply the list of members. LIST = fc0 fc1 fc2 fc3 fc4
MEMBERS = fc0
# Chunk size unit. STRING = hour, day, month, year
CHUNKSIZEUNIT = month
# Chunk size. NUMERIC = 4, 6, 12
CHUNKSIZE = 1
# Total number of chunks in experiment. NUMERIC = 30, 15, 10
NUMCHUNKS = 2
# Calendar used. LIST: standard, noleap
CALENDAR = standard
[rerun]
# Is a rerun or not? [Default: Do set FALSE]. BOOLEAN = TRUE, FALSE
RERUN = FALSE
# If RERUN = TRUE then supply the list of chunks to rerun
# LIST = "[ 19601101 [ fc0 [1 2 3 4] fc1 [1] ] 19651101 [ fc0 [16-30] ] ]"
```

[project]

CHUNKLIST =

```
# Select project type. STRING = git, svn, local, none
# If PROJECT_TYPE is set to none, Autosubmit self-contained dummy templates will be used
PROJECT_TYPE = git
# Destination folder name for project. type = STRING, default = leave empty,
PROJECT_DESTINATION = model
# If PROJECT_TYPE is not git, no need to change
[git]
# Repository URL STRING = 'https://github.com/torvalds/linux.git'
PROJECT_ORIGIN = https://gitlab.cfu.local/cfu/auto-ecearth3.git
# Select branch or tag, STRING, default = 'master',
# help = {'master' (default), 'develop', 'v3.1b', ...}
PROJECT_BRANCH = develop
# type = STRING, default = leave empty, help = if model branch is a TAG leave empty
PROJECT_COMMIT =
# If PROJECT_TYPE is not svn, no need to change
# type = STRING, help = 'https://svn.ec-earth.org/ecearth3'
PROJECT_URL =
# Select revision number. NUMERIC = 1778
PROJECT REVISION =
# If PROJECT_TYPE is not local, no need to change
[local]
# type = STRING, help = /foo/bar/ecearth
PROJECT_PATH =
# If PROJECT_TYPE is none, no need to change
[project_files]
# Where is PROJECT CONFIGURATION file location relative to project root path
FILE_PROJECT_CONF = templates/ecearth3/ecearth3.conf
# Where is JOBS CONFIGURATION file location relative to project root path
FILE_JOBS_CONF = templates/common/jobs.conf
vi <experiments_directory>/cxxx/conf/jobs_cxxx.conf
# Example job with all options specified
## Job name
# [JOBNAME]
## Script to execute. If not specified, job will be omited from workflow.
## Path relative to the project directory
# FILE =
## Platform to execute the job. If not specificied, defaults to HPCARCH in expedf file.
## LOCAL is always defined and referes to current machine
# PLATFORM =
## Queue to add the job to. If not specificied, uses PLATFORM default.
# OUEUE =
## Defines dependencies from job as a list of parents jobs separed by spaces.
## Dependencies to jobs in previous chunk, member o startdate, use -(DISTANCE)
# DEPENDENCIES = INI SIM-1 CLEAN-2
## Define if jobs runs once, once per stardate, once per member or once per chunk.
## Options: once, date, member, chunk.
## If not specified, defaults to once
# RUNNING = once
## Specifies that job has only to be run after X dates, members or chunk.
## A job will always be created for the last
```

```
## If not specified, defaults to once
# FREQUENCY = 3
## Defines if job is only to be executed in reruns. If not specified, defaults to false.
# RERUN_ONLY = False
## Defines jobs needed to be rerun if this job is going to be rerunned
# RERUN_DEPENDENCIES = RERUN INI LOCAL_SETUP REMOTE_SETUP TRANSFER
## Wallclock to be submitted to the HPC queue in format HH:MM
# WALLCLOCK = 00:05
## Processors number to be submitted to the HPC. If not specified, defaults to 1.
# PROCESSORS = 1
## Threads number to be submitted to the HPC. If not specified, defaults to 1.
# THREADS = 1
## Tasks number to be submitted to the HPC. If not specified, defaults to 1.
\# TASKS = 1
[LOCAL_SETUP]
FILE = templates/common/common.localsetup
PLATFORM = LOCAL
[REMOTE_SETUP]
FILE = templates/common/common.remotesetup
DEPENDENCIES = LOCAL_SETUP
WALLCLOCK = 03:00
[INI]
FILE = templates/ecearth3/ecearth3.ini
DEPENDENCIES = REMOTE_SETUP
RUNNING = member
WALLCLOCK = 01:00
[SIM]
FILE = templates/ecearth3/ecearth3.sim
DEPENDENCIES = INI SIM-1 CLEAN-2
RUNNING = chunk
WALLCLOCK = 04:00
PROCESSORS = 1616
THREADS = 1
TASKS = 1
FILE = templates/ecearth3/ecearth3.post
DEPENDENCIES = SIM
RUNNING = chunk
WALLCLOCK = 06:00
[CLEAN]
FILE = templates/ecearth3/ecearth3.clean
DEPENDENCIES = POST
RUNNING = chunk
WALLCLOCK = 01:00
[TRANSFER]
FILE = templates/common/common.localtrans
PLATFORM = LOCAL
DEPENDENCIES = CLEAN
RUNNING = member
```

```
vi <experiments_directory>/cxxx/conf/platforms_cxxx.conf
# Example queue with all options specified
## Platform name
# [PLAFORM]
## Queue type. Options: PBS, SGE, PS, LSF, ecaccess, SLURM
# TYPE =
## Version of queue manager to use. Needed only in PBS (options: 10, 11, 12)
## and ecaccess (options: pbs, loadleveler)
# VERSION =
## Hostname of the HPC
# HOST =
## Project for the machine scheduler
# PROJECT =
## Budget account for the machine scheduler. If omited, takes the value defined in PROJECT
# BUDGET =
## Option to add project name to host. This is required for some HPCs
# ADD_PROJECT_TO_HOST = False
## User for the machine scheduler
# USER =
## Path to the scratch directory for the machine
# SCRATCH_DIR = /scratch
## If true, autosubmit test command can use this queue as a main queue. Defaults to false
# TEST_SUITE = False
## If given, autosubmit will add jobs to the given queue
\# QUEUE =
## If specified, autosubmit will run jobs with only one processor in the specified platform.
# SERIAL_PLATFORM = SERIAL_PLATFORM_NAME
## If specified, autosubmit will run jobs with only one processor in the specified queue.
## Autosubmit will ignore this configuration if SERIAL PLATFORM is provided
# SERIAL_QUEUE = SERIAL_QUEUE_NAME
[ithaca]
# Queue type. Options: ps, SGE, LSF, SLURM, PBS, eceaccess
TYPE = SGE
HOST = ithaca
PROJECT = cfu
ADD_PROJECT_TO_HOST = true
USER = dmanubens
SCRATCH_DIR = /scratch/cfu
TEST_SUITE = True
vi <experiments_directory>/cxxx/conf/autosubmit_cxxx.conf
[config]
# Experiment identifier
# No need to change
EXPID = cxxx
# No need to change.
# Autosubmit version identifier
AUTOSUBMIT_VERSION = 3.0.0rc1
# Maximum number of jobs to be waiting in the HPC queue
# Default = 3
MAXWAITINGJOBS = 3
# Maximum number of jobs to be running at the same time at the HPC
# Default = 6
TOTALJOBS = 6
```

```
# Time (seconds) between connections to the HPC queue scheduler to poll already
# submitted jobs status
# Default = 10
SAFETYSLEEPTIME = 10
# Number of retrials if a job fails
# Default = 4
RETRIALS = 4
```

Then, Autosubmit *create* command uses the expdef_cxxx.conf and generates the experiment:

```
autosubmit create cxxx
```

cxxx is the name of the experiment.

In the process of creating the new experiment a plot has been created.

It can be found in <experiments_directory>/cxxx/plot/

2.1.3 Third Step: Experiment run

After filling the experiment configuration and create, user can go into proj which has a copy of the model.

A short reference on how to prepare the experiment project is detailed in the following section of this documentation:

Developing a project

The experiment project contains the scripts specified in jobs_xxxx.conf and a copy of model source code and data specified in expdef_xxxx.conf.

To configure experiment project parameters for the experiment, edit proj_cxxx.conf.

proj_cxxx.conf contains:

• The project dependant experiment variables that Autosubmit will substitute in the scripts to be run.

Example:

```
vi <experiments_directory>/cxxx/conf/proj_cxxx.conf
```

[common]

