ESM Tools r6.19 UserManual

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CHAPTER

ONE

INTRODUCTION

This is the user manual for the esm-tools. To contribute to this document, please contact the authors for feedback.

The esm-tools are a collection of scripts to download, compile, configure different simulation models for the Earth system, such as atmosphere, ocean, geo-biochemistry, hydrology, sea-ice and ice-sheet models, as well as coupled Earth System Models (ESMs). They include functionality to write unified runscripts to carry out model simulations for different model setups (standalone and ESMs) on different HPC systems.

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 *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).
- 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 \sim /.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 (*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

10. Run the experiment:

```
$ esm_runscripts fesom2-ollie-initial-monthly.yaml -e my_first_test
```

That should really be it. Good luck!

CHAPTER

THREE

INSTALLATION

3.1 Downloading

esm_tools is hosted on https://github.com/esm-tools. To get access to the software you need to be able to log into GitHub.

Then you can start by cloning the repository esm_tools.git:

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

This gives you 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.

3.2 Installing in an encapuslated environment

Based on an alternative installation procedure, that provides an esm-tools installation employing direnv (https://direnv.net/), you can now install various encapsulated versions of esm-tools alongside each other. These different installations do not impact each others' configuration. Consequently, they can coexist in peaceful harmony. In the suggested alternative installation method all configurations will reside within the base folder of a specific esm-tools version that you install. There is no dependency on configurations outside the installation directory of a specific esm-tools version, mitigating the potential for side effects if another version of esm tools is installed in parallel. To install esm-tools as suggested here, just follow the procedure outlined below. The steps to create the installation involve preparation of direnv, including setting up an environment that encapsulates potentially version-specific settings, creating a dedicated directory to which a specific version of esm-tools will be installed, and installing the the esm-tools via pip. The commands to be executed are (note comments for further explanation):

```
$ curl -sfL https://direnv.net/install.sh | bash # install direnv if not yet done - this...
--enables encapsulation and parallel use of different esm-tools versions

$ mkdir esm_tools_v6.1.10 #adjust version number as appropriate

$ cd esm_tools_v6.1.10/
#create .envrc (e.g. via direnv edit .) and add information matching the result of the...
--cat command below

$ cat .envrc
module load python3
layout python
module load gcc

$ pip install -U pip wheel

$ pip install esm-tools
```

3.3 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. Become a member of the group esm_tools. Either look for the group and request membership, or directly contact dirk.barbi@awi.de.
- 3. Request access from the corresponding author of the component. Feel free to contact us if you don't know who the model developers are or check the *Supported Models* section.

CHAPTER

FOUR

ESM TOOLS

For our complete documentation, please check https://esm-tools.readthedocs.io/en/latest/index.html.

4.1 Before you continue

You will need python 3 (possibly version 3.6 or newer), 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:

ollie.awi.de:

```
$ module load git
$ module load python3
```

levante.dkrz.de:

```
$ module load git
$ module load python3
```

glogin.hlrn.de / blogin.hlrn.de:

```
$ module load git
$ module load anaconda3
```

juwels.fz-juelich.de:

```
$ module load git
$ module load Python-3.6.8
```

aleph:

```
$ module load git
$ module load python
```

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:

```
$ module unload netcdf_c
$ module load anaconda3
```

4.2 Installing

1. First, make sure you 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. Inside the same login or profile file, add also the module commands necessary for the HPC system you are using (find the lines in the section above).
- 3. You can choose to source now your login or profile file, so that the module and export commands are run (e.g. \$ source ~/.bash_profile).
- 4. To use the new version of the ESM-Tools, now rewritten in Python, clone this repository:

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

5. Then, run the install.sh:

```
$ ./install.sh
```

You should now have the command line tools esm_master and esm_runscripts, which replace the old version.

4.3 Upgrade ESM-Tools

To upgrade all the ESM-Tools packages you can run:

```
$ esm_versions upgrade
```

This will only upgrade the packages that are not installed in editable mode. Those, installed in editable mode will need to be upgraded using git.

