ESM Tools r5.0 UserManual

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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.

TWO

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. You might want to add the following line to one of your login or profile files, e.g. ~/.bash_profile, ~/.bashrc, ~/. profile, etc.:

```
$ export PATH=$PATH:~/.local/bin
```

- 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. Also, a new file called \sim /.esmtoolsrc is added to your HOME, which contains some very few details about the installation.

- 5. Run esm_master once and answer the questions to setup the tool completely. You should see a long list of available targets if everything works. Note that you will need to manually edit the file ~/.esmtoolsrc, if you mistakenly spelled any of the user names required for accessing the repositories, or you selected the default user name (anonymous).
- 6. Go to the toplevel folder into which you want to install your model codes, and run <code>esm_master install-</code>, followed by the name and the version of the model you want to install. As an example, if we want to install FESOM2:

```
$ 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, <code>esm_master</code> 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.

Note: An error may occur in case you have performed a fresh install of ESM-Tools version 5 after having version 4 installed. In this known error, esm master crashes with a FileNotFoundError with regard to esm master.

yaml. Try to fix this by updating your ~/.esmtoolsrc, removing lines that define paths for runscripts, namelists, and functions. Then try again (RUNSCRIPT_PATH, NAMELIST_PATH and FUNCTION_PATH).

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 ../esm_tools/runscripts/fesom2
$ (your_favourite_editor) fesom2-ollie-initial-monthly.yaml
```

Notice that the examples exist with the endings .run and .yaml. It doesn't matter what you pick. The files ending in .run are looking more like conventional shell scripts that you might be better used to, the .yaml-files are written as yaml configuration files, which makes things much nicer and more elegant to write down. We strongly encourage you to give the yaml-version a try.

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 .sad 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!

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 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 <code>esm_tools</code>. Either look for the group and request membership, or directly <code>contact dirk.barbi@awi.de</code>.
- 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.

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
```

mistral.awi.de:

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

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
```

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 swap netcdf_c anaconda3
```

4.2 Installing

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
```

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.

You may have to add the installation path to your PATH variable:

```
$ export PATH=~/.local/bin:$PATH
```

4.3 Configuration

If you have installed <code>esm_tools</code> you need to configure it before the first use to setup the hidden file <code>\$HOME/.esmtoolsrc</code> correctly. This configuration will set required user information that are needed by both <code>esm_master</code> and <code>esm_runscripts</code> to work correctly. Such information are your user accounts on the different software repositories, your account on the machines you want to compute on, and some basic settings for the esm runscripts.

To configure esm_master you should run the executable:

```
$ esm_master
```

Running it for the first time after installation, you will be asked to type in your user settings. This interactive configuration includes the following steps:

```
$ Please enter your username for gitlab.dkrz.de (default: anonymous)
$ Please enter your username for swrepol.awi.de (default: anonymous)
```

Note that you will need to manually edit the file ~/.esmtoolsrc, if you mistakenly spelled any of the user names required for accessing the repositories, or you selected the default user name (anonymous).

4.4 Uninstall ESM-tools

To uninstall your current installation of ESM-Tools you can use the following command:

```
$ esm_versions clean
```

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 ~/.local/bin/esm*
$ rm ~/.local/lib/python3.6/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.

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:
                                                                      (to get the list of_
make
                                      esm_master
-available
                                                                      targets)
make get-fesom-1.4
                                      esm_master get-fesom-1.4
                                                                      (download)
make conf-...
                                      esm_master conf-...
                                                                      (configure)
make comp-...
                                                                      (compile)
                                      esm_master comp-...
make clean-...
                                                                      (clean)
                                      esm_master clean-...
```

Apart from that, the new esm_master offers certain new functionality:

```
esm_master fesom
esm_master install-...
esm_master recomp-...
esm_master log-...
esm_master status-...

(lists all available targets containing the string "fesom")
(shortcut for: get-, then conf-, then comp-)
(shortcut for: conf-, then clean-, then comp-)
(overview over last commits of the model, e.g. git log)
(changes in the model repository since last commit, e.g.__

git status)
```

If the user wants to define own shortcut commands, that can be done by editing <code>esm_tools/configs/esm_master.yaml</code>. New wrappers for the version control software can be e.g. added in <code>esm_tools/configs/vcs/git.yaml</code>. 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 <code>esm_tools/configs/esm_master/setups2models.yaml</code>. 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 <code>ESM Master</code> 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, <code>load_all_functions</code> and <code>general_do_it_all</code>, 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 <code>esm_tools/namelists</code>.

5.5. Namelists

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. <code>general</code>, <code>ollie</code>, <code>fesom</code>, <code>awicm</code>, ...). 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:

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 " \star " or \star 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/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:
    [ ... ]
HIST:
    forcing_files:
```

(continues on next page)

(continued from previous page)

```
[ ... ]

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:

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 .:

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 operations			
calendar units			
	seconds		
	minutes		
	days		
	months		
	years		

Extraction of Date Components from a Date

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

```
"${variable!date_component}"
```

An example to extract the year from the initial_time variable:

```
yearnew: "${initial_date!syear}"
```

If initial_date was 2001-01-01T00:00:00, then yearnew would be 2001.

The date components available are:

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

6.2.6 Globbing

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

```
file_list: common_pathname*common_pathname
```

Note that this also works together with the *List Loops*.

Example

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

This will include inside the restart_in_sources and restart_out_sources lists, all the files sharing the specified common name around the position of the * symbol, following the same rules used by the Unix shell.

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
environment	_Changesefor both the compilation and the runtime environments.
compiletime	Changesotontheten_virtemmentsapplied only during compilation.
runtime_env	i@hangesto_theremojrenament 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.

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:
```

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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):

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```
clonp = -0.008
```

Note that, although we set <code>l_orbsvop87</code> to be false, it is translated to the namelist as a fortran boolean (. false.). This occurs because <code>ESM-Tools</code> "understands" that it is writing a fortan namelist and transforms the <code>yaml</code> 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-6.3.04pl.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 source elements defined in sources. files is optional				
	If not present, all source files are copied to the target directory, and the source tags need to				
	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>				
	directory. 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>
	<pre><experiment_name>/</experiment_name></pre>	<pre><experiment_name>/</experiment_name></pre>	<experiment_name>/</experiment_name>
	run_date1_date2/work	run_date1_date2/work	outdata/ <model></model>
restart_in			
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.

YAML FILE HIERARCHY

7.1 Hierarchy of YAML configuration files

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

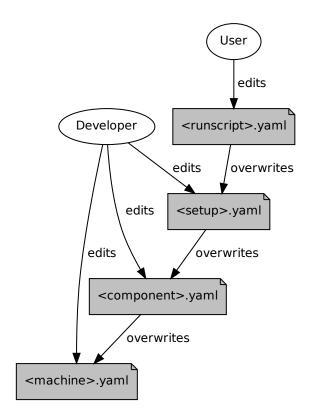


Fig. 1: ESM-Tools configuration files hierarchy

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>/<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).
available_version	nList of supported versions of the component or coupled setup.
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>

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</component>
	after compilation.
compute_time	Estimated computing time for a run, used for submitting a job with the job scheduler.
time_step	Time step of the component in seconds.
lresume	Boolean to indicate whether the run is an initial run or a restart.
pool_dir	Path to the pool directory to read in mesh data, forcing files, inputs, etc.
namelists	List of namelist files required for the model.
namelist_change	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	
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).
execution_comr	nandmmand for executing the component, including \${executable} and the necessary flags.

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
nmonth,	implies 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.).	
coupling_fields	List of coupling field dictionaries containing coupling field variables.	
nx	When using oasis3mct, used inside grids to define the first dimension of the grid.	
ny	When using oasis3mct, used inside grids to define the second dimension of the grid.	
coupling_metho	dList of coupling methods and their parameters (i.e. time_transformation, remapping,	
	etc.).	
time_transforma	time_transformation used by oasis3mct, defined inside coupling_methods.	
remapping	Remappings and their parameters, used by oasis3mct, 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 Supported Models. This information
	should be organized in nested keys followed by the corresponding description. Nested keys do not
	receive a special treatment meaning that you can include here any kind of information about the
	model. Only the <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. https://doi.org/>).

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. In case you are unsure, please contact
	redmine

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
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	The Finite-volumE Sea ice-Ocean Model (FESOM2)
	Scalability and some optimization of the Finite-volumE Sea ice-Ocean Model, Version 2.0
	(FESOM2)
License	Please make sure you have a licence to use FESOM. In case you are unsure, please contact
	redmine

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, Rein-
	hard 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		
	modelling framework for research activities and forecasting services in ocean and climate		
	sciences, 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 OIFS

Institute	ECMWF	
Description	OpenIFS provides research institutions with an easy-to-use version of the ECMWF IFS	
	(Integrated 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 OIFS. In case you are unsure, please contact	
	redmine	

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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

9.16 **RECOM**

Institute	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	Please make sure you have a licence to use REcoM. In case you are unsure, please contact	
	redmine	

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 VILMA

9.21 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

9.22 YAC

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

9.20. VILMA 39

TEN

ESM MASTER

10.1 Usage: esm master

To use the command line tool esm_master, just enter at a prompt:

```
$ esm_master
```

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

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

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

```
$ esm_master operation-software-version,
```

e.g.:

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

By default, esm_master supports the following operations:

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

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

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

clean: Remove all the compiled object files.

install: Shortcut to get, then conf, then comp.

recomp: Shortcut to conf, then clean, then comp.

update: Get the newest commit of the software from the repository.

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

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

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

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

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

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

You can get further help with:

```
$ esm_master --help
```

10.2 Configuring esm-master for Compile-Time Overrides

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

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

The same is also possible for specifying runtime_environment_changes.

ELEVEN

ESM-VERSIONS

New with the Tools version 3.1.5, you will find an executable in your path called <code>esm_version</code>. This was added by Paul Gierz to help the user / developer to keep track of / upgrade the python packages belonging to ESM Tools.

11.1 Usage

It doesn't matter from which folder you call <code>esm_versions</code>. 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.

11.2 Getting ESM-Versions

As was said before, if you have the Tools with a version newer than 3.1.4, you should already have esm_versions in your path. In case you are on an older version of the Tools, or it is missing because of problems, you need to remove the installed python packages by hand one last time, and then reinstall them using the installer:

- 1. Make sure to push all your local changes to branches of the repos, or save them otherwise!
- 2. Remove the installed python libs:

```
$ rm -rf ~/.local/lib/python-whatever_your_version/site-packages/esm*
```

3. Remove the installed executables:

```
$ rm -rf ~/.local/bin/esm*
```

4. Upgrade the repository esm_tools:

ESM Tools r5.0 UserManual

```
$ cd path/to/esm_tools
$ git checkout release
$ git pull
```

5. Re-install the python packages:

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

You should now be on the most recent released version of the tools, and esm_versions should be in your PATH.

TWELVE

ESM RUNSCRIPTS

12.1 Usage

```
esm_runscripts [-h] [-d] [-v] [-e EXPID] [-c] [-P] [-j LAST_JOBTYPE]

[-t TASK] [-p PID] [-x EXCLUDE] [-0 ONLY]

[-r RESUME_FROM] [-U]

runscript
```

12.2 Arguments

Optional	Description
argu-	
ments	
-h, –help	Show this help message and exit.
-d, -de-	Print lots of debugging statements.
bug	
-v, -ver-	Be verbose.
bose	
-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-	Write profiling information (esm-tools).
file -j	Write the jobtype this run was called from (esm-tools internal).
-J LAST_JOI	,
-last_jobty	
LAST_JOH	
-t TASK,	The task to run. Choose from: compute, post, couple, tidy_and_resubmit.
-task	The task to rain. Choose from: compace, pose, coapie, cray_ana_resusmic.
TASK	
-p PID,	The PID of the task to observe.
-pid PID	
-X	E[x]clude this step.
EXCLUDE,	
-exclude	
EXCLUDE	
-o ONLY,	[o]nly do this step.
-only	
ONLY	
-r	[r]esume from this step.
RESUME_I	FROM,
-resume-	
from RESUME_I	ZDOM
-U, -up-	[U]pdate the runscript in the experiment folder and associated files
date	[O]puate the funscript in the experiment folder and associated mes
-i, -in-	This option can be used to [i]nspect the results of a previous run, for example one prepared with -c.
spect	This argument needs an additional keyword. Choose among: overview (gives you the same litte
-r	message you see at the beginning of each run, lastlog (displays the last log file), explog (the
	overall experiment logfile), datefile (the overall experiment logfile), config (the Python dict
	that contains all information), size (the size of the experiment folder), a filename or a directory name
	output the content of the file /directory if found in the last run_folder.)

12.3 Running a Model/Setup

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

```
$ esm_runscripts <runscript.yaml/.run> -e <experiment_ID>
```

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

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

12.4 Job Phases

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

12.5 Running only part of a job

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

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

```
esm_runscripts ${PATH_TO_USER_CONFIG} -t tidy_and_resubmit
```

12.6 Experiment Directory Structure

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

The path of the *Experiment Directory* is composed by the general.base_dir path specified in the runscript (see yaml:Runscripts syntax) followed by the given experiment_ID during the esm_runscripts call:

```
<general.base_dir>/<experiment_ID>
```

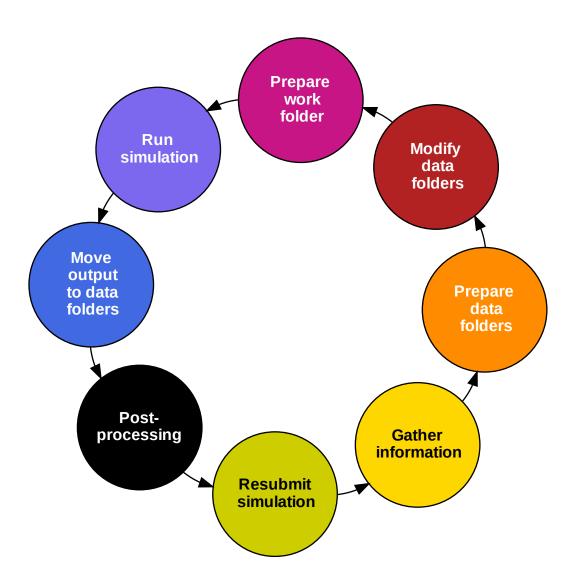


Fig. 1: ESM-Tools job phases

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

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

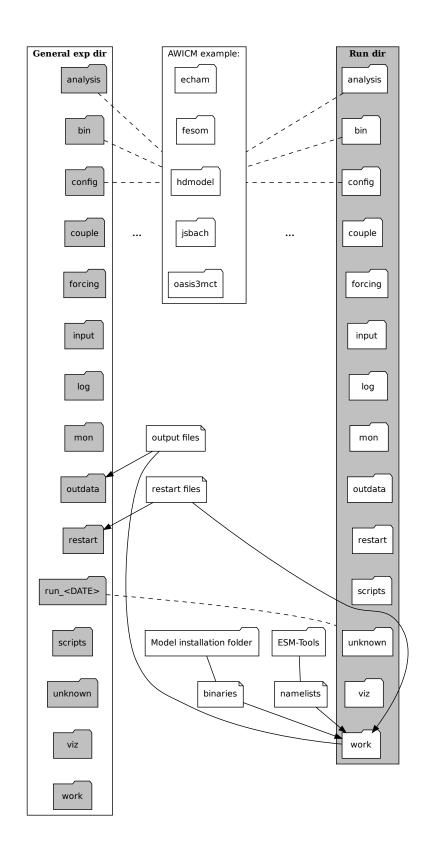


Fig. 2: Experiment directory structure

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 ex-
		periment.
config	• <experiment_id>_ fin-</experiment_id>	Configuration files for the ex-
	ished_config.yaml	periment including namelists
	• namelists	and other files specified in
	• other configuration files	the component's configuration
	other configuration mes	files (<path>/esm_tools/</path>
		configs/ <component>/</component>
		<pre><component>.yaml, see</component></pre>
		File Dictionaries). The file
		<pre><experiment_id>_finished_com</experiment_id></pre>
		yaml is located at the base of the
		config folder and contains the
		whole ESM-Tools variable space
		for the experiment, resulting from
		combining the variables of the
		runscript, setup and component
		configuration files, and the machine
		environment file.
couple	coupling related files	Necessary files for model couplings.
forcing	forcing files	Forcing files for the experiment.
		Only copied here when specified by
		the user in the runscript or in the
		configuration files (File Dictionar-
		ies).
input	input files	Input files for the experiment. Only
		copied here when specified by the
		user in the runscript or in the con-
		figuration files (File Dictionaries).
log	• <experiment_id>_</experiment_id>	Experiment log files. The com-
	<pre><setup_name>.log</setup_name></pre>	ponent specific log files are
	• component log files	placed in their respective sub-
	component log mes	folder. The general log file
		<pre><experiment_id>_<setup_name:< pre=""></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 ₀ 6. Expeniment Dire	Province files	Run folder containing all the file § 1
		for a given run. Folders contained
		here have the same names as the
		anas contained in the concept or

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

12.8 Debugging an Experiment

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

- The ESM-Tools variable space file config/<experiment_ID>_finished_config.yaml.
- The run log file run_YYYYMMDD-YYYYMMDD/<experiment_ID>_compute_YYYYMMDD-YYYYMMDD_<JobID>. log`.

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

```
general:
    debug_recipe: True
```

12.9 Setting the file movement method for filetypes in the runscript

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

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

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

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

THIRTEEN

ESM MOTD

The package <code>esm_motd</code> 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 <code>esm_runscripts</code>.

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/ree/release/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;-)

FOURTEEN

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"].

14.1 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	
single_proc_sub	n B iy_flagault defined asntasks-per-node=1
additional_flags	To add any additional flag that is not predefined in ESM-Tools

14.1.1 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"
```

14.2 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.

