



**Barcelona
Supercomputing
Center**
Centro Nacional de Supercomputación



EXCELENCIA
SEVERO
OCHOA

Autosubmit Tutorial 2021

**Hands-on: How to run
experiments using Autosubmit**

The Autosubmit Team

Autosubmit Introduction



**Barcelona
Supercomputing
Center**

Centro Nacional de Supercomputación

Autosubmit - Summary

- **Automatization:** Orchestrating different kind of tasks in homogeneous or heterogeneous environments. No user intervention needed.
- **Provenance and reproducibility:** Unique identifier per experiment, storing all the parameters needed to reproduce it (Autosubmit version, model version, configuration, etc.). Linked with CVS.
- **Failure tolerance:** Automatic retrials and ability to rerun chunks in case of corrupted or missing data, repeating postprocessing and transfers if needed. Recovery capabilities.
- **Versatility:** Different workflows including Auto-Models (EC-Earth, MONARCH, CALIOPE), data downloading (Auto-MARS), machine learning, performance analysis... Providing specialized features for each case (different kind of wrappers, using MPI machine files or masks to handle resources affinity).

Autosubmit basic usage

How to create a dummy experiment



**Barcelona
Supercomputing
Center**

Centro Nacional de Supercomputación

Before start - Initialization

- Ensure that you have password less ssh to esarchive.
 - You can generate a ssh keygen by `ssh-keygen -t rsa -b 4096 -C “email@bsc.es” -m PEM`
 - Then you will need to perform an `scp ~/.ssh/id_rsa.pub user@bscautosubmit02.bsc.es`
 - Repeat the same for **marenostrum4** if not already done.
 - ForwardX11 yes
- Load autosubmit in two terminals (follow the colors to know where put each

```
# Terminal 1 (workstation)
• ssh -XY workstation
• module load autosubmit
```

```
# Terminal 2 (AS machine)
1) ssh bscautosubmit02.bsc.es
2) module load autosubmit
```

```
# Terminal 3 (workstation)
• Edit files there.
```

Basic Workflow - Initialization

- **Create a new experiment** -> Automatically stores fundamental info in a database.

```
Terminal 1
```

```
autosubmit expid -dm -H "marenostrum4" -d "AS-Tutorial 2021"
```

```
The new experiment "<expid>" has been registered.
```

- Creates the **folder structure** with the **basic configuration**.

```
/esarchive/autosubmit/<expid>/conf    -> Config files  
/esarchive/autosubmit/<expid>/pkl      -> Workflow  
/esarchive/autosubmit/<expid>/plot     -> Visualization  
/esarchive/autosubmit/<expid>/tmp      -> Logs, templates
```

Basic Workflow - Configuration

conf/expdef

- Default platform (-H).
- Start dates, members and chunks.
- Experiment project source (git, local, svn, dummy).
- Project configuration file path.

conf/platforms

- Manage cluster, Fat-nodes and Support computers.
- Multiple computers are allowed (even unused).

Basic Workflow - Configuration(cont.)

conf/jobs

- Scripts to execute.
- Dependencies between jobs.
- Job requirements.
- Platform and queue to use.

conf/autosubmit

- Total jobs limitation (waiting, total).
- Version info, Retrials, Mail notification and storage systems.
- Wrappers, presubmission and migrate.

Basic Workflow - Create

- Create an experiment using terminal 1 (workstation)

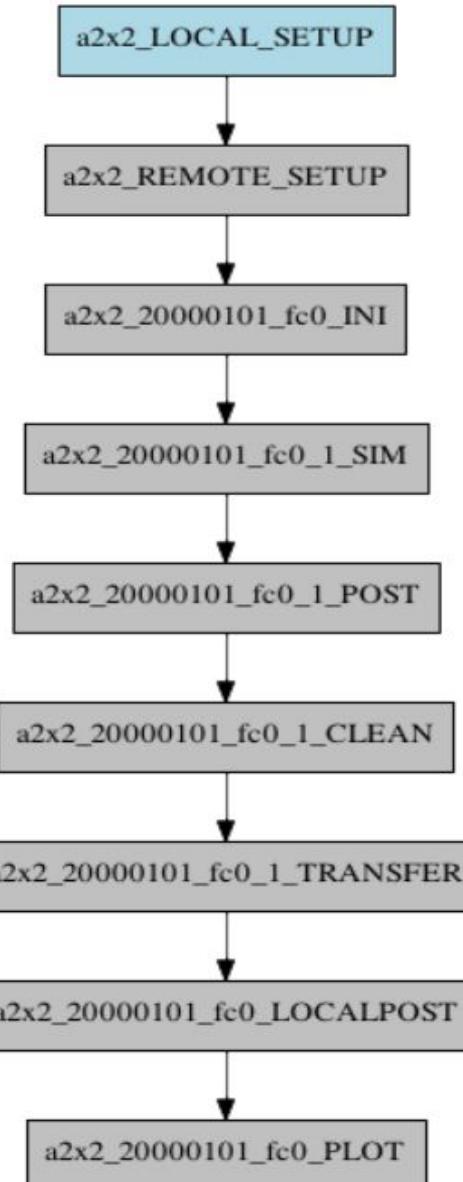
```
autosubmit create <expid>
```

#Each one will have a different expid

Generates plot/expid_timestamp_hour.pdf =>

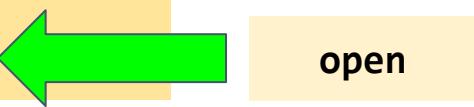
Generates tmp/Log_<expid> <= template logs