You can also choose to upgrade specific packages by adding the package name to the previous command, i.e. to upgrade esm_master:

```
$ esm_versions upgrade esm_parser
```

Note: If there are version conflicts reported back at this point with some of the Python modules (i.e. pkg_resources. ContextualVersionConflict: (<package name>)), try reinstalling that package: pip install <package>--upgrade --ignore-installed.

4.4 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).

CHAPTER

FIVE

TRANSITIONING FROM THE SHELL VERSION

5.1 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:
                                      NEW WAY:
make
                                                                      (to get the list of ⊔
                        -->
                                      esm_master
→available
                                                                       targets)
make get-fesom-1.4
                                                                      (download)
                        -->
                                      esm_master get-fesom-1.4
make conf-...
                        -->
                                      esm_master conf-...
                                                                      (configure)
make comp-...
                                                                      (compile)
                                      esm_master comp-...
make clean-...
                        -->
                                      esm_master clean-...
                                                                      (clean)
```

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)
esm_master status-... (changes in the model repository since last commit, e.g. git_
```

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.

5.2 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.

5.3 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 normal 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.

 $(\dots to be continued\dots)$

5.4 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.

5.5 Namelists

No changes. Namelists can be found in esm_tools/namelists.

5.5. Namelists

CHAPTER

SIX

YAML FILE SYNTAX

6.1 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*').

6.1.1 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.:

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.:

```
config_files:
    config: config
    forcing: forcing
    ice: ice
```

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).

6.2 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.

6.2.1 Variable Calls

Variables defined in a *YAML* file can be invoked on the same file or in oder 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> ...).

6.2.2 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:

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:

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.

6.2.3 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.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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```

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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:

6.2.4 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 .:

```
remove_<model>.<dictionary>.<subkey1>.<subkey2>: [<element_to_remove1>, <element_to_

→remove2>, ... ]
```

6.2.5 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 opera | LIUII3 | |
|-------------------------------------|---------|--|
| calendar units | | |
| | seconds | |
| | minutes | |
| | days | |
| | months | |
| | years | |
| | jours | |

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. | |

6.2.6 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):

```
restart_in_sources:
    restart_in: ${expid}_${prevstep_formatted}_restart*_${start_date_m1!syear!smonth!}
    sday}_*.nc
restart_out_sources:
    restart_out: ${expid}_${newstep_formatted}_restart*_${end_date_m1!syear!smonth!sday}_
    *.nc

[ ... ]
```

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.

6.2.7 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 |
|--------------|--|
| | changes for both the compilation and the runtime environments. |
| compiletime_ | enChiangementhehanigement applied only during compilation. |
| runtime_envi | rochmenges chaheges vironment 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.

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/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}
```

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```
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:

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
```

6.2.8 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:

```
outdata_sources:
    "[[outputs-->OUTPUT]]": OUTPUT.fesom.${start_date!syear}.nc
```

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*:

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.

6.2.9 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 <i>Experiment</i> | |
| | Directory Structure), during the beginning of the computing phase (e.g. to copy restart files from | |
| | the previous step into the new run folder). | |
| restart_out | Restart files to be copied from the run directory into the experiment directory (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 experiment directory 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 into | | | |
| | 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 <i>source</i> 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 <i>source</i> files included in files | | | |
| | will be copied (see the <i>ECHAM</i> forcing files example below). | | | |
| in_work | Files inside the work directory of a run (<base_dir>/<experiment_name>/</experiment_name></base_dir> | | | |
| | run_date1_date2/work) to be transferred to the target 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 <i>sources</i> directory to the <i>target</i> 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 | <pre><base_dir>/</base_dir></pre> | <pre><base_dir>/</base_dir></pre> | <pre><base_dir>/</base_dir></pre> |
| | <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_o | ut | | |

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:

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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:

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:

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.

