# ESM Tools r6.27 UserManual

Dirk Barbi, Nadine Wieters, Paul Gierz, Fatemeh Chegini, Miguel Andrés-Martínez, Deniz Ural

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# INTRODUCTION

Welcome to the user documentation of the ESM-Tools software.

*ESM-Tools* is a collection of command-line tools to download and build different simulation models for the Earth system, such as atmosphere, ocean, biogeochemistry, hydrology, sea-ice and ice-sheet models, as well as coupled Earth System Models (ESMs). It also includes the functionality to write unified runscripts to carry out model simulations for different model setups (standalone and ESMs) on different High Performance Computing (HPC) systems.

*ESM-Tools* consists of the following command line tools:

Tool	Description	Documenta-
		tion
esm_tools	Basic command to return information about <i>ESM-Tools</i> and create config files.	ESM Tools
esm_master	Command to download and build a model or ESM	ESM Master
esm_runscripts	Command to execute a simulation	ESM Runscripts

A short roadmap on how to run a model or ESM with ESM-Tools is given in the section Ten Steps to a Running Model.

*ESM-Tools* strongly seperates back-end code and the configuration of model or machine dependent information. A description about the syntax of these configuration files is given in the section *YAML File Syntax*.

A list of supported model components are given in the section *Supported Models*.

You are very welcome to contribute to this document. Please find more information on how to contribute here and contact the authors for feedback.

# **GET ESM-TOOLS**

# 2.1 Downloading

*ESM-Tools* is hosted on https://github.com/esm-tools/esm\_tools. To get access to the software you need to be able to log into https://github.com.

Then you can start by cloning the repository esm\_tools.git. Type into a terminal of the HPC or computer of your choice the following command line:

\$ git clone https://github.com/esm-tools/esm\_tools.git

This will create a local repository of *ESM-Tools* in a folder named esm\_tools. This repository includes a collection of *yaml* configuration files containing all the information on models, coupled setups, machines, etc. in the subfolder config, default namelists in the folder namelists, example runscripts for a large number of models on different HPC systems in subfolder runscripts, and this documention in docs. Also you will find the installer install.sh used to install the python packages.

More information on the installation of *ESM-Tools* can be found in the section *Installation* or also in the section *Ten Steps to a Running Model*.

# 2.2 Accessing components in DKRZ server

Some of the *ESM-Tools* components are hosted in the gitlab.dkrz.de servers. To be able to reach these components you will need:

- 1. A DKRZ account (https://www.dkrz.de/up/my-dkrz/getting-started/account/DKRZ-user-account).
- 2. Request access to the repository from the corresponding author of the component if necessary. Feel free to contact us if you don't know who the model developers are or check the *Supported Models* section.

# THREE

# **BEFORE YOU CONTINUE**

You will need python version 3.7 or later, a version of git that is not ancient (everything newer than 2.10 should be good), and up-to-date pip (pip install -U pip) to install the *ESM-Tools*. That means that on the supported machines, you could for example use the following settings:

machine	Settings
albedo	
	<pre>\$ module load git</pre>
	<pre>\$ module load python</pre>
levante.dkrz.de	
	<pre>\$ module load git</pre>
	<pre>\$ module load python3</pre>
glogin.hlrn.de/blogin.hlrn.de	
	<pre>\$ module load git</pre>
	<pre>\$ module load anaconda3</pre>
juwels.fz-juelich.de	
	<pre>\$ module load Stages/2022</pre>
	<pre>\$ module load git</pre>
	<pre>\$ module load Python/3.9.6</pre>
aleph	
	<pre>\$ module load git</pre>
	<pre>\$ module load python</pre>

**Note:** Note that some machines might raise an error conflict netcdf\_c when loading anaconda3. In that case you will need to swap netcdf\_c with anaconda3:

# **TEN STEPS TO A RUNNING MODEL**

1. Make sure you have git installed with version newer than 2.13, that the python version is 3.6 or later (see also *Before you continue*), and that pip is up-to-date (pip install -U pip). Also make sure that the location to which the python binaries will be installed (which is ~/.local/bin by default) is in your PATH. For that purpose, add the following lines to one of your login or profile files, i.e. ~/.bash\_profile, ~/.bashrc, ~/.profile, etc.:

```
$ export PATH=$PATH:~/.local/bin
$ export LC_ALL=en_US.UTF-8
$ export LANG=en_US.UTF-8
```

- 2. Make sure you have a GitHub account and check our GitHub repository (https://github.com/esm-tools/ esm\_tools).
- 3. Download the git repository esm\_tools.git from GitHub:

```
$ git clone https://github.com/esm-tools/esm_tools.git
```

4. In the new folder esm\_tools, run the installer:

\$ cd esm\_tools
\$ ./install.sh

This should install the python packages of *ESM-Tools*. If you wonder where they end up, take a look at ~/. local/lib/python%versionnumber%/site-packages.

- 5. Run esm\_master once. You should see a long list of available targets if everything works.
- 6. Go to the toplevel folder into which you want to install your model codes, and run esm\_master install-, followed by the name and the version of the model you want to install. As an example, if we want to install FESOM2:

```
$ cd /some/folder/you/wish/to/work/in
$ mkdir model_codes
$ cd model_codes
$ esm_master install-fesom-2.0
```

You will be asked for your password to the repository of the model you are trying to install. If you don't have access to that repo yet, esm\_master will not be able to install the model; you will have to contact the model developers to be granted access. A list of supported model can be found in the section *Supported Models*. Feel free to contact us if you don't know who the model developers are.

7. Check if the installation process worked; if so, you should find the model executable in the subfolder bin of the model folder. E.g.:

```
$ ls fesom-2.0/bin
```

8. Go back to the esm\_tools folder, and pick a sample runscript from the runscripts subfolder. These examples are very short and can be easily adapted. Pick one that is for the model you want to run, and maybe already adapted to the HPC system you are working on. Make sure to adapt the paths to your personal settings, e.g. model\_dir, base\_dir etc.:

```
$ cd <PATH TO ESM TOOLS>/esm_tools/runscripts/fesom2
$ (your_favourite_editor) fesom2-ollie-initial-monthly.yaml
```

Notice that the examples exist with the endings .yaml.

9. Run a check of the simulation to see if all needed files are found, and everything works as expected:

\$ esm\_runscripts fesom2-ollie-initial-monthly.yaml -e my\_first\_test -c

The command line option -c specifies that this is a check run, which means that all the preparations, file system operations, ... are performed as for a normal simulation, but then the simulation will stop before actually submitting itself to the compute nodes and executing the experiment. You will see a ton of output on the screen that you should check for correctness before continuing, this includes:

- information about missing files that could not be copied to the experiment folder
- namelists that will be used during the run
- the miniature .run script that is submitted the compute nodes, which also shows the environment that will be used

You can also check directly if the job folder looks like expected. You can find it at \$BASE\_DIR/\$EXP\_ID/ run\_xxxxxxxxx, where BASE\_DIR was set in your runscript, EXP\_ID (probably) on the command line, and run\_xxxxxxxxx stands for the first chunk of your chain job. You can check the work folder, which is located at \$BASE\_DIR/\$EXP\_ID/run\_xxxxxxxx/work, as well as the complete configuration used to generate the simulation, located at \$BASE\_DIR/\$EXP\_ID/run\_xxxxxxxxx/log.

10. Run the experiment:

\$ esm\_runscripts fesom2-ollie-initial-monthly.yaml -e my\_first\_test

That should really be it. Good luck!

FIVE

### INSTALLATION

### 5.1 Prerequisite

Make sure you have installed or loaded a python version that is 3.7 or later but not newer than 3.10 (see also *Before you continue*). Use a pip version that is up-to-date (to update run pip install -U pip). Also make sure that the location to which the python binaries of *ESM-Tools* will be installed (which is ~/.local/bin by default) is in your PATH. For that purpose, add the following lines to one of your login or profile files, i.e. ~/.bash\_profile, ~/.bashrc, ~/.profile, etc.:

```
$ export PATH=$PATH:~/.local/bin
$ export LC_ALL=en_US.UTF-8
```

\$ export LANG=en\_US.UTF-8

# 5.2 Installing in local environment

After downloading the *ESM-Tools* software (see *Get ESM-Tools*) you have a new folder named esm\_tools. In this new folder you find the script to install *ESM-Tools* on the HPC your are running this install script on.

To change into the new folder and execute the instalation script, execute the following commands:

```
$ cd esm_tools
$ ./install.sh
```

This should install all necessary python packages of *ESM-Tools*. If you wonder where they end up, take a look at ~/.local/lib/python%versionnumber%/site-packages.

To see where ESM-Tools are installed, run the following command:

```
$ which esm_tools
```

A possible (default) output can be ~/.local/bin/esm\_tools.

# 5.3 Installing using pip

tbd

# 5.4 Installing in a conda environment

Work in progress. We are still testing it.

# 5.5 Update ESM-Tools

If you installed in editable mode as described above, you can update ESM-Tools by using git:

```
$ cd esm_tools
$ git pull origin release
```

# 5.6 Uninstall ESM-Tools

We are sorry to see you go! To uninstall your current installation make sure you have the most recent version of pip available for your system:

```
$ python3 -m pip install -U pip
```

Then, you can use use the following command to uninstall all *ESM-Tools* packages:

\$ pip freeze | grep esm | xargs pip uninstall -y

You can also choose to manually uninstall. In order to do that, remove the installed Python packages and delete the esm\_\* executables. The following commands will do the trick if you installed with the install.sh script or installed using pip with user mode

```
$ rm -ri ~/.local/bin/esm*
$ rm -ri ~/.local/lib/python3.<version>/site-packages/esm*
```

Note that you may have a different Python version, so the second command might need to be adapted. You may also use pip to uninstall any of the packages:

```
$ pip uninstall [--user] esm-tools
```

The --user flag may be required when using pip if you are not uninstalling in either a virtual environment or a global install (you would need to be root in that case).

# **ESM TOOLS**

*ESM-Tools* includes also a command line tool named esm\_tools. It can be used to interact with several parts of our software. esm\_tools can be used with the following options and subcommands:

# 6.1 Options

esm_tools options	Description
version	Shows the version of the currently used esm-tools.
help	Prints usage information about esm_tools

# 6.2 Subcommands

esm_tools sub-	Options	Argu-	Descritpion
command		ments	
create-new-	help, -t ortype [component	NAME	Opens your \$EDITOR and creates a
config	(default) setup machine]		new file for NAME
test-state	help		Prints the state of the last tested ex-
			periments.

### 6.2.1 Usage: Top level command

To show all top-level command options and subcommands:

```
$ esm_tools --help
Usage: esm_tools [OPTIONS] COMMAND [ARGS]...
Options:
    --version Show the version and exit.
    --help Show this message and exit.
Commands:
    create-new-config Opens your $EDITOR and creates a new file for NAME
    test-state Prints the state of the last tested experiments.
```

### 6.2.2 Usage: Getting the Version

You can get the version number of the currently used esm\_tools installation with:

```
$ esm_tools --version
esm_tools, version 6.20.1
```

### 6.2.3 Usage: Checking current testing state

You can get the current state of our automatic tests with:

```
$ esm_tools test-state
```

### 6.2.4 Usage: Create a new configuration

You can get a pre-generated template to add a new component with:

```
$ esm_tools create-new-config <MY_NEW_CONFIG_NAME>
Creating a new component configuration for my_new_thing
```

```
...EDITOR OPENS....
```

```
Thank you! The new configuration has been saved. Please commit it (and get in touch with

→ the

ESM-Tools team if you need help)!
```

You can also specify if you want to create a new setup, component or machine configuration file by giving the option -t or --type to the subcommand:

\$ esm\_tools create-new-config --type setup <MY\_NEW\_SETUP\_NAME>

Note however that there is (as of this writing) no template available for setups!

### SEVEN

## YAML FILE SYNTAX

### 7.1 What Is YAML?

*YAML* is a structured data format oriented to human-readability. Because of this property, it is the chosen format for configuration and runscript files in *ESM-Tools* and the recommended format for runscripts (though bash runscripts are still supported). These *YAML* files are read by the *esm\_parser* and then converted into a Python dictionary. The functionality of the *YAML* files is further expanded through the *esm\_parser* and other *ESM-Tools* packages (i.e. calendar math through the *esm\_calendar*). The idea behind the implementation of the *YAML* format in *ESM-Tools* is that the user only needs to create or edit easy-to-write *YAML* files to run a model or a coupled setup, speeding up the configuration process, avoiding bugs and complex syntax. The same should apply to developers that would like to implement their models in *ESM-Tools*: the implementation consists on the configuration of a few *YAML* files.

**Warning:** *Tabs* are not allowed as *yaml* indentation, and therefore, *ESM-Tools* will return an error every time a *yaml* file with *tabs* is invoked (e.g. *runscripts* and *config* files need to be '*tab-free*').

### 7.1.1 YAML-Specific Syntax

The main YAML elements relevant to ESM-Tools are:

• Scalars: numbers, strings and booleans, defined by a key followed by : and a value, i.e.:

```
model: fesom
version: "2.0"
time_step: 1800
```

• Lists: a collection of elements defined by a *key* followed by : and an indented list of *elements* (numbers, strings or booleans) starting with -, i.e.:

```
namelists:
    - namelist.config
    - namelist.forcing
    - namelist.oce
```

or a list of the same *elements* separated by , inside square brackets [elem1, elem2]:

namelists: [namelist.config, namelist.forcing, namelist.oce]

• Dictionaries: a collection of scalars, lists or dictionaries nested inside a general key, i.e.:

Some relevant **properties** of the YAML format are:

- Only white spaces can be used for indentation. Tabs are not allowed.
- Indentation can be used to structure information in as many levels as required, i.e. a dictionary choose\_resolution that contains a list of dictionaries (T63, T31 and T127):

- This data can be easily imported as Python dictionaries, which is part of what the esm\_parser does.
- : should always be followed by a *white space*.
- Strings can be written both inside quotes (key: "string" or key: 'string') or unquoted (key: string).
- *YAML* format is **case sensitive**.
- It is possible to add **comments** to YAML files using **#** before the comment (same as in Python).

# 7.2 ESM-Tools Extended YAML Syntax

Warning: Work in progress. This chapter might be incomplete. Red statements might be imprecise or not true.

*ESM-Tools* offers extended functionality of the *YAML* files through the *esm\_parser*. The following subsections list the extended *ESM-Tools* syntax for *YAML* files including calendar and math operations (see *Math and Calendar Operations*). The yaml:YAML Elements section lists the *YAML* elements needed for configuration files and runscripts.

### 7.2.1 Variable Calls

Variables defined in a *YAML* file can be invoked on the same file or in other files provided that the file where it is defined is read for the given operation. The syntax for calling an already defined variable is:

"\${name\_of\_the\_variable}"

Variables can be nested in sections. To define a variable using the value of another one that is nested on a section the following syntax is needed:

```
"${<section>.<variable>}"
```

When using *esm\_parser*, variables in components, setups, machine files, general information, etc., are grouped under sections of respective names (i.e. general, ollie, fesom, awicm, ...). To access a variable from a different file than the one in which it is declared it is necessary to reference the file name or label as it follows:

"\${<file\_label>.<section>.<variable>}"

#### Example

Lets take as an example the variable ini\_parent\_exp\_id inside the general section in the *FESOM-REcoM* runscript runscripts/fesom-recom/fesom-recom-ollie-restart-daily.yaml:

```
general:
```

```
setup_name: fesom-recom
[ ... ]
ini_parent_exp_id: restart_test
ini_restart_dir: /work/ollie/mandresm/esm_yaml_test/${ini_parent_exp_id}/restart/
[ ... ]
```

Here we use ini\_parent\_exp\_id to define part of the restart path ini\_restart\_dir. general.ini\_restart\_dir is going to be called from the *FESOM-REcoM* configuration file configs/setups/fesom-recom/fesom-recom. yaml to define the restart directory for *FESOM* fesom.ini\_restart\_dir:

```
[ ... ]
ini_restart_dir: "${general.ini_restart_dir}/fesom/"
[ ... ]
```

Note that this line adds the subfolder /fesom/ to the subdirectory.

If we would like to invoke from the same runscript some of the variables defined in another file, for example the useMPI variable in configs/machines/ollie.yaml, then we would need to use:

a\_new\_variable: "\${ollie.useMPI}"

Bare in mind that these examples will only work if both *FESOM* and *REcoM* are involved in the *ESM-Tool* task triggered and if the task is run in *Ollie* (i.e. it will work for esm\_runscripts fesom-recom-ollie-restart-daily.yaml -e <experiment\_id> ...).

### 7.2.2 Switches (choose\_)

A *YAML* list named as choose\_<variable> function as a *switch* that evaluates the given variable. The nested element *keys* inside the choose\_<variable> act as *cases* for the switch and the *values* of this elements are only defined outside of the choose\_<variable> if they belong to the selected case\_key:

```
variable_1: case_key_2
choose_variable_1:
    case_key_1:
        configuration_1: value
        configuration_2: value
        [ ... ]
        case_key_2:
        configuration_1: value
        configuration_2: value
        [ ... ]
    "*":
        configuration_1: value
        configuration_2: value
        [ ... ]
```

The key "\*" or \* works as an *else*.

#### Example

An example that can better illustrate this general description is the *FESOM 2.0* resolution configuration in <PATH>/ esm\_tools/configs/fesom/fesom-2.0.yaml:

```
resolution: CORE2
choose_resolution:
    CORE2:
    nx: 126858
    mesh_dir: "${pool_dir}/meshes/mesh_CORE2_final/"
    nproc: 288
GLOB:
    nx: 830305
```

Here we are selecting the CORE2 as default configuration set for the resolution variable, but we could choose the GLOB configuration in another *YAML* file (i.e. a runscript), to override this default choice.

In the case in which resolution: CORE2, then nx, mesh\_dir and nproc will take the values defined inside the choose\_resolution for CORE2 (126858, runscripts/fesom-recom/fesom-recom-ollie-restart-daily. yaml, and 288 respectively), once resolved by the *esm\_parser*, at the same **nesting level** of the choose\_resolution.

**Note:** choose\_versions inside configuration files is treated in a special way by the *esm\_master*. To avoid conflicts in case an additional choose\_versions is needed, include the compilation information inside a compile\_infos section (including the choose\_versions switch containing compilation information). Outside of this exception, it is possible to use as many choose\_<variable> repetitions as needed.

### 7.2.3 Append to an Existing List (add\_)

Given an existing list list1 or dictionary:

list1:
 - element1
 - element2

it is possible to add members to this list/dictionary by using the following syntax:

```
add_list1:
        - element3
        - element4
```

so that the variable list1 at the end of the parsing will contain [element1, element2, element3, element4]. This is not only useful when you need to build the list piecewise (i.e. and expansion of a list inside a choose\_ switch) but also as the *YAML File Hierarchy* will cause repeated variables to be overwritten. Adding a nested dictionary in this way merges the add\_<dictionary> content into the <dictionary> with priority to add\_<dictionary> elements inside the same file, and following the *YAML File Hierarchy* for different files.

#### **Properties**

• It is possible to have multiple add\_ for the same variable in the same or even in different files. That means that all the elements contained in the multiple add\_ will be added to the list after the parsing.

#### Exceptions

Exceptions to add\_ apply only to the environment and namelist \_changes (see *Environment and Namelist Changes* (*\_changes*)). For variables of the type \_changes, an add\_ is only needed if the same \_changes block repeats inside the same file. Otherwise, the \_changes block does not overwrite the same \_changes block in other files, but their elements are combined.

#### Example

In the configuration file for *ECHAM* (configs/components/echam/echam.yaml) the list input\_files is declared as:

```
[ ... ]
input_files:
    "cldoptprops": "cldoptprops"
    "janspec": "janspec"
    "jansurf": "jansurf"
    "rrtmglw": "rrtmglw"
    "rrtmgsw": "rrtmgsw"
    "tslclim": "tslclim"
    "vgratclim": "vgratclim"
    "vltclim": "vltclim"
```

[ ... ]

However different *ECHAM* scenarios require additional input files, for example the HIST scenario needs a MAC-SP element to be added and we use the add\_ functionality to do that:

[ ... ] choose\_scenario: [ ... ]

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```
HIST:
	forcing_files:
		[ ... ]
		add_input_files:
		MAC-SP: MAC-SP
	[ ... ]
```

An example for the \_changes exception can be also found in the same ECHAM configuration file. Namelist changes necessary for *ECHAM* are defined inside this file as:

```
[ ... ]
namelist_changes:
namelist.echam:
runctl:
    out_expname: ${general.expid}
    dt_start:
        - ${pseudo_start_date!year}
        - ${pseudo_start_date!month}
        [ ... ]
```

This changes specified here will be combined with changes in other files (i.e. echam.namelist\_changes in the coupled setups *AWICM* or *AWIESM* configuration files), not overwritten. However, *ECHAM*'s version 6.3. 05p2-concurrent\_radiation needs of further namelist changes written down in the same file inside a choose\_ block and for that we need to use the add\_ functionality:

```
[ ... ]
choose_version:
  [ ... ]
  6.3.05p2-concurrent_radiation:
     [ ... ]
     add_namelist_changes:
        namelist.echam:
        runctl:
            npromar: "${npromar}"
        parctl:
     [ ... ]
```

### 7.2.4 Remove Elements from a List/Dictionary (remove\_)

It is possible to remove elements inside list or dictionaries by using the remove\_ functionality which syntax is:

```
remove_<dictionary>: [<element_to_remove1>, <element_to_remove2>, ... ]
```

or:

```
remove_<dictionary>:
    - <element_to_remove1>
    - <element_to_remove2>
    - ...
```

You can also remove specific nested elements of a dictionary separating the keys for the path by .:

#### 7.2.5 Math and Calendar Operations

The following math and calendar operations are supported in YAML files:

#### **Arithmetic Operations**

An element of a *YAML* file can be defined as the result of the addition, subtraction, multiplication or division of variables with the format:

key: "\$(( \${variable\_1} operator \${variable\_2} operator ... \${variable\_n} ))"

The *esm\_parser* supports calendar operations through *esm\_calendar*. When performing calendar operations, variables that are not given in date format need to be followed by their unit for the resulting variable to be also in date format, i.e.:

runtime: \$(( \${end\_date} - \${time\_step}seconds ))

time\_step is a variable that is not given in date format, therefore, it is necessary to use seconds for runtime to be in date format. Another example is to subtract one day from the variable end\_date:

\$(( \${end\_date} - 1days ))

The units available are:

Units supported by arithmetic operations			
calendar units			
	seconds		
	minutes		
	days		
	months		
	years		

#### Extraction of Date Components from a Date

It is possible to extract date components from a *date variable*. The syntax for such an operation is:

"\${variable!date\_component}"

An example to extract the year from the initial\_time variable:

yearnew: "\${initial\_date!syear}"

If initial\_date was 2001-01-01T00:00:00, then yearnew would be 2001.

The date components available are:

Date components		
ssecond	Second from a given date.	
sminute Minute from a given date.		
shour Hour from a given date.		
sday Day from a given date.		
smonth	Month from a given date.	
syear	Year from a given date.	
sdoy	Day of the year, counting from Jan. 1.	

### 7.2.6 Globbing

Globbing allows to use \* as a wildcard in filenames for restart, input and output files. With this feature files can be copied from/to the work directory whose filenames are not completely known. The syntax needed is:

```
file_list: common_pathname*common_pathname
```

Note that this also works together with the List Loops.

#### Example

The component *NEMO* produces one restart file per processor, and the part of the file name relative to the processor is not known. In order to handle copying of restart files under this circumstances, globbing is used in *NEMO*'s configuration file (configs/components/nemo/nemo.yaml):

This will include inside the restart\_in\_sources and restart\_out\_sources lists, all the files sharing the specified common name around the position of the \* symbol, following the same rules used by the Unix shell.

### 7.2.7 Environment and Namelist Changes (\_changes)

The functionality \_changes is used to control environment, namelist and coupling changes. This functionality can be used from config files, but also runscripts. If the same type of \_changes is used both in config files and a runscript for a simulation, the dictionaries are merged following the hierarchy specified in the *YAML File Hierarchy* chapter.

#### **Environment Changes**

Environment changes are used to make changes to the default environment defined in the machine files (esm\_tools/ configs/machines/<name\_of\_the\_machine>.yaml). There are three types of environment changes:

Key	Description	
environment_	changes for both the compilation and the runtime environments.	
compiletime_	compiletime_erChiangementhchangesment applied only during compilation.	
runtime_envir@margeschahgesvironment applied only during runtime.		

Two types of *yaml* elements can be nested inside an environment changes: add\_module\_actions and add\_export\_vars.

- Use add\_module\_actions to include one *module* command or a list of them. The shell command module is already invoked by *ESM-Tools*, therefore you only need to list the options (i.e. load/unload <module\_name>).
- Use add\_export\_vars to export one or a list of environment variables. Shell command export is not needed here, just define the variable as VAR\_NAME: VAR\_VALUE or as a nested dictionary.

#### **Syntax**

add\_export\_vars can be defined as a dictionary or a list of strings (list of strings will be deprecated from version 7.0 onwards). We are strongly encourage to define the export variables as a dictionary.

#### As dictionary

```
[ ... ]
add_export_vars:
    NETCDF_DIR: /sw/dataformats/netcdf/intel.18/4.7.3/skl/
    LD_LIBRARY_PATH: '$NETCDF_DIR/lib/:$LD_LIBRARY_PATH'
```

### As list

[...]