Generates tmp/ASLOG <= command logs



Basic Workflow - Config

conf/platform.conf



```
[marenostrum]
TYPE = slurm #scheduler
HOST = mn1.bsc.es #ip or alias
PROJECT = bsc32
USER = bsc32XXX # Your username
SCRATCH_DIR = /gpfs/scratch
ADD_PROJECT_TO_HOST = false
QUEUE = debug
```

edit

conf/expdef.conf

```
[DEFAULT]
HPCARCH = marenostrum4

[experiment]
DATELIST = 20000101
MEMBERS = fc0
CHUNKSIZEUNIT = month
CHUNKSIZE = 4
MEMBERS = fc0
NUMCHUNKS = 1
CHUNKINI =

[project]
# Select project type. STRING = git,
# svn, local, none
PROJECT_TYPE = none
PROJECT_DESTINATION = proj
```

Basic Workflow - Run

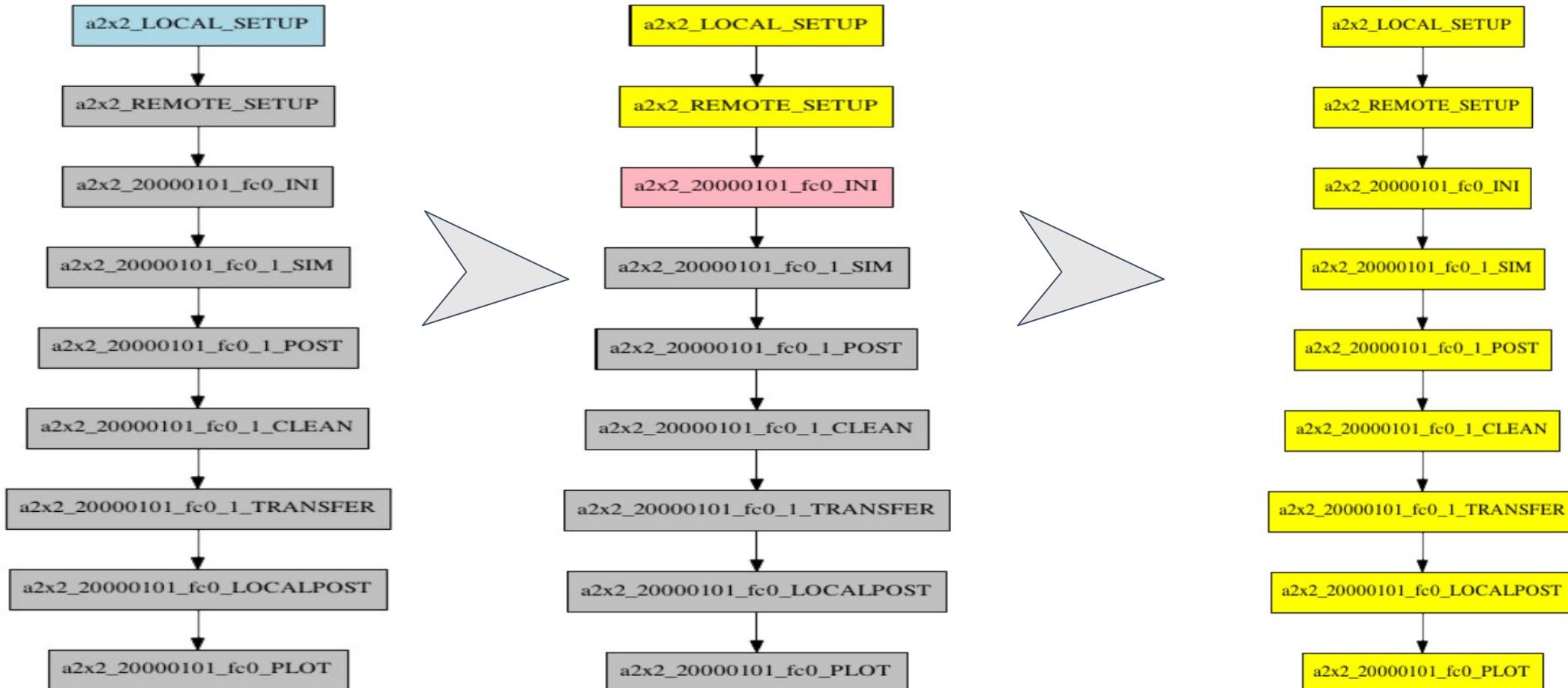
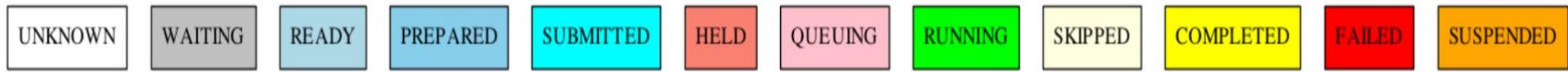
```
autosubmit run <expid>
```

- Generates **tmp/Log_<expid>** <= template logs (per each completed job)
- Generates **tmp/ASLOG** <= command log
- Runs the experiment.