6.2.10 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:

6.2.11 Error-handling and warning syntax

This syntax allows for error-handling and raising of warnings from the configuration files (i.e. *yaml* 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:

- <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

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 ${\bf continue}$ (set general.ignore_config_warnings: False to avoid_

→quesitoning)?

YAML FILE HIERARCHY

7.1 Hierarchy of YAML configuration files

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

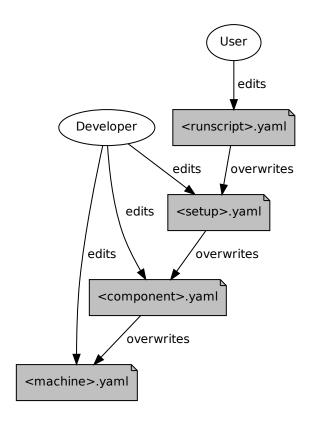


Fig. 1: ESM-Tools configuration files hierarchy

EIGHT

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.

8.1 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/).

8.1.1 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 | |
| | <pre><component setup_path="">/bin folder.</component></pre> | |
| source_code_pe | source_code_perr8istsicthe file permisions for the source code using `chmod <source_code_permissions> -R</source_code_permissions> | |
| | <source_code_folder>.</source_code_folder> | |

8.1.2 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 compilation.</component> |
| 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 | esFunctionality 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 | ationallelization. When false OpenMP is not used for any component, independently of the value |
| | 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 <i>Heterogeneous Paral-</i> |
| | lelization Run (MPI/OpenMP) 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. |

8.1.3 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 simulation in the format YYYY-MM-DD. |
| start_date | Date of the beginning of the current run . |
| end_date | Date of the end of the current run. |
| 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. |

8.1.4 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_transforma | tion transformation used by <i>oasis3mct</i> , defined inside coupling_methods. |
| remapping | Remappings and their parameters, used by <i>oasis3mct</i> , defined inside coupling_methods. |

8.1.5 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 <i>Supported Models</i> . This information should |
| | be organized in nested <i>keys</i> followed by the corresponding description. Nested <i>keys</i> do not receive |
| | a special treatment meaning that you can include here any kind of information about the model. |
| | Only the <i>Publications key</i> 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, |
| | Journal, Year. |

NINE

SUPPORTED MODELS

9.1 **AMIP**

9.2 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 |

9.3 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 gitlab.dkrz.de/modular_esm/echam.git, regis- |
| | ter for the MPI-ESM user forum at https://mpimet.mpg.de/en/science/modeling-with-icon/ |
| | code-availability/mpi-esm-users-forum and send a screenshot to either dirk.barbi@awi.de, |
| | deniz.ural@awi.de or miguel.andres-martinez@awi.de |

9.4 ESM_INTERFACE

| Institute | Alfred Wegener Institute |
|--------------|---|
| Description | Coupling interface for a modular coupling approach of ESMs. |
| Authors | Nadine Wieters (nadine.wieters@awi.de) |
| Publications | `None`_ |
| License | None |

9.5 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 |

9.6 FESOM_MESH_PART

| Description | The FESOM Mesh Partioner (METIS) |
|-------------|----------------------------------|
|-------------|----------------------------------|

9.7 HDMODEL

9.8 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 |

9.9 JSBACH

9.10 **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 |

9.11 **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 | |

9.12 NEMOBASEMODEL

9.13 OASIS3MCT

9.14 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 | |

9.15 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 | |

9.11. NEMO 41

9.16 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 | |

9.17 RNFMAP

9.18 SAMPLE

9.19 **SCOPE**

| Institute | Alfred Wegener Institute |
|-------------|----------------------------|
| Description | The Script-Based Coupler |
| Authors | Paul Gierz (pgierz@awi.de) |

9.20 TUX

| Institute | wiki |
|--------------|---------------------|
| Description | Tux image |
| Authors | who knows |
| Publications | `are you serious?`_ |
| License | GPL |

9.21 VILMA

9.22 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 | |

9.23 YAC

| Information | For more information about YAC please go to the webpage: https://dkrz-sw.gitlab-pages. |
|-------------|--|
| | dkrz.de/yac/index.html |

9.24 YAXT

| Information | For more information about YAXT please |
|--------------|--|
| Description | yaxt |
| Authors | |
| Publications | _ |
| License | |

9.23. YAC 43

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-TOOLS VERSION

Use esm_tools --version to get the version of *ESM-Tools*.