```
[ ... ]
add_export_vars:
    "NETCDF_DIR=/sw/dataformats/netcdf/intel.18/4.7.3/skl/"
    "LD_LIBRARY_PATH=$NETCDF_DIR/lib/:$LD_LIBRARY_PATH"
    "NETCDF_CXX_LIBRARIES=$NETCDF_DIR/lib"
[ ... ]
```

**Note:** It is also possible here to use variables that are defined in a yaml file (see also *Variable Calls*). If you need to mix environment variables and *ESM-Tools* variables (defined in a yaml file), please note the following syntax:

• put *ESM-Tools* variables in curly braces (see also *Variable Calls*)

• give the environment variable without curly braces

#### Example

```
[ ... ]
model_dir: "some_path_to_model_dir"
[ ... ]
add_export_vars:
LD_LIBRARY_PATH: '$LD_LIBRARY_PATH:${model_dir}/build/lib'
```

For more information about esm\_environment package, please check ESM Environment.

#### Example

fesom.yaml

The model *FESOM* needs some environment changes for compiling in *Mistral* and *Blogin* HPCs, which are included in *FESOM*'s configuration file (esm\_tools/configs/components/fesom.yaml):

```
[...]
compiletime_environment_changes:
        add_export_vars:
                takenfrom:
                                fesom1
choose_computer.name:
       mistral:
                add_compiletime_environment_changes:
                        add_module_actions:
                                - "unload gcc"
                                - "load gcc/4.8.2"
       blogin:
                add_compiletime_environment_changes:
                        add_export_vars:
                                - "NETCDF_DIR=/sw/dataformats/netcdf/intel.18/4.7.3/skl/"
                                - "LD_LIBRARY_PATH=$NETCDF_DIR/lib/:$LD_LIBRARY_PATH"
                                - "NETCDF_CXX_INCLUDE_DIRECTORIES=$NETCDF_DIR/include"
                                - "NETCDF_CXX_LIBRARIES=$NETCDF_DIR/lib"
                                - "takenfrom='fesom1'"
runtime_environment_changes:
        add_export_vars:
                AWI_FESOM_YAML:
                        output_schedules:
                                        vars: [restart]
                                        unit: ${restart_unit}
                                        first: ${restart_first}
                                        rate: ${restart_rate}
                                         [ ... ]
```

Independently of the computer, fesom.yaml exports always the takenfrom variable for compiling. Because compiletime\_environment\_changes is already defined for that purpose, any compiletime\_environment\_changes in a choose\_ block needs to have an add\_ at the beginning. Here we see that a choose\_ block is used to select which changes to apply compile environment (add\_compiletime\_environment\_changes) depending on the HPC system we are in (*Mistral* or *Blogin*). For more details on how to use the choose\_ and add\_ functionalities see *Switches* (choose\_) and Append to an *Existing List* (add\_).

We also see here how runtime\_environment\_changes is used to add nested information about the output schedules for *FESOM* into an AWI\_FESOM\_YAML variable that will be exported to the runtime environment.

#### **Changing Namelists**

It is also possible to specify namelist changes to a particular section of a namelist:

```
echam:

namelist_changes:

namelist.echam:

runctl:

l_orbvsop87: false

radctl:

co2vmr: 217e-6

ch4vmr: 540e-9

n2ovmr: 245e-9

cecc: 0.017

cobld: 23.8

clonp: -0.008

yr_perp: "remove_from_namelist"
```

In the example above, the *namelist.echam* file is changed in two specific chapters, first the section runctrl parameter l\_orbsvop87 is set to false, and appropriate gas values and orbital values are set in radctl. Note that the special entry "remove\_from\_namelist is used to delete entries. This would translate the following fortran namelist (trucated):

```
&runctl
    l_orbvsop87 = .false.
/

&radctl
    co2vmr = 0.000217
    ch4vmr = 5.4e-07
    n2ovmr = 2.45e-07
    cecc = 0.017
    cobld = 23.8
    clonp = -0.008
/
```

Note that, although we set 1\_orbsvop87 to be false, it is translated to the namelist as a fortran boolean (.false.). This occurs because *ESM-Tools* "understands" that it is writing a fortan namelist and transforms the *yaml* booleans into fortran.

For more examples, check the recipe in the cookbook (Changing Namelist Entries from the Runscript).

#### **Coupling changes**

Coupling changes (coupling\_changes) are typically invoked in the coupling files (esm\_tools/configs/ couplings/), executed before compilation of coupled setups, and consist of a list of shell commands to modify the configuration and make files of the components for their correct compilation for coupling.

For example, in the fesom-1.4+echam-6.3.04p1.yaml used in *AWICM-1.0*, coupling\_changes lists two sed commands to apply the necessary changes to the CMakeLists.txt files for both *FESOM* and *ECHAM*:

```
components:
- echam-6.3.04p1
- fesom-1.4
- oasis3mct-2.8
coupling_changes:
- sed -i '/FESOM_COUPLED/s/OFF/ON/g' fesom-1.4/CMakeLists.txt
- sed -i '/ECHAM6_COUPLED/s/OFF/ON/g' echam-6.3.04p1/CMakeLists.txt
```

### 7.2.8 List Loops

This functionality allows for basic looping through a YAML list. The syntax for this is:

"[[list\_to\_loop\_through-->ELEMENT\_OF\_THE\_LIST]]"

where ELEMENT\_OF\_THE\_LIST can be used in the same line as a variable. This is particularly useful to handle files which names contain common strings (i.e. *outdata* and *restart* files, see *File Dictionaries*).

The following example uses the list loop functionality inside the fesom-2.0.yaml configuration file to specify which files need to be copied from the *work* directory of runs into the general experiment *outdata* directory. The files to be copied for runs modeling a couple of months in year 2001 are a\_ice.fesom.2001.nc, alpha.fesom.2001. nc, atmice\_x.fesom.2001.nc, etc. The string .fesom.2001.nc is present in all files so we can use the list loop functionality together with calendar operations (*Math and Calendar Operations*) to have a cleaner and more generalized configure file. First, you need to declare the list of unshared names:

```
outputs: [a_ice,alpha,atmice_x, ... ]
```

Then, you need to declare the outdata\_sources dictionary:

Here, "[[outputs-->OUTPUT]]": provides the *keys* for this dictionary as a\_ice, alpha, atmice\_x, etc., and OUTPUT is later used in the *value* to construct the complete file name (a\_ice.fesom.2001.nc, alpha.fesom.2001.nc, atmice\_x.fesom.2001.nc, etc.).

Finally, outdata\_targets dictionary can be defined to give different names to *outdata* files from different runs using *calendar operations*:

```
outdata_targets:
    "[[outputs-->OUTPUT]]": OUTPUT.fesom.${start_date!syear!smonth}.${start_date!sday}.
    onc
```

The values for the *keys* a\_ice, alpha, atmice\_x, ..., will be a\_ice.fesom.200101.01.nc, alpha.fesom. 200101.01.nc, atmice\_x.fesom.200101.01.nc, ..., for a January run, and a\_ice.fesom.200102.01.nc, alpha.fesom.200102.01.nc, atmice\_x.fesom.200102.01.nc, ..., for a February run.

### 7.2.9 File Dictionaries

File dictionaries are a special type of *YAML* elements that are useful to handle input, output, forcing, logging, binary and restart files among others (see *File Dictionary Types* table), and that are normally defined inside the *configuration files* of models. File dictionary's *keys* are composed by a file dictionary type followed by \_ and an option, and the *elements* consist of a list of file\_tags as *keys* with their respective file\_paths as *values*:

```
type_option:
    file_tag1: file_path1
    file_tag2: file_path2
```

The file\_tags need to be consistent throughout the different options for files to be correctly handled by ESM-Tools. Exceptionally, sources files can be tagged differently but then the option files is required to link sources tags to general tags used by the other options (see *File Dictionary Options* table below).

### **File Dictionary Types**

Key	Description		
analysis	User's files for their own analysis tools (i.e. to be used in the pre-/postprocessing).		
bin	Binary files.		
config	Configure sources.		
couple	Coupling files.		
ignore	Files to be ignored in the copying process.		
forcing	Forcing files. An example is described at the end of this section.		
log	Log files.		
mon	Monitoring files.		
outdata	Output configuration files. A concise example is described in <i>List Loops</i> .		
restart_in	Restart files to be copied from the experiment directory into the run directory (see Experiment		
	<i>Directory Structure</i> ), during the beginning of the <i>computing phase</i> (e.g. to copy restart files from		
	the previous step into the new run folder).		
restart_out	Restart files to be copied from the <b>run directory</b> into the <b>experiment directory</b> (see <i>Experiment</i>		
	Directory Structure), during the tidy and resubmit phase (e.g. to copy the output restart files from		
	a finished run into the <b>experiment directory</b> for later use the next run).		
viz	Files for the visualization tool.		

#### **File Dictionary Options**

Key	Description		
sources	Source file paths or source file names to be copied to the target path. Without this option no		
	files will be handled by ESM-Tools. If targets option is not defined, the files are copied int		
	the default <i>target</i> directory with the same name as in the <i>source</i> directory. In that case, if two		
	files have the same name they are both renamed to end in the dates corresponding to their run		
	(file_name.extension_YYYYMMDD_YYYYMMDD).		
files	Links the general file tags (key) to the source elements defined in sources. files is optional.		
	If not present, all <i>source</i> files are copied to the <i>target</i> directory, and the <i>source tags</i> need to be the		
	same as the ones in in_work and targets. If present, only the source files included in files		
	will be copied (see the ECHAM forcing files example below).		
in_work	Files inside the <i>work</i> directory of a run ( <base_dir>/<experiment_name>/</experiment_name></base_dir>		
	run_date1_date2/work) to be transferred to the <i>target</i> directory. This files copy to the		
	target path even if they are not included inside the files option. in_work is optional.		
targets	Paths and new names to be given to files transferred from the sources directory to the target di-		
_	rectory. A concised example is described in <i>List Loops</i> . targets is optional.		

File paths can be absolute, but most of the type\_option combinations have a default folder assigned, so that you can choose to specify only the file name. The default folders are:

Default	sources	in_work	targets	
folders				
bin				
config				
ignore				
forcing				
log				
outdata	<base_dir>/</base_dir>	<base_dir>/</base_dir>	<base_dir>/</base_dir>	
	<experiment_name>/</experiment_name>	<experiment_name>/</experiment_name>	<experiment_name>/</experiment_name>	
	run_date1_date2/work	run_date1_date2/work	outdata/ <model></model>	
restart_ir				
restart_out				

#### Example for ECHAM forcing files

The *ECHAM* configuration file (<PATH>/configs/echam/echam.yaml) allows for choosing different scenarios for a run. These scenarios depend on different combinations of forcing files. File sources for all cases are first stored in echam.datasets.yaml (a further\_reading file) as:

```
forcing_sources:
    # sst
    "amipsst":
        "${forcing_dir}/amip/${resolution}_amipsst_@YEAR@.nc":
            from: 1870
            to: 2016
    "pisst": "${forcing_dir}/${resolution}${ocean_resolution}_piControl-LR_sst_1880-
    $2379.nc"
    # sic
    "amipsic":
        "${forcing_dir}/amip/${resolution}_amipsic_@YEAR@.nc":
        "${forcing_dir}/amip/${forcing_dir}}
        "${forcing_dir}/amip/${forcing_dir}}
        "${forcing_dir}/amip/${forcing_dir}}
        "${forcing_dir}/amip/${forcing_dir}}
        "${forcing_dir}/amip/${forcing_dir}}
        "${forcing_dir}/amip/${forcing_dir}}
        "${forcing_dir}/amip/${forcing_dir}}
        "${forcing_dir}
        "${forcing_dir}}
        "${forcing_dir}/amip/${forcing_dir}}
        "${forcing_dir}
        "${forcing_dir}}
        "${forcing_dir}
        "${forcing_dir}}
        "${forcing_dir}
        "${forcing_dir}}
        "${forcing_dir}]
        "${forcing_dir}
        "${forcing_dir}]
        "${forcing_dir}
        "${forcing_dir}]
        "${forcin
```

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```
from: 1870
    to: 2016
    "pisic": "${forcing_dir}/${resolution}${ocean_resolution}_piControl-LR_sic_1880-
    ...]
```

Here forcing\_sources store all the sources necessary for all *ECHAM* scenarios, and tag them with source *keys* (amipsst, pisst, ...). Then, it is possible to choose among these source files inside the scenarios defined in echam. yaml using forcing\_files:

```
choose scenario:
      "PI-CTRL":
              forcing_files:
                      sst: pisst
                      sic: pisic
                      aerocoarse: piaerocoarse
                      aerofin: piaerofin
                      aerofarir: piaerofarir
                      ozone: piozone
     PALEO:
              forcing_files:
                      aerocoarse: piaerocoarse
                      aerofin: piaerofin
                      aerofarir: piaerofarir
                      ozone: piozone
      [ ... ]
```

This means that for a scenario PI-CTRL the files that are handled by ESM-Tools will be **exclusively** the ones specified inside forcing\_files, defined in the forcing\_sources as pisst, pisic, piaerocoarse, piaerofin, piaerofarir and piozone, and they are tagged with new general *keys* (sst, sic, ...) that are common to all scenarios. The source files not included in forcing\_files won't be used.

#### **File movements**

Inside the file dictionaries realm, it is possible to specify the type of movement you want to carry out (among copy, link and move), for a specific file or file type, and for a given direction. By default all files are copied in all directions.

The syntax for defining a file movement for a given file type is:

```
<model>:
file_movements:
<file_type>:
<direction1>: <copy/link/move>
<direction2>: <copy/link/move>
[ ... ]
```

where the file\_type in one among the File Dictionary Types, and the direction one of the following ones:

Movement file directions			
init_to_exp	Initial files to the corresponding general folder		
exp_to_run	From general to the corresponding run folder		
run_to_work	From run to the work folder on that run		
work_to_run	From the work folder to the corresponding run folder		
all_directions	Directions not specifically defined, use this movement		

It is also possible to do the same for specific files instead of for all files inside a file\_type. The syntax logic is the same:

```
<model>:
file_movements:
    <file_key>:
        <direction1>: <copy/link/move>
        <direction2>: <copy/link/move>
        [ ... ]
```

where file\_key is the key you used to identify your file inside the <file\_type>\_files, having to add to it \_in or \_out if the file is a restart, in order to specify in which direction to apply this.

Movements specific to files are still compatible with the file\_type option, and only the moves specifically defined for files in the file\_movements will differ from those defined using the file\_type.

### 7.2.10 Accessing Variables from the Previous Run (prev\_run)

It is possible to use the prev\_run dictionary, in order to access values of variables from the previous run, in the current run. The idea behind this functionality is that variables from the previous run can be called from the yaml files with a very similar syntax to the one that would be used for the current run.

The syntax for that is as follows:

<your\_var>: \${prev\_run.<path>.<to>.<the>.<var>.<in>.<the>.<previous>.<run>}

For example, let's assume we want to access the *time\_step* from the previous run of a *FESOM* simulation and store it in a variable called *prev\_time\_step*:

prev\_time\_step: \${prev\_run.fesom.time\_step}

Note: Only the single previous simulation loaded

**Warning:** Use this feature only when there is no other way of accessing the information needed. Note that, for example, dates of the previous run are already available in the current run, under variables such as last\_start\_date, parent\_start\_date, etc.

#### Branchoff experiments with prev\_run

If you use prev\_run variables in your model configuration files, esm\_runscripts will require that you define a prev\_run\_config\_file variable in your runscript when you try to run a branchoff experiment. As a branchoff is a way of restarting, esm\_runscripts needs to know which file should use to load the prev\_run information, but (contrary to the regular restarts within the same experiment) finding that file name is a non-trivial task: being a different experiment, the datestamps and restart frequency can differ from the parent experiment to the branchoff experiment. To overcome this problem the user needs to specify the full path to the finished\_config.yaml to be used on the first run of the branchoff experiment:

### 7.2.11 Error-handling and warning syntax

This syntax allows for error-handling and raising of warnings from the configuration files (i.e. *yanl* files in esm\_tools/ configs). For including an error or a warning under a given condition (e.g. choose\_ block for a given selection) use the key words error or warning respectively (if more than one error/warning is present in the section of your file, use add\_error/warning to combine them).

The syntax in the yaml files for triggering warnings or errors is as follows:

```
warning/error:
        <name>: # Name for the specific warning or error
        message: "the message of the warning/error"
        esm_tools_version: ">/</=/!=/version_number" # trigger it under certain ESM-
        →Tools version conditions
        ask_user_to_continue: True/False # Ask user about continuing or stopping the
        →process, only for warnings, errors always kill the process
```

- <name>: what is displayed on the title of the error/warning
- message: the detailed message of the error/warning. You can use *ESM-Tools* variables here (\${<variable>})
- esm\_tools\_version: only trigger this error/warning under given ESM-Tools versions
- ask\_user\_to\_continue: if true, it asks the user whether they want to continue, after displaying the warning. Only works for warnings as errors halt the simulation without asking

Example

```
recom:
choose_scenario:
HIST:
    [ ... ]
PI-CTRL:
    [ ... ]
    "*":
    add_warning:
    "wrong scenario type":
    message: "The scenario you specified (``${recom.scenario}``) is not_
    ...supported!"
    ask_user_to_continue: True
```

If you then define recom.scenario: hist instead of HIST then you'll get the following:

wrong scenario type WARNING \_\_\_\_\_\_\_Section: recom Wrong scenario, scenario hist does not exist ? Do you want to continue (set general.ignore\_config\_warnings: False to avoid\_ \_\_\_quesitoning)?

EIGHT

## **YAML FILE HIERARCHY**

## 8.1 Hierarchy of YAML configuration files

The following graph illustrates the hierarchy of the different YAML configuration files.

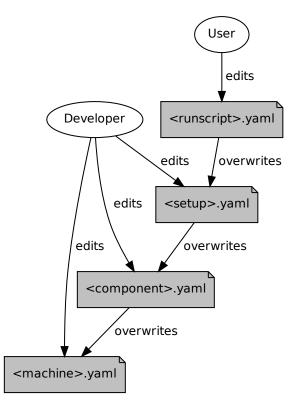


Fig. 1: ESM-Tools configuration files hierarchy

## **ESM-TOOLS VARIABLES**

The *esm\_parser* is used to read the multiple types of *YAML* files contained in *ESM-Tools* (i.e. model and coupling configuration files, machine configurations, runscripts, etc.). Each of these *YAML* files can contain two type of *YAML* elements/variables:

- **Tool-specific elements**: *YAML-scalars*, *lists* or *dictionaries* that include instructions and information used by *ESM-Tools*. These elements are predefined inside the *esm\_parser* or other packages inside *ESM-Tools* and are used to control the *ESM-Tools* functionality.
- Setup/model elements: YAML-scalars, lists of dictionaries that contain information defined in the model/setup config files (i.e. awicm.yaml, fesom.yaml, etc.). This information is model/setup-specific and causes no effect unless it is combined with the tool-specific elements. For example, in fesom.yaml for FESOM-1.0 the variable asforcing exists, however this means nothing to ESM-Tools by its own. In this case, this variable is used in namelist\_changes (a tool-specific element) to state the type of forcing to be used and this is what actually makes a difference to the simulation. The advantage of having this variable already defined and called in namelist\_changes, in the fesom.yaml is that the front-end user can simply change the forcing type by changing the value of asforcing (no need for the front-end user to use namelist\_changes).

The following subsection lists and describes the Tool-specific elements used to operate ESM-Tools.

**Note:** Most of the **Tool-specific elements** can be defined in any file (i.e. *configuration file, runscript, ...*) and, if present in two files used by ESM-Tools at a time, the value is chosen depending on the ESM-Tools file priority/read order (*YAML File Hierarchy*). Ideally, you would like to declare as many elements as possible inside the *configuration files*, to be used by default, and change them in the *runscripts* when necessary. However, it is ultimately up to the user where to setup the Tool-specific elements.

# 9.1 Tool-Specific Elements/Variables

The following keys should/can be provided inside configuration files for models (<PATH>/esm\_tools/configs/ components/<name>.yaml), coupled setups (<PATH>/esm\_tools/configs/setups/<name>.yaml) and runscripts. You can find runscript templates in esm\_tools/runscripts/templates/).

## 9.1.1 Installation variables

Key	Description
model	Name of the model/setup as listed in the config files (esm_tools/configs/components for
	models and esm_tools/configs/setups for setups).
setup_name	Name of the coupled setup.
version	Version of the model/setup (one of the available options in the available_versions list).
avail-	List of supported versions of the component or coupled setup.
able_versions	
git-repository	Address of the model's git repository.
branch	Branch from where to clone.
destination	Name of the folder where the model is downloaded and compiled, in a coupled setup.
comp_command	Command used to compile the component.
install_bins	Path inside the component folder, where the component is compiled by default. This path is
	necessary because, after compilation, ESM-Tools needs to copy the binary from this path to the
	<component setup_path="">/bin folder.</component>
source_code_permissions for the source code using `chmod <source_code_permissions> -R</source_code_permissions>	
	<source_code_folder>.</source_code_folder>

## 9.1.2 Runtime variables

Key	Description	
account	User account of the HPC system to be used to run the experiment.	
model_dir	Absolute path of the model directory (where it was installed by <i>esm_master</i> ).	
setup_dir	Absolute path of the setup directory (where it was installed by <i>esm_master</i> ).	
executable	Name of the component executable file, as it shows in the <component setup_path="">/bin after</component>	
	compilation.	
compute_time	Estimated computing time for a run, used for submitting a job with the job scheduler.	
time_step	Time step of the component in seconds.	
lresume	Boolean to indicate whether the run is an initial run or a restart.	
pool_dir	Path to the pool directory to read in mesh data, forcing files, inputs, etc.	
namelists	List of namelist files required for the model.	
namelist_change	sFunctionality to handle changes in the namelists from the yaml files (see <i>Changing Namelists</i> ).	
nproc	Number of processors to use for the model.	
nproca/nprocb	Number of processors for different MPI tasks/ranks. Incompatible with nproc.	
base_dir	Path to the directory that will contain the experiment folder (where the experiment will be run and	
	data will be stored).	
post_processing	Boolean to indicate whether to run postprocessing or not.	
File Dictio-	YAML dictionaries used to handle input, output, forcing, logging, binary and restart files (see File	
naries	Dictionaries).	
expid	ID of the experiment. This variable can also be defined when calling esm_runscripts with the	
	-e flag.	
ini_restart_exp_	idD of the restarted experiment in case the current experiment has a different expid. For this	
	variable to have an effect lresume needs to be true (e.g. the experiment is a restart).	
ini_restart_dir	Path of the restarted experiment in case the current experiment runs in a different directory. For	
	this variable to have an effect lresume needs to be true (e.g. the experiment is a restart).	
execu-	Command for executing the component, including \${executable} and the necessary flags.	
tion_command		
heteroge-	A boolean that controls whether the simulation needs to be run with or without heterogeneous	
neous_paralleliz	ation approximation and the second se	
	of omp_num_threads defined in the components. When true, open_num_threads needs to	
	be specified for each component using OpenMP. heterogeneous_parallelization variable	
	needs to be defined inside the computer section of the runscript. See Heterogeneous Paral-	
	<i>lelization Run (MPI/OpenMP)</i> for examples.	
omp_num_threa	dA variable to control the number of OpenMP threads used by a component during an hetero-	
	geneous parallelization run. This variable has to be defined inside the section of the com-	
	ponents for which OpenMP needs to be used. This variable will be ignored if computer.	
	heterogeneous_parallelization is not set to true.	
gen-	A boolean to indicate whether esm_runscripts needs to install missing plugins (True, default)	
eral.install_miss	ing_potugfralse). Implemented to solve a problem with the esm_tests CI in GitHub where we	
	might not have access to some repositories.	

## 9.1.3 Calendar variables

Key	Description	
initial_date	Date of the beginning of the simulation in the format YYYY-MM-DD. If the simulation is a	
	restart, initial_date marks the beginning of the restart.	
final_date	Date of the end of the <b>simulation</b> in the format YYYY-MM-DD.	
start_date	Date of the beginning of the <b>current run</b> .	
end_date	Date of the end of the <b>current run</b> .	
current_date	Current date of the run.	
next_date	Next run initial date.	
nyear,	Number of time unit per run. They can be combined (i.e. nyear: 1 and nmonth: 2 implies	
nmonth,	that each run will be 1 year and 2 months long).	
nday, nhour,		
nminute		
parent_date	Ending date of the previous run.	