Run log:

```
[marenostrum4] Connection successful to host mn1.bsc.es
[marenostrum4] Correct user privileges for host mn1.bsc.es
[local] Connection successful to host localhost
[local] Correct user privileges for host localhost
```

Basic Workflow - Monitor



autosubmit monitor <expid>

Basic workflow - Common commands

autosubmit refresh

Update project experiment folder.

autosubmit inspect

Generates a preview of the job scripts combined with AS settings (templates).

autosubmit recovery

Synchronizes the status of the remote platform with the local platform.

autosubmit setstatus

Allows to change the status of the workflow.

Practical Example: Running MONARCH with Autosubmit



*Barcelona
Supercomputing
Center*

Centro Nacional de Supercomputación

Monarch - Creation of a new experiment

```
dbeltran@bscesautosubmit01:~$ autosubmit expid --copy t0lk -H marenostrum4 -d "Test for MONARCH & Autosubmit training - DUST mode"
```

The new experiment "**<expid>**" has been registered.

Copying previous experiment config directories

Experiment registered successfully

The experiment folder will be created in: /esarchive/autosubmit

```
dbeltran@bscesautosubmit01:~$ cd /esarchive/autosubmit/<expid>
```

Monarch - Platforms.conf

Configure the main HPC platform, and the transfer machine.

Edit the platforms configuration file: /esarchive/autosubmit/<expid>/conf/platforms_<expid>.conf

```
[marenostrum]
TYPE = slurm
HOST = mn1.bsc.es
PROJECT = bsc32
USER = bsc32NNN
QUEUE = debug
SCRATCH_DIR = /gpfs/scratch
ADD_PROJECT_TO_HOST = false
PROCESSORS_PER_NODE = 48
MAX_PROCESSORS = 768
MAX_WALLCLOCK = 48:00
#DISABLE_RECOVERY_THREADS = FALSE
```

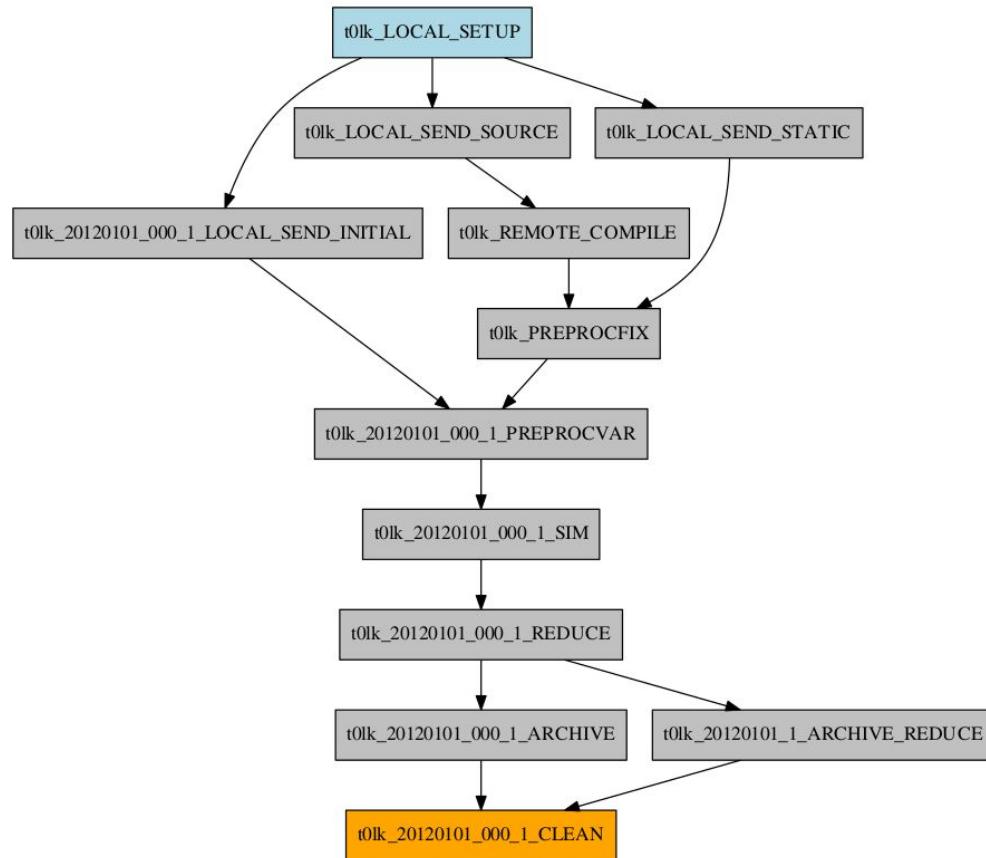
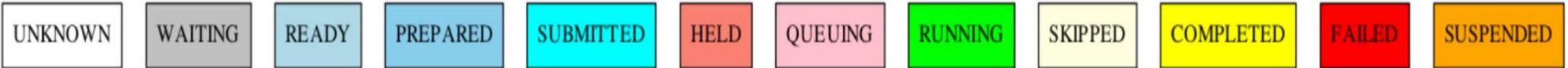
```
[marenostrum_archive]
TYPE = ps
HOST = dt02.bsc.es
PROJECT = bsc32
USER = bsc32NNN
SCRATCH_DIR = /gpfs/scratch
ADD_PROJECT_TO_HOST = False
TEST_SUITE = False
```