14.2.1 **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
```

14.2.2 See also

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

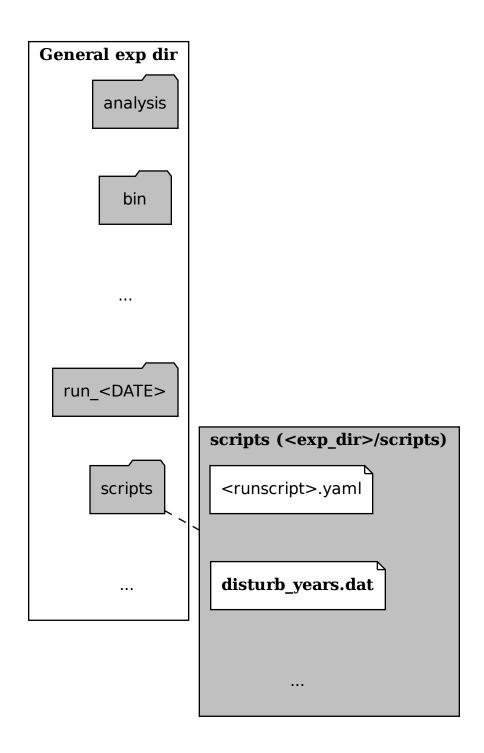


Fig. 1: disturb_years.dat location

14.3 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>
```

14.3.1 Example

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

Snippet

Full Runscript

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

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

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

```
general:
    setup_name: "awiesm"
    compute_time: "02:30:00"
    initial_date: "2000-01-01"
    final_date: "2002-12-31"
   base_dir: "/work/ab0246/a270077/For_Christian/experiments/"
   nmonth: 0
   nyear: 1
   account: "ab0246"
echam:
   restart_unit: "years"
   nprocar: 0
   nprocbr: 0
   namelist_changes:
            namelist.echam:
                    radctl:
                             co2vmr: 1137.e-6
                    parctl:
                            nprocar: 0
                            nprocbr: 0
```

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```
runct1:
                            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"
```

14.3.2 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*).

14.3.3 See also

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

14.4 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>
```

14.4.1 See also

- ESM-Tools Variables
- What Is YAML?

14.5 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 *esm_master* can find them once compiled. The available_versions key is needed for *esm_master* to list the versions of your model. The comp_command key indicates the command needed to compile your model, and can be set as \${defaults.comp_command} for a default command (mkdir -p

build; cd build; cmake ..; make install -j `nproc --all`), or you can define your own list of compiling commands separated with; ("command1; command2").

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

Single file

Multiple version files

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

```
choose_version:
    "1.0.0":
        branch: "1.0.0"
    "1.0.1":
        branch: "1.0.1"
    "1.0.2":
        branch: "develop"
```

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

```
$ touch <PATH>/esm_tools/configs/<model>/<model-version>.yaml
```

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

```
branch: "develop"
```

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

fesom.yaml

fesom-2.0.yaml

```
[ ... ]
available_versions:
- 2.0-0
- 2.0-esm-interface
- '1.4'
- '1.4-recom-mocsy-slp'
- 2.0-esm-interface-yac
- 2.0-paleodyn
- 1.4-recom-awicm
- '2.0'
- '2.0-r' # OG: temporarily here
choose version:
  '1.4-recom-awicm':
   destination: fesom-1.4
   branch: co2_coupling
  '1.4-recom-mocsy-slp':
```

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```
branch: fesom-recom-mocsy-slp
  destination: fesom-1.4
[ ... ]
```

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

9. You can now check if *esm_master* can list and install your model correctly:

```
$ esm_master
```

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

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

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

```
$ flake8 <PATH>/esm_tools/configs/components/<model>.yaml
```

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

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

Note: You can include all the compiling information inside a compile_infos section to avoid conflicts with other choose_version switches present in your configuration file.

14.5.1 See also

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

14.6 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).

- 1. 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 <code>esm_tools/configs/setups</code> 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:

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:

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```
- "model1-1.1+model2-1.1"
```

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>.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*).

14.6.1 Example

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

fesom-1.4+echam-6.3.04p1.yaml

awicm.yaml

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

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

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

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```
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"
available_versions:
- '1.0'
- '1.0-recom'
- CMIP6
choose version:
  '1.0':
    couplings:
    - fesom-1.4+echam-6.3.04p1
  '1.0-recom':
    couplings:
    - fesom-1.4+recom-2.0+echam-6.3.04p1
  CMIP6:
    couplings:
    - fesom-1.4+echam-6.3.04p1
```

14.6.2 See also

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

14.7 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.

14.7.1 Source Path Already Defined in a Config File

- 1. Make sure the source of the file is already specified inside the forcing_sources or input_sources file dictionaries in the configuration file of the setup or model you are running, or on the further_reading files
- 2. In your runscript, include the *key* of the source file you want to include inside the forcing_files or input_files section.

Note: Note that the *key* containing the source in the forcing_sources or input_sources can be different than the key specified in forcing_files or input_files.

Example

ECHAM

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

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

```
forcing_files:
    sst: pisst
```

14.7.2 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:

14.7.3 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

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

"PI-CTRL" then scenario: the source selected will \${forcing_dir}/ \${resolution}\${ocean_resolution}_piControl-LR_sst_1880-2379. 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.

14.7.4 See also

- What Is YAML?
- File Dictionaries

14.8 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>
    - ...
```

14.8.1 Example

ECHAM

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

14.8.2 See also

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

14.9 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>].

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.

14.9.1 **Example**

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

ECHAM

FESOM

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

```
# 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:

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.

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.

14.9.2 See also

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

14.10 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 ${\tt T}$ is the old dimension and time is the new dimension.

14.10.1 See also

• cookbook: How to run a branch-off experiment

CHAPTER

FIFTEEN

FREQUENTLY ASKED QUESTIONS

15.1 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.

15.2 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 <code>esm_runscripts</code> 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.

15.3 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

15.4 Frequent Errors

1. **Q**: When I use esm_versions I get the following error:

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

A: Some systems have C.UTF-8 as locale default (i.e. \$LC_ALL, \$LANG). This issue is solved by setting up the locales respectively to en_US and en_US.utf-8, either manually or adding them to the local bash configuration file (i.e. ~/.bash_profile):

```
$ export LC_ALL=en_US
$ export LANG=en_US.utf-8
```

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

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

CHAPTER

SIXTEEN

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:

16.1 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).

16.2 esm master.git

This repository contains the python files that give the <code>esm_master</code> executable in the subfolder <code>esm_master</code>.

16.3 esm_runscripts.git

The python package of the <code>esm_runscripts</code> executable. The main routines can be found in <code>esm_runscripts/esm_sim_objects.py</code>.

16.4 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.

16.5 esm_calendar.git

ESM TOOLS CODE DOCUMENTATION

17.1 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

Returns

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

Returns

Return type None

esm_archiving.determine_datestamp_location(files)

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

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

Returns A slice object giving the location of the datestamp

Return type slice

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

esm_archiving.determine_potential_datestamp_locations(filepattern)

For a filepattern, gives back index of potential date locations

Parameters filepattern (str) – The filepattern to check.

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

Return type list

```
esm_archiving.find_indices_of (char, in_string)
Finds indicies of a specific character in a string
```

Parameters

- char (str) The character to look for
- in_string (str) The string to look in

Yields *int* – Each round of the generator gives you the next index for the desired character.