## 9.1.4 Coupling variables

Key	Description
grids	List of grids and their parameters (i.e. name, nx, ny, etc.).
cou-	List of coupling field dictionaries containing coupling field variables.
pling_fields	
nx	When using <i>oasis3mct</i> , used inside grids to define the first dimension of the grid.
ny	When using <i>oasis3mct</i> , used inside grids to define the second dimension of the grid.
cou-	List of coupling methods and their parameters (i.e. time_transformation, remapping, etc.).
pling_methods	
time_transformation used by <i>oasis3mct</i> , defined inside coupling_methods.	
remapping	Remappings and their parameters, used by <i>oasis3mct</i> , defined inside coupling_methods.

## 9.1.5 Other variables

Key	Description		
metadata	List to incude descriptive information about the model (i.e. Authors, Institute,		
	Publications, etc.) used to produce the content of Supported Models. This information should		
	be organized in nested keys followed by the corresponding description. Nested keys do not receive		
	a special treatment meaning that you can include here any kind of information about the model.		
	Only the Publications key is treated in a particular way: it can consist of a single element or a		
	<i>list</i> , in which each element contains a link to the publication inside <> (i.e Title, Authors,		
	<pre>Journal, Year. <https: doi.org=""></https:>).</pre>		

### TEN

# ESM MASTER

## 10.1 Usage: esm\_master

To use the command line tool esm\_master, just enter at a prompt:

\$ esm\_master

The tool may ask you to configure your settings; which are stored in your home folder under \${HOME}/.esmtoolsrc. A list of available models, coupled setups, and available operations are printed to the screen, e.g.:

```
setups:
    awicm:
        1.0: ['comp', 'clean', 'get', 'update', 'status', 'log', 'install', 'recomp']
        CMIP6: ['comp', 'clean', 'get', 'update', 'status', 'log', 'install', 'recomp']
        2.0: ['comp', 'clean', 'get', 'update', 'status', 'log', 'install', 'recomp']
[...]
```

As can be seen in this example, esm\_master supports operations on the coupled setup awicm in the versions 1.0, CMIP6 and 2.0; and what the tool can do with that setup. You execute esm\_master by calling:

\$ esm\_master operation-software-version,

e.g.:

```
$ esm_master install-awicm-2.0
```

By default, esm\_master supports the following operations:

get:

Cloning the software from a repository, currently supporting git and svn

conf:

Configure the software (only needed by mpiesm and icon at the moment)

comp:

Compile the software. If the software includes libraries, these are compiled first. After compiling the binaries can be found in the subfolders bin and lib.

### clean:

Remove all the compiled object files.

### install:

Shortcut to get, then conf, then comp.

#### recomp:

Shortcut to conf, then clean, then comp.

### update:

Get the newest commit of the software from the repository.

#### status:

Get the state of the local database of the software (e.g. git status)

log:

Get a list of the last commits of the local database of the software (e.g. git log)

To download, compile, and install awicm-2.0; you can say:

```
$ esm_master install-awicm-2.0
```

This will trigger a download, if needed a configuration, and a compilation process. Similarly, you can recompile with recomp-XXX, clean with clean-XXX, or do individual steps, e.g. get, configure, comp.

The download and installation will always occur in the current working directory.

You can get further help with:

\$ esm\_master --help

## 10.2 Configuring esm-master for Compile-Time Overrides

It is possible that some models have special compile-time settings that need to be included, overriding the machine defaults. Rather than placing these changes in configs/machines/NAME.yaml, they can be instead placed in special blocks of the component or model configurations, e.g.:

```
compiletime_environment_changes:
    add_export_vars:
        [ ... ]
```

The same is also possible for specifying runtime\_environment\_changes.

## **ELEVEN**

# **ESM-VERSIONS (DEPRECATED)**

**Note:** Deprecated since version 6.0.0: This feature is deprecated since 2022 (version 6.0.0). If you are using a more recent version of ESM-Tools, please use esm\_tools --version instead, to get the version of *ESM-Tools*. See also section *ESM Tools* and *Usage: Getting the Version*. Please also find further information for e.g. upgrading ESM-Tools here ....

Above version 3.1.5 and below 6.0.0, you will find an executable in your path called esm\_version. This was added by Paul Gierz to help the user / developer to keep track of / upgrade the python packages belonging to ESM Tools.

## 11.1 Usage

It doesn't matter from which folder you call esm\_versions. You have two subcommands:

esm_versions check	gives you the version number of each
	installed esm python package
esm_versions upgrade	upgrades all installed esm python
	packages to the newest version
	of the release branch

Notice that you can also upgrade single python packages, e.g.:

esm_versions upgrade esm_parser	upgrades only the package esm_parser to the newest version of the release branch	
---------------------------------	----------------------------------------------------------------------------------------	--

And yes, esm\_versions can upgrade itself.

## TWELVE

## **ESM RUNSCRIPTS**

# 12.1 Usage

esm\_runscripts [-h] [-d] [-v] [-e EXPID] [-c] [-P] [-j LAST\_JOBTYPE] [-t TASK] [-p PID] [-x EXCLUDE] [-o ONLY] [-r RESUME\_FROM] [-U] runscript

# **12.2 Arguments**

Optional ar-	Description
guments	
-h,help	Show this help message and exit.
-d,debug	Print lots of debugging statements.
-v,	Be verbose.
verbose	
-e EXPID,	The experiment ID to use. Default test.
expid	
EXPID	
-c,check	Run in check mode (don't submit job to supercomputer).
-P,	Write profiling information (esm-tools).
profile	
-j	Write the jobtype this run was called from (esm-tools internal).
LAST_JOBTYP	E,
last_jobt	vpe
LAST_JOBTYP	E
-t TASK,	The task to run. Choose from: compute, post, couple, tidy_and_resubmit.
task	
TASK	
-p PID,	The PID of the task to observe.
pid PID	
-X	E[x]clude this step.
EXCLUDE,	
exclude	
EXCLUDE	
-o ONLY,	[o]nly do this step.
only	
ONLY	
-r	[r]esume from the specified run/step (i.e. to resume a second run you'll need to use -r 2).
RESUME_FROM,	
resume-fro	Dm Contraction of the second se
RESUME_FROM	
-U,	[U]pdate the runscript in the experiment folder and associated files
update	
update-fi	dtypetes the requested files from external sources in a currently ongoing simulation. For example,
	<b>TYPES</b> u want to update the binaries and the configs (namelists) in a resubmission of a experiment you
[UPDATE_FIL	ETAPER this by addingupdate-filetypes bin config to your esm_runscripts command.
]	We strongly advise against using this option unless you really know what you are doing.
-i,	This option can be used to [i]nspect the results of a previous run, for example one prepared with
inspect	-c. This argument needs an additional keyword. Choose among: overview (gives you the same
	litte message you see at the beginning of each run, lastlog (displays the last log file), explog (the
	overall experiment logfile), datefile (the overall experiment logfile), config (the Python dict
	that contains all information), size (the size of the experiment folder), a filename or a directory
	name output the content of the file /directory if found in the last run_ folder.)

## 12.3 Running a Model/Setup

*ESM-Runscripts* is the *ESM-Tools* package that allows the user to run the experiments. *ESM-Runscripts* reads the runscript (either a *bash* or *yaml* file), applies the required changes to the namelists and configuration files, submits the runs of the experiment to the compute nodes, and handles and organizes restart, output and log files. The command to run a runscript is:

\$ esm\_runscripts <runscript.yaml/.run> -e <experiment\_ID>

The runscript.yaml/.run should contain all the information regarding the experiment paths, and particular configurations of the experiment (see the yaml:Runscripts section for more information about the syntax of *yaml* runscripts). The experiment\_ID is used to identify the experiment in the scheduler and to name the experiment's directory (see *Experiment Directory Structure*). Omitting the argument -e <experiment\_ID> will create an experiment with the default experiment ID test.

*ESM-Runscript* allows to run an experiment check by adding the -c flag to the previous command. This check performs all the system operations related to the experiment that would take place on a normal run (creates the experiment directory and subdirectories, copies the binaries and the necessary restart/forcing files, edits the namelists, ...) but stops before submitting the run to the compute nodes. We strongly recommend **running first a check before submitting an experiment to the compute nodes**, as the check outputs contains already valuable information to understand whether the experiment will work correctly or not (we strongly encourage users to pay particular attention to the *Namelists* and the *Missing files* sections of the check's output).

## 12.4 Job Phases

The following table summarizes the job phases of ESM-Runscripts and gives a brief description. ...

# 12.5 Running only part of a job

It's possible to run only part of a job. This is particularly interesting for development work; when you might only want to test a specific phase without having to run a whole simulation.

As an example; let's say you only want to run the tidy phase of a particular job; which will move things from the particular run folder to the overall experiment tree. In this example; the experiment will be called test001:

esm\_runscripts \${PATH\_TO\_USER\_CONFIG} -t tidy\_and\_resubmit

# **12.6 Experiment Directory Structure**

All the files related to a given experiment are saved in the *Experiment Directory*. This includes among others model binaries, libraries, namelists, configuration files, outputs, restarts, etc. The idea behind this approach is that all the necessary files for running an experiment are contained in this folder (the user can always control through the runscript or configuration files whether the large forcing and mesh files also go into this folder), so that the experiment can be reproduced again, for example, even if there were changes into one of the model's binaries or in the original runscript.

The path of the *Experiment Directory* is composed by the general.base\_dir path specified in the runscript (see yaml:Runscripts syntax) followed by the given experiment\_ID during the esm\_runscripts call:

<general.base\_dir>/<experiment\_ID>

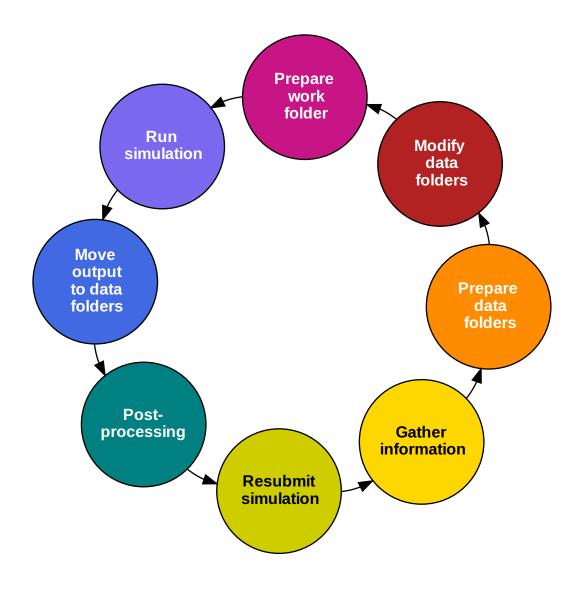
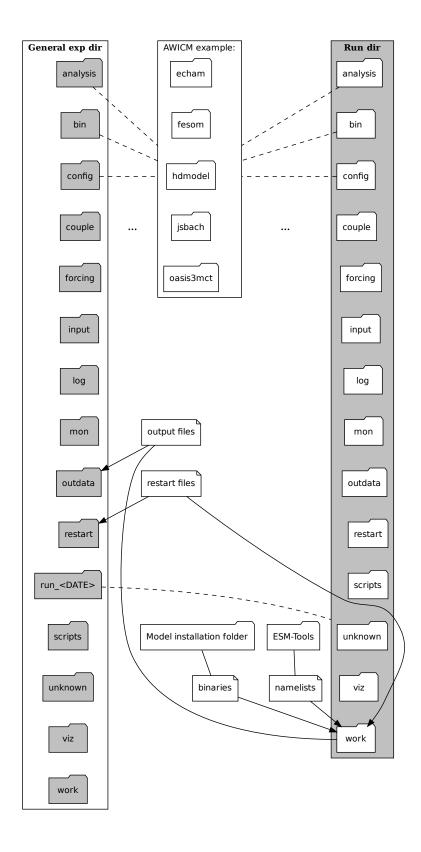


Fig. 1: ESM-Tools job phases

The **main experiment folder** (General exp dir) contains the subfolders indicated in the graph and table below. Each of these subfolders contains a folder for each component in the experiment (i.e. for an AWI-CM experiment the outdata folder will contain the subfolders echam, fesom, hdmodel, jsbach, oasis3mct).

The structure of the **run folder** run\_YYYYMMDD-YYYYMMDD (Run dir in the graph) replicates that of the general experiment folder. *Run* directories are created before each new run and they are useful to debug and restart experiments that have crashed.



Subfolder	Files	Description
analysis	user's files	Results of user's "by-hand" analysis
		can be placed here.
bin	component binaries	Model binaries needed for the exper-
		iment.
config	• <experiment_id>_ fin</experiment_id>	Configuration files for the ex-
	ished_config.yaml	periment including namelists
	namelists	and other files specified in
	other configuration files	the component's configuration
		files ( <path>/esm_tools/</path>
		configs/ <component>/</component>
		<pre><component>.yaml, see</component></pre>
		File Dictionaries). The file
		<pre><experiment_id>_finished_cont</experiment_id></pre>
		yaml is located at the base of the
		config folder and contains the
		whole ESM-Tools variable space
		for the experiment, resulting from
		combining the variables of the
		runscript, setup and component
		configuration files, and the machine
		environment file.
couple	coupling related files	Necessary files for model couplings.
forcing	forcing files	Forcing files for the experiment.
		Only copied here when specified by
		the user in the runscript or in the
		configuration files (File Dictionar-
		ies).
input	input files	Input files for the experiment. Only
		copied here when specified by the
		user in the runscript or in the con-
		figuration files ( <i>File Dictionaries</i> ).
log	• counceriment ID	Experiment log files. The com-
	<ul> <li><experiment_id>_</experiment_id></li> <li><setup_name>.log</setup_name></li> </ul>	ponent specific log files are
	component log files	placed in their respective sub-
	• component log mes	folder. The general log file
		<pre><experiment_id>_<setup_name></setup_name></experiment_id></pre>
		log reports on the ESM-Runscripts
		Job Phases and is located at the base
		of the log folder. Log file names
		and copying instructions should be
		included in the configuration files
		of components (File Dictionaries).
mon	user's files	Monitoring scripts created by the
		user can be placed here.
outdata	outdata files	Outdata files are placed here. Out-
		data file names and copying instruc-
		tions should be included in the con-
		figuration files of components (File
		Dictionaries).
restart	restart files	Restart files are placed here. Restart
		file names and copying instructions
		should be included in the configura-
		tion files of components (File Dic-
		tionaries).
2.6. Experiment Direc	ctory Structure files	Run folder containing all the file
YYYYMMDD		for a given run. Folders contained
		here have the same names as the
		ones contained in the general ex-

If one file was to be copied in a directory containing a file with the same name, both files get renamed by the addition of their start date and end dates at the end of their names (i.e. fesom.clock\_YYYYMMDD-YYYYMMDD).

**Note:** Having a *general* and several *run* subfolders means that files are duplicated and, when models consist of several runs, the *general* directory can end up looking very untidy. *Run* folders were created with the idea that they will be deleted once all files have been transferred to their respective folders in the *general* experiment directory. The default is not to delete this folders as they can be useful for debugging or restarting a crashed simulation, but the user can choose to delete them (see *Cleanup of run\_ directories*).

## 12.7 Cleanup of run\_ directories

This plugin allows you to clean up the run\_\${DATE} folders. To do that you can use the following variables under the general section of your runscript (documentation follows order of code as it is executed):

- clean\_runs: This is the most important variable for most users. It can take the following values:
  - True: removes the run\_ directory after each run (overrides every other clean\_ option).
  - False: does not remove any run\_ directory (default) if no clean\_ variable is defined.
  - <int>: giving an integer as a value results in deleting the run\_ folders except for the last <int> runs (recommended option as it allows for debugging of crashed simulations).

**Note:** clean\_runs: (bool) is incompatible with clean\_this\_rundir and clean\_runs: (int) is incompatible with clean\_old\_rundirs\_except (an error will be raised after the end of the first simulation). The functionality of clean\_runs variable **alone will suffice most of the standard user requirements**. If finer tunning for the removal of **run\_** directories is required you can used the following variables instead of clean\_runs.

- clean\_this\_rundir: (bool) Removes the entire run directory (equivalent to clean\_runs: (bool)). clean\_this\_rundir: True overrides every other clean\_ option.
- clean\_old\_rundirs\_except: (int) Removes the entire run directory except for the last <x> runs (equivalent to clean\_runs: (int)).
- clean\_old\_rundirs\_keep\_every: (int) Removes the entire run directory except every <x>th run. Compatible with clean\_old\_rundirs\_except or clean\_runs: (int).
- clean\_<filetype>\_dir: (bool) Erases the run directory for a specific filetype. Compatible with all the other options.
- clean\_size: (int or float) Erases all files with size greater than clean\_size, must be specified in bytes! Compatible with all the other options.

### Example

To delete all the run\_ directories in your experiment include this into your runscript:

To keep the last 2 run\_ directories:

To keep the last 2 runs and every 5 runs:

# 12.8 Debugging an Experiment

To debug an experiment we recommend checking the following files that you will find, either in the *general* experiment directory or in the *run* subdirectory:

- The ESM-Tools variable space file config/<experiment\_ID>\_finished\_config.yaml.
- The run log file run\_YYYYMMDD-YYYYMMDD/<experiment\_ID>\_compute\_YYYYMMDD-YYYYMMDD\_<JobID>. log`.

For interactive debugging, you may also add the following to the general section of your configuration file. This will enable the pdb Python debugger, and allow you to step through the recipe.

```
general:
    debug_recipe: True
```

## 12.9 Setting the file movement method for filetypes in the runscript

By default, esm\_runscripts copies all files initially into the first run\_-folder, and from there to work. After the run, outputs, logs, restarts etc. are copied from work to run\_, and then moved from there to the overall experiment folder. We chose that as the default setting as it is the safest option, leaving the user with everything belonging to the experiment in one folder. It is also the most disk space consuming, and it makes sense to link some files into the experiment rather than copy them.

As an example, to configure esm\_runscripts for an echam-experiment to link the forcing and inputs, one can add the following to the runscript yaml file:

```
echam:
    file_movements:
        forcing:
            all_directions: "link"
            input:
                 init_to_exp: "link"
                 exp_to_run: "link"
                run_to_work: "link"
                work_to_run: "link"
```

Both ways to set the entries are doing the same thing. It is possible, as in the input case, to set the file movement method independently for each of the directions; the setting all\_directions is just a shortcut if the method is identical for all of them.

## 12.10 Running an experiment with a virtual environment

Running jobs can optionally be encapsulated into a virtual environment.

To use a virtual environment run esm\_runscripts with the flag --contained-run or set use\_venv within the general section of your runscript to True:

general: use\_venv: True

This shields the run from changes made to the remainder of the ESM-Tool installation, and it's strongly recommended for production runs.

**Warning:** Refrain from using this feature if you have installed ESM-Tools within a conda environment. Conda environment installation is still in its testing phase and we cannot evaluate yet which conflicts might arise from combining both the venv of this feature and the environment from conda.

If you choose to use a virtual environment, a local installation will be created in the experiment tree at the begining of the first run into the folder named .venv\_esmtools. That installation will be used for the experiment. It will be installed at the root of your experiment and contains all the Python libraries used by ESM-Tools. The installation at the beginning of the experiment will induce a small overhead (~2-3 minutes).

For example, for a user miguel with a run with expid test ESM-Tools will be installed here:

/scratch/miguel/test/.venv\_esmtools/lib/python3.10/site-packages/esm\_tools

instead of:

/albedo/home/miguel/.local/lib/site-packages/esm\_tools

The virtual environment installs by default the **release** branch, pulling it directly from our GitHub repository. You can choose to override this default by specifying another branch, adding to your runscript:

general: install\_esm\_tools\_branch: '<your\_branch\_name>'

**Warning:** The branch **needs to exist on GitHub** as it is cloned form there, and **not from your local folder**. If you made any changes in your local branch make sure they are pushed before running esm\_runscripts with a virtual environment, so that your changes are included in the virtual environment installation.

You may also select to install esm\_tools in *editable mode*, in which case they will be installed in a folder src/ esm\_tools/ in the root of your experiment. Any changes made to the code in that folder will influence how ESM-Tools behave. To create a virtual environment with ESM-Tools installed in *editable* mode use:

general: install\_<esm\_package>\_editable: true/false

**Note:** When using a virtual environment, config files and namelists will come of the folder .venv\_esmtools listed above and **not** from your user install directory. You should make **all** changes to the namelists and config files via your user runscript (*Changing Namelists*). This is recommended in all cases!!!

THIRTEEN

# **ESM RUNSCRIPTS - USING THE WORKFLOW MANAGER**

## **13.1 Introduction**

Starting with Release 6.0, esm\_runscripts allows the user to define additional subjobs for data processing, arrange them in clusters, and set the order of execution of these and the standard runjob parts in a flexible and short way from the runscript. This is applicable for both pre- and postprocessing, but especially useful for iterative coupling jobs, like e.g. coupling pism to vilma (see below). In this section we explain the basic concept, and the keywords that have to be set in the runscript to make use of this feature.

## 13.2 Subjobs of a normal run

Even before the addition of the workflow manager, the run jobs of esm\_runscript were split into different subjobs, even though that was mostly hidden from the user's view. Before Release 6.0, these subjobs were:

compute --> tidy\_and\_resubmit (incl. wait\_and\_observe + resubmit next run)

Technically, wait\_and\_observe was part of the tidy\_and\_resubmit job, as was the resubmission, including above only for the purpose of demonstrating the difference to the new standard workflow, which is now (post-Release 6.0):

newrun --> prepcompute --> compute --> observe\_compute --> tidy (+ resubmit next run)

Other than before adding the workflow manager, these standard subjobs are all separated and independant subjobs, each submitted (or started) by the previous subjob in one of three ways (see below). The splitting of the old compute job into newrun, prepcompute and compute on one side, and tidy\_and\_resubmit into observe and tidy, was necessary to enable the user to insert coupling subjobs for iterative coupling at the correct places. Here is what each of the standard subjobs does:

Subjob	Function	
newrun	Initializes a new experiment, only very basic stuff, like creating (empty) folders needed by any of the	
	following subjobs. NEEDS TO BE THE FIRST SUBJOB OF ANY EXPERIMENT.	
prepcom-	Prepares the compute job. All the (Python) functionality that needs to be run, up to the job submission.	
pute	Includes copying files, editing namelists, write batch scripts, etc.	
compute	Actual model integration, nothing else. No Python codes involved.	
ob-	Python job running at the same time as compute, checking if the compute job is still running, looking	
serve_computer some known errors for monitoring / job termination.		
tidy	Sorts the produced outputs, restarts and log files into the correct folders, checks for missing and un-	
	known files, builds coupler restart files if not present	

It is important to understand that none of this has to be edited by the users, this is the default setup.

# 13.3 Keywords available for defining additional data processing subjobs

The workflow manager is intended to include shell scripted data processing jobs into the esm\_runscripts workflow, so several things have to be defined:

- Name of the script to be run
- Name of the python script used for setting up the environment
- Name of the folder in which both of the above scripts can be found
- Information on how often the subjob should be called
- Information on between which other subjobs the new subjob should be inserted into the workflow
- In case it isn't clear: Which subjob should resubmit the next run.