Swap User bsc32NNN for your marenostrum user.

MONARCH - Create Workflow

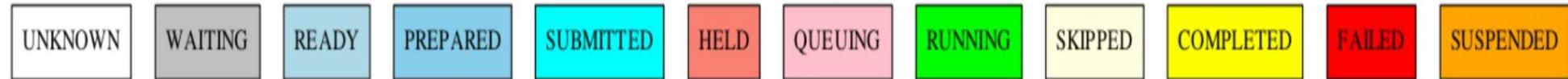
```
autosubmit create <expid> -np
```

```
autosubmit setstatus <expid> -t SUSPENDED -ft CLEAN -s
```



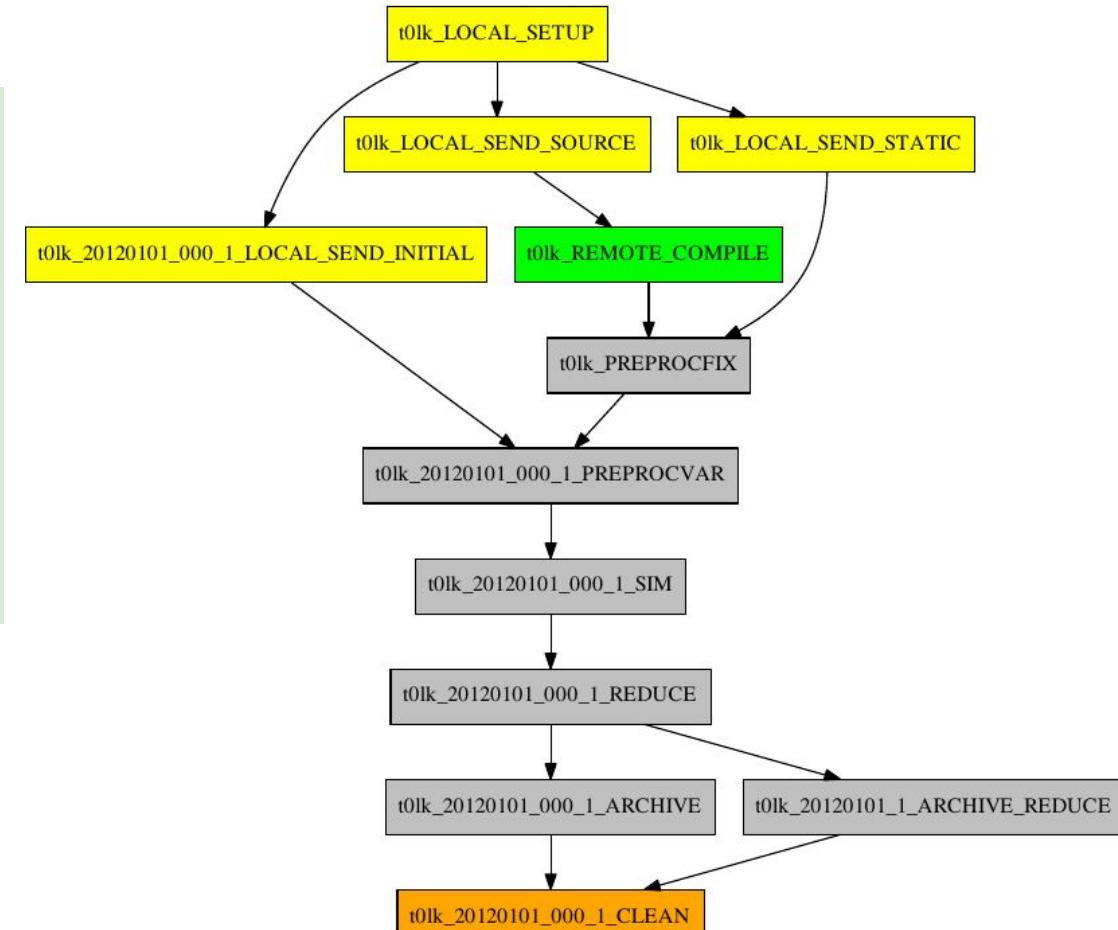
Monarch - Run and monitor

autosubmit run <expid>



autosubmit monitor <expid>

[marenostrum4] Connection successful to host mn1.bsc.es
[marenostrum4] Correct user privileges for host mn1.bsc.es
[local] Connection successful to host localhost
[local] Correct user privileges for host localhost
[marenostrum_archive] Connection successful to host dt02.bsc.es
[marenostrum_archive] Correct user privileges for host dt02.bsc.es