```
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"
>>> get_files_for_date_range(filepattern, "1890-07", "1891-11", "1M", date_format=

→ "%Y%m")

   "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",
```

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

Returns

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.

17.1.1 Subpackages

esm_archiving.database package

The database module for archiving.

The database extension allows you keep track of which experiments are on the tape, which files are in which tarball, along with some experiment meta-data.

Submodules

esm_archiving.database.model module

The database module for archiving.

The database extension allows you keep track of which experiments are on the tape, which files are in which tarball, along with some experiment meta-data.

```
class esm_archiving.database.model.Archive(**kwargs)
    Bases: sqlalchemy.ext.declarative.api.Base
    exp_ref
    expid_id
    id
    tarballs
class esm_archiving.database.model.ArchivedFile(**kwargs)
    Bases: sqlalchemy.ext.declarative.api.Base
    fname
    id
    on disk
    on tape
    tarball
    tarball id
class esm_archiving.database.model.Experiments(**kwargs)
    Bases: sqlalchemy.ext.declarative.api.Base
    archive
    created_at
    expid
    id
class esm_archiving.database.model.Tarball(**kwargs)
    Bases: sqlalchemy.ext.declarative.api.Base
    archive
    archive id
    files
```

```
fname
     id
esm archiving.database.utils module
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"

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

makedirs (path)

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)
```

17.1.2 Submodules

17.1.3 esm_archiving.cli module

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

```
esm_archive
```

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

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

Console script for esm_archiving.

Options:

--version Show the version and exit.

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

--write_config Write a global configuration YAML file in

-/.config/esm_archiving/

--help Show this message and exit.
```

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```
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:

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

17.1.4 esm_archiving.config module

When run from either the command line or in library mode (note **not** as an ESM Plugin), <code>esm_archiving</code> can be configured to how it looks for specific files. The configuration file is called <code>esm_archiving_config</code>, 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)
```

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```
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)
```

17.1.5 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

Returns

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

Returns

Return type None

esm_archiving.esm_archiving.determine_datestamp_location(files)

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

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

Returns A slice object giving the location of the datestamp

Return type slice

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

esm_archiving.esm_archiving.determine_potential_datestamp_locations (filepattern) For a filepattern, gives back index of potential date locations

Parameters filepattern (str) – The filepattern to check.

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

Return type list

esm_archiving.esm_archiving.find_indices_of (char, in_string)
Finds indicies of a specific character in a string

Parameters

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

Yields *int* – Each round of the generator gives you the next index for the desired character.

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"
>>> get_files_for_date_range(filepattern, "1890-07", "1891-11", "1M", date_format=
→ "%Y%m")
    "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",
```

```
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)]
```

 $\verb|esm_archiving.esm_archiving.log_tarfile_contents| (\textit{tfile}) \\$

Generates a log of the tarball contents

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

Returns

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

 $\verb|esm_archiving.esm_archiving.purify_expid_in (\textit{model_files}, \textit{expid}, \textit{restore} = False)|$

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.

17.2 esm_calendar package

Top-level package for ESM Calendar.

17.2.1 Submodules

17.2.2 esm calendar.esm calendar module

```
Module Docstring.,..?
```

```
\verb|class| esm_calendar.esm_calendar.Calendar| (calendar_type=1)
```

Bases: object

Class to contain various types of calendars.

Parameters calendar_type (int) – The type of calendar to use.

Supported calendar types: 0

no leap years

- 1 proleptic greogrian calendar (default)
- **n** equal months of n days

timeunits

A list of accepted time units.

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', 'N
     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.
            Returns
            Return type
               ??
class esm calendar.esm calendar.Dateformat (form=1, printhours=True, printminutes=True,
                                               printseconds=True)
    Bases: object
    timesep = ['', ':', ':', ':', ':', ':', ':', '',
esm_calendar.esm_calendar.find_remaining_hours (seconds)
    Finds the remaining full minutes of a given number of seconds
        Parameters seconds (int) – The number of seconds to allocate
        Returns The leftover seconds once new minutes have been filled.
        Return type int
esm calendar.esm calendar.find remaining minutes (seconds)
    Finds the remaining full minutes of a given number of seconds
        Parameters seconds (int) - The number of seconds to allocate
        Returns The leftover seconds once new minutes have been filled.
        Return type int
```

17.3 esm_database package

Top-level package for ESM Database.

17.3.1 Submodules

17.3.2 esm_database.cli module

A small wrapper that combines the shell interface and the Python interface

17.3.3 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()
```

17.3.4 esm_database.getch module

```
esm_database.getch.get_one_of (testlist)
```

17.3.5 esm database.location database module

```
class esm_database.location_database.database_location(**kwargs)
    Bases: sqlalchemy.ext.declarative.api.Base
    class_in
    id
    location
    table_name
    static topline()
esm_database.location_database.register(table_name, given_location, class_in)
```

17.4 esm_environment package

Top-level package for ESM Environment.

17.4.1 Submodules

17.4.2 esm environment.esm environment module

Main module for EsmEnvironment.

```
class esm_environment.esm_environment.EnvironmentInfos(run_or_compile,
                                                                                            com-
                                                                       plete config=None,
                                                                       model=None)
     Bases: object
     static add_commands (commands, name)
          Writes all commands in a list to a file named <name>_script.sh, located in the current working
          directory. The header from this script is read from dummy script.sh, also in the current working
          directory.
              Parameters
                  • commands (list of str) - List of the commands to write to the file after the header
                  • name (str) - Name of the script, generally something like comp echam-6.3.05
              Returns name + "_script.sh"
              Return type str
     add_esm_var()
          Adds the ENVIRONMENT_SET_BY_ESMTOOLS=TRUE to the config, for later dumping to the shell
     apply_config_changes (run_or_compile, config, model)
     apply_model_changes (model, run_or_compile='runtime', modelconfig=None)
     static cleanup_dummy_script()
          Removes the dummy script.sh if it exists.
     get shell commands()
          Gathers module actions and export variables from the config to a list, prepending appropriate shell com-
          mand words (e.g. module and export)
              Returns
              Return type list
     output()
     replace_model_dir (model_dir)
          Replaces any instances of ${model_dir} in the config section "export_vars" with the argument
              Parameters model_dir (str) – The replacement string for $\{\text{model_dir}\}
```

at the beginning of the script. This causes the shell to stop as soon as an error is encountered.

Writes a dummy script containing only the header information, module commands, and export variables.

Parameters include set e (bool) – Default to True, whether or not to include a set -e

write_dummy_script (include_set_e=True)

The actual compile/configure commands are added later.

```
class esm_environment.esm_environment.environment_infos(*args, **kwargs)
    Bases: esm_environment.esm_environment.EnvironmentInfos
```

17.5 esm master package

Top-level package for ESM Master.

17.5.1 Submodules

17.5.2 esm_master.cli module

```
Console script for esm_master.
esm_master.cli.main()
```

17.5.3 esm_master.compile_info module

17.5.4 esm_master.database module

```
class esm_master.database.installation (**kwargs)
    Bases: sqlalchemy.ext.declarative.api.Base
    action
    folder
    id
    static nicer_output(run)
    setup_name
    timestamp
    static topline()
```

17.5.5 esm master.database actions module

```
esm_master.database_actions.database_entry(action, setup_name, base_dir)
```

17.5.6 esm master.esm master module

17.5.7 esm master.general stuff module

17.5.8 esm master.software package module

```
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 ()
```

17.5.9 esm_master.task module

```
class esm_master.task.Task(raw, setup_info, vcs, general, complete_config)
    Bases: object
    What you can do with a software_package, e.g. comp-awicm-2.0
    assemble_command_list()
    check_if_download_task(setup_info)
    check_if_target (setup_info)
    check_requirements()
    cleanup_script()
    compile_binaries()
    download_folders()
    execute()
    get_subtasks (setup_info, vcs, general, complete_config)
    list_required_dirs()
    order_subtasks (setup_info, vcs, general)
    output()
    output_steps()
    validate()
    validate_only_subtask()
esm_master.task.install(package)
```

17.6 esm parser package

Top-level package for ESM Parser.

17.6.1 Submodules

17.6.2 esm_parser.esm_parser module

YAML Parser for Earth System Models

One core element of the esm-tools is the description of model configurations and experiments with the aid of YAML files. Beyond the standard features of YAML, several specific conventions have been implemented to ease the description of your simulations. These conventions are described below, and the functions which implement them are documented with minimal examples. Internally, after parsing the YAML files are converted into a single Python dictionary.

Parsing takes place by initializing objects which represent either an entire setup, ConfigSetup, or a specific component, ConfigComponent. Both of these objects base off of GeneralConfig, which is a dictionary subclass performing specific parsing steps during the object's creation. The parsing steps are presented in the order that they are resolved:

When initializing a ConfigSetup or ConfigComponent, a name of the desired setup or component must be given, e.g. "awicm" or "echam". This configuration is immediately loaded along with any further configs listed in the section "further_reading". Note that this means that any configuration listed in "further_reading" must not contain any variables!!

Following this step, a method called _config_init is run for all classes based off of GeneralConfig. For components, any entries listed under "include_submodels" are attached and registed under a new keyword "submodels".

For setups, the next step is to determine the computing host and load the appropriate configuration files. Setups divide their configuration into 3 specific parts:

- 1. Setup information, contained under <code>config['setup']</code>. This includes, e.g. information regarding a standalone setup, possible coupling, etc.
- 2. Model Information, under <code>config['model']</code>. This contains specific information for all models and submodels, such as resolution, input file names, namelists, etc.
- 3. User information, under <code>config['model']</code>. The user can specify to override any of the defaults with their own choices.

In the next step, all keys starting with "choose_" are determined, along with any information they set. This is done first for the setup, and then for the models. These are filtered to determine an independent choice, and if cyclic dependencies occur, an error is raised. All choices are then resolved until nothing is left.

Specific documentation for classes and functions are given below:

```
class esm_parser.esm_parser.ConfigSetup (model, version, user_config)
    Bases: esm_parser.esm_parser.GeneralConfig

    Config Class for Setups
    finalize()
    run_recursive_functions (config, isblacklist=True)
```

```
exception esm_parser.esm_parser.EsmParserError
     Bases: Exception
     Raise this error when the parser has problems
class esm_parser.esm_parser.GeneralConfig(model, version, user_config)
     Bases: dict
     All configs do this!
esm_parser.esm_parser.actually_find_variable(tree, rhs, full_config)
esm_parser.esm_parser.add_entries_from_chapter(config, add_chapter, add_entries)
esm_parser.esm_parser.add_entries_to_chapter_in_config(model_config,
                                                                  valid model names,
                                                                  setup_config,
                                                                  valid_setup_names)
esm_parser.esm_parser.add_entry_to_chapter(add_chapter, add_entries, model_to_add_to,
                                                    model_with_add_statement,
                                                                              model_config,
                                                    setup_config)
esm_parser.esm_parser.add_more_important_tasks(choose_keyword,
                                                                           all_set_variables,
                                                        task list)
     Determines dependencies of a choose keyword.
```

Parameters

- **choose_keyword** (str) The keyword, starting with choose, which is looked through to check if there are any dependencies that must be resolved first to correctly resolve this one.
- all_set_variables (dict) All variables that can be set
- task_list (list) A list in the order in which tasks must be resolved for choose keyword to make sense.

Returns A list of choices which must be made in order for choose_keyword to make sense.

Return type task_list

Parameters

- **config_to_read_from** (dict) The configuration dictionary from which information is read from. The keyword from which additional YAML files are read from should be on the top level of this dictionary.
- config_to_write_to (dict) The dictionary where the contents of config_to_read_from[full_keyword] is written in.
- **full keyword** The keyword where contents are extracted from

Attaches a new dictionary to the config, and registers it as the value of reduced_keyword.

• reduced_keyword — The keyword where the contents of config_to_read_from[full_keyword] are written to

• level_to_write_to - If this is specified, the attached entries are written here instead of in the top level of config_to_write_to. Note that only one level down is currently supported.

The purpose behind this is to have a chapter in config "include_submodels" = ["echam", "fesom"], which would then find the "echam.yaml" and "fesom.yaml" configs, and attach them to "config" under config[submodels], and the entire config for e.g. echam would show up in config[echam

Since config_to_read_from and config_to_write_to are dict objects, they are modified in place. Note also that the entry config to read from [full keyword] is deleted at the end of the routine.

If the entry in config_to_read_from[full_keyword] is a list, each item in that list is split into two parts: model and model_part. For example:

The first part, in the example echam is used to determine where to look for new YAML files. Then, a yaml file corresponding to a file called echam.datasets.yaml is loaded, and attached to the config.

Warning: Both config_to_read_from and config_to_write_to are modified in place!

```
\verb|esm_parser.esm_parser.attach_to_config_and_remove| (config, attach\_key)|
```

Attaches extra dict to this one and removes the chapter

Updates the dictionary on config with values from any file found under a listing specified by attach key.

Parameters

- **config** (*dict*) The configuration to update
- attach_key (str) A key who's value points to a list of various yaml files to update config with.

Warning: The config is modified in place!

Determines dependencies of a choose keyword.

Parameters

- **choose_keyword** (str) The keyword, starting with choose, which is looked through to check if there are any dependencies that must be resolved first to correctly resolve this one.
- all_set_variables (dict) All variables that can be set
- task_list (list) A list in the order in which tasks must be resolved for choose_keyword to make sense.

Returns A list of choices which must be made in order for choose_keyword to make sense.

Return type task list

```
esm_parser.esm_parser.basic_choose_blocks(config_to_resolve, config_to_search, isblack-list=True)

esm_parser.esm_parser.basic_determine_set_variables_in_choose_block(config)

esm_parser.esm_parser.basic_find_add_entries_in_config(mapping)

esm_parser.esm_parser.basic_find_one_independent_choose(all_set_variables)

Given a dictionary of all_set_variables, which comes out of the function determine_set_variables_in_choose_block, gives a list of task/variable dependencies to resolve in order to figure out the variable.
```

Parameters all_set_variables(dict)-

Returns task_list - A list of tuples comprising (model_name, var_name) in order to resolve one choose_ block. This list is built in such a way that the beginning of the list provides dependencies for later on in the list.

Return type list

```
esm_parser.esm_parser.basic_find_remove_entries_in_config(mapping)

esm_parser.esm_parser.basic_list_all_keys_starting_with_choose(mapping, ignore_list, isblacklist)

esm_parser.esm_parser.basic_remove_entries_from_chapter_in_config(config)

esm_parser.esm_parser.choose_blocks(config, blackdict={}}, isblacklist=True)

esm_parser.esm_parser.complete_config(user_config)

esm_parser.esm_parser.convert(value)

esm_parser.esm_parser.could_be_bool(value)

esm_parser.esm_parser.could_be_float(value)

esm_parser.esm_parser.could_be_float(value)

esm_parser.esm_parser.could_be_int(value)

esm_parser.esm_parser.deep_update(chapter, entries, config, blackdict={}})

esm_parser.esm_parser.del_value_for_nested_key(config, key)

In a dict of dicts, delete a key/value pair.
```

Parameters

- config(dict) The dict to delete in.
- **key** (*str*) The key to delete.

Warning: The config is modified in place!

```
esm_parser.esm_parser.determine_computer_from_hostname()
    Determines which yaml config file is needed for this computer
```

Notes

The supercomputer must be registered in the all_machines.yaml file in order to be found.

Returns A string for the path of the computer specific yaml file.

Return type str

Given a config, figures out which variables are resolved in a choose block.

In order to avoid cyclic dependencies, it is necessary to figure out which variables are set in which choose block. This function recurses over all key/value pairs of a configuration, and for any key which is a model name, it determines which variables are set in it's choose_blocks. Tuples of (model_name, var_name) are appended to a list, which is returned with all it's duplicates removed.

Parameters

- config(dict)-
- valid model names (list) -
- model_name (list) -

Returns set_variables – A list of tuples of model_name and corresponding variable that are determined in config

Return type list

```
esm_parser.esm_parser.dict_merge(dct, merge_dct)
```

Recursive dict merge. Inspired by :meth:dict.update(), instead of updating only top-level keys, dict_merge recurses down into dicts nested to an arbitrary depth, updating keys. The merge_dct is merged into dct.:param dct: dict onto which the merge is executed:param merge_dct: dct merged into dct:return: None

Searches for a key inside a nested dictionary. It can search for an integer, or a piece of string. A list of strings can be given as an input to search for keys containing all of them. An additional list of strings can be specified for keys containing them be excluded from the findings. This is a recursive function.

Note: Always define paths2finds, to avoid expansion of this list with consecutive calls.

Parameters

- **d_search** (*dict*) The dictionary to be explored recursively.
- **k_search** (*list*, *str*, *int*) String, integer or list of strings to be search for in d_search.
- **exc_strings** (*list*, *str*) String or list of strings for keys containing them to be excluded from the finds. When set to an empty string, nothing is excluded.
- **level** (string) String specifying the full path to the currently evaluated dictionary. Each dictionary level in these strings is separated by a ...

- paths2finds (list) List of strings specifying the full path to the found keys in d_search. Each dictionary level in these strings is separated by a the specified string in sep (default is ".").
- **sep** (*string*) String separator used in between each path component in paths2finds.

Returns paths2finds – List of strings specifying the full path to the found keys in d_search. Each dictionary level in these strings is separated by a ...

Return type list