The keywords used to define that are:

word         work-       Chapter headline in a model's section, indicating that alterations to the standard workflow will be defined         flow       here         sub-       Section in the workflow chapter, containing the information on additional subjob_clusters. A sub-         job_cluster is a collection of subjobs run from the same batch script. Each subjob needs to belong to         one cluster, if none is defined, each subjob will automatically get assigned to its own cluster. Each entry         in subjob_clusters is a dict, with the outermost key being the (arbitrary) name of the cluster.         sub-         Section in the workflow chapter, containing the information on additional subjobs.         jobs         run_afterEntry in spevifications of a subjob_cluster, to define before or after which other cluster of the workflow this         /       cluster is supposed to run. Only one of the two should be specified. Can also be used in the specifications         run_beformef subjobs if these subjobs get a corresponding cluster auto-assigned.         script:       script_dir:         call_function:       env_preparation:         next_run_triggered_by:       next_run_triggered_by:	Key-	Function
work- flowChapter headline in a model's section, indicating that alterations to the standard workflow will be defined heresub- job_cluster is a collection of subjobs run from the same batch script. Each subjob needs to belong to one cluster, if none is defined, each subjob will automatically get assigned to its own cluster. Each entry in subjob_clusters is a dict, with the outermost key being the (arbitrary) name of the cluster.sub- jobsSection in the workflow chapter, containing the information on additional subjobs.sub- jobsSection in the workflow chapter, containing the information on additional subjobs.sub- jobsSection in the workflow chapter, containing the information on additional subjobs.run_afterEntry in spevifications of a subjob_cluster, to define before or after which other cluster of the workflow this cluster is supposed to run. Only one of the two should be specified. Can also be used in the specifications run_beformer subjobs if these subjobs get a corresponding cluster auto-assigned.script: call_function: env_preparation:script	-	Tunction .
flow       here         sub-       Section in the workflow chapter, containing the information on additional subjob_clusters. A sub- job_cluster is a collection of subjobs run from the same batch script. Each subjob needs to belong to one cluster, if none is defined, each subjob will automatically get assigned to its own cluster. Each entry in subjob_clusters is a dict, with the outermost key being the (arbitrary) name of the cluster.         sub-       Section in the workflow chapter, containing the information on additional subjobs.         jobs       run_afterEntry in spevifications of a subjob_cluster, to define before or after which other cluster of the workflow this cluster is supposed to run. Only one of the two should be specified. Can also be used in the specifications run_beform subjobs if these subjobs get a corresponding cluster auto-assigned.         script:	word	
sub- job_clusterSection in the workflow chapter, containing the information on additional subjob_clusters. A sub- job_cluster is a collection of subjobs run from the same batch script. Each subjob needs to belong to one cluster, if none is defined, each subjob will automatically get assigned to its own cluster. Each entry in subjob_clusters is a dict, with the outermost key being the (arbitrary) name of the cluster.sub- jobsSection in the workflow chapter, containing the information on additional subjobs.sub- jobsSection in the workflow chapter, containing the information on additional subjobs.run_afterEntry in spevifications of a subjob_cluster, to define before or after which other cluster of the workflow this cluster is supposed to run. Only one of the two should be specified. Can also be used in the specifications run_beforef subjobs if these subjobs get a corresponding cluster auto-assigned.script_dir: call_function: env_preparation:call_function: env_preparation:	work-	Chapter headline in a model's section, indicating that alterations to the standard workflow will be defined
job_cluster is a collection of subjobs run from the same batch script. Each subjob needs to belong to one cluster, if none is defined, each subjob will automatically get assigned to its own cluster. Each entry in subjob_clusters is a dict, with the outermost key being the (arbitrary) name of the cluster. sub- jobs run_afterEntry in spevifications of a subjob_cluster, to define before or after which other cluster of the workflow this cluster is supposed to run. Only one of the two should be specified. Can also be used in the specifications run_beformer subjobs if these subjobs get a corresponding cluster auto-assigned. script: call_function: env_preparation:	flow	here
one cluster, if none is defined, each subjob will automatically get assigned to its own cluster. Each entry in subjob_clusters is a dict, with the outermost key being the (arbitrary) name of the cluster.         sub- jobs       Section in the workflow chapter, containing the information on additional subjobs.         run_afterEntry in spevifications of a subjob_cluster, to define before or after which other cluster of the workflow this cluster is supposed to run. Only one of the two should be specified. Can also be used in the specifications run_before f subjobs if these subjobs get a corresponding cluster auto-assigned.         script:	sub-	Section in the workflow chapter, containing the information on additional subjob_clusters. A sub-
in subjob_clusters is a dict, with the outermost key being the (arbitrary) name of the cluster. Sub- jobs run_afterEntry in spevifications of a subjob_cluster, to define before or after which other cluster of the workflow this cluster is supposed to run. Only one of the two should be specified. Can also be used in the specifications run_beform subjobs if these subjobs get a corresponding cluster auto-assigned. script: script_dir: call_function: env_preparation:	job_clu	stoop_cluster is a collection of subjobs run from the same batch script. Each subjob needs to belong to
sub- jobs       Section in the workflow chapter, containing the information on additional subjobs.         jobs       run_afterEntry in spevifications of a subjob_cluster, to define before or after which other cluster of the workflow this cluster is supposed to run. Only one of the two should be specified. Can also be used in the specifications run_beforef subjobs if these subjobs get a corresponding cluster auto-assigned.         script:       script_dir:         call_function:       env_preparation:		
jobs         run_afterEntry in spevifications of a subjob_cluster, to define before or after which other cluster of the workflow this         /       cluster is supposed to run. Only one of the two should be specified. Can also be used in the specifications         run_beforef subjobs if these subjobs get a corresponding cluster auto-assigned.         script.         script_dir:         call_function:         env_preparation:		
run_aft       rEntry in spevifications of a subjob_cluster, to define before or after which other cluster of the workflow this cluster is supposed to run. Only one of the two should be specified. Can also be used in the specifications run_before subjobs if these subjobs get a corresponding cluster auto-assigned.         script:	sub-	Section in the workflow chapter, containing the information on additional subjobs.
/       cluster is supposed to run. Only one of the two should be specified. Can also be used in the specifications         run_beform f subjobs if these subjobs get a corresponding cluster auto-assigned.         script:         script_dir:         call_function:         env_preparation:	jobs	
run_beforcef subjobs if these subjobs get a corresponding cluster auto-assigned.         script:         script_dir:         call_function:         env_preparation:	run_afte	erEntry in spevifications of a subjob_cluster, to define before or after which other cluster of the workflow this
script: script_dir: call_function: env_preparation:	/	cluster is supposed to run. Only one of the two should be specified. Can also be used in the specifications
script_dir: call_function: env_preparation:	run_bef	or subjobs if these subjobs get a corresponding cluster auto-assigned.
call_function: env_preparation:	script:	
env_preparation:	script_d	ir:
· ·	call_fur	ction:
next_run_triggered_by:	env_pre	paration:
	next_ru	n_triggered_by:

# 13.4 Example 1: Adding an additional postprocessing subjob

In the case of a simple echam postprocessing job, the corresponding section in the runscript could look like this:

```
echam:

[...other information...]

workflow:

next_run_triggered_by: tidy

subjobs:

my_new_subjob:

nproc: 1
```

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<pre>run_after: tidy script_dir: script: call_function:</pre>
env_preparation:

# 13.5 Example 2: Adding an additional preprocessing subjob

A preprocessing job basically is configured the same way as a postprocessing job, but the run\_after entry is repl

# 13.6 Example 3: Adding a iterative coupling job

Writing a runscript for iterative coupling using the workflow manager requires some more changes. The principal idea is that each coupling step consists of two data processing jobs, one pre- and one postprocessing job. This is done this way as to make the coupling modular, and enable the modeller to easily replace one of the coupled components by a different implementation. This is of course up to the user to decide, but we generally advise to do so, and the iterative couplings distributed with ESM-Tools are organized this way.

CHAPTER FOURTEEN

## **ESM ENVIRONMENT**

The package esm\_environment takes care of generating the environments for the different HPCs supported by *ESM*-*Tools*. This is done through the use of the EnvironmentInfos class inside the different *ESM*-*Tools* packages.

For the correct definition of an environment for an HPC a *yaml* file for that system needs to be included inside the esm\_tools package inside the configs/machines/ folder (e.g. ollie.yaml). This file should contain all the required preset variables for that system and the environment variables module\_actions and export\_vars.

## 14.1 Environment variables

#### module\_actions (list)

A list of module actions to be included in the compilation and run scripts generated by esm\_master and esm\_runscripts respectively, such as module load netcdf, module unload netcdf, module purge, etc. The syntax of this list is such as that of the command that would be normally used in shell, but omitting the module word, for example:

```
module_actions:
    - "purge"
    - "load netcdf"
```

This variable also allows for sourcing files by adding a member to the list such as source <file\_to\_be\_sourced>.

#### export\_vars (dict)

A dictionary containing all the variables (and their values) to be exported. The syntax is as follows:

The previous example will result in the following export in the script produced by esm\_master or esm\_runscripts:

export A\_VAR\_TO\_BE\_EXPORTED=the\_value

As a dictionary, export\_vars is not allowed to have repeated keys. This could be a problem when environments are required to redefine a variable at different points of the script. To overcome this limitation, repetitions of the same variable are allowed if the key is followed by an integer contained inside [(int)]:

The resulting script will contain the following exports:

export A\_VAR\_TO\_BE\_EXPORTED=the\_value
export A\_VAR\_TO\_BE\_EXPORTED=\$A\_VAR\_TO\_BE\_EXPORTED:another\_value

Note that the index is removed once the exports are transferred into the script.

## 14.2 Modification of the environment through the model/setup files

As previously mentioned, the default environment for a HPC system is defined inside its machine file (in esm\_tools/machines/<machine\_name>.yaml). However, it is possible to modify this environment through the model and/or coupled setup files (or even inside the runscript) to adjust to the model/setup requirements. For this purpose, the variables environment\_changes, compiletime\_environment\_changes and runtime\_environment\_changes can be used.

#### environment\_changes (dict)

Allows for modifications of the machine module\_actions and export\_vars, both during compilation and runtime.

#### compiletime\_environment\_changes (dict)

Allows for modifications of the machine module\_actions and export\_vars, only applied during compilation time.

#### compiletime\_environment\_changes (dict)

Allows for modifications of the machine module\_actions and export\_vars, only applied during run time.

The syntax for this dictionary is the same as that defined in Environment variables, but using add\_ in front of the environment variables (add\_module\_actions and add\_export\_vars). Furthermore, the environment variables can be nested inside choose\_ blocks:

```
environment_changes:
    choose_computer:
    ollie:
        add_export_vars:
            COMPUTER_VAR: 'ollie'
        juwels:
            add_export_vars:
            COMPUTER_VAR: 'mistral'
```

**Note:** This changes are model-specific for compilation, meaning that **the changes will only occur for the compilation script of the model containing those changes**. For runtime, all the environments of the components will be added together into the same **.run** script. Please, refer to *Coupled setup environment control* for an explanation on how to control environments for a whole setup.

# 14.3 Coupled setup environment control

There are two ways in which the environments for the coupled setups can be modified: defining environment\_changes for each component or defining a general environment\_changes for the whole setup:

### 14.3.1 Component-by-component

The environment\_changes are taken from the standalone component files. It is possible to modify these environment\_changes through the setup file by including environment\_changes inside the chapter of that component.

**Warning:** Handling environment\_changes in this fashion implies that compilation scripts can potentially end up containing different environments.

### 14.3.2 General environment for setups

To define a general environment\_changes for all the components of a setup, include the environment\_changes inside the general section of the setup file. This will ignore all the environment\_changes defined by the standalone files. It is still possible to add component-specific environment\_changes from the component chapter inside the setup file.

### FIFTEEN

## **ESM-TESTS**

**Note:** This is a feature aimed for advance users and developers who work in preparing default configurations of experiments, or who implement a model/coupled-setup in ESM-Tools.

*ESM-Tests* is the integration testing suite from *ESM-Tools*. Its aim is to test a set of selected runscripts and model builds just by using one single command: esm\_tests. It can also perform dry actions (i.e. check compilations and check runs).

## 15.1 Glossary

### actual vs check test

An *actual test* is a test where the model has been compiled and run in one of the supported HPCs. A *check test* is a dry test, meaning, no compilation or run takes place, but instead, the configuration files and scripts are generated. Both *actual* and *check* tests compare their output configuration files and scripts to the *last-state*, and offer the possibility to update the *last-state* of those files at the end of the test.

### esm\_tests\_info

The repository where the files of the last-state and the runscripts for testing are stored. This repository is clone as a submodel of *ESM-Tools* whenever esm\_tests command is run for the first time. The repository is cloned locally into the esm\_tools/src/esm\_tests/resources folder. You can activate the submodule manually via git submodule init followed by git submodule sync.

#### last-state

Set of configuration files, both from compilation and runtime, that represent the last approved configuration of the testing runscripts. This set of files is kept for comparison with the equivalent files of future pull-requests, to ensure the stability of the configurations. *ESM-Tests* always compares the new files to the last-state files automatically, both in actual compilation/runs or check compilation/runs. See *Last-state*.

#### runscripts

The runscripts to run the tests. Runscripts define the test simulation details as in regular *ESM-Tools* runscripts, but are also used for *ESM-Tests* to understand what needs to be compiled. Runscripts are part of the esm\_tests\_info submodule, and can be found (if the submodule was initiated via esm\_tests -u) in esm\_tools/src/esm\_tests/resources/runscripts. Runscripts need to be generalized (i.e. choose\_computer.name) for the different HPCs where you want to run the tests.

### state.yaml

In this document some times referred only as state, is a *YAML* file that includes information about the status of the tests (actual tests or check tests) in different computers. It also includes the date of the last actual test.

# 15.2 Usage

*ESM-Tests* is designed to compile and run tests **just with one single command**, without additional arguments: esm\_tests, so that launching a suite of tests in a supported HPC is straight forward. Higher granularity in the control of the tests is enabled via:

- Arguments
- Runscripts via the usual esm\_parser syntax (e.g. choose\_computer.name)
- Model control file (config.yaml)
- *Local test configuration (test\_config.yaml)*

The commands syntax is as follows:

	E 1.7 E		-7 [7	E 41 E		F . 7 F	- T E 1. T	E T E .	
esm tests	-n	-n     -	C     -11		S NAVHI	- T     -	$-0 \mid  -n $	1-01 I-e	e] [-r BRANCH]
	L ++J L		C] [ u]			L 4J L		L 91 L 9	

## **15.3 Arguments**

Optional argu-	Description
ments	
-h, -help	Show this help message and exit
-n, –no-user	Avoid loading user config (for check tests in GitHub)
-c, –check	Check mode on (does not compile or run, but produces some files that can be compared to
	previous existing files in last_tested folder)
-u, –update	Updates the resources with the release branch, including runscripts and last_tested files
-d, -delete	Delete previous tests
-s SAVE, -save SAVE	Save files for comparisson in last_tested folder. The values can be True/False
-t, -state	Print the state stored in state.yaml
-o, -hold	Hold before operation, to give time to check the output
-b, -bulletpoints	Bullet points for printing the state and copy/paste as markdown text
-g, –github	Use this flag when running in GitHub servers (i.e. adds syntax for collapsing compare
	sections of the output for GitHub Actions)
-e, -system-exit-on-	Trigger a system exit on errors or file differences so that GitHub actions can catch that as a
errors	failing test
-r BRANCH, -branch	use the given esm_tests_info branch
BRANCH	

## 15.4 Last-state

The last-state files are https://github.com/esm-tools/esm\_tets\_info repository, in the release branch. The files stored in the last-state are: \* compilation scripts (comp-\*.sh) \* namelists \* namcouple \* finished\_config \* batch scripts (.run)

## 15.5 Check test status

As a user, you can check the last-state status (the online one of the esm\_tests\_info repo, release branch) by running:

esm\_tools test-state

This will give you a summary of the state of compilation and running tests for different models, in different computers, and also a date of when the latest actual compilation and run tests were carried out.

If you are testing locally in an HPC, you can get the same information about your local state by running:

```
esm_tests -t
```

## 15.6 Model control file (config.yaml)

File location: esm\_tools/src/esm\_tests/resources/runscripts/<model>/config.yaml Versioned: Yes,
distributed with esm\_tests\_info

The *Model control file* gives you control over *ESM-Tests* setups for the set of runscripts for a given model (the model which name is the same as the folder where the config.yaml is contained: esm\_tools/src/esm\_tests/ resources/runscripts/<model>/).

Within this file you can control:

- which files need to be present for considering an actual compilation test successful (comp.actual. files)
- which files need to be present for considering an actual run test successful (run.actual.files)
- which messages from the execution of esm\_runscripts should trigger an error in an actual run test (run. actual.errors)
- which computers are supported for this set of tests (computers)

The file should contain this structure:

```
comp:
        actual:
                files:
                    - "file/path" # Typically the binaries
        check: {}
run:
        actual:
                errors:
                    - "error message to mark the test as not successful # Typically
→"MISSING FILES"
                files: # Typically restart files and outdata files
                    - "path/to/file1"
                    - "globbing/path/*/to*files"
        check: {}
computers:
        - <computer1>
        - <cimputer2>
```

In the files sections, globbing is supported.

The file's paths should be relative to the compilation folder or the experiment folder.

Each file name can be followed by the syntax in/except [<model\_version1>, <model\_version2>, ...] to only check for that file in that set of model versions, or to exclude (except) that file from being check for a set of model versions.

Example

```
comp:
        actual:
                files:
                    - "bin/fesom*"
                    - "bin/oifs"
                    - "bin/rnfma"
        check: {}
run:
        actual:
                errors:
                    - "MISSING FILES"
                files:
                    - "restart/fesom/fesom.*.oce.restart/hnode.nc*"
                    - "restart/fesom/fesom.*.oce.restart/salt.nc*"
                    - "restart/fesom/fesom.*.oce.restart/ssh_rhs_old.nc*"
                    - "restart/fesom/fesom.*.oce.restart/temp.nc*"
                    - "restart/fesom/fesom.*.oce.restart/urhs_AB.nc*"
                    - "restart/fesom/fesom.*.oce.restart/vrhs_AB.nc*"
                    - "restart/fesom/fesom.*.oce.restart/w_impl.nc*"
                    - "restart/fesom/fesom.*.ice.restart/area.nc*"
                    - "restart/fesom/fesom.*.ice.restart/hice.nc*"
                    - "restart/fesom/fesom.*.ice.restart/hsnow.nc*"
                    - "restart/fesom/fesom.*.ice.restart/ice_albedo.nc*"
                    - "restart/fesom/fesom.*.ice.restart/ice_temp.nc*"
                    - "restart/fesom/fesom.*.ice.restart/uice.nc*"
                    - "restart/fesom/fesom.*.ice.restart/vice.nc*"
                    - "restart/oasis3mct/rmp_*"
                    - "restart/oasis3mct/rstas.nc*"
                    - "restart/oasis3mct/rstos.nc*"
                    - "restart/oifs/*/BLS*"
                    - "restart/oifs/*/LAW*"
                    - "restart/oifs/*/rcf"
                    - "restart/oifs/*/srf*"
                    - "restart/oifs/*/waminfo*"
                    - "outdata/oifs/*/ICMGG* except [frontiers-xios, v3.1]"
                    - "outdata/oifs/*/ICMSH* except [frontiers-xios, v3.1]"
                    - "outdata/oifs/*/ICMUA* except [frontiers-xios, v3.1]"
                    - "outdata/oifs/atm_remapped* in [frontiers-xios, v3.1]"
                    - "outdata/fesom/*.fesom.*.nc"
        check: {}
computers:
        - ollie
        - mistral

    juwels

        - aleph
```

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```
- blogin
- levante
```

## 15.7 Local test configuration (test\_config.yaml)

File location: esm\_tools/src/esm\_tests/test\_config.yaml Versioned: No, user specific, git-ignored

This file gives you control on which tests esm\_tests will run in the current machine, independently of what tests are defined in the *Model control files*. The current machine needs to be included in the *Model control file* for the test to run (i.e. test\_config.yaml runs only the tests included there and supported on the current platform). The syntax is as follows:

```
<model1>:

- <runscript1_name>.yaml

- <runscript2_name>.yaml

- [ ... ]

<model2>: all

[ ... ]
```

The model sections need to be named after the folders in esm\_tools/src/esm\_tests/resources/runscripts. If you want to run all the suported runscripts for a model in this platform, make the model section have the value all. If you want to select a set of **supported runscripts** make the model be a list of runscripts (this runscripts need to be in esm\_tools/src/esm\_tests/resources/runscripts/<model>/). If you want to run all the supported runscripts for all supported runscripts, commented most of the contents), make the file content be an empty dictionary ({}).

Example

```
#{}
awiesm: #all
    - all_awiesm-2.1-recom.yaml
     - awiesm-2.1_icebergs.yaml
#
    - bootstrap.yaml
    - pico.yaml
    - PI_ctrl_awiesm-2.1-wiso.yaml
    - pi.yaml
    - pi-wiso.yaml
echam: all
fesom: all
awicm: all
     - awicm1-CMIP6-initial-monthly.yaml
#
#
     - awicm2-initial-monthly.yaml
fesom-recom:
   - fesom-recom1.4-initial-daily.yaml
awicm3: all
#
     - awicm3-v3.1-TC095L91-CORE2_initial
     - awicm3-frontiers-TC0159L91-CORE2_initial.yaml
#
#oifsamip: all
#vilma-pism: all
```

# 15.8 ESM-Tests cookbook

### 15.8.1 How to include a new model/runscript

- 1. Add the given runscript to esm\_tools/src/esm\_tests/resources/runscripts/<model>/
- 2. Make sure your runscript has a meaningful name
- 3. Make sure your runscript has the correct model version defined, for a standalone model in the section of the model (not in general), and for a coupled setup, both in the general section and in the coupled setup section (e.g. awiesm section). This version will be used by *ESM-Test* for the esm\_master command to compile
- 4. Modify the following variables to take the environment variables setup by *ESM-Tests*:

```
general:
    account: !ENV ${ACCOUNT}
    base_dir: !ENV ${ESM_TESTING_DIR}
<standalone-model/setup>:
    model_dir: !ENV ${MODEL_DIR}
```

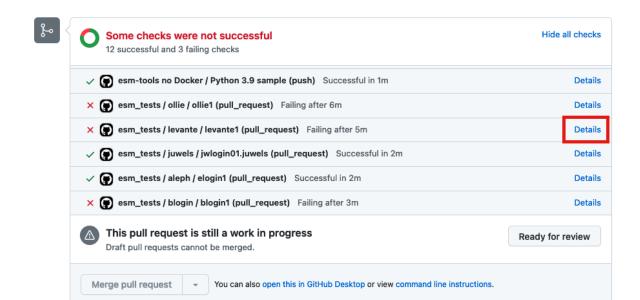
- 5. Generalize the runscript to be able to run in the computers where you'd want it to be supported (i.e. add the necessary choose\_computer.name switches)
- 6. Create the *Model control file* (esm\_tools/src/esm\_tests/resources/runscripts/<model>/config. yaml). See ref:*esm\_tests:Model control file* (``*config.yaml*``) for details about the content
- 7. If you are using the Local test configuration (``test\_config.yaml``) to exclude some models, make sure the current model is included, so that your tests can be run locally.

### 15.8.2 How to include a new platform for in an existing model

- 1. In the corresponding *Model control file* (esm\_tools/src/esm\_tests/resources/runscripts/<model>/ config.yaml), add the name of the platform to the computers list
- 2. In the runscripts (esm\_tools/src/esm\_tests/resources/runscripts/<model>/<runscript>.yaml), add the necessary case to the choose\_computer.name to specify pool directories, forcing files, nproc, etc.

### 15.8.3 How to approve changes on a GitHub Pull-Request

- 1. In the pull-request, if all the tests passed you don't need to approve any changes, you can jump directly to step 4.
- 2. If any of the tests labelled as esm\_tests failed (click on the triangles to expand screen captures):



1412	awi	lesm:
1413	I.	2.1:
1414	T	awiesm-2.1_icebergs:
1415	- I	ollie: comp files identical run files differ
1416	- I	pico:
1417	1	ollie: comp files identical run files differ
1418	1	bootstrap:
1419	1	ollie: comp files identical run files differ
1420	1	pi:
1421	1	ollie: comp files identical run files differ
1422	1	pi-wiso:
1423	1	ollie: comp files identical run files differ
1424	1	2.1-wiso:
1425	1	PI_ctrl_awiesm-2.1-wiso:
1426	1	ollie: comp files identical run files differ
1427	1	2.1-recom:
1428		all_awiesm-2.1-recom:
1429	Ι	ollie: comp files identical run files differ

52	► COMPILING (5.9%) vilma-pism-1.0vld
57	► COMPILING (11.8%) fesom-recom-1.4
62	► COMPILING (17.6%) fesom-2.0
66	► COMPILING (23.5%) fesom-2.1
70	► COMPILING (29.4%) echam-6.3.04p1
74	► COMPILING (35.3%) awiesm-2.1
80	► COMPILING (41.2%) awiesm-2.1
86	► COMPILING (47.1%) awiesm-2.1-wiso
92	► COMPILING (52.9%) awiesm-2.1
98	► COMPILING (58.8%) awiesm-2.1
104	► COMPILING (64.7%) awiesm-2.1
110	► COMPILING (70.6%) awiesm-2.1-recom
116	► COMPILING (76.5%) awicm-CMIP6
122	► COMPILING (82.4%) <b>awicm-2.0</b>
128	► COMPILING (88.2%) <b>awicm3-v3.0</b>
135	► COMPILING (94.1%) awicm3-frontiers-xios
143	► COMPILING (100.0%) awicm3-v3.1
151	▶ SUBMITTING (5.9%) vilma-pism/vilmald_1ky-pism_1y
152	► SUBMITTING (11.8%) fesom-recom/fesom-recoml.4-initial-daily
161	► SUBMITTING (17.6%) fesom/fesom2.0-initial-monthly
169	► SUBMITTING (23.5%) fesom/fesom2.1-initial-monthly
179	SUBMITTING (29.4%) echam/echam6.3.04p1-initial-monthly
230	► SUBMITTING (35.3%) awiesm/awiesm-2.1_icebergs
372	► SUBMITTING (41.2%) awiesm/pico
514	► SUBMITTING (47.1%) awiesm/PI_ctrl_awiesm-2.1-wiso
662	► SUBMITTING (52.9%) awiesm/bootstrap
805	► SUBMITTING (58.8%) awiesm/pi
947	► SUBMITTING (64.7%) awiesm/pi-wiso
1095	► SUBMITTING (70.6%) awiesm/all_awiesm-2.1-recom
1238	SUBMITTING (76.5%) awicm/awicm1-CMIP6-initial-monthly
1295	► SUBMITTING (82.4%) awicm/awicm2-initial-monthly
1352	SUBMITTING (88.2%) awicm3/awicm3-v3.0-TC0159L91-CORE2_initial
1364	SUBMITTING (94.1%) awicm3/awicm3-frontiers-xios-TC0159L91-CORE2_initial
1376	► SUBMITTING (100.0%) awicm3/awicm3-v3.1-TC095L91-CORE2_initial



3. If there are no problematic differences, and the pull-request has been already reviewed and is just ready to be merged, write a message on the PR containing #approve-changes. This will commit the new files from the tests as the last-state, in the esm\_tests\_info repository.

**Warning:** Currently, **#approve-changes** does not update the test status on GitHub, once the operation finishes. If you want to see whether **#approve\_changes** finished or not you have to navigate to the Actions tab in GitHub. If you want to see all tests green, wait until **#approve-changes** finishes, and relaunch the tests for the last failed set of tests in the PR. Miguel - I know this is a pain, but I could not figure out how to do all this automatically (I wasted enough time on GitHub Actions for years to come).

- 4. Bump the version and wait that the bumpversion commit shows up.
- 5. You can now merge.

### CHAPTER

## SIXTEEN

## **ESM MOTD**

The package esm\_motd is an *ESM-Tools* integrated *message-of-the-day* system, intended as a way for the *ESM-Tools Development Team* to easily announce new releases and bug fixes to the users without the need of emailing.

It checks the versions of the different *ESM-Tools* packages installed by the user, and reports back to the user (writing to *stdout*) about packages that have available updates, and what are the new improvements that they provide (i.e. reports back that a bug in a certain package has been solved).

This check occurs every time the user uses esm\_runscripts.

The messages, their corresponding versions and other related information is stored online in GitHub and accessed by *ESM-Tools* also online to produce the report. The user can look at this file if necessary here: <<u>https://github.com/esm-tools/ree/release/esm\_tools/motd/motd.yaml>\_</u>.

**Warning:** The motd.yaml file is to be modified exclusively by the ESM-Tools Core Development Team, so... stay away from it ;-)

### CHAPTER

### SEVENTEEN

## COOKBOOK

In this chapter you can find multiple recipes for different ESM-Tools functionalities, such running a model, adding forcing files, editing defaults in namelists, etc.

If you'd like to contribute with your own recipe, or ask for a recipe, please open a documentation issue on our GitHub repository.

**Note:** Throughout the cookbook, we will sometimes refer to a nested part of a configuration via dot notation, e.g. a.b.c. Here, we mean the following in a YAML config file:

```
a:
b:
c: "foo"
```

This would indicate that the value of a.b.c is "foo". In Python, you would access this value as a["b"]["c"].

## 17.1 Change/Add Flags to the sbatch Call

#### Feature available since version: 4.2

If you are using *SLURM* batch system together with *ESM-Tools* (so far the default system), you can modify the sbatch call flags by modifying the following variables from your runscript, inside the computer section:

Key	Description
mail_type,	Define these two variables to get updates about your slurm-job through email.
mail_user	
sin-	By default defined asntasks-per-node=1
gle_proc_submit_flag	
addi-	To add any additional flag that is not predefined in ESM-Tools
tional_flags	

### 17.1.1 Example

Assume you want to run a simulation using the Quality of Service flag (--qos) of *SLURM* with value 24h. Then, you'll need to define the additional\_flags inside the computer section of your runscript. This can be done by adding the following to your runscript:

```
computer:
    additional_flags: "--qos=24h"
```

### 17.1.2 Adding more than one flag

Alternatively, you can include a list of additional flags:

```
computer:
    additional_flags:
    - "--qos=24h"
    - "--comment='My Slurm Comment'"
```

See the documentation for the batch scheduler on your HPC system to see the allowed options.

## 17.2 Applying a temporary disturbance to ECHAM to overcome numeric instability (lookup table overflows of various kinds)

Feature available since version: esm\_runscripts v4.2.1

From time to time, the ECHAM family of models runs into an error resulting from too high wind speeds. This may look like this in your log files:

```
30:
30:
30:
30: FATAL ERROR in cuadjtq (1): lookup table overflow
30: FINISH called from PE: 30
```

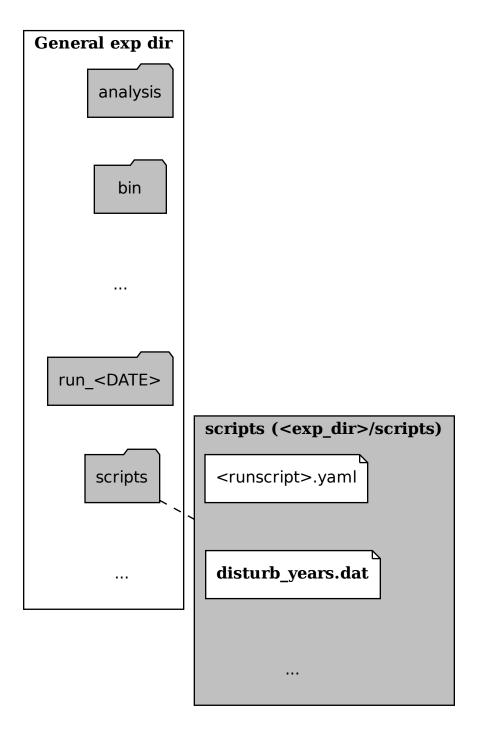
To overcome this problem, you can apply a small change to the factor "by which stratospheric horizontal diffussion is increased from one level to the next level above." (mo\_hdiff.f90), that is the namelist parameter enstdif, in the dynctl section of the ECHAM namelist. As this is a common problem, there is a way to have the run do this for specific years of your simulation. Whenever a model year crashes due to numeric instability, you have to apply the method outlined below.

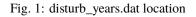
1. Generate a file to list years you want disturbed.

In your experiment script folder (**not** the one specific for each run), you can create a file called disturb\_years. dat. An abbreviated file tree would look like:

2. Add years you want disturbed.

The file should contain a list of years the disturbance should be applied to, seperated by new lines. In practice, you will add a new line with the value of the model year during which the model crashes whenever such a crash occurs.





17.2. Applying a temporary disturbance to ECHAM to overcome numeric instability (lookup table73 overflows of various kinds)

### 17.2.1 Example

In this example, we disturb the years 2005, 2007, and 2008 of an experiment called EXAMPLE running on ollie:

```
$ cat /work/ollie/pgierz/test_esmtools/EXAMPLE/scripts/disturb_years.dat
2005
2007
2008
```

You can also set the disturbance strength in your configuration under echam.disturbance. The default is 1.000001. Here, we apply a 200% disturbance whenever a "disturb\_year" is encountered.

```
echam:
disturbance: 2.0
```

### 17.2.2 See also

- ECHAM6 User Handbook, Table 2.4, dynctl
- Relevant source code

## **17.3 Changing Namelist Entries from the Runscript**

#### Feature available since version: 4.2

You can modify namelists directly from your user yaml runscript configuration.

- 1. Identify which namelist you want to modify and ensure that it is in the correct section. For example, you can only modify ECHAM specific namelists from an ECHAM block.
- 2. Find the subsection ("chapter") of the namelist you want to edit.
- 3. Find the setting ("key") you want to edit
- 4. Add a namelist\_changes block to your configuration, specify next the namelist filename you want to modify, then the chapter, then the key, and finally the desired value.

In dot notation, this will look like: <model\_name>.namelist\_changes.<namelist\_name>.<chapter\_name>.
<key\_name> = <value>

### 17.3.1 Example

Here are examples for just the relevant YAML change, and for a full runscript using this feature.

Snippet

Full Runscript

In this example, we modify the co2vmr of the radctl section of namelist.echam.

```
echam:
namelist_changes:
namelist.echam:
radctl:
co2vmr: 1200e-6
```

In this example, we set up AWI-ESM 2.1 for a 4xCO2 simulation. You can see how multiple namelist changes are applied in one block.

```
general:
           setup_name: "awiesm"
           compute_time: "02:30:00"
           initial_date: "2000-01-01"
           final_date: "2002-12-31"
           base_dir: "/work/ab0246/a270077/For_Christian/experiments/"
           nmonth: 0
           nyear: 1
           account: "ab0246"
echam:
           restart_unit: "years"
           nprocar: 0
           nprocbr: 0
           namelist_changes:
                                    namelist.echam:
                                                            radctl:
                                                                                     co2vmr: 1137.e-6
                                                            parctl:
                                                                                    nprocar: 0
                                                                                     nprocbr: 0
                                                            runctl:
                                                                                     default_output: True
awiesm:
           version: "2.1"
           postprocessing: true
           scenario: "PALEO"
           model_dir: "/work/ab0246/a270077/For_Christian/model_codes/awiesm-2.1/"
fesom:
           version: "2.0"
           res: "CORE2"
           pool_dir: "/pool/data/AWICM/FESOM2"
           mesh_dir: "/work/ba1066/a270061/mesh_CORE2_finaltopo_mean/"
           restart_rate: 1
           restart_unit: "y"
           restart_first: 1
           lresume: 0
           namelist_changes:
                       namelist.config:
                                   paths:
                                                ClimateDataPath: "/work/ba0989/a270077/AWIESM_2_1_LR_concurrent_rad/

where the second 
jsbach:
           input_sources:
                        jsbach_1850: "/work/ba1066/a270061/mesh_CORE2_finaltopo_mean/tarfilesT63/input/
 →jsbach/jsbach_T63CORE2_11tiles_5layers_1850.nc"
```

### 17.3.2 Practical Usage

It is generally a good idea to run your simulation once in **check** mode before actually submitting and examining the resulting namelists:

\$ esm\_runscripts <your\_config.yaml> -e <expid> -c

The namelists are printed in their final form as part of the log during the job submission and can be seen on disk in the work folder of your first run\_XZY folder.

Note that you can have several chapters for one namelist or several namelists included in one namelist\_changes block, but you can only have one namelist\_changes block per model or component (see *Changing Namelists*).

### 17.3.3 Unusual Namelists

Some times, you have strange namelists of the form:

```
= 'DET'
                         , 'Detritus
                                                                              .false.
sn_tracer(1)
                                                             'mmole-N/m3',
                          , 'Zooplankton concentration
                                                        1
                                                             'mmole-N/m3',
sn_tracer(2)
               = 'Z00'
                                                                              .false.
               = 'PHY'
                         , 'Phytoplankton concentration'
                                                             'mmole-N/m3',
                                                                              .false.
sn_tracer(3)
```

To correctly insert this via esm-tools, you can use:

```
namelist_changes:
    namelist_top_cfg:
    namtrc:
    sn_tracer: "remove_from_namelist"
    sn_tracer(1)%clsname: DET
    sn_tracer(2)%clsname: Z00
    sn_tracer(3)%clsname: PHY
    sn_tracer(3)%clsname: "Detritus"
    sn_tracer(2)%cllname: "Zooplankton concentration"
    sn_tracer(3)%cllname: "Phytoplankton concentration"
    sn_tracer(1:3)%clunit: "mmole-N/m3"
```

### 17.3.4 See also

- Default namelists on GitHub
- Changing Namelists
- What Is YAML?

## 17.4 Heterogeneous Parallelization Run (MPI/OpenMP)

#### Feature available since version: 5.1

In order to run a simulation with hybrid MPI/OpenMP parallelization include the following in your runscript:

- 1. Add heterogenous\_parallelization: true in the computer section of your runscript. If the computer section does not exist create one.
- 2. Add omp\_num\_threads: <number> to the sections of the components you'd like to have OpenMP parallelization.

### 17.4.1 Example

#### AWICM3

In *AWICM3* we have 3 components: *FESOM-2*, *OpenIFS* and *RNFMAP*. We want to run *OpenIFS* with 8 OpenMP threads, *RNFMAP* with 48, and *FESOM-2* with 1. Then, the following lines need to be added to our runscript:

```
general:
   [ ... ]
computer:
   heterogeneous_parallelization: true
   [ ... ]
fesom:
   omp_num_threads: 1
   [ ... ]
oifs:
   omp_num_threads: 8
   [ ... ]
rnfmap:
   omp_num_threads: 48
   [ ... ]
```

### 17.4.2 See also

• Runtime variables

## 17.5 How to setup runscripts for different kind of experiments

This recipe describes how to setup a runscript for the following different kinds of experiments. Besides the variables described in *ESM-Tools Variables*, add the following variables to your runscript, as described below.

• Initial run: An experiment from initial model conditions.

```
general:
lresume: 0
```

• Restart: An experiment that restarts from a previous experiment with the same experiment id.

```
general:
    lresume: 1
```

• Branching off: An experiment that restarts from a previous experiment but with a different experiment id.

```
general:
    lresume: 1
    ini_parent_exp_id: <old-experiment-id>
    ini_restart_dir: <path-to-restart-dir-of-old-experiment>/restart/
```

• **Branching off and redate**: An experiment that restarts from a previous experiment with a different experiment id and if this experiment should be continued with a different start date.

```
general:
    lresume: 1
    ini_parent_exp_id: <old-experiment-id>
    ini_restart_dir: <path-to-restart-dir-of-old-experiment>/restart/
    first_initial_year: <year>
```

### 17.5.1 See also

- ESM-Tools Variables
- What Is YAML?

## 17.6 Implement a New Model

Feature available since version: 4.2

**Note:** since version 6.20.2 a template is available in esm\_tools/configs/templates/component\_template. yaml

- 1. Upload your model into a repository such us *gitlab.awi.de*, *gitlab.dkrz.de* or *GitHub*. Make sure to set up the right access permissions, so that you comply with the licensing of the software you are uploading.
- 2. If you are interested in implementing more than one version of the model, we recommend you to commit them to the master branch in the order they were developed, and that you create a tag per version. For example:
  - a. Clone the empty master branch you just created and add your model files to it:

```
$ git clone https://<your_repository>
$ cp -rf <your_model_files_for_given_version> <your_repository_folder>
$ git add .
```

b. Commit, tag the version and push the changes to your repository:

```
$ git commit -m "your comment here"
$ git tag -a <version_id> -m "your comment about the version"
$ git push -u origin <your_master_branch>
$ git push origin <version_id>
```

- c. Repeat steps a and b for all the versions that you would like to be present in ESM-Tools.
- 3. Now that you have your model in a repository you are ready to implement it into *esm\_tools*. First, you will need to create your own branch of *esm\_tools*, following the steps 1-4 in *Contribution to esm\_tools Package*. The recommended name for the branch would be feature/<name\_of\_your\_model>.
- 4. Then you will need to create a folder for your model inside esm\_tools/configs/components and create the model's yaml file:

```
$ mkdir <PATH>/esm_tools/configs/components/<model>
$ touch <PATH>/esm_tools/configs/components/<model>.yaml
```

5. Use your favourite text editor to open and edit your <model>.yaml in the esm\_tools/configs/components/ <model> folder:

\$ <your\_text\_editor> <PATH>/esm\_tools/configs/components/<model>/<model>.yaml

6. Complete the following information about your model:

```
# YOUR_MODEL YAML CONFIGURATION FILE
#
model: your_model_name
type: type_of_your_model  # atmosphere, ocean, etc.
version: "the_default_version_of_your_model"
```

7. Include the names of the different versions in the available\_versions section and the compiling information for the default version:

```
[...]
available_versions:
- "1.0.0"
- "1.0.1"
- "1.0.2"
git-repository: "https://your_repository.git"
branch: your_model_branch_in_your_repo
install_bins: "path_to_the_binaries_after_comp"
comp_command: "your_shell_commands_for_compiling"
                                                      # You can use the defaults "$
→{defaults.comp_command}"
clean_command: "your_shell_commands_for_cleaning"
                                                     # You can use the defaults "$

→{defaults.clean_command}"
executable: your_model_command
setup_dir: "${model_dir}"
bin_dir: "${setup_dir}/name_of_the_binary"
```

In the install\_bins key you need to indicate the path inside your model folder where the binaries are compiled to, so that *esm\_master* can find them once compiled. The available\_versions key is needed for *esm\_master* to list the versions of your model. The comp\_command key indicates the command needed to compile your model, and can be set as \${defaults.comp\_command} for a default command (mkdir -p build; cd build; cmake ...; make install -j `nproc --all`), or you can define your own list of compiling commands separated with; ("command1; command2").

8. At this point you can choose between including all the version information inside the same <model>.yaml file, or to distribute this information among different version files:

Single file

Multiple version files

In the <model>.yaml, use a choose\_ switch (see *Switches (choose\_)*) to modify the default information that you added in step 7 to meet the requirements for each specific version. For example, each different version has its own git branch:

```
choose_version:
    "1.0.0":
    branch: "1.0.0"
    "1.0.1":
```

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```
branch: "1.0.1"
"1.0.2":
branch: "develop"
```

a. Create a *yaml* file per version or group of versions. The name of these files should be the same as the ones in the available\_versions section, in the main <model>.yaml file or, in the case of a file containing a group of versions, the shared name among the versions (i.e. fesom-2.0.yaml):

\$ touch <PATH>/esm\_tools/configs/<model>/<model-version>.yaml

b. Open the version file with your favourite editor and include the version specific changes. For example, you want that the version 1.0.2 from your model pulls from the develop git branch, instead of from the default branch. Then you add to the <model>-1.0.2.yaml version file:

branch: "develop"

Another example is the fesom-2.0.yaml. While fesom.yaml needs to contain all available\_versions, the version specific changes are split among fesom.yaml (including information about versions 1) and fesom-2.0.yaml (including information about versions 2):

fesom.yaml

fesom-2.0.yaml

```
[ ... ]
```

```
available_versions:
- '2.0-o'
- '2.0-esm-interface'
- '1.4'
- '1.4-recom'
- '1.4-recom-awicm'
 '2.0-esm-interface-yac'
- '2.0-paleodyn'
- '2.0'
- '2.0-r' # OG: temporarily here
choose version:
  '1.4-recom-awicm':
    branch: fesom_recom_1.4_master
    destination: fesom-1.4
  '1.4-recom':
    branch: fesom_recom_1.4_master
    destination: fesom-1.4
```

```
[ ... ]
```

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```
- github.com/FESOM/fesom2.git
install_bins: bin/fesom.x
2.0-esm-interface:
branch: fesom2_using_esm-interface
destination: fesom-2.0
git-repository:
- https://gitlab.dkrz.de/a270089/fesom-2.0_yac.git
install_bins: bin/fesom.x
```

**Note:** These are just examples of model configurations, but the parser used by *ESM-Tools* to read *yaml* files (*esm\_parser*) allows for a lot of flexibility in their configuration; i.e., imagine that the different versions of your model are in different repositories, instead of in different branches, and their paths to the binaries are also different. Then you can include the git-repository and install\_bins variables inside the corresponding version case for the choose\_version.

9. You can now check if esm\_master can list and install your model correctly:

\$ esm\_master

This command should return, without errors, a list of available models and versions including yours. Then you can actually try installing your model in the desired folder:

```
$ mkdir ~/model_codes
$ cd ~/model_codes
$ esm_master install-your_model-version
```

10. If everything works correctly you can check that your changes pass flake8:

\$ flake8 <PATH>/esm\_tools/configs/components/<model>.yaml

Use this link to learn more about flake8 and how to install it.

11. Commit your changes, push them to the origin remote repository and submit a pull request through GitHub (see steps 5-7 in *Contribution to esm\_tools Package*).

**Note:** You can include all the compiling information inside a compile\_infos section to avoid conflicts with other choose\_version switches present in your configuration file.

#### 17.6.1 See also

- ESM-Tools Variables
- Switches (choose\_)
- What Is YAML?

## 17.7 Implement a New Coupled Setup

#### Feature available since version: 4.2

An example of the different files needed for AWICM setup is included at the end of this section (see recipes/add\_model\_setup:Example).

- Make sure the models, couplers and versions you want to use, are already available for *esm\_master* to install them
   (\$ esm\_master and check the list). If something is missing you will need to add it following the instructions in
   *Implement a New Model*.
- 2. Once everything you need is available to *esm\_master*, you will need to create your own branch of *esm\_tools*, following the steps 1-4 in *Contribution to esm\_tools Package*.
- 3. Setups need two types of files: 1) **coupling files** containing information about model versions and coupling changes, and 2) **setup files** containing the general information about the setup and the model changes. In this step we focus on the creation of the **coupling files**.
  - a. Create a folder for your couplings in esm\_tools/configs/couplings:

```
$ cd esm_tools/configs/couplings/
$ mkdir <coupling_name1>
$ mkdir <coupling_name2>
...
```

The naming convention we follow for the coupling files is component1-version+component2-version+.

b. Create a *yaml* file inside the coupling folder with the same name:

```
$ touch <coupling_name1>/<coupling_name1>.yaml
```

c. Include the following information in each coupling file:

```
components:
- "model1-version"
- "model2-version"
- [ ... ]
- "coupler-version"
coupling_changes:
- sed -i '/MODEL1_PARAMETER/s/OFF/ON/g' model1-1.0/file_to_change
- sed -i '/MODEL2_PARAMETER/s/OFF/ON/g' model2-1.0/file_to_change
- [ ... ]
```

The components section should list the models and couplers used for the given coupling including, their required version. The coupling\_changes subsection should include a list of commands to make the necessary changes in the component's compilation configuration files (CMakeLists.txt, configure, etc.), for a correct compilation of the coupled setup.

4. Now, it is the turn for the creation of the **setup file**. Create a folder for your coupled setup inside esm\_tools/ configs/setups folder, and create a *yaml* file for your setup:

```
$ mkdir <PATH>/esm_tools/configs/setups/<your_setup>
$ touch <PATH>/esm_tools/configs/setups/<your_setup>/<setup>.yaml
```

5. Use your favourite text editor to open and edit your <setup>.yaml in the esm\_tools/configs/setups/ <your\_setup> folder:

\$ <your\_text\_editor> <PATH>/esm\_tools/configs/setups/<your\_setup>/<setup>.yaml

6. Complete the following information about your setup:

```
→#####
→#####
→#####
general:
    model: your_setup
    version: "your_setup_version"
    coupled_setup: True
    include_models:
                 # List of models, couplers and componentes of the_
\rightarrow setup.
        - component_1
                 # Do not include the version number
        - component_2
        - [ ... ]
```

Note: Models do not have a general section but in the setups the general section is mandatory.

7. Include the names of the different versions in the available\_versions section:

```
general:
    [ ... ]
    available_versions:
        - "1.0.0"
        - "1.0.1"
```

The available\_versions key is needed for *esm\_master* to list the versions of your setup.

8. In the <setup>.yaml, use a choose\_ switch (see *Switches (choose\_)*) to assign the coupling files (created in step 3) to their corresponding setup versions:

9. You can now check if esm\_master can list and install your coupled setup correctly:

\$ esm\_master

This command should return, without errors, a list of available setups and versions including yours. Then you can actually try installing your setup in the desire folder:

```
$ mkdir ~/model_codes
$ cd ~/model_codes
$ esm_master install-your_setup-version
```

10. If everything works correctly you can check that your changes pass flake8:

```
$ flake8 <PATH>/esm_tools/configs/setups/<your_setup>/<setup>.yaml
$ flake8 <PATH>/esm_tools/configs/couplings/<coupling_name>/<coupling_name>.yaml
```

Use this link to learn more about flake8 and how to install it.

11. Commit your changes, push them to the origin remote repository and submit a pull request through GitHub (see steps 5-7 in *Contribution to esm\_tools Package*).

### 17.7.1 Example

Here you can have a look at relevant snippets of some of the AWICM-1.0 files.

fesom-1.4+echam-6.3.04p1.yaml

awicm.yaml

One of the coupling files for *AWICM-1.0* ( esm\_tools/configs/couplings/fesom-1.4+echam-6.3.04p1/ fesom-1.4+echam-6.3.04p1.yaml):

```
components:
- echam-6.3.04p1
- fesom-1.4
- oasis3mct-2.8
coupling_changes:
- sed -i '/FESOM_COUPLED/s/OFF/ON/g' fesom-1.4/CMakeLists.txt
- sed -i '/ECHAM6_COUPLED/s/OFF/ON/g' echam-6.3.04p1/CMakeLists.txt
```

Setup file for AWICM (esm\_tools/configs/setups/awicm/awicm.yaml):

(continued from previous page)