Monarch - Jobs.<expid>.conf

```
[LOCAL_SETUP]
FILE = templates/local_setup.sh
PLATFORM = LOCAL
RUNNING = once
NOTIFY_ON = FAILED
```

```
[LOCAL_SEND_INITIAL]
FILE = templates/00_local_send_initial.sh
PLATFORM = marenostrum_archive
DEPENDENCIES = LOCAL_SETUP
#because different dates (chunk = day):
RUNNING = chunk
NOTIFY_ON = FAILED
```

```
[LOCAL_SEND_SOURCE]
FILE = templates/01_local_send_source.sh
PLATFORM = marenostrum_archive
DEPENDENCIES = LOCAL_SETUP
RUNNING = once
NOTIFY_ON = FAILED
```

```
[LOCAL_SEND_STATIC]
FILE = templates/01b_local_send_static.sh
PLATFORM = marenostrum_archive
DEPENDENCIES = LOCAL_SETUP
RUNNING = once
NOTIFY_ON = FAILED
```

Monarch - Jobs.conf

[REMOTE_COMPILE]

```
FILE = templates/02_compile.sh
DEPENDENCIES = LOCAL_SEND_SOURCE
RUNNING = once
PROCESSORS = 4
WALLCLOCK = 00:50
CUSTOM_DIRECTIVES = ["#SBATCH -p interactive"]
NOTIFY_ON = FAILED
```

[PREPROCFIX]

```
FILE = templates/03_preproc_fix.sh
DEPENDENCIES = REMOTE_COMPILE LOCAL_SEND_STATIC
RUNNING = once
WALLCLOCK = 00:30
NOTIFY_ON = FAILED
```

[PREPROCVAR]

```
FILE = templates/04_preproc_var.sh
DEPENDENCIES = LOCAL_SEND_INITIAL PREPROCFIX
#In Autosubmit nomenclature chunk will be our days
(because days is used for start days)
RUNNING = chunk
PROCESSORS = 8
WALLCLOCK = 00:30
NOTIFY_ON = FAILED
```

[SIM]

```
FILE = templates/05b_sim.sh
DEPENDENCIES = PREPROCVAR SIM-1
RUNNING = chunk
PROCESSORS = 284
WALLCLOCK = 00:10
NOTIFY_ON = FAILED
```

Monarch - Jobs.conf

[ARCHIVE]

```
FILE = templates/06_archive.sh  
DEPENDENCIES = REDUCE ARCHIVE-1  
PLATFORM = marenostrum_archive  
RUNNING = chunk  
WALLCLOCK = 00:10  
NOTIFY_ON = FAILED
```

[REDUCE]

```
FILE = templates/07_reduce.sh  
DEPENDENCIES = SIM REDUCE-1  
RUNNING = chunk  
WALLCLOCK = 01:00  
NOTIFY_ON = FAILED
```

[ARCHIVE_REDUCE]

```
FILE = templates/06c_archive_reduce.sh  
DEPENDENCIES = REDUCE  
PLATFORM = marenostrum_archive  
RUNNING = chunk  
SYNCHRONIZE = member  
WALLCLOCK = 01:00  
NOTIFY_ON = FAILED
```

[CLEAN]

```
FILE = templates/08_clean.sh  
DEPENDENCIES = REDUCE+1 ARCHIVE ARCHIVE_REDUCE  
PLATFORM = marenostrum_archive  
RUNNING = chunk  
WALLCLOCK = 00:10  
NOTIFY_ON = FAILED
```

Monarch - project folder

Inside the **proj/auto-monarch** directory we can find the scripts, configuration files and source code to run the model:

```
$ ls -l /esarchive/autosubmit/<expid>/proj/auto-monarch
drwxr-xr-x 2 dbeltran Earth 4096 Nov  6 18:08 plugins
drwxr-xr-x 5 dbeltran Earth 4096 Nov  6 18:08 sources
drwxr-xr-x 4 dbeltran Earth 4096 Nov  6 18:08 templates
drwxr-xr-x 4 dbeltran Earth 4096 Nov  6 18:08 utils
```

```
$ ls -l /esarchive/autosubmit/<expid>/proj/auto-monarch/sources
drwxr-xr-x 3 dbeltran Earth 4096 Nov  6 18:08 monarch-DA
drwxr-xr-x 2 dbeltran Earth 4096 Nov 13 13:50 MONARCH_Reduce
drwxr-xr-x 5 dbeltran Earth 4096 Nov  6 18:08 nmmrb-monarch
```