```
# No need to change.
MODEL = ecearth
# No need to change.
VERSION = v3.1
# No need to change.
TEMPLATE_NAME = ecearth3
# Select the model output control class. STRING = Option
# listed under the section : http://ic3.cat/wikicfu/index.php/Models#Outclass.
OUTCLASS = specs
# After transferring output at /cfunas/exp remove a copy available at permanent storage of HPC
# [Default: Do set "TRUE"]. BOOLEAN = TRUE, FALSE
MODEL_output_remove = TRUE
# Activate cmorization [Default: leave empty]. BOOLEAN = TRUE, FALSE
CMORIZATION = TRUE
# Essential if cmorization is activated.
# STRING = (http://www.specs-fp7.eu/wiki/images/1/1c/SPECS_standard_output.pdf)
# Supply the name of the experiment associated (if there is any) otherwise leave it empty.
# STRING (with space) = seasonal r1p1, seaiceinit r?p?
ASSOCIATED_EXPERIMENT =
# Essential if cmorization is activated (Forcing). STRING = Nat, Ant (Nat and Ant is a single option)
```

```
FORCING =
# Essential if cmorization is activated (Initialization description). STRING = N/A
INIT_DESCR =
\# Essential if cmorization is activated (Physics description). STRING = N/A
PHYS_DESCR =
# Essential if cmorization is activated (Associated model). STRING = N/A
ASSOC_MODEL =
[grid]
# AGCM grid resolution, horizontal (truncation T) and vertical (levels L).
# STRING = T159L62, T255L62, T255L91, T511L91, T799L62 (IFS)
IFS_resolution = T511L91
# OGCM grid resolution. STRING = ORCA1L46, ORCA1L75, ORCA025L46, ORCA025L75 (NEMO)
NEMO_resolution = ORCA025L75
[oasis]
# Coupler (OASIS) options.
OASIS3 = yes
# Number of pseduo-parallel cores for coupler [Default: Do set "7"]. NUMERIC = 1, 7, 10
OASIS_nproc = 7
# Handling the creation of coupling fields dynamically [Default: Do set "TRUE"].
# BOOLEAN = TRUE, FALSE
OASIS_flds = TRUE
[ifs]
# Atmospheric initial conditions ready to be used.
# STRING = ID found here: http://ic3.cat/wikicfu/index.php/Initial_Conditions/Atmospheric
ATM ini =
# A different IC member per EXPID member ["PERT"] or which common IC member
# for all EXPID members ["fc0" / "fc1"]. String = PERT/fc0/fc1...
ATM_ini_member =
# Set timestep (in sec) w.r.t resolution.
# NUMERIC = 3600 (T159), 2700 (T255), 900 (T511), 720 (T799)
IFS_timestep = 900
# Number of parallel cores for AGCM component. NUMERIC = 28, 100
IFS_nproc = 640
# Coupling frequency (in hours) [Default: Do set "3"]. NUMERIC = 3, 6
RUN_coupFreq = 3
# Post-procssing frequency (in hours) [Default: Do set "6"]. NUMERIC = 3, 6
# [Default: Do set "TRUE"]. BOOLEAN = TRUE, FALSE
LCMIP5 = TRUE
# Choose RCP value [Default: Do set "2"]. NUMERIC = 0, 1=3-PD, 2=4.5, 3=6, 4=8.5
NRCP = 0
# [Default: Do set "TRUE"]. BOOLEAN = TRUE, FALSE
LHVOLCA = TRUE
# [Default: Do set "0"]. NUMERIC = 1850, 2005
NFIXYR = 0
# Save daily output or not [Default: Do set "FALSE"]. BOOLEAN = TRUE, FALSE
SAVEDDA = FALSE
# Save reduced daily output or not [Default: Do set "FALSE"]. BOOLEAN = TRUE, FALSE
ATM_REDUCED_OUTPUT = FALSE
# Store grib codes from SH files [User need to refer defined ppt* files for the experiment]
ATM SH CODES =
# Store levels against "ATM_SH_CODES" e.g: level1, level2, level3, ...
ATM_SH_LEVELS =
# Store grib codes from GG files [User need to refer defined ppt* files for the experiment]
ATM GG CODES =
```

```
# Store levels against "ATM_GG_CODES" (133.128, 246.128, 247.128, 248.128)
# e.g: level1, level2, level3, ...
ATM_GG_LEVELS =
# SPPT stochastic physics active or not [Default: set "FALSE"]. BOOLEAN = TRUE, FALSE
LSPPT = FALSE
# Write the perturbation patterns for SPPT or not [Default: set "FALSE"].
# BOOLEAN = TRUE, FALSE
LWRITE_ARP =
# Number of scales for SPPT [Default: set 3]. NUMERIC = 1, 2, 3
NS_SPPT =
# Standard deviations of each scale [Default: set 0.50, 0.25, 0.125]
# NUMERIC values separated by ,
SDEV_SPPT =
# Decorrelation times (in seconds) for each scale [Default: set 2.16E4, 2.592E5, 2.592E6]
# NUMERIC values separated by ,
TAU_SPPT =
# Decorrelation lengths (in meters) for each scale [Default: set 500.E3,1000.E3,2000.E3]
# NUMERIC values separated by ,
XLCOR_SPPT =
# Clipping ratio (number of standard deviations) for SPPT [Default: set 2] NUMERIC
XCLIP SPPT =
# Stratospheric tapering in SPPT [Default: set "TRUE"]. BOOLEAN = TRUE, FALSE
LTAPER_SPPT =
# Top of stratospheric tapering layer in Pa [Default: set to 50.E2] NUMERIC
# Bottom of stratospheric tapering layer in Pa [Default: set to 100.E2] NUMERIC
PTAPER BOT =
## ATMOSPHERIC NUDGING PARAMETERS ##
# Atmospheric nudging towards reinterpolated ERA-Interim data. BOOLEAN = TRUE, FALSE
ATM_NUDGING = FALSE
# Atmospheric nudging reference data experiment name. [T255L91: b0ir]
ATM_refnud =
# Nudge vorticity. BOOLEAN = TRUE, FALSE
NUD VO =
# Nudge divergence. BOOLEAN = TRUE, FALSE
NUD_DI =
# Nudge temperature. BOOLEAN = TRUE, FALSE
NUD_TE =
# Nudge specific humidity. BOOLEAN = TRUE, FALSE
NUD O =
# Nudge liquid water content. BOOLEAN = TRUE, FALSE
NUD_QL =
# Nudge ice water content. BOOLEAN = TRUE, FALSE
NUD_QI =
# Nudge cloud fraction. BOOLEAN = TRUE, FALSE
NUD_QC =
# Nudge log of surface pressure. BOOLEAN = TRUE, FALSE
NUD LP =
# Relaxation coefficient for vorticity. NUMERIC in ]0, inf[;
# 1 means half way between model value and ref value
ALPH_VO =
# Relaxation coefficient for divergence. NUMERIC in ]0,inf[;
# 1 means half way between model value and ref value
ALPH DT =
# Relaxation coefficient for temperature. NUMERIC in ]0, inf[;
# 1 means half way between model value and ref value
ALPH_TE =
# Relaxation coefficient for specific humidity. NUMERIC in ]0, inf[;
```