```
- echam
        - fesom
        - oasis3mct
version: "1.1"
scenario: "PI-CTRL"
resolution: ${echam.resolution}_${fesom.resolution}
postprocessing: false
post_time: "00:05:00"
choose_general.resolution:
        T63_CORE2:
                 compute_time: "02:00:00"
        T63_REF87K:
                 compute_time: "02:00:00"
        T63_REF:
                compute_time: "02:00:00"
available_versions:
- '1.0'
- '1.0-recom'
- CMIP6
choose_version:
  '1.0':
    couplings:
    - fesom-1.4+echam-6.3.04p1
  '1.0-recom':
    couplings:
    - fesom-1.4+recom-2.0+echam-6.3.04p1
  CMIP6:
    couplings:
    - fesom-1.4+echam-6.3.04p1
```

### 17.7.2 See also

- ESM-Tools Variables
- Switches (choose\_)
- What Is YAML?

## 17.8 Implement a New HPC Machine

To implement a new HPC machine to ESM-Tools, two files need to be updated and created, respectively:

- <PATH>/esm\_tools/configs/machines/all\_machines.yaml
- <PATH>/esm\_tools/configs/machines/<new\_machine>.yaml
- 1. Add an additional entry for the new machine.

Use your favourite text editor and open the file <PATH>/esm\_tools/configs/machines/all\_machines. yaml: \$ <your\_text\_editor> <PATH>/esm\_tools/configs/machines/all\_machines.yaml

and add a new entry for the new machine (replace placeholders indicated by <...>)

```
<new_machine>:
    login_nodes: '<hostname>*' # A regex pattern that matches the hostname of login_
    ondes
    compute_nodes: '<compute_notes>' # A regex pattern that matches the hostname of_
    ocompute nodes
```

2. Create a new machine file.

Use your favourite text editor to create and edit a new machine file <new\_machine>.yaml in the esm\_tools/ configs/machines/ folder:

\$ <your\_text\_editor> <PATH>/esm\_tools/configs/machines/<new\_machine>.yaml

A template file (machine\_template.yaml) is available in configs/templates, so you can alternatively copy this file into the configs/machines folder edit the relevant entries:

```
$ cp <PATH>/esm_tools/configs/templates/machine_template.yaml <PATH>/esm_tools/

oconfigs/machines/<new_machine>.yaml
$ <your_text_editor> <PATH>/esm_tools/configs/machines/<new_machine>.yaml
```

You can also reproduce the two steps above simply by running the following esm\_tools command:

This will copy the machine\_template.yaml in the target location and open the file in your default editor.

### 17.8.1 See also

- ESM-Tools Variables
- Switches (choose\_)
- What Is YAML?

## 17.9 Include a New Forcing/Input File

#### Feature available since version: 4.2

The next sections illustrate some of the many options to handle forcing and input files.

### 17.9.1 Source Path Already Defined in a Config File

- 1. Make sure the source of the file is already specified inside the forcing\_sources or input\_sources *file dictionaries* in the configuration file of the setup or model you are running, or on the further\_reading files.
- 2. In your runscript, include the *key* of the source file you want to include inside the forcing\_files or input\_files section.

**Note:** Note that the *key* containing the source in the forcing\_sources or input\_sources can be different than the key specified in forcing\_files or input\_files.

#### Example

#### ECHAM

In ECHAM, the source and input file paths are specified in a separate file (<PATH>/esm\_tools/configs/ components/echam/echam.datasets.yaml) that is reached through the further\_reading section of the echam. yaml. This file includes a large number of different sources for input and forcing contained in the pool directories of the HPC systems Ollie and Mistral. Let's have a look at the sst forcing file options available in this file:

This means that from our runscript we will be able to select either amipsst or pisst as *sst* forcing files. If you define scenario in *ECHAM* be PI-CTRL the correct file source (pisst) is already selected for you. However, if you would like to select this file manually you can just simply add the following to your runscript:

```
forcing_files:
    sst: pisst
```

### 17.9.2 Modify the Source of a File

To change the path of the source for a given forcing or input file from your runscript:

1. Include the source path under a key inside forcing\_sources or input\_sources in your runscript:

```
<forcing/input>_sources:
<key_for_your_file>: <path_to_your_file>
```

If the source is not a single file, but there is a file per year use the @YEAR@ and from: to: functionality in the path to copy only the files corresponding to that run's year:

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```
from: <first_year>
to: <last_year>
```

2. Make sure the *key* for your path is defined in one of the config files that you are using, inside of either forcing\_files or input\_files. If it is not defined anywhere you will have to include it in your runscript:

```
<forcing/input>_files:
<key_for_your_file>: <key_for_your_source>
```

### 17.9.3 Copy the file in the work folder and/or rename it

To copy the files from the forcing/input folders into the work folder (<base\_dir>/<exp\_id>/run\_<DATE>/work) or rename them:

- 1. Make sure your file and its source is defined somewhere (either in the config files or in your runscript) in <forcing/input>\_sources and <forcing/input>\_files (see subsections *Source Path Already Defined in a Config File* and *Modify the Source of a File*).
- 2. In your runscript, add the *key* to the file you want to **copy** with *value* the same as the *key*, inside <forc-ing/input>\_in\_work:

```
<forcing/input>_in_work:
<key_for_your_file>: <key_for_your_file>
```

3. If you want to **rename** the file set the *value* to the desired name:

#### Example

#### ECHAM

In *ECHAM* the sst forcing file depends in the scenario defined by the user:

#### esm\_tools/config/component/echam/echam.datasets.yaml

```
forcing_sources:
    # sst
    "amipsst":
        "${forcing_dir}/amip/${resolution}_amipsst_@YEAR@.nc":
            from: 1870
            to: 2016
        "pisst": "${forcing_dir}/${resolution}${ocean_resolution}_piControl-LR_sst_1880-
            ~2379.nc"
```

esm\_tools/config/component/echam/echam.yaml

```
choose_scenario:
    "PI-CTRL":
    forcing_files:
    sst: pisst
    [ ... ]
```

If scenario: "PI-CTRL" then the source selected will be \${forcing\_dir}/ \${resolution}\${ocean\_resolution}\_piControl-LR\_sst\_1880-2379.nc and the name of the file copied to the experiment forcing folder will be \${resolution}\${ocean\_resolution}\_piControl-LR\_sst\_1880-2379. nc. However, *ECHAM* needs this file in the same folder as the binary (the work folder) under the name unit.20. To copy and rename this file into the work folder the following lines are used in the echam.yaml configuration file:

```
forcing_in_work:
    sst: "unit.20"
```

You can use the same syntax **inside your runscript** to copy into the **work** folder any forcing or input file, and rename it.

### 17.9.4 See also

- What Is YAML?
- File Dictionaries

## 17.10 Exclude a Forcing/Input File

#### Feature available since version: 4.2

To exclude one of the predefined forcing or input files from being copied to your experiment folder:

- 1. Find the key of the file to be excluded inside the config file, <forcing/input>\_files file dictionary.
- 2. In your runscript, use the remove\_ functionality to exclude this *key* from the <forcing/input>\_files *file dictionary*:

```
remove_<input/forcing>_files:
        - <key_of_the_file1>
        - <key_of_the_file2>
        - ...
```

### 17.10.1 Example

### ECHAM

To exclude the sst forcing file from been copied to the experiment folder include the following lines in your runscript:

### 17.10.2 See also

- What Is YAML?
- Remove Elements from a List/Dictionary (remove\_)
- File Dictionaries

## 17.11 Using your own namelist

#### Feature available since version: 4.2

**Warning:** This feature is only recommended if the number of changes that need to be applied to the default namelist is very large, otherwise we recommend to use the feature namelist\_changes (see *Changing Namelist Entries from the Runscript*). You can check the default namelists here.

In your runscript, you can instruct ESM-Tools to substitute a given default namelist by a namelist of your choice.

- 1. Search for the config\_sources variable inside the configuration file of the model you are trying to run, and then, identify the "key" containing the path to the default namelist.
- 2. In your runscript, indented in the corresponding model section, add an add\_config\_sources section, containing a variable whose "key" is the one of step 1, and the value is the path of the new namelist.
- 3. Bare in mind, that namelists are first loaded by *ESM-Tools*, and then modified by the default namelist\_changes in the configuration files. If you want to ignore all those changes for the your new namelist you'll need to add remove\_namelist\_changes: [<name\_of\_your\_namelist>].

In dot notation both steps will look like: <model\_name>.<add\_config\_sources>.<key\_of\_the\_namelist>:
 cpath\_of\_your\_namelist> <model\_name>.<remove\_namelis\_changes>: [<name\_of\_your\_namelist>]

**Warning:** Use step 3 at your own risk! Many of the model specific information and functionality is transferred to the model through namelist\_changes, and therefore, we discourage you from using remove\_namelist\_changes unless you have a very deep understanding of the configuration file and the model. Following *Changing Namelist Entries from the Runscript* would be a safest solution.

### 17.11.1 Example

In this example we show how to use an *ECHAM* namelist.echam and a *FESOM* namelist.ice that are not the default ones and omit the namelist\_changes present in echam.yaml and fesom.yaml configuration files.

ECHAM

FESOM

Following step 1, search for the config\_sources dictionary inside the echam.yaml:

In this case the "key" is "namelist.echam" and the "value" is "\${namelist\_dir}/namelist.echam". Let's assume your namelist is in the directory /home/ollie/<usr>/my\_namelists. Following step 2, you will need to include the following in your runscript:

echam:

```
add_config_sources:
```

"namelist.echam": /home/ollie/<usr>/my\_namelists/namelist.echam

If you want to omit the namelist\_changes in echam.yaml or any other configuration file that your model/couple setup is using, you'll need to add to your runscript remove\_namelist\_changes: [namelist.echam] (step 3):

echam:

```
add_config_sources:
    "namelist.echam": /home/ollie/<usr>/my_namelists/namelist.echam
    remove_namelist_changes: [namelist.echam]
```

**Warning:** Many of the model specific information and functionality is transferred to the model through namelist\_changes, and therefore, we discourage you from using this unless you have a very deep understanding of the echam.yaml file and the ECHAM model. For example, using remove\_namelist\_changes: [namelist. echam] will destroy the following lines in the echam.yaml:

This lines are relevant for correctly performing restarts, so if remove\_namelist\_changes is used, make sure to have the appropriate commands on your runscript to remove dt\_start from your namelist in case of a restart.

Following step 1, search for the config\_sources dictionary inside the fesom.yaml:

```
config_sources:
    config: "${namelist_dir}/namelist.config"
    forcing: "${namelist_dir}/namelist.forcing"
    ice: "${namelist_dir}/namelist.ice"
    oce: "${namelist_dir}/namelist.oce"
    diag: "${namelist_dir}/namelist.diag"
```

In this case the "key" is ice and the "value" is  ${\text{mmelist_dir}/\text{namelist.ice. Let's assume your namelist is in the directory /home/ollie/<usr>/my_namelists. Following step 2, you will need to include the following in your runscript:$ 

fesom:
 add\_config\_sources:
 ice: "/home/ollie/<usr>/my\_namelists/namelist.ice"

If you want to omit the namelist\_changes in fesom.yaml or any other configuration file that your model/couple setup is using, you'll need to add to your runscript remove\_namelist\_changes: [namelist.ice] (step 3):

```
fesom:
    add_config_sources:
        ice: "/home/ollie/<usr>/my_namelists/namelist.ice"
```

remove\_namelist\_changes: [namelist.ice]

**Warning:** Many of the model specific information and functionality is transferred to the model through namelist\_changes, and therefore, we discourage you from using this unless you have a very deep understanding of the fesom.yaml file and the FESOM model.

### 17.11.2 See also

- Default namelists on GitHub
- Append to an Existing List (add\_)
- Changing Namelists
- What Is YAML?

## 17.12 How to branch-off FESOM from old spinup restart files

When you branch-off from very old FESOM ocean restart files, you may encounter the following runtime error:

read ocean restart file Error: NetCDF: Invalid dimension ID or name

This is because the naming of the NetCDF time dimension variable in the restart file has changed from T to time during the development of *FESOM* and the different *FESOM* versions. Therefore, recent versions of *FESOM* expect the name of the time dimension to be time.

In order to branch-off experiments from spinup restart files that use the old name for the time dimension, you need to rename this dimension before starting the branch-off experiment.

**Warning:** The following work around will change the restart file permanently. Make sure you do not apply this to the original file.

To rename a dimension variable of a NetCDF file, you can use ncrename:

ncrename -d T,time <copy\_of\_restart\_spinup\_file>.nc

where T is the old dimension and time is the new dimension.

## 17.12.1 See also

• cookbook:How to run a branch-off experiment

CHAPTER

### EIGHTEEN

## FREQUENTLY ASKED QUESTIONS

## **18.1 Installation**

1. Q: My organization is not in the pull-down list I get when trying the Federated Login to gitlab.awi.de.

A: Then maybe your institution just didn't join the DFN-AAI. You can check that at https://tools.aai.dfn.de/ entities/.

2. **Q**: I am trying to use the Federated Login, and that seems to work fine. When I should be redirected to the gitlab server though, I get the error that my uid is missing.

A: Even though your organization joined the DFN-AAI, gitlab.awi.de needs your organization to deliver information about your institutional e-mail address as part of the identity provided. Please contact the person responsible for shibboleth in your organization.

## **18.2 ESM Runscripts**

1. Q: I get the error: load\_all\_functions: not found [No such file or directory] when calling my runscript like this:

\$ ./my\_run\_script.sh -e some\_expid

A: You are trying to call your runscript the old-fashioned way that worked with the shell-script version, until revision 3. With the new python version, you get a new executable esm\_runscripts that should be in your PATH already. Call your runscript like this:

\$ esm\_runscripts my\_run\_script.sh -e some\_expid

All the command line options still apply. By the way, "load\_all\_function" doesn't hurt to have in the runscript, but can savely be removed.

2. Q: What should I put into the variable FUNCTION\_PATH in my runscript, I can't find the folder functions/all it should point to.

A: You can safely forget about FUNCTION\_PATH, which was only needed in the shell script version until revision 3. Either ignore it, or better remove it from the runscript.

3. Q: When I try to branch-off from a spinup experiment using FESOM, I get the following runtime error:

```
read ocean restart file
Error:
NetCDF: Invalid dimension ID or name
```

A: See How to branch-off FESOM from old spinup restart files.

## 18.3 ESM Master

1. Q: How can I define different environments for different models / different versions of the same model?

A: You can add a choose-block in the models yaml-file (esm\_tools/configs/model\_name.yaml), e.g.:

choose_version:	
<b>40r1</b> :	
	environment_changes:
	add_export_vars:
	<pre>- 'MY_VAR="something"'</pre>
	add_module_actions:
	<pre>- load my_own_module</pre>
43r3:	
	environment_changes:
	add_export_vars:
	- 'MY_VAR="something_else"'

2. Q: How can I add a new model, setup, and coupling strategy to the esm\_master tool?

A: Add your configuration in the file configs/esm\_master/setups2models.yaml

## **18.4 Frequent Errors**

1. Q: When I try to install *ESM-Tools* or use esm\_versions I get the following error:

RuntimeError: Click will abort further execution because Python 3 was configured to →use ASCII as encoding for the environment. Consult https://click.palletsprojects. →com/en/7.x/python3/ for mitigation steps.

or something on the following lines:

```
ERROR: Command errored out with exit status 1:
command: /sw/rhel6-x64/conda/anaconda3-bleeding_edge/bin/python -c 'import sys,
→setuptools, tokenize; sys.argv[0] = '''''/tmp/pip-install-0y687gmq/esm-master/setup.py'
___''''; _file__='''''/tmp/pip-install-0y687gmq/esm-master/setup.py''''';
→f=getattr(tokenize, '"'"'open'"''', open)(__file__);code=f.read().replace('"'''\r\n'"'"
→egg-base /tmp/pip-install-0y687gmq/esm-master/pip-egg-info
cwd: /tmp/pip-install-0y687gmq/esm-master/
Complete output (7 lines):
Traceback (most recent call last):
  File "<string>", line 1, in <module>
  File "/tmp/pip-install-0y687gmq/esm-master/setup.py", line 8, in <module>
    readme = readme_file.read()
  File "/sw/rhel6-x64/conda/anaconda3-bleeding_edge/lib/python3.6/encodings/ascii.py",
\rightarrow line 26, in decode
    return codecs.ascii_decode(input, self.errors)[0]
```

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```
UnicodeDecodeError: 'ascii' codec can't decode byte 0xf0 in position 1468: ordinal not_

in range(128)

ERROR: Command errored out with exit status 1: python setup.py egg_info Check the logs_

for full command output.

**A**: Some systems have ``C.UTF-8`` as locale default (i.e. ``$LC_ALL``, ``$LANG``)._

This issue is solved by setting up the locales respectively to ``en_US.UTF-8`` and_

...

*`en_US.UTF-8``, either manually or adding them to the local bash configuration file_

(i.e. ``~/.bash_profile``)::

$ export LC_ALL=en_US.UTF-8

$ export LANG=en_US.UTF-8
```

2. Q: How can I add a new model, setup, and coupling strategy to the esm\_master tool?

A: Add your configuration in the file configs/esm\_master/setups2models.yaml (see contributing:Implementing a New Model and *Implement a New Coupled Setup*)

### CHAPTER

### NINETEEN

## **PYTHON PACKAGES**

The ESM-Tools are divided into a number of python packages / git repositories, both to ensure stability of the code as well as reusability:

## 19.1 esm\_tools.git

The only repository to clone by hand by the user, esm\_tools.git contains the subfolders

**configs**: A collection of yaml configuration files, containing all the information needed by the python packages to work properly. This includes machine specific files (e.g. machines/mistral.yaml), model specific files (e.g fesom/fesom-2.0.yaml), configurations for coupled setups (e.g. foci/foci.yaml), but also files with the information on how a certain software works (batch\_systems/slurm.yaml), and finally, how the esm\_tools themselves are supposed to work (e.g. esm\_master/esm\_master.yaml).

## 19.2 esm\_master.git

This repository contains the python files that give the esm\_master executable in the subfolder esm\_master.

## 19.3 esm\_runscripts.git

The python package of the esm\_runscripts executable. The main routines can be found in esm\_runscripts/ esm\_sim\_objects.py.

## 19.4 esm\_parser.git

In order to provide the additional functionality to the yaml+ configuration files (like choose blocks, simple math operations, variable expansions etc.). esm\_parser is an extension of the pyyaml package, it needs the esm\_calendar package to run, but can otherwise easily be used to add yaml+ configurations to any python software.

# 19.5 esm\_calendar.git

### CHAPTER

### TWENTY

## ESM TOOLS CODE DOCUMENTATION

## 20.1 esm\_archiving package

Top-level package for ESM Archiving.

esm\_archiving.archive\_mistral(tfile, rtfile=None)

Puts the tfile to the tape archive using tape\_command

#### **Parameters**

- tfile (str) The full path of the file to put to tape
- **rtfile** (*str*) The filename on the remote tape server. Defaults to None, in which case a replacement is performed to keep as much of the filename the same as possible. Example: /work/ab0246/a270077/experiment.tgz -> /hpss/arch/ab0246/a270077/experiment.tgz

#### **Return type**

None

esm\_archiving.check\_tar\_lists(tar\_lists)

#### esm\_archiving.delete\_original\_data(tfile, force=False)

Erases data which is found in the tar file.

#### Parameters

- **tfile** (*str*) Path to the tarfille whose data should be erased.
- **force** (*bool*) If False, asks the user if they really want to delete their files. Otherwise just does this silently. Default is False

#### **Return type**

None

#### esm\_archiving.determine\_datestamp\_location(files)

Given a list of files; figures where the datestamp is by checking if it varies.

#### Parameters

files (list) – A list (longer than 1!) of files to check

#### Returns

A slice object giving the location of the datestamp

#### **Return type**

slice

#### Raises

**DatestampLocationError** : – Raised if there is more than one slice found where the numbers vary over different files -or- if the length of the file list is not longer than 1.

#### esm\_archiving.determine\_potential\_datestamp\_locations(filepattern)

For a filepattern, gives back index of potential date locations

#### Parameters

**filepattern** (*str*) – The filepattern to check.

#### Returns

A list of slice object which you can use to cut out dates from the filepattern

#### **Return type**

list

#### esm\_archiving.find\_indices\_of(char, in\_string)

Finds indicies of a specific character in a string

#### Parameters

- char (str) The character to look for
- **in\_string** (*str*) The string to look in

Yields

int - Each round of the generator gives you the next index for the desired character.

Creates a list of files for specified start/stop dates

#### Parameters

- **filepattern** (*str*) A filepattern to replace dates in
- start\_date (str) The starting date, in a pandas-friendly date format
- stop\_date (str) Ending date, pandas friendly. Note that for end dates, you need to add
  one month to assure that you get the last step in your list!
- frequency (str) Frequency of dates, pandas friendly
- date\_format (str) How dates should be formatted, defaults to %Y%m%d

#### Returns

A list of strings for the filepattern with correct date stamps.

#### **Return type**

list

#### Example

```
>>> filepattern = "LGM_24hourly_PMIP4_echam6_BOT_mm_>>>DATE<<<<.nc"
>>> LGM_files = get_files_for_date_range(filepattern, "1890-07", "1891-11", "1M",_
__date_format="%Y%m")
>>> LGM_files == [
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189007.nc",
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189008.nc",
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189009.nc",
```

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"LGM_24hourly_PMIP4_echam6_BOT_mm_189010.nc",
"LGM_24hourly_PMIP4_echam6_BOT_mm_189011.nc",
<pre> "LGM_24hourly_PMIP4_echam6_BOT_mm_189012.nc",</pre>
<pre> "LGM_24hourly_PMIP4_echam6_BOT_mm_189101.nc",</pre>
<pre> "LGM_24hourly_PMIP4_echam6_BOT_mm_189102.nc",</pre>
<pre> "LGM_24hourly_PMIP4_echam6_BOT_mm_189103.nc",</pre>
<pre> "LGM_24hourly_PMIP4_echam6_BOT_mm_189104.nc",</pre>
"LGM_24hourly_PMIP4_echam6_BOT_mm_189105.nc",
"LGM_24hourly_PMIP4_echam6_BOT_mm_189106.nc",
"LGM_24hourly_PMIP4_echam6_BOT_mm_189107.nc",
<pre> "LGM_24hourly_PMIP4_echam6_BOT_mm_189108.nc",</pre>
<pre> "LGM_24hourly_PMIP4_echam6_BOT_mm_189109.nc",</pre>
<pre> "LGM_24hourly_PMIP4_echam6_BOT_mm_189110.nc",</pre>
]
True

#### esm\_archiving.get\_list\_from\_filepattern(filepattern)

#### esm\_archiving.group\_files(top, filetype)

Generates quasi-regexes for a specific filetype, replacing all numbers with #.

#### Parameters

- top (str) Where to start looking (this should normally be top of the experiment)
- **filetype** (*str*) Which files to go through (e.g. outdata, restart, etc...)

#### Returns

A dictonary containing keys for each folder found in filetype, and values as lists of files with strings where numbers are replaced by #.

#### **Return type**

dict

```
esm_archiving.group_indexes(index_list)
```

Splits indexes into tuples of monotonically ascending values.

#### Parameters

**list** – The list to split up

#### Returns

A list of tuples, so that you can get only one group of ascending tuples.

#### **Return type**

list

#### Example

```
>>> indexes = [0, 1, 2, 3, 12, 13, 15, 16]
>>> group_indexes(indexes)
[(0, 1, 2, 3), (12, 13), (15, 16)]
```

#### esm\_archiving.log\_tarfile\_contents(tfile)

Generates a log of the tarball contents

Parameters

tfile (str) – The path for the tar file to generate a log for

Return type

None

**Warning:** Note that for this function to work, you need to have write permission in the directory where the tarball is located. If not, this will probably raise an OSError. I can imagine giving the location of the log path as an argument; but would like to see if that is actually needed before implementing it...

#### esm\_archiving.pack\_tarfile(flist, wdir, outname)

Creates a compressed tarball (outname) with all files found in flist.

#### **Parameters**

- **flist** (*list*) A list of files to include in this tarball
- wdir (*str*) The directory to "change" to when packing up the tar file. This will (essentially) be used in the tar command as the -C option by stripping off the beginning of the flist
- **outname** (*str*) The output file name

#### Returns

The output file name

#### **Return type**

str

esm\_archiving.purify\_expid\_in(model\_files, expid, restore=False)

Puts or restores >>>EXPID<<< marker in filepatterns

#### **Parameters**

- **model\_files** (*dict*) The model files for archiving
- **expid** (*str*) The experiment ID to purify or restore
- restore (bool) Set experiment ID back from the temporary marker

#### Returns

Dictionary containing keys for each model, values for file patterns

#### **Return type**

dict

esm\_archiving.sort\_files\_to\_tarlists(model\_files, start\_date, end\_date, config)

esm\_archiving.split\_list\_due\_to\_size\_limit(in\_list, slimit)

esm\_archiving.stamp\_filepattern(filepattern, force\_return=False)

Transforms # in filepatterns to >>>DATE<<< and replaces other numbers back to original

#### **Parameters**

- filepattern (str) Filepattern to get date stamps for
- **force\_return** (*bool*) Returns the list of filepatterns even if it is longer than 1.

#### Returns

New filepattern, with >>>DATE<<<

#### Return type

str

#### esm\_archiving.stamp\_files(model\_files)

Given a strandard file dictioanry (keys: model names, values: filepattern); figures out where the date probably is, and replaces the # sequence with a >>>DATE<<< stamp.

#### Parameters

**model\_files** (*dict*) – Dictionary of keys (model names) where values are lists of files for each model.

#### Returns

As the input, but replaces the filepatterns with the >>>DATE<<< stamp.

#### **Return type**

dict

#### esm\_archiving.sum\_tar\_lists(tar\_lists)

Sums up the amount of space in the tar lists dictionary

Given tar\_lists, which is generally a dicitonary consisting of keys (model names) and values (files to be tarred), figures out how much space the **raw, uncompressed** files would use. Generally the compressed tarball will take up less space.

#### **Parameters**

**tar\_lists** (*dict*) – Dictionary of file lists to be summed up. Reports every sum as a value for the key of that particular list.

#### Returns

Keys are the same as in the input, values are the sums (in bytes) of all files present within the list.

### **Return type**

dict

#### esm\_archiving.sum\_tar\_lists\_human\_readable(tar\_lists)

As sum\_tar\_lists but gives back strings with human-readable sizes.

### 20.1.1 Subpackages

#### esm\_archiving.external package

#### **Submodules**

#### esm\_archiving.external.pypftp module

class esm\_archiving.external.pypftp.Pftp(username=None, password=None)

Bases: object

HOST = 'tape.dkrz.de'

PORT = 4021

close()

cwd(path)

change working directory

#### directories(path=None)

gather directories at the given path

#### static download(source, destination)

uses pftp binary for transfering the file

#### exists(path)

check if a path exists

### files(path=None)

gather files at the given path

#### is\_connected()

check if the connection is still active

#### isdir(pathname)

Returns true if pathname refers to an existing directory

#### isfile(pathname)

Returns true if pathname refers to an existing file

#### islink(pathname)

#### listdir(path=None)

list directory contents

#### listing(path=None)

list directory contents

#### listing2(path=None)

directory listing in long form. similar to "Is -l"

#### makedirs(path)

Recursively create dirs as required walking up to an existing parent dir

#### mkdir(path)

mlsd(path)

#### pwd()

present working directory

#### quit()

#### reconnect()

reconnects to the ftp server

#### remove(filename)

removedirs(path)

rename(from\_name, to\_name)

#### rmdir(path)

remove directory

#### size(pathname)

Returns size of path in bytes

stat(pathname)
 Returns stat of the path

static upload(source, destination)

uses pftp binary for transfering the file

walk(path=None)

recursively walk the directory tree from the given path. Similar to os.walk

walk\_for\_directories(path=None)
recursively gather directories

walk\_for\_files(path=None)

recursively gather files

esm\_archiving.external.pypftp.download(source, destination)

esm\_archiving.external.pypftp.upload(source, destination)

## 20.1.2 Submodules

### 20.1.3 esm\_archiving.cli module

After installation, you have a new command in your path:

esm\_archive

Passing in the argument --help will show available subcommands:

```
Usage: esm_archive [OPTIONS] COMMAND [ARGS]...