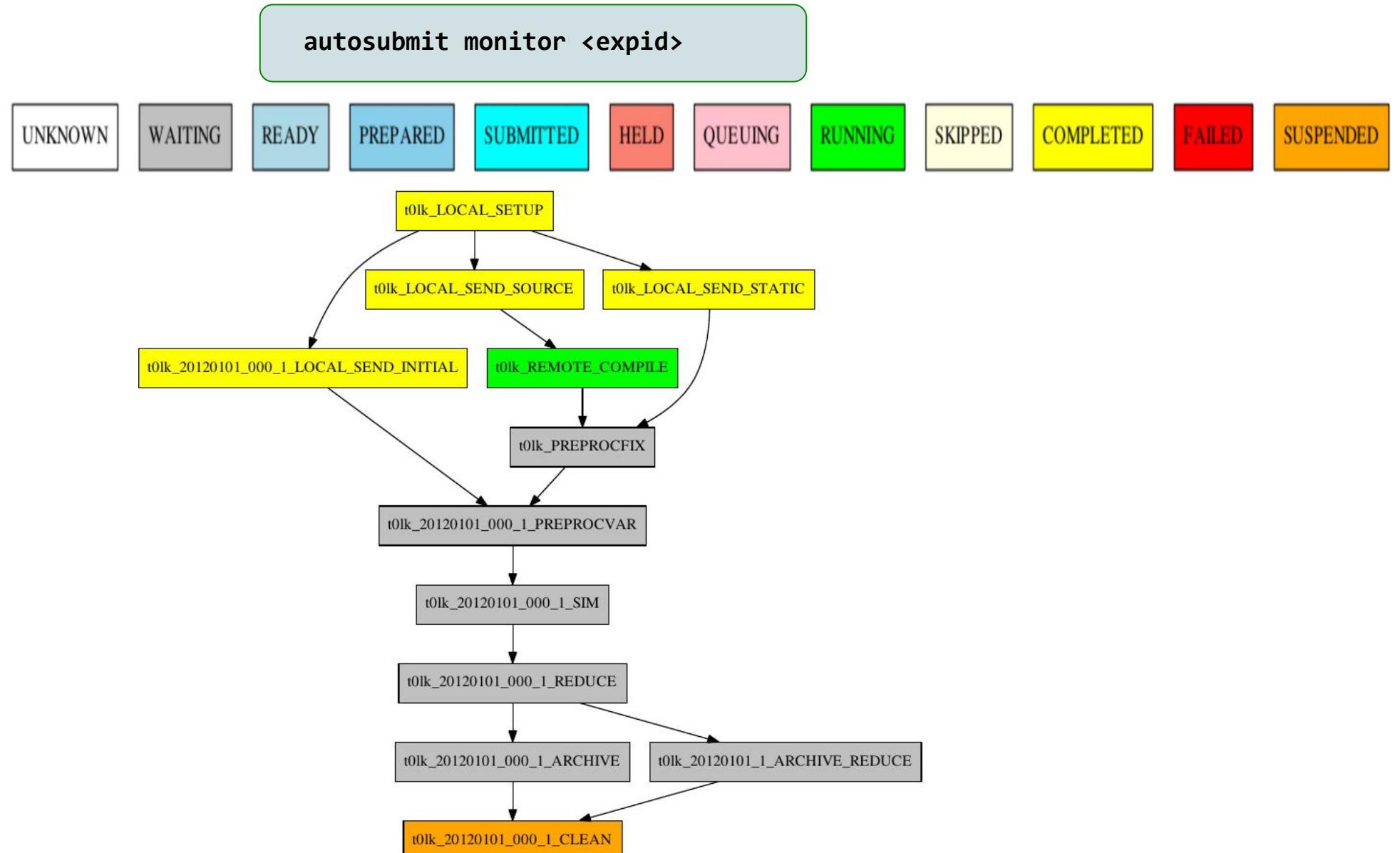
Monarch - proj conf and folder

Inside the **proj/auto-monarch** directory we can find the scripts, configuration files and source code to run the model:

```
$ ls -l /esarchive/autosubmit/<expid>/proj/auto-monarch/templates
-rw-r--r-- 1 dbeltran Earth 5.1K Nov  6 18:08 clean.sh
-rw-r--r-- 1 dbeltran Earth 12K Nov  6 18:08 compile.sh
drwxr-xr-x 2 dbeltran Earth 4.0K Nov  6 18:08 conf
-rw-r--r-- 1 dbeltran Earth 2.3K Nov  6 18:08 cp_compiled.sh
-rw-r--r-- 1 dbeltran Earth 6.2K Nov  6 18:08 da.sh
-rw-r--r-- 1 dbeltran Earth 1.2K Nov  6 18:08 get_out_files.sh
-rw-r--r-- 1 dbeltran Earth 1.5K Nov  6 18:08 local_send_initial_DA.sh
-rw-r--r-- 1 dbeltran Earth 2.9K Nov  6 18:08 local_send_source.sh
-rw-r--r-- 1 dbeltran Earth 4.6K Nov  6 18:08 local_send_static.sh
-rw-r--r-- 1 dbeltran Earth 5.5K Nov  6 18:08 reduce.sh
drwxr-xr-x 2 dbeltran Earth 4.0K Nov 13 16:15 remoteselectup
-rw-r--r-- 1 dbeltran Earth 41K Nov  6 18:08 sim.sh
```

open file **conf/proj_XXXX.conf**. You will find there several MONARCH configuration parameters and values.