```
# 1 means half way between model value and ref value
ALPH_Q =
# Relaxation coefficient for log surface pressure. NUMERIC in ]0,inf[;
# 1 means half way between model value and ref value
ALPH_LP =
# Nudging area Northern limit [Default: Do set "90"]
NUD_NLAT =
# Nudging area Southern limit [Default: Do set "-90"]
NUD SLAT =
# Nudging area Western limit NUMERIC in [0,360] [Default: Do set "0"]
NUD_WLON =
# Nudging area Eastern limit NUMERIC in [0,360] [Default: Do set "360"; E<W will span Greenwich]
NUD_ELON =
# Nudging vertical levels : lower level [Default: Do set "1"]
NUD_VMIN =
# Nudging vertical levels : upper level [Default: Do set to number of vertical levels]
NUD_VMAX =
[nemo]
# Ocean initial conditions ready to be used. [Default: leave empty].
# STRING = ID found here : http://ic3.cat/wikicfu/index.php/Initial_Conditions/Oceanic
OCEAN_ini =
# A different IC member per EXPID member ["PERT"] or which common IC member
# for all EXPID members ["fc0" / "fc1"]. String = PERT/fc0/fc1...
OCEAN_ini_member =
# Set timestep (in sec) w.r.t resolution. NUMERIC = 3600 (ORCA1), 1200 (ORCA025)
NEMO timestep = 1200
# Number of parallel cores for OGCM component. NUMERIC = 16, 24, 36
NEMO_nproc = 960
# Ocean Advection Scheme [Default: Do set "tvd"]. STRING = tvd, cen2
ADVSCH = cen2
# Nudging activation. BOOLEAN = TRUE, FALSE
OCEAN_NUDGING = FALSE
# Toward which data to nudge; essential if "OCEAN_NUDGING" is TRUE.
# STRING = fa9p, s4, glorys2v1
OCEAN_NUDDATA = FALSE
# Rebuild and store restarts to HSM for an immediate prediction experiment.
# BOOLEAN = TRUE, FALSE
OCEAN STORERST = FALSE
[ice]
# Sea-Ice Model [Default: Do set "LIM2"]. STRING = LIM2, LIM3
# Sea-ice initial conditions ready to be used. [Default: leave empty].
# STRING = ID found here : http://ic3.cat/wikicfu/index.php/Initial_Conditions/Sea-Ice
ICE_ini =
# A different IC member per EXPID member ["PERT"] or which common IC member
# for all EXPID members ["fc0" / "fc1"]. String = PERT/fc0/fc1...
ICE_ini_member =
# Set timestep (in sec) w.r.t resolution. NUMERIC = 3600 (ORCA1), 1200 (ORCA025)
LIM_timestep = 1200
[pisces]
# Activate PISCES (TRUE) or not (FALSE) [Default: leave empty]
PISCES = FALSE
# PISCES initial conditions ready to be used. [Default: leave empty].
# STRING = ID found here : http://ic3.cat/wikicfu/index.php/Initial_Conditions/Biogeochemistry
PISCES ini =
```

```
\# Set timestep (in sec) w.r.t resolution. NUMERIC = 3600 (ORCA1), 3600 (ORCA025) PISCES_timestep = 3600
```

Finally, you can launch Autosubmit *run* in background and with nohup (continue running although the user who launched the process logs out).

```
nohup autosubmit run cxxx &
```

2.1.4 Fourth Step: Experiment monitor

The following procedure could be adopted to generate the plots for visualizing the status of the experiment at any instance. With this command we can generate new plots to check which is the status of the experiment. Different job status are represented with different colors.

```
autosubmit monitor cxxx
```

The location where user can find the generated plots with date and timestamp can be found below:

```
<experiments_directory>/cxxx/plot/cxxx_<date>_<time>.pdf
```

CHAPTER

THREE

INSTALLATION

3.1 How to install

The Autosubmit code is maintained in *PyPi*, the main source for python packages.

• Pre-requisties: These packages (bash, python2, sqlite3, git-scm > 1.8.2, subversion) must be available at local host machine. These packages (argparse, dateutil, pyparsing, numpy, pydotplus, matplotlib, paramiko) must be available for python runtime.

Important: The host machine has to be able to access HPC's/Clusters via password-less ssh.

To install autosubmit just execute:

pip install autosubmit

or download, unpack and:

python setup.py install

Hint: To check if autosubmit has been installed run autosubmit -v. This command will print autosubmit's current version

Hint: To read autosubmit's readme file, run autosubmit readme

Hint: To see the changelog, use autosubmit changelog

3.2 How to configure

After installation, you have to configure database and path for Autosubmit. It can be done at host, user or local level (by default at host level). If it does not exist, create a repository for experiments: Say for example /cfu/autosubmit

Then follow the confingre instructions after executing:

```
autosubmit configure
```

and introduce path to experiment storage and database. Folders must exit.

For installing the database for Autosubmit on the configured folder, when no database is created on the given path, execute:

autosubmit install

Danger: Be careful! autosubmit install will create a blank database.

Now you are ready to use Autosubmit!

CHAPTER

FOUR

USAGE

4.1 Command list

-expid Create a new experiment

-create Create specified experiment workflow

-check Check configuration for specified experiment

-run Run specified experiment

-test Test experiment

-monitor Plot specified experiment

-stats Plot statistics for specified experiment

-setstatus Sets job status for an experiment
 -recovery Recover specified experiment
 -clean Clean specified experiment

-refresh Refresh project directory for an experiment

-delete Delete specified experiment

-configure Configure database and path for autosubmit

-install Install database for Autosubmit on the configured folder

-refresh Refresh project directory for an experiment

-archive Clean, compress and remove from the experiments' folder a finalized experiment

-unarchive Restores an archived experiment

4.2 How to create an experiment

To create a new experiment, just run the command:

```
autosubmit expid -H HPCname -d Description
```

HPCname is the name of the main HPC platform for the experiment: it will be the default platform for the tasks. *Description* is a brief experiment description.

Options:

```
usage: autosubmit expid [-h] [-y COPY | -dm] -H HPC -d DESCRIPTION

-h, --help show this help message and exit
-y COPY, --copy COPY makes a copy of the specified experiment
-dm, --dummy creates a new experiment with default values, usually for testing
-H HPC, --HPC HPC specifies the HPC to use for the experiment
-d DESCRIPTION, --description DESCRIPTION
sets a description for the experiment to store in the database.
```

Example:

```
autosubmit expid --HPC ithaca --description "experiment is about..."
```

4.3 How to create a copy of an experiment

This option makes a copy of an existing experiment. It registrates a new unique identifier and copies all configuration files in the new experiment folder:

```
autosubmit expid -H HPCname -y COPY -d Description
```

HPCname is the name of the main HPC platform for the experiment: it will be the default platform for the tasks. COPY is the experiment identifier to copy from. Description is a brief experiment description.

Example:

```
autosubmit expid -H ithaca -y cxxx -d "experiment is about..."
```

Warning: You can only copy experiments created with Autosubmit 3.0 or above.

4.4 How to create a dummy experiment

This command creates a new experiment with default values, useful for testing:

```
autosubmit expid -H HPCname -dm -d Description
```

HPCname is the name of the main HPC platform for the experiment: it will be the default platform for the tasks. *Description* is a brief experiment description.

Example:

```
autosubmit expid -H ithaca -dm "experiment is about..."
```

4.5 How to configure the experiment

Edit expdef_cxxx.conf, jobs_cxxx.conf and platforms_cxxx.conf in the conf folder of the experiment.

expdef_cxxx.conf contains:

- Start dates, members and chunks (number and length).
- Experiment project source: origin (version control system or path)

• Project configuration file path.

jobs_cxxx.conf contains the workflow to be run:

- Scripts to execute.
- Dependencies between tasks.
- Task requirements (processors, wallclock time...).
- · Platform to use.

platforms_cxxx.conf contains:

• HPC, fat-nodes and supporting computers configuration.

Note: *platforms_cxxx.conf* is usually provided by technicians, users will only have to change login and accounting options for HPCs.

You may want to configure Autosubmit parameters for the experiment. Just edit autosubmit_cxxx.conf.

autosubmit_cxxx.conf contains:

- Maximum number of jobs to be running at the same time at the HPC.
- Time (seconds) between connections to the HPC queue scheduler to poll already submitted jobs status.
- Number of retrials if a job fails.

Then, Autosubmit *create* command uses the $expdef_cxxx.conf$ and generates the experiment: After editing the files you can proceed to the experiment workflow creation. Experiment workflow, which contains all the jobs and its dependencies, will be saved as a pkl file:

```
autosubmit create EXPID
```

EXPID is the experiment identifier.

Options:

```
usage: autosubmit create [-h] [-np] expid
expid experiment identifier
-h, --help show this help message and exit
-np, --noplot omit plot
```

Example:

```
autosubmit create cxxx
```

More info on pickle can be found at http://docs.python.org/library/pickle.html

4.6 How to check the experiment configuration

To check the configuration of the experiment, use the command:

```
autosubmit check EXPID
```

EXPID is the experiment identifier.

It checks experiment configuration and warns about any detected error or inconsistency.

Options:

```
usage: autosubmit check [-h] expid
expid experiment identifier
-h, --help show this help message and exit
```

Example:

autosubmit check cxxx

4.7 How to run the experiment

Launch Autosubmit with the command:

```
autosubmit run EXPID
```

EXPID is the experiment identifier.

Options:

```
usage: autosubmit run [-h] expid
expid experiment identifier
-h, --help show this help message and exit
```

Example:

autosubmit run cxxx

Hint: It is recommended to launch it in background and with nohup (continue running although the user who launched the process logs out).

Example:

```
nohup autosubmit run cxxx &
```

Important: Before launching Autosubmit check password-less ssh is feasible (*HPCName* is the hostname):

ssh HPCName

More info on password-less ssh can be found at: http://www.linuxproblem.org/art_9.html

Caution: After launching Autosubmit, one must be aware of login expiry limit and policy (if applicable for any HPC) and renew the login access accordingly (by using token/key etc) before expiry.

4.8 How to test the experiment

This method is to conduct a test for a given experiment. It creates a new experiment for a given experiment with a given number of chunks with a random start date and a random member to be run on a random HPC.

To test the experiment, use the command:

```
autosubmit test CHUNKS EXPID
```

EXPID is the experiment identifier. CHUNKS is the number of chunks to run in the test.

Options

Example:

```
autosubmit test -c 1 -s 19801101 -m fc0 -H ithaca -b develop cxxx
```

4.9 How to monitor the experiment

To monitor the status of the experiment, use the command:

```
autosubmit monitor EXPID
```

EXPID is the experiment identifier.

Options:

Example:

```
autosubmit monitor cxxx
```

The location where user can find the generated plots with date and timestamp can be found below:

```
<experiments_directory>/cxxx/plot/cxxx_<date>_<time>.pdf
```

Hint: Very large plots may be a problem for some pdf and image viewers. If you are having trouble with your usual monitoring tool, try using svg output and opening it with Google Chrome with the SVG Navigator extension installed.

4.10 How to monitor job statistics

The following command could be adopted to generate the plots for visualizing the jobs statistics of the experiment at any instance:

```
autosubmit stats EXPID
```

EXPID is the experiment identifier.

Options:

```
usage: autosubmit stats [-h] [-o {pdf,png,ps,svg}] expid
expid experiment identifier

-h, --help show this help message and exit
-o {pdf,png,ps,svg}, --output {pdf,png,ps,svg}
type of output for generated plot
```

Example:

```
autosubmit stats cxxx
```

The location where user can find the generated plots with date and timestamp can be found below:

```
<experiments_directory>/cxxx/plot/cxxx_statistics_<date>_<time>.pdf
```

4.11 How to stop the experiment

You can stop Autosubmit by sending a signal to the process. To get the process identifier (PID) you can use the ps command on a shell interpreter/terminal.

To send a signal to a process you can use kill also on a terminal.

To stop immediately experiment cxxx:

```
kill -9 22835
```

Important: In case you want to restart the experiment, you must follow the *How to restart the experiment* procedure, explained below, in order to properly resynchronize all completed jobs.

4.12 How to restart the experiment

This procedure allows you to restart an experiment.

You must execute:

```
autosubmit recovery EXPID
```

EXPID is the experiment identifier.

Options:

```
usage: autosubmit recovery [-h] [-all] [-s] expid

expid experiment identifier

-h, --help show this help message and exit
-all Get all completed files to synchronize pkl
-s, --save Save changes to disk
```

Example:

```
autosubmit recovery cxxx -s
```

Hint: When we are satisfied with the results we can use the parameter -s, which will save the change to the pkl file and rename the update file.

The -all flag is used to synchronize all jobs of our experiment locally with the information available on the remote platform (i.e.: download the COMPLETED files we may not have). In case new files are found, the pkl will be updated.

Example:

```
autosubmit recovery cxxx -all -s
```

4.13 How to rerun a part of the experiment

This procedure allows you to create automatically a new pickle with a list of jobs of the experiment to rerun.

Using the <code>expdef_<expid>.conf</code> the <code>create</code> command will generate the rerun if the variable RERUN is set to TRUE and a CHUNKLIST is provided.

```
autosubmit create cxxx
```

It will read the list of chunks specified in the CHUNKLIST and will generate a new plot.

Note: The results are saved in the new pkl rerun_job_list.pkl.

Example:

```
vi <experiments_directory>/cxxx/conf/expdef_cxxx.conf

[...]

[rerun]
# Is a rerun or not? [Default: Do set FALSE]. BOOLEAN = TRUE, FALSE
RERUN = TRUE
# If RERUN = TRUE then supply the list of chunks to rerun
# LIST = "[ 19601101 [ fc0 [1 2 3 4] fc1 [1] ] 19651101 [ fc0 [16-30] ] ]"
CHUNKLIST = [ 19601101 [ fc1 [1] ]
```

Then you are able to start again Autosubmit for the rerun of cxxx 19601101, chunk 1, member 1:

```
nohup autosubmit run cxxx &
```

4.14 How to clean the experiment

This procedure allows you to save space after finalising an experiment. You must execute:

```
autosubmit clean EXPID
```

Options:

• The -p and -s flag are used to clean our experiment plot folder to save disk space. Only the two latest plots will be kept. Older plots will be removed.

Example:

```
autosubmit clean cxxx -p
```

• The -pr flag is used to clean our experiment proj locally in order to save space (it could be particularly big).

Caution: Bear in mind that if you have not synchronized your experiment project folder with the information available on the remote repository (i.e.: commit and push any changes we may have), or in case new files are found, the clean procedure will be failing although you specify the -pr option.

Example:

```
autosubmit clean cxxx -pr
```

A bare copy (which occupies less space on disk) will be automatically made.

Hint: That bare clone can be always reconverted in a working clone if we want to run again the experiment by using git clone bare_clone original_clone.

Note: In addition, every time you run this command with -pr option, it will check the commit unique identifier for local working tree existing on the proj directory. In case that commit identifier exists, clean will register it to the expdef_cxxx.conf file.

4.15 How to refresh the experiment project

To refresh the project directory of the experiment, use the command:

```
autosubmit refresh EXPID
```

EXPID is the experiment identifier.

It checks experiment configuration and copy code from original repository to project directory.

Warning: DO NOT USE THIS COMMAND IF YOU ARE NOT SURE! Project directory will be overwritten and you may loose local changes.

Options:

Example:

autosubmit refresh cxxx

4.16 How to delete the experiment

To delete the experiment, use the command:

```
autosubmit delete EXPID
```

EXPID is the experiment identifier.

Warning: DO NOT USE THIS COMMAND IF YOU ARE NOT SURE! It deletes the experiment from database and experiment's folder.

Options:

```
usage: autosubmit delete [-h] [-f] expid
expid experiment identifier

-h, --help show this help message and exit
-f, --force deletes experiment without confirmation
```

Example:

autosubmit delete cxxx

Warning: Be careful! force option does not ask for your confirmation.

4.17 How to add a new job

To add a new job, open the <experiments_directory>/cxxx/conf/jobs_cxxx.conf file where cxxx is the experiment identifier and add this text:

```
[new_job]
FILE = <new_job_template>
```

This will create a new job named "new_job" that will be executed once at the default platform. This job will user the template located at <new job template> (path is relative to project folder).

This is the minimun job definition and usually is not enough. You usually will need to add some others parameters:

- PLATFORM: allows you to execute the job in a platform of yout choice. It must be defined in the experiment's platforms.conf file or to have the value 'LOCAL' that always refer to the machine running Autosubmit
- RUNNING: defines if jobs runs only once or once per stardate, member or chunk. Options are: once, date, member, chunk
- DEPENDENCIES: defines dependencies from job as a list of parents jobs separed by spaces. For example, if 'new_job' has to wait for "old_job" to finish, you must add the line "DEPENDENCIES = old_job". For dependencies to jobs running in previous chunks, members or startdates, use -(DISTANCE). For example, for a job "SIM" waiting for the previous "SIM" job to finish, you have to add "DEPENDENCIES = SIM-1"

For jobs running in HPC platforms, usually you have to provide information about processors, wallclock times and more . To do this use:

- WALLCLOCK: wallclock time to be submitted to the HPC queue in format HH:MM
- PROCESSORS: processors number to be submitted to the HPC. If not specified, defaults to 1.
- THREADS: threads number to be submitted to the HPC. If not specified, defaults to 1.
- TASKS: tasks number to be submitted to the HPC. If not specified, defaults to 1.
- QUEUE: queue to add the job to. If not specificied, uses PLATFORM default.

There are also another, less used features that you can use:

- FREQUENCY: specifies that a job has only to be run after X dates, members or chunk. A job will always be created for the last one. If not specified, defaults to 1
- RERUN_ONLY: determines if a job is only to be executed in reruns. If not specified, defaults to false.
- RERUN_DEPENDENCIES: defines the jobs to be rerun if this job is going to be rerunned. Syntax is identical to the used in DEPENDENCIES

Example:

THREADS = 1 TASKS = 1

```
[SIM]
FILE = templates/ecearth3/ecearth3.sim
DEPENDENCIES = INI SIM-1 CLEAN-2
RUNNING = chunk
WALLCLOCK = 04:00
PROCESSORS = 1616
```

4.18 How to add a new platform

To add a new platform, open the <experiments_directory>/cxxx/conf/platforms_cxxx.conf file where cxxx is the experiment identifier and add this text:

[new platform]