Console script for esm_archiving.

Options:

--version Show the version and exit.

--write_local_config Write a local configuration YAML file in the current

working directory

--write_config Write a global configuration YAML file in

~/.config/esm_archiving/

--help Show this message and exit.

Commands:

create

upload
```

To use the tool, you can first create a tar archive and then use upload to put it onto the tape server.

#### **Creating tarballs**

Use esm\_archive create to generate tar files from an experiment:

```
esm_archive create /path/to/top/of/experiment start_date end_date
```

The arguments start\_date and end\_date should take the form YYYY-MM-DD. A complete example would be:

```
esm_archive create /work/ab0246/a270077/from_ba0989/AWICM/LGM_6hours 1850-01-01 1851-01-
```

The archiving tool will automatically pack up all files it finds matching these dates in the outdata and restart directories and generate logs in the top of the experiment folder. Note that the final date (1851-01-1 in this example) is **not included**. During packing, you get a progress bar indicating when the tarball is finished.

Please be aware that are size limits in place on DKRZ's tape server. Any tar files **larger than 500 Gb will be trucated**. For more information, see: https://www.dkrz.de/up/systems/hpss/hpss

#### **Uploading tarballs**

A second command esm\_archive upload allows you to put tarballs onto to tape server at DKRZ:

```
esm_archive upload /path/to/top/of/experiment start_date end_date
```

The signature is the same as for the create subcommand. Note that for this to work; you need to have a properly configured .netrc file in your home directory:

```
$ cat ~/.netrc
machine tape.dkrz.de login a270077 password OMITTED
```

This file needs to be readable/writable **only** for you, e.g. **chmod 600**. The archiving program will then be able to automatically log into the tape server and upload the tarballs. Again, more information about logging onto the tape server without password authentication can be found here: https://www.dkrz.de/up/help/faq/hpss/ how-can-i-use-the-hpss-tape-archive-without-typing-my-password-every-time-e-g-in-scripts-or-jobs

### 20.1.4 esm\_archiving.config module

When run from either the command line or in library mode (note **not** as an ESM Plugin), esm\_archiving can be configured to how it looks for specific files. The configuration file is called esm\_archiving\_config, should be written in YAML, and have the following format:

```
echam: # The model name
archive: # archive seperator **required**
    # Frequency specification (how often
    # a datestamp is generated to look for)
    frequency: "1M"
    # Date format specification
    date_format: "%Y%m"
```

By default, esm\_archive looks in the following locations:

- 1. Current working directory
- 2. Any files in the XDG Standard:

https://specifications.freedesktop.org/basedir-spec/basedir-spec-latest.html

If nothing is found, the program reverts to the hard-coded defaults, found in esm\_archiving/esm\_archiving/ config.py

**Note:** In future, it might be changed that the program will look for an experiment specific configuration based upon the path it is given during the create or upload step.

#### Generating a configuration

You can use the command line switches --write\_local\_config and --write\_config to generate configuration files either in the current working directory, or in the global directory for your user account defined by the XDG standard (typically ~/.config/esm\_archiving):

```
$ esm_archive --write_local_config
Writing local (experiment) configuration...
$ esm_archive --write_config
Writing global (user) configuration...
```

#### esm\_archiving.config.load\_config()

Loads the configuration from one of the default configuration directories. If none can be found, returns the hard-coded default configuration.

#### Returns

A representation of the configuration used for archiving.

Return type

esm\_archiving.config.write\_config\_yaml(path=None)

### 20.1.5 esm\_archiving.esm\_archiving module

This is the esm\_archiving module.

#### exception esm\_archiving.esm\_archiving.DatestampLocationError

Bases: Exception

esm\_archiving.esm\_archiving.archive\_mistral(tfile, rtfile=None)

Puts the tfile to the tape archive using tape\_command

#### Parameters

- **tfile** (*str*) The full path of the file to put to tape
- **rtfile** (*str*) The filename on the remote tape server. Defaults to None, in which case a replacement is performed to keep as much of the filename the same as possible. Example: /work/ab0246/a270077/experiment.tgz -> /hpss/arch/ab0246/a270077/experiment.tgz

#### **Return type**

None

esm\_archiving.esm\_archiving.check\_tar\_lists(tar\_lists)

#### esm\_archiving.esm\_archiving.delete\_original\_data(tfile, force=False)

Erases data which is found in the tar file.

#### Parameters

- tfile (str) Path to the tarfille whose data should be erased.
- **force** (*bool*) If False, asks the user if they really want to delete their files. Otherwise just does this silently. Default is False

#### **Return type**

None

#### esm\_archiving.esm\_archiving.determine\_datestamp\_location(files)

Given a list of files; figures where the datestamp is by checking if it varies.

#### Parameters

files (list) – A list (longer than 1!) of files to check

#### Returns

A slice object giving the location of the datestamp

#### **Return type**

slice

#### Raises

**DatestampLocationError** : – Raised if there is more than one slice found where the numbers vary over different files -or- if the length of the file list is not longer than 1.

#### esm\_archiving.esm\_archiving.determine\_potential\_datestamp\_locations(filepattern)

For a filepattern, gives back index of potential date locations

#### Parameters

**filepattern** (*str*) – The filepattern to check.

#### Returns

A list of slice object which you can use to cut out dates from the filepattern

#### **Return type**

list

#### esm\_archiving.esm\_archiving.find\_indices\_of(char, in\_string)

Finds indicies of a specific character in a string

#### Parameters

- char (str) The character to look for
- **in\_string** (*str*) The string to look in

#### Yields

int - Each round of the generator gives you the next index for the desired character.

esm\_archiving.esm\_archiving.get\_files\_for\_date\_range(filepattern, start\_date, stop\_date, frequency,

date\_format='%Y%m%d')

Creates a list of files for specified start/stop dates

#### Parameters

- **filepattern** (*str*) A filepattern to replace dates in
- start\_date (str) The starting date, in a pandas-friendly date format

- stop\_date (str) Ending date, pandas friendly. Note that for end dates, you need to add one month to assure that you get the last step in your list!
- frequency (str) Frequency of dates, pandas friendly
- date\_format (str) How dates should be formatted, defaults to %Y%m%d

#### Returns

A list of strings for the filepattern with correct date stamps.

#### **Return type**

list

#### Example

```
>>> filepattern = "LGM_24hourly_PMIP4_echam6_BOT_mm_>>>DATE<<<.nc"</pre>
>>> LGM_files = get_files_for_date_range(filepattern, "1890-07", "1891-11", "1M",.
→date_format="%Y%m")
>>> LGM_files == [
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189007.nc",
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189008.nc"
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189009.nc"
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189010.nc",
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189011.nc",
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189012.nc"
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189101.nc"
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189102.nc",
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189103.nc",
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189104.nc"
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189105.nc"
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189106.nc",
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189107.nc"
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189108.nc"
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189109.nc".
... "LGM_24hourly_PMIP4_echam6_BOT_mm_189110.nc",
...]
True
```

#### esm\_archiving.esm\_archiving.get\_list\_from\_filepattern(filepattern)

#### esm\_archiving.esm\_archiving.group\_files(top, filetype)

Generates quasi-regexes for a specific filetype, replacing all numbers with #.

#### Parameters

- top (str) Where to start looking (this should normally be top of the experiment)
- **filetype** (*str*) Which files to go through (e.g. outdata, restart, etc...)

#### Returns

A dictonary containing keys for each folder found in filetype, and values as lists of files with strings where numbers are replaced by #.

#### **Return type**

dict

esm\_archiving.esm\_archiving.group\_indexes(index\_list)

Splits indexes into tuples of monotonically ascending values.

Parameters

**list** – The list to split up

#### Returns

A list of tuples, so that you can get only one group of ascending tuples.

**Return type** 

list

#### Example

>>> indexes = [0, 1, 2, 3, 12, 13, 15, 16]
>>> group\_indexes(indexes)
[(0, 1, 2, 3), (12, 13), (15, 16)]

#### esm\_archiving.esm\_archiving.log\_tarfile\_contents(tfile)

Generates a log of the tarball contents

#### **Parameters**

tfile (str) – The path for the tar file to generate a log for

Return type

None

**Warning:** Note that for this function to work, you need to have write permission in the directory where the tarball is located. If not, this will probably raise an OSError. I can imagine giving the location of the log path as an argument; but would like to see if that is actually needed before implementing it...

#### esm\_archiving.esm\_archiving.pack\_tarfile(flist, wdir, outname)

Creates a compressed tarball (outname) with all files found in flist.

#### Parameters

- flist (list) A list of files to include in this tarball
- wdir (*str*) The directory to "change" to when packing up the tar file. This will (essentially) be used in the tar command as the -C option by stripping off the beginning of the flist
- **outname** (*str*) The output file name

#### Returns

The output file name

#### **Return type**

str

esm\_archiving.esm\_archiving.purify\_expid\_in(model\_files, expid, restore=False)

Puts or restores >>>EXPID<<< marker in filepatterns

#### Parameters

- model\_files (dict) The model files for archiving
- **expid** (*str*) The experiment ID to purify or restore
- restore (bool) Set experiment ID back from the temporary marker

#### Returns

Dictionary containing keys for each model, values for file patterns

# Return type

esm\_archiving.esm\_archiving.query\_yes\_no(question, default='yes')

Ask a yes/no question via input() and return their answer.

"question" is a string that is presented to the user. "default" is the presumed answer if the user just hits <Enter>.

It must be "yes" (the default), "no" or None (meaning an answer is required of the user).

The "answer" return value is True for "yes" or False for "no".

Note: Shamelessly stolen from StackOverflow It's not hard to implement, but Paul is lazy...

#### Parameters

• question (str) – The question you'd like to ask the user

• default (str) – The presumed answer for question. Defaults to "yes".

#### Returns

True if the user said yes, False if the use said no.

**Return type** 

bool

#### esm\_archiving.esm\_archiving.run\_command(command)

Runs command and directly prints output to screen.

#### **Parameters**

**command** (str) – The command to run, with pipes, redirects, whatever

#### Returns

rc – The return code of the subprocess.

#### **Return type**

int

esm\_archiving.esm\_archiving.sort\_files\_to\_tarlists(model\_files, start\_date, end\_date, config)

```
esm_archiving.esm_archiving.split_list_due_to_size_limit(in_list, slimit)
```

#### esm\_archiving.esm\_archiving.stamp\_filepattern(filepattern, force\_return=False)

Transforms # in filepatterns to >>>DATE<<< and replaces other numbers back to original

#### **Parameters**

- filepattern (str) Filepattern to get date stamps for
- **force\_return** (*bool*) Returns the list of filepatterns even if it is longer than 1.

#### Returns

New filepattern, with >>>DATE<<<

#### **Return type**

str

#### esm\_archiving.esm\_archiving.stamp\_files(model\_files)

Given a strandard file dictioanry (keys: model names, values: filepattern); figures out where the date probably is, and replaces the # sequence with a >>>DATE<<< stamp.

#### **Parameters**

**model\_files** (*dict*) – Dictionary of keys (model names) where values are lists of files for each model.

#### Returns

As the input, but replaces the filepatterns with the >>>DATE<<< stamp.

### **Return type**

dict

esm\_archiving.esm\_archiving.sum\_tar\_lists(tar\_lists)

Sums up the amount of space in the tar lists dictionary

Given tar\_lists, which is generally a dicitonary consisting of keys (model names) and values (files to be tarred), figures out how much space the **raw, uncompressed** files would use. Generally the compressed tarball will take up less space.

#### Parameters

**tar\_lists** (*dict*) – Dictionary of file lists to be summed up. Reports every sum as a value for the key of that particular list.

#### Returns

Keys are the same as in the input, values are the sums (in bytes) of all files present within the list.

#### **Return type**

dict

esm\_archiving.esm\_archiving.sum\_tar\_lists\_human\_readable(tar\_lists)

As sum\_tar\_lists but gives back strings with human-readable sizes.

## 20.2 esm\_calendar package

Top-level package for ESM Calendar.

## 20.2.1 Submodules

### 20.2.2 esm\_calendar.esm\_calendar module

Module Docstring.,..?

```
class esm_calendar.esm_calendar.Calendar(calendar_type=1)
```

Bases: object

Class to contain various types of calendars.

#### **Parameters**

**calendar\_type** (*int*) – The type of calendar to use.

Supported calendar types: 0

no leap years

1

proleptic greogrian calendar (default)

n

equal months of n days

#### timeunits

A list of accepted time units.

### Туре

list of str

#### monthnames

A list of valid month names, using 3 letter English abbreviation.

#### Type

list of str

### isleapyear(year)

Returns a boolean testing if the given year is a leapyear

#### day\_in\_year(year)

Returns the total number of days in a given year

#### day\_in\_month(year, month)

Returns the total number of days in a given month for a given year (considering leapyears)

#### day\_in\_month(year, month)

Finds the number of days in a given month

#### Parameters

• year (*int*) – The year to check

• month (int or str) – The month number or short name.

#### Returns

The number of days in this month, considering leapyears if needed.

#### **Return type**

int

#### Raises

TypeError - Raised when you give an incorrect type for month

#### day\_in\_year(year)

Finds total number of days in a year, considering leapyears if the calendar type allows for them.

#### Parameters

**year** (*int*) – The year to check

#### Returns

The total number of days for this specific calendar type

### **Return type**

int

#### isleapyear(year)

Checks if a year is a leapyear

#### Parameters

**year** (int) – The year to check

#### Returns

True if the given year is a leapyear

#### **Return type**

bool

```
monthnames = ['Jan', 'Feb', 'Mar', 'Apr', 'May', 'Jun', 'Jul', 'Aug', 'Sep', 'Oct',
'Nov', 'Dec']
```

```
timeunits = ['years', 'months', 'days', 'hours', 'minutes', 'seconds']
```

**class** esm\_calendar.esm\_calendar.**Date**(*indate*, *calendar=esm\_calendar(calendar\_type=1*))

Bases: object

A class to contain dates, also compatiable with paleo (negative dates)

#### Parameters

• **indate** (*str*) – The date to use.

See *pyesm.core.time\_control.esm\_calendar.Dateformat* for available formatters.

• **calendar** (*Calendar*`, *optional*) – The type of calendar to use. Defaults to a greogrian proleptic calendar if nothing is specified.

#### year

The year

Type int

#### month

The month

Type int

#### day

The day

Type int

#### hour

The hour

Type int

minute

The minute

Туре

int

#### second

The second

Type int

\_calendar

The type of calendar to use

Type

Calendar`

#### $add(to\_add)$

Adds another date to this one.

#### Parameters

**to\_add** (*Date*`) – The other date to add to this one.

#### Returns

new\_date - A new date object with the added dates

### Return type

Date`

### day\_of\_year()

Gets the day of the year, counting from Jan. 1

#### Returns

The day of the current year.

# Return type int

format(form='SELF', givenph=None, givenpm=None, givenps=None)

Beautifully returns a Date object as a string.

#### **Parameters**

- form (str or int) Logic taken from MPI-Met
- givenph (bool-ish) Print hours
- givenpm (bool-ish) Print minutes
- givenps (bool-ish) Print seconds

#### Note:

#### How to use the ``form`` argument

The following forms are accepted: + SELF: uses the format which was given when constructing the date + 0: A Date formatted as YYYY

- In [5]: test.format(form=1) Out[5]: '1850-01-01\_00:00:00'
- In [6]: test.format(form=2) Out[6]: '1850-01-01T00:00:00'
- In [7]: test.format(form=3) Out[7]: '1850-01-01 00:00:00'
- In [8]: test.format(form=4) Out[8]: '1850 01 01 00 00 00'
- In [9]: test.format(form=5) Out[9]: '01 Jan 1850 00:00:00'
- In [10]: test.format(form=6) Out[10]: '18500101\_00:00:00'
- In [11]: test.format(form=7) Out[11]: '1850-01-01\_000000'
- In [12]: test.format(form=8) Out[12]: '18500101000000'
- In [13]: test.format(form=9) Out[13]: '18500101\_000000'
- In [14]: test.format(form=10) Out[14]: '01/01/1850 00:00:00'

#### classmethod from\_list(\_list)

Creates a new Date from a list

Parameters

\_list (list of ints) – A list of [year, month, day, hour, minute, second]

Returns

date - A new date of year month day, hour minute, second

Return type

Date`

#### classmethod fromlist(\_list)

Creates a new Date from a list

#### Parameters

\_list (list of ints) – A list of [year, month, day, hour, minute, second]

#### Returns

date - A new date of year month day, hour minute, second

#### **Return type**

Date

#### makesense(ndate)

Puts overflowed time back into the correct unit.

When manipulating the date, it might be that you have "70 seconds", or something similar. Here, we put the overflowed time into the appropriate unit.

output(form='SELF')

- property sday
- property sdoy
- property shour
- property sminute
- property smonth
- property ssecond
- sub\_date(other)
- sub\_tuple(to\_sub)

Adds another date to from one.

#### **Parameters**

**to\_sub** (*Date*`) – The other date to sub from this one.

#### Returns

new\_date - A new date object with the subtracted dates

Return type Date`

#### property syear

#### time\_between(date, outformat='seconds')

Computes the time between two dates

#### Parameters

**date** (*date*`) – The date to compare against.

Return type

??

**class** esm\_calendar.esm\_calendar.**Dateformat**(*form=1*, *printhours=True*, *printminutes=True*, *printseconds=True*)

Bases: object

esm\_calendar.esm\_calendar.date\_range(start\_date, stop\_date, frequency)

esm\_calendar.esm\_calendar.find\_remaining\_hours(seconds)

Finds the remaining full minutes of a given number of seconds

#### Parameters

seconds (int) – The number of seconds to allocate

Returns

The leftover seconds once new minutes have been filled.

Return type

int

esm\_calendar.esm\_calendar.find\_remaining\_minutes(seconds)

Finds the remaining full minutes of a given number of seconds

#### Parameters

seconds (int) – The number of seconds to allocate

#### Returns

The leftover seconds once new minutes have been filled.

Return type int

## 20.3 esm\_cleanup package

Cleanup tool for ESM-Tools simulations

### 20.3.1 Submodules

#### 20.3.2 esm\_cleanup.cli module

```
esm_cleanup.cli.evaluate_arguments()
```

The arg parser for interactive use

```
esm_cleanup.cli.main()
```

```
esm_cleanup.cli.main_loop(folder)
```

### 20.3.3 esm\_cleanup.esm\_cleanup module

esm\_cleanup.esm\_cleanup.add\_size\_information(toplevel, item) esm\_cleanup.esm\_cleanup.ask\_for\_action(folder) esm\_cleanup.esm\_cleanup.assert\_question(question) esm\_cleanup.esm\_cleanup.check\_if\_folder\_exists(folder) esm\_cleanup.esm\_cleanup.dir\_size(somepath) esm\_cleanup.esm\_cleanup.file\_size(somepath) esm\_cleanup.esm\_cleanup.format\_size(total\_size) esm\_cleanup.esm\_cleanup.inspect\_size(thisfile) esm\_cleanup.esm\_cleanup.is\_experiment\_folder(checkpath) esm\_cleanup.esm\_cleanup.pick\_experiment\_folder(folder) esm\_cleanup.esm\_cleanup.pick\_subfolder(folder) esm\_cleanup.esm\_cleanup.print\_disclaimer() esm\_cleanup.esm\_cleanup.print\_folder\_content(checkpath, saved\_space) esm\_cleanup.esm\_cleanup.read\_in\_yaml\_file(filename) esm\_cleanup.esm\_cleanup.remove\_post\_subfolders(folder, saved\_space) esm\_cleanup.esm\_cleanup.remove\_run\_subfolders(folder, saved\_space) esm\_cleanup.esm\_cleanup.remove\_size\_information(name\_with\_file) esm\_cleanup.esm\_cleanup.remove\_some\_files(folder, saved\_space) esm\_cleanup.esm\_cleanup.remove\_subfolder(folder, saved\_space)

## 20.4 esm\_database package

Top-level package for ESM Database.

### 20.4.1 Submodules

### 20.4.2 esm\_database.cli module

A small wrapper that combines the shell interface and the Python interface esm\_database.cli.main()

```
esm_database.cli.parse_shargs()
```

The arg parser for interactive use

### 20.4.3 esm\_database.esm\_database module

class esm\_database.esm\_database.DisplayDatabase(tablename=None)

```
Bases: object
ask_column()
ask_dataset()
decision_maker()
edit_dataset()
output_writer()
remove_datasets()
select_stuff()
```

### 20.4.4 esm\_database.getch module

```
esm_database.getch.get_one_of(testlist)
```

### 20.4.5 esm\_database.location\_database module

```
class esm_database.location_database.database_location(**kwargs)
Bases: Base
class_in
id
location
table_name
static topline()
```

```
esm_database.location_database.register(table_name, given_location, class_in)
```

## 20.5 esm\_environment package

### 20.5.1 Submodules

## 20.5.2 esm\_environment.esm\_environment module

## 20.6 esm\_master package

Top-level package for ESM Master.

### 20.6.1 Submodules

- 20.6.2 esm\_master.cli module
- 20.6.3 esm\_master.compile\_info module

### 20.6.4 esm\_master.database module

```
class esm_master.database.installation(**kwargs)
    Bases: Base
    action
    folder
    id
    static nicer_output(run)
    setup_name
    timestamp
    static topline()
```

### 20.6.5 esm\_master.database\_actions module

esm\_master.database\_actions.database\_entry(config, action, setup\_name, base\_dir)

### 20.6.6 esm\_master.esm\_master module

### 20.6.7 esm\_master.general\_stuff module

### 20.6.8 esm\_master.software\_package module

esm\_master.software\_package.replace\_var(var, tag, value)

# class esm\_master.software\_package.software\_package(raw, setup\_info, vcs, general, no\_infos=False) Bases: object

complete\_targets(setup\_info)

fill\_in\_infos(setup\_info, vcs, general)

get\_command\_list(setup\_info, vcs, general)

get\_comp\_type(setup\_info)

get\_coupling\_changes(setup\_info)

get\_repo\_info(setup\_info, vcs)

get\_subpackages(setup\_info, vcs, general)