Monarch - Monitor



Monarch - Expand Workflow

Edit `expdef_<expid>.conf` and add an higher Number of chunks

`NUMCHUNKS = 4`

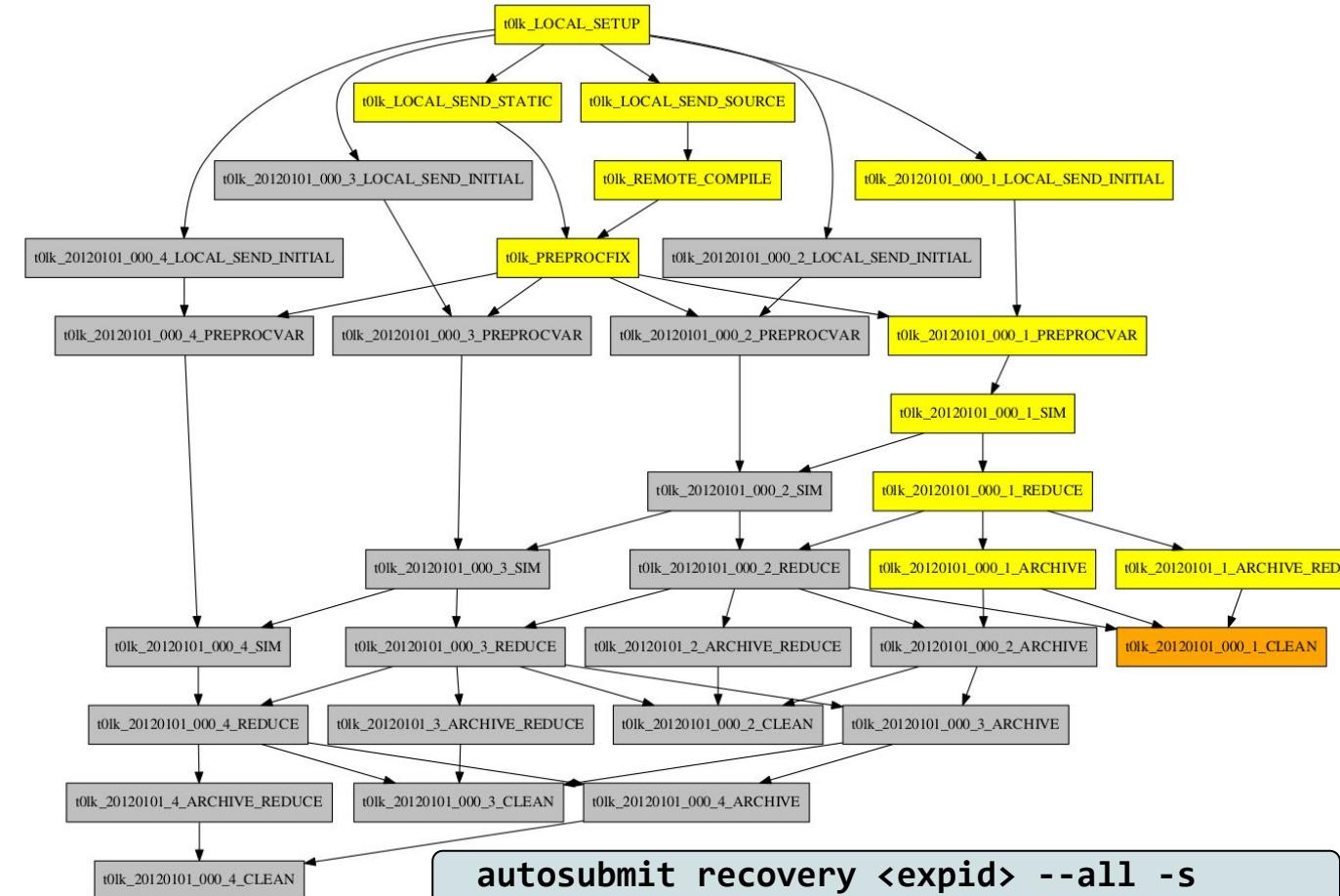
Jobs affected:

- [LOCAL_SEND_INITIAL]
- [PREPROCVAR]
- [SIM]
- [ARCHIVE]
- [REDUCE]
- [ARCHIVE_REDUCER]
- [CLEAN]