```
TYPE = <plantform_type>
HOST = <host_name>
PROJECT = <project>
USER = <user>
SCRATCH = <scratch_dir>
```

This will create a platform named "new_platform". The options specified are all mandatory:

- TYPE: queue type for the platform. Options supported are PBS, SGE, PS, LSF, ecaccess and SLURM
- HOST: hostname of the platform
- PROJECT: project for the machine scheduler.
- USER: user for the machine scheduler
- SCRATCH DIR: path to the scratch directory of the machine

Warning: With some platform types, Autosubmit may also need the version, forcing you to add the parameter VERSION. These platforms are PBS (options: 10, 11, 12) and ecaccess (options: pbs, loadleveler)

Some platforms may require to run serial jobs in a different queue or platform. To avoid changing the job configuration, you can specify what platform or queue to use to run serial jobs assigned to this platform:

- SERIAL_PLATFORM: if specified, Autosubmit will run jobs with only one processor in the specified platform.
- SERIAL_QUEUE: if specified, Autosubmit will run jobs with only one processor in the specified queue. Autosubmit will ignore this configuration if SERIAL_PLATFORM is provided

There are some other paramaters that you must need to specify:

- BUDGET: budget account for the machine scheduler. If omited, takes the value defined in PROJECT
- ADD_PROJECT_TO_HOST = option to add project name to host. This is required for some HPCs
- · QUEUE: if given, Autosubmit will add jobs to the given queue instead of platformn's default queue
- TEST_SUITE: if true, autosubmit test command can use this queue as a main queue. Defaults to false
- MAX_WAITING_JOBS: maximum number of jobs to be waiting in this platform.
- TOTAL_JOBS: maximum number of jobs to be running at the same time in this platform.

Example:

[platform]

```
TYPE = SGE
HOST = hostname
PROJECT = my_project
ADD_PROJECT_TO_HOST = true
USER = my_user
```

SCRATCH_DIR = /scratch TEST_SUITE = True

4.19 How to refresh an experiment

To refresh the project folder after creating the experiment use the command:

```
autosubmit refresh EXPID
```

EXPID is the experiment identifier.

Options:

```
usage: autosubmit refresh [-h] [-mc] expid refresh project directory for an experiment
```

4.20 How to archive an experiment

To archive the experiment, use the command:

```
autosubmit archive EXPID
```

EXPID is the experiment identifier.

Warning: this command calls implicitly the clean command. Check clean command documentation.

Warning: experiment will be unusable after archiving. If you want to use it, you will need to call first the unarchive command

Options:

```
usage: autosubmit archive [-h] expid
expid experiment identifier
-h, --help show this help message and exit
Example:
```

autosubmit archive cxxx

Hint: Archived experiment will be stored as a tar.gz file on a folder named after the year of the last COMPLETED file date. If not COMPLETED file is present, it will be stored in the folder matching the date at the time the archive command was run.

4.21 How to unarchive an experiment

To unarchive an experiment, use the command:

```
autosubmit unarchive EXPID
```

EXPID is the experiment identifier.

Options:

```
usage: autosubmit unarchive [-h] expid
expid experiment identifier
```

-h, --help show this help message and exit

Example:

autosubmit unarchive cxxx

CHAPTER

FIVE

TROUBLESHOOTING

5.1 How to change the job status stopping autosubmit

This procedure allows you to modify the status of your jobs.

Warning: Beware that Autosubmit must be stopped to use setstatus. Otherwise a running instance of Autosubmit, at some point, will overwritte any change you may have done.

You must execute:

```
autosubmit setstatus EXPID -fs STATUS_ORIGINAL -t STATUS_FINAL -s
```

EXPID is the experiment identifier. STATUS_ORIGINAL is the original status to filter by the list of jobs. STATUS_FINAL the desired target status.

Options:

```
usage: autosubmit setstatus [-h] [-s] -t
    {READY, COMPLETED, WAITING, SUSPENDED, FAILED, UNKNOWN, QUEUING, RUNNING}
    (-fl LIST
    | -fc FILTER_CHUNKS
    | -fs {Any, READY, COMPLETED, WAITING, SUSPENDED, FAILED, UNKNOWN}
    | -ft FILTER_TYPE)
    expid
expid
                      experiment identifier
                      show this help message and exit
-h, --help
-s, --save
                      Save changes to disk
-t {READY, COMPLETED, WAITING, SUSPENDED, FAILED, UNKNOWN},
            --status_final {READY, COMPLETED, WAITING, SUSPENDED, FAILED, UNKNOWN}
                         Supply the target status
    -fl LIST, --list LIST Supply the list of job names to be changed. Default =
                        "Any". LIST = "cxxx_20101101_fc3_21_sim
                        cxxx_20111101_fc4_26_sim"
    -fc FILTER_CHUNKS, --filter_chunks FILTER_CHUNKS
                         Supply the list of chunks to change the status.
                        Default = "Any". LIST = "[ 19601101 [ fc0 [1 2 3 4]
                        fc1 [1] ] 19651101 [ fc0 [16-30] ] "
    -fs {Any, READY, COMPLETED, WAITING, SUSPENDED, FAILED, UNKNOWN},
            --filter_status {Any, READY, COMPLETED, WAITING, SUSPENDED, FAILED, UNKNOWN}
                         Select the original status to filter the list of jobs
    -ft FILTER_TYPE, --filter_type FILTER_TYPE
                         Select the job type to filter the list of jobs
```

Examples:

```
autosubmit setstatus cxxx -fl "cxxx_20101101_fc3_21_sim cxxx_20111101_fc4_26_sim" -t READY -s autosubmit setstatus cxxx -fc [ 19601101 [ fc1 [1] ] ] -t READY -s autosubmit setstatus cxxx -fs FAILED -t READY -s autosubmit setstatus cxxx -ft TRANSFER -t SUSPENDED -s
```

This script has two mandatory arguments.

The -t where you must specify the target status of the jobs you want to change to:

```
{READY, COMPLETED, WAITING, SUSPENDED, FAILED, UNKNOWN}
```

The second argument has four alternatives, the -fl, -fc, -fs and -ft; with those we can apply a filter for the jobs we want to change:

• The -fl variable recieves a list of jobnames separated by blank spaces: e.g.:

```
"cxxx_20101101_fc3_21_sim cxxx_20111101_fc4_26_sim"
```

If we supply the key word "Any", all jobs will be changed to the target status.

• The variable -fc should be a list of individual chunks or ranges of chunks in the following format:

```
[ 19601101 [ fc0 [1 2 3 4] fc1 [1] ] 19651101 [ fc0 [16-30] ] ]
```

• The variable -fs can be one of the following status for job:

```
{Any, READY, COMPLETED, WAITING, SUSPENDED, FAILED, UNKNOWN}
```

• The variable -ft can be one of the defined types of job.

Hint: When we are satisfied with the results we can use the parameter -s, which will save the change to the pkl file.

5.2 How to change the job status without stopping autosubmit

This procedure allows you to modify the status of your jobs without having to stop Autosubmit.

You must create a file in <experiments_directory>/<expid>/pkl/ named:

```
updated_list_<expid>.txt
```

Format:

This file should have two columns: the first one has to be the job_name and the second one the status.

Options:

```
READY, COMPLETED, WAITING, SUSPENDED, FAILED, UNKNOWN
```

Example:

```
vi updated_list_cxxx.txt

cxxx_20101101_fc3_21_sim READY
cxxx_20111101_fc4_26_sim READY
```

If Autosubmit finds the above file, it will process it. You can check that the processing was OK at a given date and time, if you see that the file name has changed to:

update_list_<expid>_<date>_<time>.txt

Note: A running instance of Autosubmit will check the existance of avobe file after checking already submitted jobs. It may take some time, depending on the setting SAFETYSLEEPTIME.

Warning: Keep in mind that autosubmit reads the file automatically so it is suggested to create the file in another location like /tmp or /var/tmp and then copy/move it to the pkl folder. Alternatively you can create the file with a different name an rename it when you have finished.

DEVELOPING A PROJECT

Autosubmit is used at IC3 to run EC-Earth. To do that, a git repository has been created that contains the model source code and the scripts used to run the tasks.

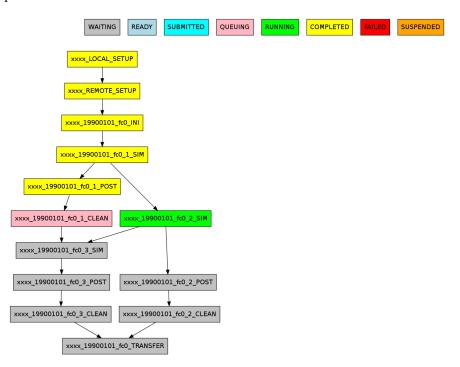


Figure 6.1: Example of monitoring plot for EC-Earth run with Autosubmit for 1 start date, 1 member and 3 chunks.

The workflow is defined using seven job types, as shown in the figure above. These job types are:

- Local_setup: prepares a patch for model changes and copies it to HPC.
- Remote_setup: creates a model copy and applies the patch to it.
- Ini: prepares model to start the simulation of one member.
- Sim: runs a simulation chunk (usually 1 to 3 months).
- Post: post-process outputs for one simulation chunk.
- Clean: removes unnecessary outputs from the simulated chunk.
- Transfer: transfers post-processed outputs to definitive storage.

Since Autosubmit 2.2 the user can select the desired source repository for the experiment project and using a given concrete branch is possible. This introduce a better version control system for project and more options to create new experiments based on different developments by the user. The different projects contain the shell script to run, for each job type (local setup, remote setup, ini, sim, post, clean and transfer) that are platform independent. Additionally the user can modify the sources under proj folder. The executable scripts are created at runtime so the modifications on the sources can be done on the fly.

Warning: Autosubmit automatically adds small shell script code blocks in the header and the tailer of your scripts, to control the workflow. Please, remove any exit command in the end of your scripts, e.g. exit 0.

Important: For a complete reference on how to develop an EC-Earth project, please have a look in the following wiki page: http://ic3.cat/wikicfu/index.php/Models

VARIABLES REFERENCE

Autosubmit uses a variable substitution system to facilitate the development of the templates. This variables can be used on the template in the form %VARIABLE NAME%.

7.1 Job variables

This variables are relatives to the current job.

- TASKTYPE: type of the job, as given on job configuration file.
- JOBNAME: current job full name.
- FAIL_COUNT: number of failed attempts to run this job.
- SDATE: current startdate.
- MEMBER: current member.
- CHUNK: current chunk.
- DAY_BEFORE: day before the startdate
- Chunk_End_IN_DAYS: chunk's length in days
- Chunk_START_DATE: chunk's start date
- Chunk_START_YEAR: chunk's start year
- Chunk_START_MONTH: chunk's start month
- Chunk_START_DAY: chunk's start day
- Chunk_START_HOUR: chunk's start hout
- Chunk_END_DATE: chunk's end date
- Chunk_END_YEAR: chunk's end year
- Chunk_END_MONTH: chunk's end month
- Chunk_END_DAY: chunk's end day
- Chunk_END_HOUR: chunk's end hour
- PREV: days since startdate at the chunk's start
- Chunk_FIRST: True if the current chunk is the first, false otherwise.
- Chunk_LAST: True if the current chunk is the last, false otherwise.
- NUMPROC: Number of processors that the job will use.

- **NUMTHREADS**: Number of threads that the job will use.
- NUMTASK: Number of tasks that the job will use.
- WALLCLOCK: Number of processors that the job will use.

7.2 Platform variables

This variables are relative to the platoforms defined on the jobs conf. A full set of the next variables are defined for each platform defined on the platforms configuration file, substituting {PLATFORM_NAME} for each platform's name. Also, a suite of variables is defined for the current platform where {PLATFORM_NAME} is substituted by CURRENT.

- {PLATFORM_NAME}_ARCH: Platform name
- {PLATFORM_NAME}_HOST: Platform url
- {PLATFORM_NAME}_USER: Platform user
- {PLATFORM_NAME}_PROJ: Platform project
- {PLATFORM_NAME}_BUDG: Platform budget
- {PLATFORM_NAME}_TYPE: Platform scheduler type
- {PLATFORM_NAME}_VERSION: Platform scheduler version
- {PLATFORM_NAME}_SCRATCH_DIR: Platform's scratch folder path
- {PLATFORM_NAME}_ROOTDIR: Platform's experiment folder path

It is also defined a suite of variables for the experiment's default platform:

- HPCARCH: Default HPC platform name
- HPCHOST: Default HPC platform url
- HPCUSER: Default HPC platform user
- HPCPROJ: Default HPC platform project
- HPCBUDG: Default HPC platform budget
- HPCTYPE: Default HPC platform scheduler type
- HPCVERSION: Default HPC platform scheduler version
- SCRATCH_DIR: Default HPC platform scratch folder path
- HPCROOTDIR: Default HPC platform experiment's folder path

7.3 Project variables

- NUMCHUNKS: number of chunks of the experiment
- CHUNKSIZE: size of each chunk
- CHUNKSIZEUNIT: unit of the chuk size. Can be hour, day, month or year.
- CALENDAR: calendar used for the experiment. Can be standard or noleap.
- ROOTDIR: local path to experiment's folder
- PROJDIR: local path to experiment's proj folder

MODULE DOCUMENTATION

8.1 autosubmit

8.2 autosubmit.config

8.2.1 autosubmit.config.basicConfig

```
class autosubmit.config.basicConfig.BasicConfig
```

Class to manage configuration for autosubmit path, database and default values for new experiments

static read()

Reads configuration from .autosubmitrc files, first from /etc, then for user directory and last for current path.

8.2.2 autosubmit.config.config_common

8.2.3 autosubmit.config.log

```
class autosubmit.config.log.Log
```

Static class to manage the log for the application. Messages will be sent to console and to file if it is configured. Levels can be set for each output independently. These levels are (from lower to higher priority):

- •EVERYTHING: this level is just defined to show every output
- •DEBUG
- •INFO
- •RESULT
- •USER_WARNING
- •WARNING
- •ERROR
- •CRITICAL
- •NO_LOG: this level is just defined to remove every output

static critical (msg, *args)

Sends critical errors to the log. It will be shown in red in the console.

Parameters

- msg message to show
- args arguments for message formating (it will be done using format() method on str)

static debug (msg, *args)

Sends debug information to the log

Parameters

- msg message to show
- args arguments for message formating (it will be done using format() method on str)

static error (msg, *args)

Sends errors to the log. It will be shown in red in the console.

Parameters

- msg message to show
- args arguments for message formating (it will be done using format() method on str)

static info (msg, *args)

Sends information to the log

Parameters

- msg message to show
- args arguments for message formating (it will be done using format() method on str)

static result (msg, *args)

Sends results information to the log. It will be shown in green in the console.

Parameters

- msg message to show
- args arguments for message formating (it will be done using format() method on str)

static set_console_level (level)

Sets log level for logging to console. Every output of level equal or higher to parameter level will be printed on console

Parameters level – new level for console

Returns None

static set_file (file_path)

Configure the file to store the log. If another file was specified earlier, new messages will only go to the new file.

Parameters file_path (*str*) – file to store the log

static set_file_level (level)

Sets log level for logging to file. Every output of level equal or higher to parameter level will be added to log file

Parameters level – new level for log file

static user_warning (msg, *args)

Sends warnings for the user to the log. It will be shown in yellow in the console.

Parameters

- msg message to show
- args arguments for message formating (it will be done using format() method on str)

```
static warning (msg, *args)
```

Sends program warnings to the log. It will be shown in yellow in the console.

Parameters

- msg message to show
- args arguments for message formating (it will be done using format() method on str)

```
class autosubmit.config.log.LogFormatter(to_file=False)
```

Class to format log output.

Parameters to_file (bool) - If True, creates a LogFormatter for files; if False, for console

format (record)

Format log output, adding labels if needed for log level. If logging to console, also manages font color. If logging to file adds timestamp

Parameters record (LogRecord) – log record to format

Returns formatted record

Return type str

8.3 autosubmit.database

Module containing functions to manage autosubmit's database.