Note: If your version is prior to 6.0.0 (before 2022) this option does not exist. You can use esm_versions instead (esm_versions:ESM-Versions)

11.1 ESM-Versions (deprecated)

Warning: This feature is deprecated since 2022 (version 6.0.0)

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.

11.1.1 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

| Ор- | Description |
|-------------------|--|
| tional | |
| argu- | |
| ments | Chang this halo manages and suit |
| -h, -help | Show this help message and exit. |
| -d, -de- bug | Print lots of debugging statements. |
| -v, -ver- | Be verbose. |
| bose | De Vereuse. |
| -e | The experiment ID to use. Default test. |
| EXPID, | • |
| -expid | |
| EXPID | |
| -c, | Run in check mode (don't submit job to supercomputer). |
| -check | |
| -P, –pro- file | Write profiling information (esm-tools). |
| -j | Write the jobtype this run was called from (esm-tools internal). |
| LAST_JOB | |
| -last_jobty | |
| LAST_JOB | |
| -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. |
| -p F1D, -pid | The FID of the task to observe. |
| PID | |
| -X | E[x]clude this step. |
| EXCLUDE, | - |
| -exclude | |
| EXCLUDE | |
| -o ONLY, | [o]nly do this step. |
| -only | |
| ONLY | |
| -r RESUME_F | [r]esume from the specified run/step (i.e. to resume a second run you'll need to use -r 2). |
| resume- | NOII, |
| from | |
| RESUME_F | ROM |
| -U, -up- | [U]pdate the runscript in the experiment folder and associated files |
| date | |
| -update- | Updates the requested files from external sources in a currently ongoing simulation. We strongly advise |
| filetypes | 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 -c. |
| -inspect | This argument needs an additional keyword. Choose among: overview (gives you the same little message you see at the heginning of each run lastleg (displays the lest log file), explag (the overall |
| | sage 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 experimant 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>
```

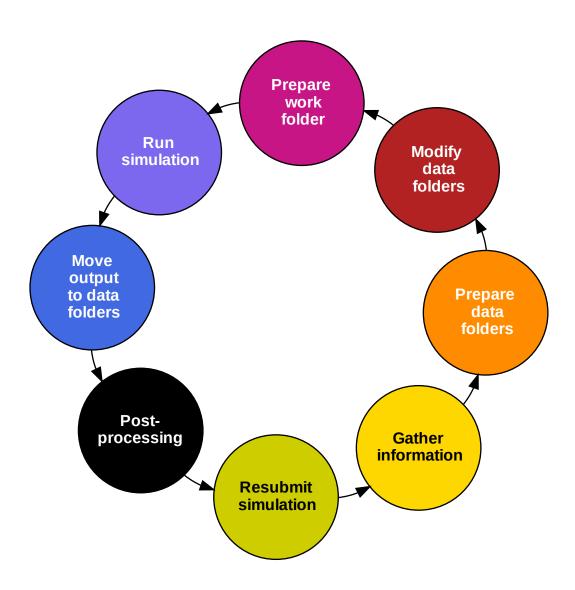


Fig. 1: ESM-Tools job phases

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.

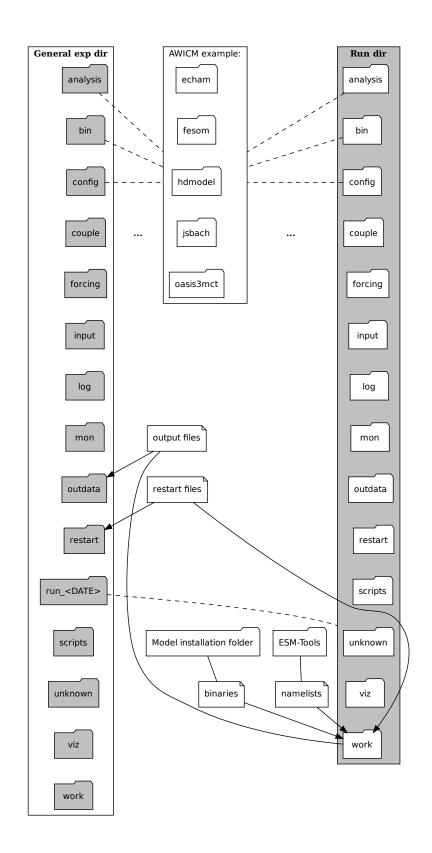


Fig. 2: Experiment directory structure

ones contained in the general ex-

| 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 experiment. |
| config | | Configuration files for the ex- |
| comig | <experiment_id>_ fin-</experiment_id> | periment including namelists |
| | ished_config.yaml | and other files specified in |
| | • namelists | the component's configuration |
| | other configuration files | files (<path>/esm_tools/</path> |
| | | configs/ <component>/</component> |
| | | <pre><component>.yaml, see</component></pre> |
| | | File Dictionaries). The file |
| | | <pre><experiment_id>_finished_con:</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. |
| Toroms | Toronig mes | 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 |
| | 1 | copied here when specified by the |
| | | user in the runscript or in the con- |
| | | figuration files (File Dictionaries). |
| log | | Experiment log files. The com- |
| | • <experiment_id>_</experiment_id> | ponent specific log files are |
| | <setup_name>.log</setup_name> | placed in their respective sub- |
| | • component log files | 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 6. Expeniment Directo | ory Structure files | Run folder containing all the file \$5 |
| YYYYMMDD | | for a given run. Folders contained |
| | | here have the same names as the |
| | | ones contained in the general av |

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:

```
general:
    clean_runs: True
```

To keep the last 2 run_ directories:

```
general:
    clean_runs: 2
```

To keep the last 2 runs and every 5 runs:

```
general:
     clean_old_rundirs_except: 2
     clean_old_rundirs_keep_every: 5
```

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:

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.

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:

| Key- | Function | |
|--|---|--|
| 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_clusting 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_before from subjobs if these subjobs get a corresponding cluster auto-assigned. | | |
| script: | | |
| script_d | ir: | |
| call_fur | ection: | |
| 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:

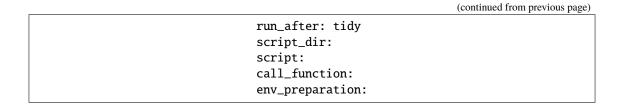
next_run_triggered_by: tidy

subjobs:

my_new_subjob:

nproc: 1
```

(continues on next page)



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.

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:

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:

```
export_vars:
A_VAR_TO_BE_EXPORTED: the_value
```

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)]:

```
export_vars:
    A_VAR_TO_BE_EXPORTED: the_value
    A_VAR_TO_BE_EXPORTED[(1)]: $A_VAR_TO_BE_EXPORTED:another_value
```

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:

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.

CHAPTER

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 <code>esm_tests</code> command is run for the first time. The repository is cloned locally into the <code>esm_tools/src/esm_tests/resources</code> 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:

```
esm_tests [-h] [-n] [-c] [-u] [-d] [-s SAVE] [-t] [-o] [-b] [-g] [-e] [-r BRANCH]
```

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 runscriptsand 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
```

(continued from previous page)

```
- 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 models in this platform, but still keep this file around (i.e. 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.