```
esm_parser.esm_parser.find_one_independent_choose(all_set_variables)
```

Given a dictionary of all_set_variables, which comes out of the function determine_set_variables_in_choose_block, gives a list of task/variable dependencies to resolve in order to figure out the variable.

Parameters all_set_variables(dict)-

Returns task_list - A list of tuples comprising (model_name, var_name) in order to resolve one choose_ block. This list is built in such a way that the beginning of the list provides dependencies for later on in the list.

Return type list

```
esm_parser.esm_parser.find_remove_entries_in_config(mapping, model_name, model_name, model_name, els=[1]
```

esm_parser.esm_parser.find_value_for_nested_key (mapping, key_of_interest, tree=[])
In a dict of dicts, find a value for a given key

Parameters

- mapping (dict) The nested dictionary to search through
- **key_of_interest** (str) The key to search for.
- tree (list) Where to start searching

Returns The value of key anywhere in the nested dict.

Return type value

Note: Behaviour of what happens when a key appears twice anywhere on different levels of the nested dict is unclear. The uppermost one is taken, but if the key appears in more than one item, I'd guess something ambigous occus...

```
esm_parser.esm_parser.find_variable (tree, rhs, full_config, white_or_black_list, isblacklist)

esm_parser.esm_parser.finish_priority_merge (config)

esm_parser.esm_parser.initialize_from_shell_script (filepath)

esm_parser.esm_parser.initialize_from_yaml (filepath)

esm_parser.esm_parser.list_all_keys_starting_with_choose (mapping, model_name, ignore_list, isblacklist)

Given a mapping (e.g. a dict-type object), list all keys that start with "choose_" on any level of the nested dictionary.
```

Parameters

• mapping (dict) - The dictionary to search through for keys starting with "choose_"

- model_name (str) -
- ignore list (list) -

Returns all_chooses – A list of tuples for A dictionary containing all key, value pairs starting with "choose_".

Return type list

```
esm_parser.esm_parser.list_all_keys_with_priority_marker(config)
```

esm_parser.esm_parser.list_to_multikey(tree, rhs, config_to_search, ignore_list, isblacklist)

A recursive_run_function conforming func which puts any list based key to a multikey elsewhere. Sorry, that sounds confusing even to me, and I wrote the function.

Parameters

- tree (list) -
- rhs (str) -
- config_to_search(dict)-

Notes

Internal variable definitions in this function; based upon the example: prefix_[[streams->STREAM]]_postfix

- ok_part: prefix_
- actual_list: streams-->STREAM
- key_in_list: streams
- value_in_list: STREAM
- entries of key: list of actual chapter streams, e.g. [accw, echam6, e6hrsp, ...]

```
esm_parser.esm_parser.look_for_file (model, item)
```

```
esm_parser.esm_parser.mark_dates(tree, rhs, config)
```

Adds the DATE_MARKER to any entry who's key ends with "date"

```
esm_parser.esm_parser.marked_date_to_date_object (tree, rhs, config)
```

Transforms a marked date string into a Date object

```
esm_parser.esm_parser.merge_dicts(*dict_args)
```

Given any number of dicts, shallow copy and merge into a new dict, precedence goes to key value pairs in latter dicts.

Note that this function only merges the first level. For deeper merging, use priority_merge_dicts.

Parameters *dict_args - Any number of dictionaries to merge together

Returns

Return type A merged dictionary (shallow)

```
esm_parser.esm_parser.new_deep_update(receiving_dict, dict_to_be_included, win-
ner='receiving', blackdict={})
```

```
esm_parser.esm_parser.new_dict_merge (dct, merge_dct, winner='to_be_included')
```

Recursive dict merge. Inspired by :meth:dict.update(), instead of updating only top-level keys, dict_merge recurses down into dicts nested to an arbitrary depth, updating keys. The merge_dct is merged into dct. :param dct: dict onto which the merge is executed :param merge_dct: dct merged into dct :param winner: should be either receiving (default) or to_be_included :return: None

```
esm_parser.esm_parser.perform_actions(tree, rhs, config)
```

```
esm_parser.esm_parser.pprint_config(config)
```

Prints the dictionary given to the stdout in a nicely formatted YAML style.

Parameters config (dict) - The configuration to print

Returns

Return type None

esm_parser.esm_parser.priority_merge_dicts (first_config, second_config, priority='first')
Given two dictionaries, merge them together preserving either first or last entries.

Parameters

- first_config(dict)-
- second_config(dict)-
- **priority** (str) One of "first" or "second". Specifies which dictionary should be given priority when merging.

Returns merged – A dictionary containing all keys, with duplicate entries reverting to the dictionary given in "priority". The merge occurs across all levels.

Return type dict

```
esm_parser.esm_parser.purify_booleans(tree, rhs, config)
```

```
esm_parser.esm_parser.recursive_get (config_to_search, config_elements)
```

Recusively gets entries in a nested dictionary in the form outer_key.middle_key.inner_key = value

Given a list of config elements in the form above (e.g. the result of splitting the string "outer_key.middle_key.inner_key".split(".")` on the dot), the value "value" of the innermost nest is returned.

Parameters

- config_to_search (dict) The dictionary to search through
- config_elements (list) Each part of the next level of the dictionary to search, as a list.

Returns

Return type The value associated with the nested dictionary specified by config_elements.

Note: This is actually just a wrapper around the function actually_recursive_get, which is needed to pop off standalone model configurations.

```
esm_parser.esm_parser.recursive_run_function (tree, right, level, func, *args, **kwargs)

Recursively runs func on all nested dicts.
```

Tree is a list starting at the top of the config dictionary, where it will be labeled "top"

Parameters

- **tree** (list) Where in the dictionary you are
- right The value of the last key in *tree*
- level (str, one of "mappings", "atomic", "always") When to perform func

- **func** (callable) An function to perform on all levels where the type of right is in level. See the Notes for how this function's call signature should look.
- *args Passed to func
- **kwargs Passed to func

Returns

Return type right

Note: The func argument must be a callable (i.e. a function) and **must** have a call signature of the following form:

```
def func(tree, right, *args, **kwargs)
```

```
esm_parser.esm_parser.remove_entries_from_chapter(config, remove_chapter, remove_entries)

esm_parser.esm_parser.remove_entries_from_chapter_in_config(model_config, valid_model_names, setup_config, valid_setup_names)

esm_parser.esm_parser.remove_entry_from_chapter(remove_chapter, remove_entries, model_to_remove_from, model_with_remove_statement, model_config, setup_config)
```

Deletes the entries specified by the user using the remove_<chapter> command contained in the chapter, that can be either a list or a dictionary. After the removals the remove_<chapter> command is cleaned up from the config.

Parameters

- **remove_chapter** (*str*) A string specifying the path inside the config to reach the chapter where the entries to be removed are. The string is composed by remove_ followed by the path where each nested chapter is separated by a . .
- remove_entries (list) The list of entries to be remove from the chapter.
- model_to_remove_from (str) Indicates the main chapter inside config where removes need to take place (i.e. computer, general, <model>,...).
- model_with_remove_statement (str) Indicates the main chapter where the remove command is defined.
- model_config (dict) Component-specific general configuration.
- **setup_config** (dict) Setup-specific general configuration.

Searches for a choose_ block inside a model configuration config, in which var is defined, and then resolves ONLY the var (the other variables in the choose_ remain untouched). Needed, for example, for being able to use include_models from a choose_ before the general choose-resolve takes place (i.e. include xios component from oifs.yaml using a choose_).

Parameters

- var (str) Name of the variable to be searched inside choose_blocks.
- **config** (*dict*) Model configuration to be changed if the var is resolved by the choose_.
- user_config (dict) User configuration, used to search for the selected case of the choose .
- model_config (dict) Component configuration, used to search for the selected case of the choose_.
- $setup_config(dict)$ Setup configuration, used to search for the selected case of the choose .

```
esm_parser.esm_parser.resolve_remove_and_add(workdict)
esm_parser.esm_parser.shell_file_to_dict(filepath)
Generates a ~`ConfigSetup` from an old shell script.