```
exception autosubmit.database.db_common.DbException (message)
```

Exception class for database errors

```
autosubmit.database.db_common.base36decode(number)
```

Converts a base36 string to a positive integer

Parameters number (*str*) – base36 string to convert

Returns number's integer value

Return type int

```
autosubmit.database.db_common.base36encode(number,
```

alpha-

bet='0123456789abcdefghijklmnopqrstuvwxyz')

Convert positive integer to a base36 string.

Parameters

- **number** (*int*) number to convert
- alphabet (str) set of characters to use

Returns number's base36 string value

Return type str

```
\verb"autosubmit.database.db_common.check_db" ()
```

Checks if database file exist

Returns None if exists, terminates program if not

```
autosubmit.database.db_common.check_experiment_exists(name,
```

ror_on_inexistence=True)

Checks if exist an experiment with the given name.

Parameters name (*str*) – Experiment name

Returns If experiment exists returns true, if not returns false

Return type bool

autosubmit.database.db_common.check_name(name)

Checks if it is a valid experiment identifier

Parameters name (*str*) – experiment identifier to check

Returns name if is valid, terminates program otherwise

Return type str

autosubmit.database.db_common.close_conn(conn, cursor)

Commits changes and close connection to database

Parameters

- conn (sqlite3.Connection) connection to close
- **cursor** (*sqlite3.Cursor*) cursor to close

autosubmit.database.db_common.copy_experiment(name, description, version, test=False)

Creates a new experiment by copying an existing experiment

Parameters

- name (str) identifier of experiment to copy
- **description** (*str*) experiment's description

Returns experiment id for the new experiment

Return type str

autosubmit.database.db_common.create_db (qry)

Creates a new database for autosubmit

Parameters qry (*str*) – query to create the new database

autosubmit.database.db_common.delete_experiment(name)

Removes experiment from database

Parameters name (*str*) – experiment identifier

Returns True if delete is succesful

Return type bool

autosubmit.database.db_common.get_autosubmit_version(expid)

Get the minimun autosubmit version needed for the experiment

Parameters expid (*str*) – Experiment name

Returns If experiment exists returns the autosubmit version for it, if not returns None

Return type str

autosubmit.database.db_common.last_name_used(test=False)

Gets last experiment identifier used

Parameters test (bool) – flag for test experiments

Returns last experiment identifier used, 'empty' if there is none

Return type str

autosubmit.database.db_common.new_experiment (description, version, test=False)

Stores a new experiment on the database and generates its identifier

Parameters

- **test** (*bool*) flag for test experiments
- **description** (*str*) experiment's description

Returns experiment id for the new experiment

Return type str

```
autosubmit.database.db_common.open_conn(check_version=True)
Opens a connection to database
```

Returns connection object, cursor object

Return type sqlite3. Connection, sqlite3. Cursor

8.4 autosubmit.date

In this python script there are tools to manipulate the dates and make mathematical operations between them.

```
autosubmit.date.chunk_date_lib.add_days (date, number_of_days, cal)
    Adds days to a date
```

Parameters

- date (datetime.datetime) base date
- number_of_days (int) number of days to add
- cal (str) calendar to use

Returns base date plus added days

Return type date

```
autosubmit.date.chunk_date_lib.add_hours (date, number_of_hours, cal)
Adds hours to a date
```

Parameters

- date (datetime.datetime) base date
- **number_of_hours** (*int*) number of hours to add
- cal (str) calendar to use

Returns base date plus added hours

Return type datetime

```
autosubmit.date.chunk_date_lib.add_months (date, number_of_months, cal)
Adds months to a date
```

Parameters

- date (datetime.datetime) base date
- number_of_months (int) number of months to add
- cal (str) calendar to use

Returns base date plus added months

Return type date

8.4. autosubmit.date 43

autosubmit.date.chunk_date_lib.add_time (date, total_size, chunk_unit, cal)
 Adds given time to a date

Parameters

- date (datetime.datetime) base date
- total size (int) time to add
- chunk_unit (str) unit of time to add
- cal (str) calendar to use

Returns result of adding time to base date

Return type datetime.datetime

autosubmit.date.chunk_date_lib.add_years (date, number_of_years)
Adds years to a date

Parameters

- date (datetime.datetime) base date
- **number_of_years** (*int*) number of years to add

Returns base date plus added years

Return type date

Gets chunk interval end date

Parameters

- **start_date** (*datetime.datetime*) chunk's start date
- **chunk_length** (*int*) length of the chunks
- **chunk_unit** (*str*) **chunk** length unit
- cal (str) calendar to use

Returns chunk's end date

Return type datetime.datetime

autosubmit.date.chunk_date_lib.chunk_start_date(date, chunk, chunk_length, chunk_unit, cal)

Gets chunk's interval start date

Parameters

- date (datetime.datetime) start date for member
- **chunk** (*int*) number of chunk
- **chunk_length** (*int*) length of chunks
- **chunk_unit** (*str*) **chunk** length unit
- cal (str) calendar to use

Returns chunk's start date

Return type datetime.datetime

```
autosubmit.date.chunk_date_lib.date2str(date, date_format='')
Converts a datetime object to a str
```

```
Parameters date (datetime.datetime) – date to convert
```

Return type str

```
autosubmit.date.chunk_date_lib.parse_date(string_date)
```

Parses a string into a datetime object

Parameters string_date (*str*) – string to parse

Return type datetime.datetime

```
autosubmit.date.chunk_date_lib.previous_day (date, cal)
    Gets previous day
```

Parameters

- date (datetime.datetime) base date
- cal (str) calendar to use

Returns base date minus one day

Return type datetime.datetime

```
autosubmit.date.chunk_date_lib.sub_days (date, number_of_days, cal) Substract days to a date
```

Parameters

- date (datetime.datetime) base date
- **number_of_days** (*int*) number of days to substract
- cal (str) calendar to use

Returns base date minus substracted days

Return type datetime.datetime

```
autosubmit.date.chunk_date_lib.subs_dates (start_date, end_date, cal)
Gets days between start_date and end_date
```

Parameters

- **start_date** (*datetime.datetime*) interval's start date
- end_date (datetime.datetime) interval's end date
- cal (str) calendar to use

Returns interval length in days

Return type int

8.5 autosubmit.git

Parameters expid (str) – experiment identifier

```
static clean_git (as_conf)
```

Function to clean space on BasicConfig.LOCAL_ROOT_DIR/git directory.

Parameters as_conf (autosubmit.config.AutosubmitConfig) - experiment configuration

8.5. autosubmit.git 45

```
static clone_repository (as_conf, force)
```

Clones a specified git repository on the project folder

Parameters

- as_conf (autosubmit.config.AutosubmitConfig) experiment configuration
- **force** (bool) if True, it will overwrite any existing clone

Returns True if clone was succesfull, False otherwise

8.6 autosubmit.job

Main module for autosubmit. Only contains an interface class to all functionality implemented on autosubmit

```
class autosubmit.job.job.job(name, jobid, status, priority)
```

Class to handle all the tasks with Jobs at HPC. A job is created by default with a name, a jobid, a status and a type. It can have children and parents. The inheritance reflects the dependency between jobs. If Job2 must wait until Job1 is completed then Job2 is a child of Job1. Inversely Job1 is a parent of Job2

Parameters

- name (str) job's name
- **jobid** (*int*) job's identifier
- status (Status) job inicial status
- **priority** (*int*) job's priority

```
add_parent (*new_parent)
```

Add parents for the job. It also adds current job as a child for all the new parents

Parameters *new_parent (*Job*) – job parent

ancestors

Returns all job's ancestors

Returns job ancestors

Return type set

```
check_completion (default_status=-1)
```

Check the presence of *COMPLETED* file and touch a Checked or failed file. Change statis to COMPLETED if *COMPLETED* file exists and to FAILED otherwise.

```
check_end_time()
```

Returns end time from completed file

Returns completed date and time

Return type str

check_fail_queued_time()

Returns total time spent waiting for failed jobs

Returns total time waiting in HPC platforms for failed jobs

Return type str

check fail run time()

Returns total time running for failed jobs

Returns total time running in HPC for failed jobs

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Return type str check_failed_times() Returns number of failed attempts before completing the job Returns failed attempts to run **Return type** str check_queued_time() Returns job's waiting time in HPC **Returns** total time waiting in HPC platforms Return type str check_run_time() Returns job's running time Returns total time running Return type str check_script (as_conf, parameters) Checks if script is well formed Parameters as_conf (AutosubmitConfig) - configuration file **Returns** true if not problem has been detected, false otherwise Return type bool children Returns a list containing all children of the job Returns child jobs Return type set compare_by_id(other) Compare jobs by ID **Parameters other** (*Job*) – job to compare **Returns** comparison result Return type bool compare_by_name (other) Compare jobs by name **Parameters other** (*Job*) – job to compare **Returns** comparison result Return type bool compare_by_status(other) Compare jobs by status value **Parameters other** (Job) – job to compare Returns comparison result

8.6. autosubmit.job

Return type bool

Creates script file to be run for the job

create_script (as_conf)