```
get_targets(setup_info, vcs)
output()
```

## 20.6.9 esm\_master.task module

## 20.7 esm\_motd package

- 20.7.1 Submodules
- 20.7.2 esm\_motd.esm\_motd module
- 20.8 esm\_parser package
- 20.8.1 Submodules
- 20.8.2 esm\_parser.esm\_parser module

### 20.8.3 esm\_parser.yaml\_to\_dict module

#### exception esm\_parser.yaml\_to\_dict.EsmConfigFileError(fpath, yaml\_error)

Bases: Exception

Exception for yaml file containing tabs or other syntax issues.

An exception used when yaml.load() throws a yaml.scanner.ScannerError. This error occurs mainly when there are tabs inside a yaml file or when the syntax is incorrect. If tabs are found, this exception returns a user-friendly message indicating where the tabs are located in the yaml file.

#### Parameters

**fpath** (*str*) – Path to the yaml file

esm\_parser.yaml\_to\_dict.check\_changes\_duplicates(yamldict\_all, fpath)

Checks for duplicates and conflicting \_changes and add\_:

- 1. Finds variables containing \_changes (but excluding add\_) and checks if they are compatible with the same \_changes inside the same file. If they are not compatible returns an error where the conflicting variable paths are specified. More than one \_changes type in a file are allowed but they need to be part of the same \_choose and not be accessible simultaneously in any situation.
- 2. Checks if there is any variable containing add\_ in the main sections of a file and labels it as incompatible if the same variable is found inside a choose\_block. add\_<variable>``s are compatible as long as they are inside ``choose\_blocks, but if you want to include something as a default, please just do it inside the <variable>.

**Warning:** add\_<variable>``s are not checked for incompatibility when they are included inside ``choose\_ blocks. Merging of these add\_<variable>``s is done using ``deep\_update, meaning that the merge is arbitrary (i.e. if two choose\_ blocks are modifying the same variable using add\_, the final value would be decided arbitrarily). It is up to the developer/user to make good use of add\_``s inside ``choose\_ blocks.

#### Parameters

- yamldict\_all (dict) Dictionary read from the yaml file
- **fpath** (*str*) Path to the yaml file

#### esm\_parser.yaml\_to\_dict.check\_duplicates(src)

Checks that there are no duplicates in a yaml file, and if there are returns an error stating which key is repeated and in which file the duplication occurs.

#### Parameters

src (object) - Source file object

Raises

ConstructorError – If duplicated keys are found, returns an error

esm\_parser.yaml\_to\_dict.check\_for\_empty\_components(yaml\_load, fpath)

esm\_parser.yaml\_to\_dict.create\_env\_loader(tag='!ENV', loader=<class 'yaml.loader.SafeLoader'>)

#### esm\_parser.yaml\_to\_dict.find\_last\_choose(var\_path)

Locates the last choose\_ on a string containing the path to a variable separated by ",", and returns the path to the choose\_ (also separated by ",") and the case that follows the choose\_.

## Parameters

**var\_path** (*str*) – String containing the path to the last choose\_ separated by ",".

#### Returns

- path2choose (str) Path to the last choose\_.
- **case** (*str*) Case after the choose.

#### esm\_parser.yaml\_to\_dict.yaml\_file\_to\_dict(filepath)

Given a yaml file, returns a corresponding dictionary.

If you do not give an extension, tries again after appending one. It raises an EsmConfigFileError exception if yaml files contain tabs.

#### Parameters

**filepath** (*str*) – Where to get the YAML file from

#### Returns

A dictionary representation of the yaml file.

#### **Return type**

dict

#### Raises

- EsmConfigFileError Raised when YAML file contains tabs or other syntax issues.
- **FileNotFoundError** Raised when the YAML file cannot be found and all extensions have been tried.

# 20.9 esm\_plugin\_manager package

- 20.9.1 Submodules
- 20.9.2 esm\_plugin\_manager.cli module
- 20.9.3 esm\_plugin\_manager.esm\_plugin\_manager module

## 20.10 esm\_profile package

Top-level package for ESM Profile.

## 20.10.1 Submodules

## 20.10.2 esm\_profile.esm\_profile module

esm\_profile.esm\_profile.timing(f)

## 20.11 esm\_runscripts package

- 20.11.1 Submodules
- 20.11.2 esm\_runscripts.assembler module
- 20.11.3 esm\_runscripts.batch\_system module
- 20.11.4 esm\_runscripts.chunky\_parts module
- 20.11.5 esm\_runscripts.cli module
- 20.11.6 esm\_runscripts.compute module
- 20.11.7 esm\_runscripts.config\_initialization module
- 20.11.8 esm\_runscripts.coupler module
- 20.11.9 esm\_runscripts.database module
- 20.11.10 esm\_runscripts.database\_actions module
- 20.11.11 esm\_runscripts.dataprocess module
- 20.11.12 esm\_runscripts.event\_handlers module
- 20.11.13 esm\_runscripts.filelists module
- 20.11.14 esm\_runscripts.helpers module
- 20.11.15 esm\_runscripts.inspect module
- 20.11.16 esm\_runscripts.last\_minute module
- 20.11.17 esm\_runscripts.logfiles module
- 20.11.18 esm\_runscripts.methods module
- 20.11.19 esm\_runscripts.mpirun module
- 20.11.20 esm\_runscripts.namelists module
- 20.11.21 esm\_runscripts.oasis module
- 20.11.22 esm\_runscripts.observe module
- 20.11.23 esm\_runscripts.pbs module
- 20.11.24 esm\_runscripts.postprocess module
- 20.111.25meamscripts package repare module
- 20.11.26 esm\_runscripts.prepcompute module

module, please refer to the handbook for user documentation as well as API documentation for the various sub-modules of the project.

#### **Accessing Configuration**

To access a particular configuration, you can use:

```
>>> from esm_tools import read_config_file
>>> ollie_config = read_config_file("machines/ollie")
```

Important note here is that the configuration file **has not yet been parsed**, so it's just the dictionary representation of the YAML.

esm\_tools.EDITABLE\_INSTALL = False

Shows if the installation is installed in editable mode or not.

Type bool

esm\_tools.caller\_wrapper(func)

esm\_tools.copy\_config\_folder(dest\_path)

esm\_tools.copy\_namelist\_folder(dest\_path)

esm\_tools.copy\_runscript\_folder(dest\_path)

esm\_tools.get\_config\_as\_str(config)

esm\_tools.get\_config\_filepath(config=")

esm\_tools.get\_namelist\_filepath(namelist=")

esm\_tools.get\_runscript\_filepath(runscript=")

```
esm_tools.list_config_dir(dirpath)
```

#### esm\_tools.read\_config\_file(config)

Reads a configuration file, which should be separated by "/". For example, "machines/ollie" will retrieve the (unparsed) configuration of the Ollie supercomputer.

#### Parameters

**config** (str) – Configuration to get, e.g. machines/ollie.yaml, or echam/echam. You may omit the ".yaml" ending if you want, it will be appended automatically if not already there.

#### Returns

A dictionary representation of the config.

#### **Return type**

dict

#### esm\_tools.read\_namelist\_file(nml)

Reads a namelist file from a path, seperated by "/". Similar to read\_config\_file

#### Parameters

nml(str) – The namelist to load

#### Returns

A string of the namelist file

Return type str

## 20.13.2 Submodules

### 20.13.3 esm\_tools.cli module

## 20.14 esm\_utilities package

Top-level package for ESM Utilities.

## 20.14.1 Submodules

### 20.14.2 esm\_utilities.cli module

Console script for esm\_utilities.

### 20.14.3 esm\_utilities.esm\_utilities module

Main module.

### 20.14.4 esm\_utilities.utils module

#### esm\_utilities.utils.check\_valid\_version(versionrange, version=")

Returns True if the version provided matches the condition of versionrange.

#### Parameters

- version (str) String specifying the version number with the format X.Y.Z.
- **versionrange** (*str*) Condition for the version range, expressed as a comparison operator followed by a version number in the format X.Y.Z.

#### Returns

True, False – True if the condition is met, False if not.

Return type

bool

esm\_utilities.utils.logfile\_stats(logfile\_to\_read)

## CHAPTER

## TWENTYONE

## SUPPORTED MODELS

## 21.1 AMIP

## 21.2 **DEBM**

Institute	AWI
Description	dEBM is a surface melt scheme to couple ice and climate models in paleo applications.
Publications	Krebs-Kanzow, U., Gierz, P., and Lohmann, G., Brief communication: An Ice surface melt scheme including the diurnal cycle of solar radiation, The Cryosphere Discuss., accepted for publication
License	MIT

# 21.3 ECHAM

Institute	MPI-Met
Description	The ECHAM atmosphere model, major version 6
Authors	Bjorn Stevens (bjorn.stevens@mpimet.mpg.de) among others at MPI-Met
Publications	Atmosphericcomponent of the MPI-M earth system model: ECHAM6
License	Please make sure you have a license to use ECHAM. Otherwise downloading ECHAM
	will already fail. To use the repository on either gitlab.dkrz.de/modular_esm/echam6.git
	or gitlab.awi.de/paleodyn/models/echam6.git, please register for the MPI-ESM user forum
	at https://code.mpimet.mpg.de/projects/mpi-esm-license and send a screenshot of yourself
	logged in to the forum to either paul.gierz@awi.de, miguel.andres-martinez@awi.de, or na-
	dine.wieters@awi.de. Note also that you can otherwise ignore the instructions on that page,
	just the registration and login screen shot is the relevant part for obtaining the license.

# 21.4 ESM\_INTERFACE

Institute	Alfred Wegener Institute
Description	Coupling interface for a modular coupling approach of ESMs.
Authors	Nadine Wieters (nadine.wieters@awi.de)
License	None

# 21.5 **FESOM**

Institute	Alfred Wegener Institute for Polar and Marine Research (AWI)
Description	Multiresolution sea ice-ocean model that solves the equations of motion on unestructured
	meshes
Authors	Dmitry Sidorenko (Dmitry.Sidorenko@awi.de), Nikolay V. Koldunov (niko-
	lay.koldunov@awi.de)
Publications	Danilov et al. 2004: A finite-element ocean model: principles and evaluation
	Wang et al. 2014: The Finite Element Sea Ice-Ocean Model (FESOM) v.1.4: formulation
	of an ocean general circulation model.
License	www.fesom.de

# 21.6 FESOM\_MESH\_PART

Description The FESOM Mesh Partioner (METIS)
----------------------------------------------

## 21.7 HDMODEL

## 21.8 ICON

Institute	MPI-Met
Description	The ICON atmosphere model, major version 2
Authors	Marco Giorgetta (marco.giorgetta@mpimet.mpg.de), Peter Korn, Christian Reick, Reinhard
	Budich
Publications	ICON-A, the Atmosphere Component of the ICON Earth System Model: I. Model Descrip-
	tion
License	Please make sure you have a license to use ICON. In case you are unsure, please contact
	redmine

## 21.9 JSBACH

# 21.10 MEDUSA

Institute	University Liege
Description	MEDUSA is Model of Early Diagenesis in the Upper Sediment with Adatable complexity.
Authors	Guy Munhoven
Publications	Model of Early Diagenesis in the Upper Sediment with Adaptable complexity – MEDUSA
	(v. 2): a time-dependent biogeochemical sediment module for Earth system models, process
	analysis and teaching
License	Please make sure you have a licence to use MEDUSA. In case you are unsure, please contact
	Guy Munhoven (guy.munhoven@uliege.be)

## 21.11 MPIOM

Institute	MPI-Met
Description	The ocean-sea ice component of the MPI-ESM. MPIOM is a primitive equation model (C-
	Grid, z-coordinates, free surface) with the hydrostatic and Boussinesq assumptions made.
Authors	Till Maier-Reimer, Helmuth Haak, Johann Jungclaus
Publications	Characteristics of the ocean simulations in the Max Planck Institute Ocean Model (MPIOM)
	the ocean component of the MPI-Earth system model
	The Max-Planck-Institute global ocean/sea ice model with orthogonal curvilinear coordi-
	nates
License	Please make sure you have a licence to use MPIOM. In case you are unsure, please contact
	redmine

# 21.12 NEMO

Organization	Nucleus for European Modelling of the Ocean
Institute	IPSL
Description	NEMO standing for Nucleus for European Modelling of the Ocean is a state-of-the-art mod-
	elling framework for research activities and forecasting services in ocean and climate sci-
	ences, developed in a sustainable way by a European consortium.
Authors	Gurvan Madec and NEMO System Team (nemo_st@locean-ipsl.umpc.fr)
Publications	NEMO ocean engine
License	Please make sure you have a license to use NEMO. In case you are unsure, please contact
	redmine

## 21.13 NEMOBASEMODEL

## 21.14 OASIS3MCT

## 21.15 OpenIFS

Institute	ECMWF
Description	OpenIFS provides research institutions with an easy-to-use version of the ECMWF IFS (In-
	tegrated Forecasting System).
Authors	Glenn Carver (openifs-support@ecmwf.int)
Website	https://www.ecmwf.int/en/research/projects/openifs
License	Please make sure you have a licence to use OpenIFS. In case you are unsure, please contact
	redmine

## 21.16 PISM

Institute	UAF and PIK
Description	The Parallel Ice Sheet Model (PISM) is an open source, parallel, high-resolution ice sheet
	model.
Authors	Ed Bueler, Jed Brown, Anders Levermann, Ricarda Winkelmann and many more (uaf-
	pism@alaska.edu)
Publications	Shallow shelf approximation as a "sliding law" in a thermomechanically coupled ice sheet
	model
	The Potsdam parallel ice sheet model (PISM-PIK) - Part 1: Model description
License	GPL 3.0

## 21.17 RECOM

Institute	Alfred Wegener Institute for Polar and Marine Research (AWI)	
Description	REcoM (Regulated Ecosystem Model) is an ecosystem and biogeochemistry model.	
Authors	Judith Hauck, Ozgur Gurses	
Publications	Seasonally different carbon flux changes in the Southern Ocean in response to the southern	
	annular mode	
	Arctic Ocean biogeochemistry in the high resolution FESOM 1.4-REcoM2 model	
License	https://recom.readthedocs.io/en/latest/index.html	

## 21.18 RNFMAP

## 21.19 SCOPE

Institute	Alfred Wegener Institute	
Description	The Script-Based Coupler	
Authors	Paul Gierz (pgierz@awi.de)	

## 21.20 TUX

Institute	
Description	
Authors	
Publications	_
License	GPL

## 21.21 VILMA

## 21.22 XIOS

Institute	IPSL and CEA
Description	A library dedicated to I/O management in climate codes.
Authors	Yann Meurdesoif (yann.meurdesoif@cea.fr)
Website	https://portal.enes.org/models/software-tools/xios
License	Please make sure you have a licence to use XIOS. In case you are unsure, please contact
	redmine

## 21.23 YAC

Information	For more information about YAC please go to the webpage: https://dkrz-sw.gitlab-pages.
	dkrz.de/yac/index.html

## 21.24 YAXT

Information	For more information about YAXT please
Description	yaxt
Authors	
License	

CHAPTER

## TWENTYTWO

## TRANSITIONING FROM THE SHELL VERSION

## 22.1 ESM-Master

The Makefile based esm\_master of the shell version has been replaced by a (python-based) executable called esm\_master that should be in your PATH after installing the new tools. The command can be called from any place now, models will be installed in the current work folder. The old commands are replaced by new, but very similar calls:

OLD WAY: make →available	>	NEW WAY: esm_master	(to get the list of $\hfill {\tt u}$
make get-fesom-1.4 make conf make comp make clean	> > >	esm_master get-fesom-1.4 esm_master conf esm_master comp esm_master clean	<pre>targets) (download) (configure) (compile) (clean)</pre>

Apart from that, the new esm\_master offers certain new functionality:

```
esm_master fesom (lists all available targets containing the string "fesom")
esm_master install-... (shortcut for: get- , then conf- , then comp-)
esm_master recomp-... (shortcut for: conf-, then clean-, then comp-)
esm_master log-... (overview over last commits of the model, e.g. git log)
(changes in the model repository since last commit, e.g. git_
status)
```

If the user wants to define own shortcut commands, that can be done by editing esm\_tools/configs/esm\_master/ esm\_master.yaml. New wrappers for the version control software can be e.g. added in esm\_tools/configs/vcs/ git.yaml. Adding commands in these configuration files is sufficient that they show up in the list of targets.

The details about models, setups, etc. are now to be found in esm\_tools/configs/esm\_master/setups2models. yaml. This file is a strucutred list instead of a barely readable, and rapidly growing, makefile. If you want to change details of your model, or add new components, this is where it should be put. Please refer to the chapter *ESM Master* for further details.

## 22.2 ESM-Environment

A visible tool, like esm-environment used to be, doesn't exist anymore. The information about the environment needed for compiling / running a model is contained:

- in the machine yaml file (e.g. esm\_tools/configs/machines/ollie.yaml): This contains a default environment that we know works for a number of models / setups, but maybe not in an optimal way,
- in the model yaml file (e.g. esm\_tools/configs/fesom/fesom-2.0.yaml): The model files are allowed to contain deviations from the default environment defined in the machine file, indicated by the keywords environment\_changes, compiletime\_environment\_changes or runtime\_environment\_changes.

Please note that even though there still is a python package called esm\_environment, this is just the collection of python routines used to assemble the environment. It does not contain anything to be configured by the user.

## 22.3 ESM-Runscripts

One main thing that has changed for the runtime tool is the way it is evoked:

OLD WAY:	NEW WAY:
./runscriptname -e experiment_id	esm_runscripts runscriptname -e experiment_id

Instead of calling your runscript directly, it is now interpreted and executed by the wrapper esm\_runscripts, the second executable to be added to your PATH when installing the Tools. Internally, esm\_runscripts reads in the script file line by line and converts it into a python dictionary. It is therefore also possible to write the "runscripts" in the form of a yaml file itself, which can be imported by python much easier. The user is invited to try the yaml-style runscripts, some example can be found in esm\_tools/runscripts.

Some of the variables which had to be set in the script when using the shell version are now deprecated, these include:

- FUNCTION\_PATH
- FPATH
- machine

Also the last two lines of the normel runscript for the shell version of the tools, load\_all\_functions and general\_do\_it\_all, don't do anything anymore, and can be safely removed. They don't hurt though.

```
(\dots to be continued...)
```

## 22.4 Functions -> Configs + Python Packages

The shell functions, which used to be in esm-runscripts/functions/all, are gone. That was basically the whole point of re-coding the tools, to get rid of this mixture of model configuration, wild shell hacks, and in general lots of annoying problems. What used to be in the functions is now seperated into python code (which is actually doing things, but doesn't have any model-, setup- or machine specific information), and yaml configurations (which are basically structured lists of all the information we have, including mesh resolutions, scenario simulation forcings,...). Anything really that you could possibly know about running a simulation belongs into the yaml configs that you can now find in esm\_runscripts/configs, while ESM-Tools functionality is coded in the python packages.

# 22.5 Namelists

No changes. Namelists can be found in esm\_tools/namelists.

# CHAPTER TWENTYTHREE

# CONTRIBUTING

Contributions are welcome, and they are greatly appreciated! Every little bit helps, and credit will always be given. You can contribute in many ways:

# 23.1 Types of Contributions

### 23.1.1 Report Bugs

Report bugs at https://github.com/esm-tools/esm\_tools/issues.

If you are reporting a bug, please include:

- Your operating system name and version.
- Any details about your local setup that might be helpful in troubleshooting.
- Detailed steps to reproduce the bug.

### 23.1.2 Fix Bugs

Look through the GitHub issues for bugs. Anything tagged with "bug" and "help wanted" is open to whoever wants to implement it.

### 23.1.3 Implement Features

Look through the GitHub issues for features. Anything tagged with "enhancement" and "help wanted" is open to whoever wants to implement it.

### 23.1.4 Write Documentation

ESM Tools could always use more documentation, whether as part of the official ESM Tools docs, in docstrings, or even on the web in blog posts, articles, and such.

### 23.1.5 Submit Feedback

The best way to send feedback is to file an issue at https://github.com/esm-tools/esm\_tools/issues.

If you are proposing a feature:

- Explain in detail how it would work.
- Keep the scope as narrow as possible, to make it easier to implement.
- Remember that this is a volunteer-driven project, and that contributions are welcome :)

## 23.2 Get Started!

Ready to contribute? Here's how to set up *esm-tools* packages for local development (see *Python Packages* for a list of available packages). Note that the procedure of contributing to the *esm\_tools* package (see *Contribution to esm\_tools Package*) is different from the one to contribute to the other packages (*Contribution to Other Packages*).

### 23.2.1 Contribution to esm\_tools Package

- 1. Fork the *esm\_tools* repo on GitHub.
- 2. Clone your fork locally:

\$ git clone https://github.com/esm-tools/esm\_tools.git

(or whatever subproject you want to contribute to).

3. By default, git clone will give you the release branch of the project. You might want to consider checking out the development branch, which might not always be as stable, but usually more up-to-date than the release branch:

\$ git checkout develop

4. Create a branch for local development:

```
$ git checkout -b name-of-your-bugfix-or-feature
```

Now you can make your changes locally.

5. When you're done making changes, check that your changes pass flake8:

\$ flake8 esm\_tools

6. Commit your changes and push your branch to GitHub:

```
$ git add .
$ git commit -m "Your detailed description of your changes."
$ git push origin name-of-your-bugfix-or-feature
```

7. Submit a pull request through the GitHub website.

### 23.2.2 Contribution to Other Packages

1. Follow steps 1-4 in Contribution to esm\_tools Package for the desired package, cloning your fork locally with:

```
$ git clone https://github.com/esm-tools/<PACKAGE>.git
```

2. Proceed to do a development install of the package in the package's folder:

```
$ cd <package´s_folder>
$ pip install -e .
```

- 3. From now on when binaries are called, they will refer to the source code you are working on, located in your local package's folder. For example, if you are editing the package *esm\_master* located in ~/esm\_master and you run \$ esm\_master install-fesom-2.0 you'll be using the edited files in ~/esm\_master to install FESOM 2.0.
- 4. Follow steps 5-7 in *Contribution to esm\_tools Package*.

#### Get Back to the Standard Distribution

Once finished with the contribution, you might want to get back to the standard non-editable mode version of the package in the release branch. To do that please follow these steps:

- 1. Uninstall all *ESM-Tools* packages (*Uninstall ESM-Tools*). This will not remove the folder where you installed the package in editable mode, just delete the links to that folder.
- 2. Navigate to the esm\_tools folder and run the ./install.sh script.
- 3. Check that your package is now installed in the folder ~/.local/lib/python3.<version>/site-packages/

**Note:** If the package is still shows the path to the editable-mode folder, try running pip install --use-feature=in-tree-build . from esm\_tools.

## 23.3 Pull Request Guidelines

Before you submit a pull request, check that it meets these guidelines:

- 1. The pull request should include tests.
- 2. If the pull request adds functionality, the docs should be updated. Put your new functionality into a function with a docstring, and add the feature to the list in README.rst.
- 3. The pull request should work for Python 3.5, 3.6, 3.7 and 3.8, and for PyPy. Check https://travis-ci.com/dbarbi/ esm\_tools/pull\_requests and make sure that the tests pass for all supported Python versions.

# 23.4 Deploying

A reminder for the maintainers on how to deploy. Make sure all your changes are committed (including an entry in HISTORY.rst). Then run:

```
$ bumpversion patch # possible: major / minor / patch
$ git push
$ git push --tags
```

CHAPTER

# TWENTYFOUR

# HOW TO CITE THE SOFTWARE

When using the *ESM-Tools*, please cite the software by using the following DOI: https://zenodo.org/doi/10.5281/ zenodo.3737927. This DOI represents all versions of the software, and will always points to the latest version on zenodo. If you navigate to that page you can also find the DOIs for each specific version, in the Versions panel.

Further information on available versions of the software can be found here.

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# TWENTYFIVE

## CREDITS

## **25.1 Development Lead**

- Dirk Barbi <dirk.barbi@awi.de>
- Paul Gierz <paul.gierz@awi.de>
- Nadine Wieters <nadine.wieters@awi.de>
- Miguel Andrés-Martínez <miguel.andres-martinez@awi.de>
- Deniz Ural <deniz.ural@awi.de>

# 25.2 Project Management

• Luisa Cristini <luisa.cristini@awi.de>

# **25.3 Contributors**

- Sara Khosravi <sara.khosravi@awi.de>
- Fatemeh Chegini <fatemeh.chegini@mpimet.mpg.de>
- Joakim Kjellsson <jkjellsson@geomar.de>
- Sebastian Wahl <swahl@geomar.de>
- ...

# 25.4 Beta Testers

- Tido Semmler <tido.semmler@awi.de>
- Christopher Danek <christopher.danek@awi.de>
- ...

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