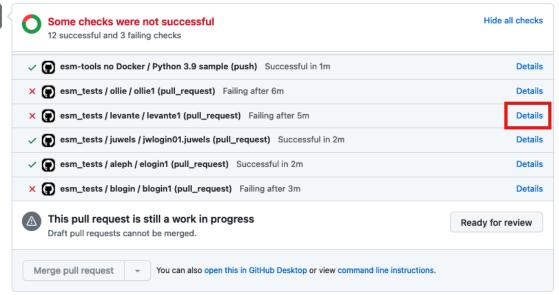
15.8.2 How to include a new platform for in an existing model

- 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):





```
awiesm:
          2.1:
              awiesm-2.1_icebergs:
                  ollie:
                              comp files identical
                                                      run files differ
              pico:
                  ollie:
                              comp files identical
                                                       run files differ
              bootstrap:
                              comp files identical
                                                       run files differ
                  ollie:
              pi:
                  ollie:
                              comp files identical
                                                       run files differ
              pi-wiso:
                              comp files identical
                                                       run files differ
                  ollie:
          2.1-wiso:
              PI_ctrl_awiesm-2.1-wiso:
                  ollie:
                              comp files identical
                                                       run files differ
          2.1-recom:
1428
              all_awiesm-2.1-recom:
                  ollie:
                              comp files identical
                                                       run files differ
```

```
► COMPILING (5.9%) vilma-pism-1.0v1d
  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%) awicm-2.0
 128 ► COMPILING (88.2%) awicm3-v3.0
 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-recom1.4-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: https://github.com/esm-tools/motd/motd.yaml.

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"
```

17.2 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:

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.

17.2.1 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
```

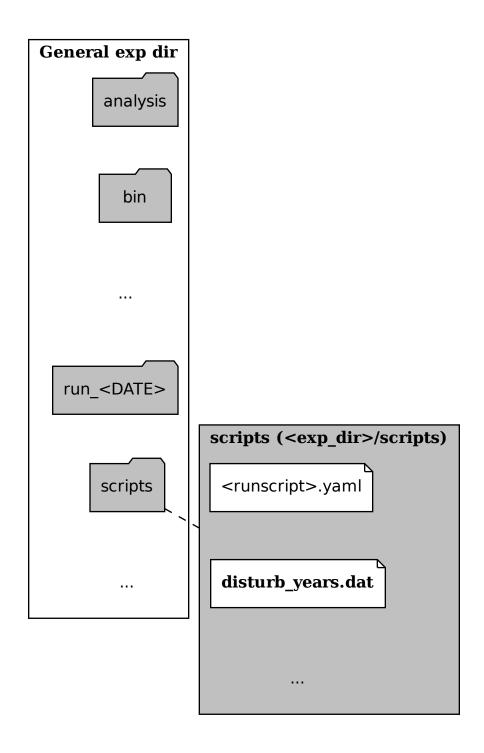


Fig. 1: disturb_years.dat location

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

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

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

Full Runscript

82

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"
```

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```
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/
→nonstandard_input_files/fesom/hydrography/"
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:

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

```
namelist_changes:
    namtrc:
        sn_tracer: "remove_from_namelist"
        sn_tracer(1)%clsname: DET
        sn_tracer(2)%clsname: Z00
        sn_tracer(3)%clsname: PHY
        sn_tracer(1)%cllname: "Detritus"
        sn_tracer(2)%cllname: "Phytoplankton concentration"
        sn_tracer(3)%cllname: "Phytoplankton 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
```

(continued from previous page)

```
[ ... ]
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

- 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>.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 <code>esm_master</code> can find them once compiled. The available_versions key is needed for <code>esm_master</code> to list the versions of your model. The <code>comp_command</code> 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

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:

Multiple version files

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

```
[ ... ]
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
[ ... ]
```

fesom-2.0.yaml

```
choose_version:
    '2.0':
    branch: 2.0.2
    git-repository:
        https://gitlab.dkrz.de/FESOM/fesom2.git
            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>/<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:

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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:

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

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
```

awicm.yaml

Setup file for AWICM (esm_tools/configs/setups/awicm/awicm.yaml):