See also ~`ShellscriptToUserConfig`
```

Parameters filepath (str) – The file to load

Returns The parsed config.

Return type ConfigSetup

```
esm_parser.esm_parser.to_boolean(value)

esm_parser.esm_parser.unmark_dates(tree, rhs, config)

Removes the DATE_MARKER to any entry who's entry contains the DATE_MARKER.

esm_parser.esm_parser.user_error(error_type, error_text, exit_code=1)
```

Parameters

- **error_type** (*str*) Error type used for the error heading.
- **text** (str) Text clarifying the error.

User-friendly error using sys.exit() instead of an Exception.

• exit_code (int) - The exit code to send back to the parent process (default to 1)

```
esm_parser.esm_parser.user_note (note_heading, note_text)
```

Notify the user about something. In the future this should also write in the log.

Parameters

- **note heading** (str) Note type used for the heading.
- **text** (*str*) Text clarifying the note.

17.6.3 esm_parser.shell_to_dict module

Backwards compatability for old runscripts

```
esm_parser.shell_to_dict.ShellscriptToUserConfig (runscript_path)
Generates a User Config from an old Shellscript

esm_parser.shell_to_dict.mini_recursive_run_func (config, func)

esm_parser.shell_to_dict.purify_cases (config)

esm_parser.shell_to_dict.remap_old_new_keys (config)
```

17.6.4 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
- Exceptions -
- -----
- ConstructorError If duplicated keys are found, returns an error

```
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.

17.7 esm_profile package

Top-level package for ESM Profile.

17.7.1 Submodules

17.7.2 esm_profile.esm_profile module

```
esm\_profile.esm\_profile.timing(f)
```

17.8 esm_rcfile package

Top-level package for ESM RCFile.

17.8.1 Submodules

17.8.2 esm rcfile.esm rcfile module

Usage

This package contains functions to set, get, and use entries stored in the esmtoolsrc file.

To use ESM RCFile in a project:

```
import esm_rcfile
```

You can set specific values in the ~/.esmtoolsrc with:

```
set_rc_entry(key, value)
```

For example:

```
>>> set_rc_entry("SCOPE_CONFIG", "/pf/a/a270077/Code/scope/configs/")
```

Retriving an entry:

```
>>> fpath = get_rc_entry("FUNCTION_PATH")
>>> print(fpath)
/pf/a/a270077/Code/esm_tools/esm_tools/configs
```

With a default value for a non-existing key:

```
>>> scope_config = get_rc_entry("SCOPE_CONFIG", "/dev/null")
>>> print(scope_config)
/dev/null
```

Without a default value, you get EsmRcfileError:

```
>>> echam_namelist = get_rc_entry("ECHAM_NMLDIR")
EsmRcFileError: No value for ECHAM_NMLDIR found in esmtoolsrc file!!
```

This error is also raised if there is no ~/.esmtoolsrc file, and no default is provided.

You can also get the entire refile as a dict:

```
>>> rcdict = import_rc_file()
```

API Documentation

```
exception esm_rcfile.esm_rcfile.EsmRcfileError
    Bases: Exception
esm_rcfile.esm_rcfile.get_rc_entry(key, default=None)
    Gets a specific entry
```

Parameters

- key (str) -
- default (str) -

Returns Value for key, or default if provided

Return type str

Raises EsmRcfileError -

Raised if key cannot be found in the refile and no default is provided * Raised if the esm-toolsrc file cannot be found and no default is provided.

```
esm_rcfile.esm_rcfile.import_rc_file()
```

Gets current values of the esmtoolsrc file

Returns A dictionary representation of the refile

Return type dict

```
esm_rcfile.esm_rcfile.set_rc_entry (key, value)
    Sets values in esmtoolsrc
```

Parameters

• key (str) -

```
• value (str) -
```

Note: Using this functions modifies the refile; which is stored in the current user's home directory.

17.9 esm_runscripts package

Top-level package for ESM Runscripts.

17.9.1 Submodules

17.9.2 esm runscripts.batch system module

```
exception esm_runscripts.batch_system.UnknownBatchSystemError
    Bases: Exception
    Raise this exception when an unknown batch system is encountered
class esm_runscripts.batch_system.batch_system(config, name)
    Bases: object
    calc_requirements(config)
    static calculate_requirements(config)
    check_if_submitted()
    static get_batch_header(config)
    static get_environment(config)
    static get_extra(config)
    get_job_state(jobid)
    get_jobid()
    static get_run_commands(config)
    static get_sad_filename(config)
    static get_submit_command(config, sadfilename)
    job_is_still_running(jobid)
    static submit(config)
    static write_simple_runscript(config)
```

17.9.3 esm runscripts.cli module

17.9.4 esm runscripts.compute module

```
esm_runscripts.compute.add_batch_hostfile(config)

esm_runscripts.compute.all_files_to_copy_append(config, model, filetype, categ, file_source, file_interm, file_target)

esm_runscripts.compute.compile_model(config)

Compiles the desired model before the run starts

esm_runscripts.compute.copy_files_to_thisrun(config)

esm_runscripts.compute.copy_files_to_work(config)

esm_runscripts.compute.copy_tools_to_thisrun(config)

Copies the tools, namelists and runscripts to the experiment directory, making sure that they don't overwrite previously existing files unless the -U flag is used. :param config: Dictionary containing the configuration information. :type config: dict
```

esm_runscripts.compute.create_new_files(config)

```
esm_runscripts.compute.initialize_experiment_logfile(config)
```

Initializes the log file for the entire experiment.

Creates a file \${BASE_DIR}/\${EXPID}/log/\${EXPID}_\${setup_name}.log to keep track of start/stop times, job id numbers, and so on. Use the function write_to_log to put information in this file afterwards.

The user can specify experiment_log_file under the general section of the configuration to override the default name. Timestamps for each message are given by the section experiment_log_file_dateformat, or defaults to Tue Mar 17 09:36:38 2020, i.e. "%c". Please use stftime compatable formats, as described here: https://strftime.org

Parameters dict – The experiment configuration

Returns As per convention for the plug-in system; this gives back the entire config.

Return type dict

Attention: Calling this has some filesystem side effects. If the run number in the general configuration is set to 1, and a file exists for general.exp_log_file; this file is removed; and re-initialized.

```
esm_runscripts.compute.modify_files(config)
esm_runscripts.compute.modify_namelists(config)
esm_runscripts.compute.prepare_coupler_files(config)
esm_runscripts.compute.run_job(config)
esm_runscripts.compute.update_runscript(fromdir, scriptsdir, tfile, gconfig, file_type)
```

Updates the script tfile in the directory scriptdir with the file in the directory fromdir if the update flag (-U) is used during the call of esm_runscripts. If that flag is not used and the source and target are different then raises a user-friendly error recommending to use the -U flag with the warning that the files will be overwritten. :param cls: Compute object. :type cls: obj :param fromdir: Path of the source. :type fromdir: str :param scriptsdir: Path of the target. :type scriptsdir: str :param tfile: Name of the script to be updated. :type tfile: str :param gconfig: Dictionary containing the general information about the compute task. :type gconfig: dict :param file_type: String specifying the nature of the file, only necessary for printing information

and for the error description.

Parameters

- Exceptions -
- ------
- **UserError** If the target and source are different and the –U flag is not used when calling esm_runscripts, returns an error.

17.9.5 esm_runscripts.coupler module

```
class esm_runscripts.coupler.coupler_class(full_config, name)
    Bases: object

add_couplings(full_config)

add_files(full_config)

finalize(destination_dir)

prepare(full_config, destination_dir)

prepare_restarts(full_config)

print_config_files()

tidy(full_config)
```

17.9.6 esm_runscripts.database module

```
class esm_runscripts.database.experiment(**kwargs)
    Bases: sqlalchemy.ext.declarative.api.Base
    archive_folder
    cpuh
    exp_folder
    expid
    gb
    id
    static nicer_output(run)
    outcome
    run_timestamp
    runtime
    setup_name
    timestamp
    static topline()
```

17.9.7 esm runscripts.database actions module

```
esm_runscripts.database_actions.database_basic_entry(config)
esm_runscripts.database_actions.database_entry(config)
esm_runscripts.database_actions.database_entry_check(config)
esm_runscripts.database_actions.database_entry_crashed(config)
esm_runscripts.database_actions.database_entry_start(config)
esm_runscripts.database_actions.database_entry_success(config)
```