Resume run with
`autosubmit run <expid>`

`autosubmit monitor <expid>`

`autosubmit setstatus <expid> -t WAITING -ft CLEAN -s`



Monarch - Integrate a wrapper

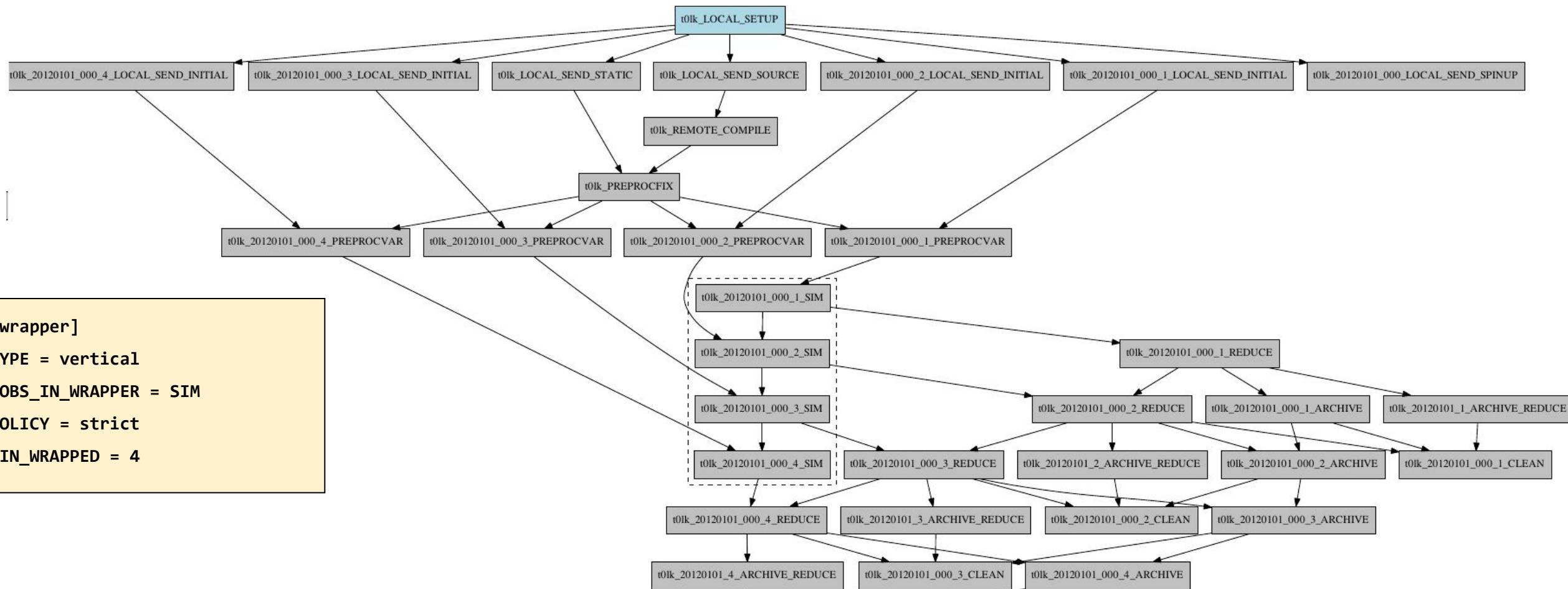
The idea is that any use case has a wrapper to speed up the workflow

Dimension	Vertical 1D	Vertical > 1D	
Horizontal 1D	-----	Vertical wrapper Speed up sequential chunks	
Horizontal > 1D	Horizontal wrapper Run independent jobs in parallel	Horizontal-vertical Speed up sequential series of parallel independent jobs	Vertical-horizontal Speed up parallel series of sequential chunks

Monarch - Wrapper

Edit `Autosubmit_<expid>.conf` and add an vertical wrapper (or just uncomment)

To previsualize the wrappers without complete them:
`autosubmit create <expid> -cw`
`autosubmit monitor <expid> -cw`



Monarch - Common commands

autosubmit refresh

Update project experiment folder.

autosubmit inspect

Generates a preview of the job scripts combined with AS settings (templates).

autosubmit recovery

Synchronizes the status of the remote platform with the local platform.

autosubmit setstatus

Allows to change the status of the workflow.

Contact

Get involved or contact us:

Autosubmit GitLab:

<https://earth.bsc.es/gitlab/es/autosubmit>

Autosubmit Mailing List:

autosubmit@bsc.es



**Barcelona
Supercomputing
Center**

Centro Nacional de Supercomputación



**Barcelona
Supercomputing
Center**
Centro Nacional de Supercomputación

Thank you for your time

daniel.beltran@bsc.es, miguel.castrillo@bsc.es, wilmer.uruchi@bsc.es

ISSUE: Clean 1 was ran

Edit proj.conf

COUPLE_DUST_INIT=1

SPINUP_FOLDER= /gpfs/archive/bsc32/esarchive/exp/monarch/<expid>/original_files