```
Parameters as_conf (AutosubmitConfig) – configuration object
         Returns script's filename
         Return type str
delete_child(child)
     Removes a child from the job
         Parameters child (Job) – child to remove
delete_parent (parent)
     Remove a parent from the job
         Parameters parent (Job) – parent to remove
get_platform()
     Returns the platforms to be used by the job. Chooses between serial and parallel platforms
     :return HPCPlatform object for the job to use :rtype: HPCPlatform
get_queue()
     Returns the queue to be used by the job. Chooses between serial and parallel platforms
     :return HPCPlatform object for the job to use :rtype: HPCPlatform
has_children()
     Returns true if job has any children, else return false
         Returns true if job has any children, otherwise return false
         Return type bool
has_parents()
     Returns true if job has any parents, else return false
         Returns true if job has any parent, otherwise return false
         Return type bool
inc_fail_count()
     Increments fail count
log_job()
    Prints job information in log
long name
     Job's long name. If not setted, returns name
         Returns long name
         Return type str
parents
     Return parent jobs list
         Returns parent jobs
         Return type set
print_job()
     Prints debug information about the job
print_parameters()
     Print sjob parameters in log
```

remove dependencies()

Checks if job is completed and then remove dependencies for childs

set_platform(value)

Sets the HPC platforms to be used by the job.

Parameters value (HPCPlatform) – platforms to set

set_queue (value)

Sets the queue to be used by the job.

Parameters value (HPCPlatform) – queue to set

short_name

Job short name

Returns short name

Return type str

update_content (project_dir)

Create the script content to be run for the job

Parameters project_dir (str) – project directory

Returns script code

Return type str

update_parameters (as_conf, parameters)

Refresh parameters value

Parameters

- as_conf (AutosubmitConfig) -
- parameters (dict) –

class autosubmit.job.job_common.StatisticsSnippetBash

Class to handle the statistics snippet of a job. It contains header and tailer for local and remote jobs

class autosubmit.job.job_common.StatisticsSnippetPython

Class to handle the statistics snippet of a job. It contains header and tailer for local and remote jobs

```
class autosubmit.job.job_common.Status
```

Class to handle the status of a job

Class to create jobs from conf file and to find jobs by stardate, member and chunk

Parameters

- **joblist** (*JobList*) joblist to use
- parser (SafeConfigParser) jobs conf file parser
- date_list (list) startdates
- **member_list** (*list*) member
- **chunk_list** (*list*) **chunks**
- date_format (str) option to formate dates

```
get_jobs (section, date=None, member=None, chunk=None)
```

Return all the jobs matching section, date, member and chunk provided. If any parameter is none, returns all the jobs without checking that parameter value. If a job has one parameter to None, is returned if all the others match parameters passed

Parameters

- **section** (*str*) section to return
- date (str) stardate to return
- **member** (*str*) member to return
- **chunk** (*int*) **chunk** to return

Returns jobs matching parameters passed

Return type list

get_option (section, option, default)

Returns value for a given option

Parameters

- **section** (*str*) section name
- **option** (*str*) option to return
- **default** (*object*) value to return if not defined in configuration file

read_section (section, priority)

Read a section from jobs conf and creates all jobs for it

Parameters

- section (str) section to read
- **priority** (*int*) priority for the jobs

```
class autosubmit.job.job_list.JobList(expid)
```

Class to manage the list of jobs to be run by autosubmit

Parameters expid (*str*) – experiment's indentifier

```
check_scripts(as_conf)
```

When we have created the scripts, all parameters should have been substituted. %PARAMETER% handlers not allowed

Parameters as_conf (AutosubmitConfig) - experiment configuration

create (date list, member list, num chunks, parameters, date format)

Creates all jobs needed for the current workflow

Parameters

- date_list (list) start dates
- member_list (list) members
- num_chunks (int) number of chunks to run
- parameters (dict) parameters for the jobs
- date_format (str) option to formate dates

expid

Returns experiment identifier

```
Returns experiment's identifier
         Return type str
get_active (platform=None)
     Returns a list of active jobs (In platforms, Ready)
         Parameters platform (HPCPlatform) – job platform
         Returns active jobs
         Return type list
get_completed(platform=None)
     Returns a list of completed jobs
         Parameters platform (HPCPlatform) – job platform
         Returns completed jobs
         Return type list
get_failed(platform=None)
     Returns a list of failed jobs
         Parameters platform (HPCPlatform) – job platform
         Returns failed jobs
         Return type list
get_finished(platform=None)
     Returns a list of jobs finished (Completed, Failed)
         Parameters platform (HPCPlatform) – job platform
         Returns finsihed jobs
         Return type list
get_in_queue (platform=None)
     Returns a list of jobs in the platforms (Submitted, Running, Queuing)
         Parameters platform (HPCPlatform) – job platform
         Returns jobs in platforms
         Return type list
get_job_by_name (name)
     Returns the job that its name matches parameter name
         Parameters name (str) – name to look for
         Returns found job
         Return type job
get_job_list()
     Get inner job list
         Returns job list
         Return type list
get_not_in_queue (platform=None)
     Returns a list of jobs NOT in the platforms (Ready, Waiting)
         Parameters platform (HPCPlatform) – job platform
```

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```
Returns jobs not in platforms

Return type list
```

get_queuing (platform=None)

Returns a list of jobs queuing

Parameters platform (*HPCPlatform*) – job platform

Returns queuedjobs

Return type list

get_ready (platform=None)

Returns a list of ready jobs

Parameters platform (*HPCPlatform*) – job platform

Returns ready jobs

Return type list

get_running(platform=None)

Returns a list of jobs running

Parameters platform (*HPCPlatform*) – job platform

Returns running jobs

Return type list

get_submitted(platform=None)

Returns a list of submitted jobs

Parameters platform (HPCPlatform) – job platform

Returns submitted jobs

Return type list

get_unknown (platform=None)

Returns a list of jobs on unknown state

Parameters platform (*HPCPlatform*) – job platform

Returns unknown state jobs

Return type list

get_waiting(platform=None)

Returns a list of jobs waiting

Parameters platform (*HPCPlatform*) – job platform

Returns waiting jobs

Return type list

load()

Recreates an stored joblist from the pickle file

Returns loaded joblist object

Return type JobList

static load_file (filename)

Recreates an stored joblist from the pickle file

Parameters filename (str) – pickle file to load

```
Return type JobList

remove_rerun_only_jobs()
Removes all jobs to be runned only in reruns

rerun (chunk_list)
Updates joblist to rerun the jobs specified by chunk_list

Parameters chunk_list (str) - list of chunks to rerun
Returns

save()
Stores joblist as a pickle file
Returns loaded joblist object
Return type JobList

sort_by_id()
Returns a list of jobs sorted by id
```

sort_by_name()

Returns a list of jobs sorted by name

Returns jobs sorted by ID

Returns jobs sorted by name

Return type list

Return type list

sort_by_status()

Returns a list of jobs sorted by status

Returns job sorted by status

Return type list

sort_by_type()

Returns a list of jobs sorted by type

Returns job sorted by type

Return type list

update_genealogy()

When we have created the joblist, every type of job is created. Update genealogy remove jobs that have no templates

update_shortened_names()

In some cases the scheduler only can operate with names shorter than 15 characters. Update the job list replacing job names by the corresponding shortened job name

8.7 autosubmit.monitor

```
class autosubmit.monitor.monitor.Monitor
```

Class to handle monitoring of Jobs at HPC.

static clean_plot (expid)

Function to clean space on BasicConfig.LOCAL_ROOT_DIR/plot directory. Removes all plots except last two.

Parameters expid (str) – experiment's identifier

static clean stats (expid)

Function to clean space on BasicConfig.LOCAL_ROOT_DIR/plot directory. Removes all stats' plots except last two.

Parameters expid (str) – experiment's identifier

static color_status (status)

Return color associated to given status

Parameters status (Status) – status

Returns color

Return type str

static create_bar_diagram (expid, joblist, output_file)

Function to plot statistics

Parameters

- **expid** (*str*) experiment's identifier
- **joblist** (*JobList*) joblist to plot
- **output_file** (*str*) path to create file

create_tree_list(expid, joblist)

Create graph from joblist

Parameters

- **expid** (*str*) experiment's identifier
- **joblist** (*JobList*) joblist to plot

Returns created graph

Return type pydotplus.Dot

generate_output (expid, joblist, output_format='pdf')

Plots graph for joblist and stores it in a file

Parameters

- **expid** (*str*) experiment's identifier
- **joblist** (*JobList*) joblist to plot
- output_format (str (png, pdf, ps)) file format for plot

generate_output_stats (expid, joblist, output_format='pdf')

Plots stats for joblist and stores it in a file

Parameters

- **expid** (*str*) experiment's identifier
- **joblist** (*JobList*) joblist to plot
- output_format (str (png, pdf, ps)) file format for plot

8.8 autosubmit.queue

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