```
general:
    model: awicm
    #model_dir: ${esm_master_dir}/awicm-${version}
    coupled_setup: True
    include_models:
         - 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"
```

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17.7.2 See also

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

17.8 Include a New Forcing/Input File

Feature available since version: 4.2

There are several ways of including a new forcing or input file into your experiment depending on the degree of control you'd like to achieve. An important clarification is that <forcing/input>_sources file dictionary specifies the sources (paths to the files in the pools or personal folders, that need to be copied or linked into the experiment folder). On the other hand <forcing/input>_files specifies which of these sources are to be included in the experiment. This allows us to have many sources already available to the user, and then the user can simply choose which of them to use by chosing from <forcing/input>_files. <forcing/input>_in_work is used to copy the files into the work folder (<base_dir>/<exp_id>/run_<DATE>/work) if necessary and change their name. For more technical details see File Dictionaries.

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

17.8.1 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 dic-tionaries* 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
```

17.8.2 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:

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:

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:

17.8.3 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 <forcing/input>_in_work:

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

esm_tools/config/component/echam/echam.yaml

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.

17.8.4 See also

- What Is YAML?
- File Dictionaries

17.9 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>
    - ...
```

17.9.1 **Example**

ECHAM

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

```
remove_forcing_files:
    - sst
```

17.9.2 See also

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

17.10 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>: <path_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.

17.10.1 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

Following step 1, search for the config_sources dictionary inside the echam.yaml:

```
# Configuration Files:
config_sources:
    "namelist.echam": "${namelist_dir}/namelist.echam"
```

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:

```
choose_lresume:
    False:
          restart_in_modifications:
```

This lines are relevant for correctly performing restarts, so if remove_namelist_changes is used, make sure to have the approrpiate commands on your runscript to remove dt_start from your namelist in case of a restart.

FESOM

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 \${namelist_dir}/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.

17.10.2 See also

- · Default namelists on GitHub
- Append to an Existing List (add_)
- Changing Namelists
- What Is YAML?

17.11 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.

17.11.1 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.:

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:

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'""
→', '"'"\n'""');f.close();exec(compile(code, _file__, '"'"'exec'"'"'))' egg_info --
→egg-base /tmp/pip-install-0y687gmq/esm-master/pip-egg-info
cwd: /tmp/pip-install-0y687qmq/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",
→line 26, in decode
    return codecs.ascii_decode(input, self.errors)[0]
```

(continued from previous page)

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

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

${\tt esm_archiving.} \textbf{determine_datestamp_location} (\mathit{files})$

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"</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.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 "ls -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:
```

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--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- {\circlearrowleft}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 dict

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

 $\verb|esm_archiving.esm_archiving.find_indices_of(\mathit{char}, \mathit{in_string})|$

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"
>>> 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 dict

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_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.

Type 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
         Type 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)
     Needs a docstring! The following forms are accepted: + SELF: uses the format which was given when
     constructing the date + 0: A Date formated 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
```

20.3 esm_cleanup package

Cleanup tool for ESM-Tools simulations

20.3.1 Submodules

20.3.2 esm_cleanup.cli module

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.inspect_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_some_files(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: sqlalchemy.orm.decl_api.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: sqlalchemy.orm.decl_api.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)
\textbf{class} \ \texttt{esm\_master.software\_package}. \textbf{software\_package}(\textit{raw}, \textit{setup\_info}, \textit{vcs}, \textit{general}, \textit{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)
```

```
\verb|esm_parser.yaml_to_dict.create_env_loader| (\textit{tag} = '!ENV', \textit{loader} = <\textit{class 'yaml.loader}. \textit{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

 ${\tt esm_profile.esm_profile.timing}(f)$

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

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 seperated 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

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:

21.1 Types of Contributions

21.1.1 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.

21.1.2 Fix Bugs

Look through the GitHub issues for bugs. Anything tagged with "bug" and "help wanted" is open to whoever wants to implement it.

21.1.3 Implement Features

Look through the GitHub issues for features. Anything tagged with "enhancement" and "help wanted" is open to whoever wants to implement it.

21.1.4 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.

21.1.5 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:)

21.2 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*).

21.2.1 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.

21.2.2 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.

21.3 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.

21.4 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

TWENTYTWO

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