17.9.8 esm_runscripts.filelists module

```
esm_runscripts.filelists.assemble(config)
esm_runscripts.filelists.assemble_intermediate_files_and_finalize_targets(config)
esm runscripts.filelists.check for unknown files(config)
esm_runscripts.filelists.choose_needed_files(config)
esm_runscripts.filelists.complete_all_file_movements(config)
esm_runscripts.filelists.complete_one_file_movement (config, model, filetype, move-
                                                        ment, movetype)
esm_runscripts.filelists.complete_restart_in(config)
esm_runscripts.filelists.complete_sources(config)
esm_runscripts.filelists.complete_targets(config)
esm_runscripts.filelists.copy_files (config, filetypes, source, target)
esm_runscripts.filelists.create_missing_file_movement_entries(config)
esm_runscripts.filelists.get_method(movement)
esm_runscripts.filelists.get_movement (config, model, filetype, source, target)
esm_runscripts.filelists.globbing(config)
esm_runscripts.filelists.log_used_files(config)
esm_runscripts.filelists.rename_sources_to_targets(config)
esm_runscripts.filelists.replace_year_placeholder(config)
esm_runscripts.filelists.report_missing_files(config)
esm_runscripts.filelists.resolve_symlinks(file_source)
esm_runscripts.filelists.reuse_sources(config)
esm_runscripts.filelists.target_subfolders(config)
```

17.9.9 esm runscripts.helpers module

```
esm_runscripts.helpers.assemble_log_message (config, message, message_sep=None, times-
tampStr_from_Unix=False)
Assembles message for log file. See doc for write_to_log
esm_runscripts.helpers.end_it_all (config)
esm_runscripts.helpers.evaluate (config, job_type, recipe_name)
esm_runscripts.helpers.vprint (message, config)
esm_runscripts.helpers.write_to_log (config, message, message_sep=None)
Puts a message into the experiment log file
```

Parameters

- message (list) A list of the message elements; which is joined by either (highest to lowest): 1) the message_sep argument passed to the method, 2) The user's chosen seperator, as written in config["general"]["experiment_log_file_message_sep"], 3) An empty space " ".
- message_sep (None) The hard-coded message seperator to use; which ignores user choices.

Note: The user can control two things regarding the logfile format:

- 1) The datestamp formatting, which is taken from the config section general. experiment_log_file_dateformat.
- 2) The message seperators; taken from general.experiment_log_file_message_sep. Note that if the programmer passes a message_sep argument; this one wins over the user choice.

17.9.10 esm_runscripts.inspect module

```
esm_runscripts.inspect.cat_file (full_filepath)
esm_runscripts.inspect.dir_size (somepath)
esm_runscripts.inspect.inspect_config (config)
esm_runscripts.inspect.inspect_file (config)
esm_runscripts.inspect.inspect_folder (config)
esm_runscripts.inspect.inspect_namelists (config)
esm_runscripts.inspect.inspect_overview (config)
esm_runscripts.inspect.inspect_size (config)
esm_runscripts.inspect.inspect_size (config)
esm_runscripts.inspect.run_job (config)
```

17.9.11 esm runscripts.last minute module

```
esm_runscripts.last_minute.apply_last_minute_changes (config)

class esm_runscripts.last_minute.last_minute_changes (config)
    Bases: object

esm_runscripts.last_minute.restore_protected_last_minute_changes (config)
```

17.9.12 esm_runscripts.methods module

esm_runscripts.methods.set_global_attr(fname, attribute, value)

17.9.13 esm_runscripts.namelists module

esm-runscripts Core Plugins for dealing with Fortran Namelists.

Provides plugins for loading, modifying, deleting, and writing Fortran Namelists as part of the esm-runscripts recipe. All plugins are found under the class Namelist as static methods. A deprecated class namelist (small "n") is provided, which warns you when it is used.

```
class esm_runscripts.namelists.Namelist
    Bases: object
```

Methods for dealing with FORTRAN namelists

```
static apply_echam_disturbance(config)
```

Applies a disturbance to the DYNCTL chapter of the echam namelist via the enstdif

Relevant configuration entries: * disturbance_years (list of int): Which year to apply the disturbance * distrubance (float): Value to apply. Default can be found in echam.yaml

```
static nmls_finalize(mconfig, verbose)
```

Writes namelists to disk after all modifications have finished.

User Information

Part of the main log output will be a section specifing the actual namelists that have been used for your simulation, including all relevant additions, removals, or changes.

Programmer Information

A copy of the f90nml object representations of the namelists is stored under the dictionary key "namelist_objs", as a dictionary of ("namelist_name", f90nml_objfect) key/value pairs.

Warning: Removing this step from your recipe might result in a broken run, as the namelists will not be present in their desired form! Even if your model runs, it might not contain all user-required changes.

Parameters mconfig (dict) - The model (e.g. ECHAM, FESOM, NEMO or OIFS) configuration

Returns mconfig – The modified configuration.

Return type dict

```
static nmls_load(mconfig)
```

Loads Fortran namelists into the configuration dictionary.

User Information

To associate namelists with a specific model, you should have a section in your configuration that lists the namelists:

```
fesom:
    namelists:
        - "namelist.config"
        - "namelist.oce"
        - "namelist.ice"
        - "namelist.diag"
```

Programmer Information

The namelists are represented by f90nml Namelist objects, and are stored under:

```
mconfig["namelists"]["namelist.echam"]``
```

This would point to the ECHAM namelist as a f90nml object, which closely resembles a dictionary.

The actual namelists to load are listed in the raw configuration as a list of strings:

```
mconfig['namelists'] = ['nml1', 'nml2', 'nml3', ...]
```

Namelists are assumed to have been copied to mconfig["thisrun_config_dir"], and are loaded from there.

If the mconfig has a key "namelist_case" equal to "uppercase", the uppercase attribute of the f90nml representation of the namelist is set to True.

Parameters mconfig (dict) - The model (e.g. ECHAM, FESOM, NEMO or OIFS) configuration

Returns mconfig – The modified configuration.

Return type dict

```
static nmls_modify(mconfig)
```

Performs namelist changes.

User Information

In the configuration file, you should have a section as:

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

This would change the value of the echam namelist (namelist.echam), subsection radctl, entry co2vmr to the value 1200e-6.

Programmer Information

IDEA(PG): Maybe we can provide examples of how these functions are used in the code?

Note: Actual changes are performed by the f90nml package patch fuction. See here: https://tinyurl.com/y4ydz363

```
 \begin{tabular}{ll} \textbf{Parameters} & \textbf{mconfig} & (\textit{dict}) - \textbf{The model (e.g. ECHAM, FESOM, NEMO or OIFS) configuration } \\ \end{tabular}
```

Returns mconfig – The modified configuration.

Return type dict

```
static nmls_output(mconfig)
static nmls_output_all(config)
static nmls_remove(mconfig)
```

Removes an element from a namelist chapter.

User Information

In the configuration file, assume you have:

In this case, the entry co2vmr would be deleted from the radctl section of namelist.echam.

Programmer Information

IDEA(PG): Maybe we can provide examples of how these functions are used in the code?

Parameters mconfig (dict) – The model (e.g. ECHAM, FESOM, NEMO or OIFS) configuration

Returns mconfig – The modified configuration.

Return type dict

```
class esm_runscripts.namelists.namelist(*args, **kwargs)
    Bases: esm_runscripts.namelists.Namelist
```

Legacy class name. Please use Namelist instead!

17.9.14 esm runscripts.oasis module

17.9.15 esm runscripts.postprocess module

```
esm_runscripts.postprocess.run_job(config)
```

17.9.16 esm runscripts.prepare module

```
esm_runscripts.prepare.add_submission_info(config)
esm_runscripts.prepare.check_model_lresume(config)
esm_runscripts.prepare.finalize_config(config)
esm_runscripts.prepare.find_last_prepared_run(config)
esm_runscripts.prepare.initialize_batch_system(config)
esm_runscripts.prepare.initialize_coupler(config)
esm_runscripts.prepare.model_env_into_computer(config)
```

This function allows to store in the computer dictionary, variables that were defined inside environment_changes or compile/runtime_environment_changes in the components.

It excludes module_actions and export_vars dictionaries as those are resolved later.

This function is necessary for controlling <code>choose_</code> blocks in the computer file from the component configuration file (i.e. add <code>useMPI</code> case to the component to control which <code>useMPI</code> case is selected in the computer file).

This function works both for compilation time and run time, and the result is that all components work under the same environment. The only exception is for the compilation of components, where add_export_vars and add_module_actions are excluded from the merging into computer, and are included individually in respective compilation scripts.

Later on, it might be desirable to always split the environments both for compiling (done by Paul Gierz, but this function would need to be adapted) and running (not done yet).

If this script gives you problems contact Miguel Andres-Martinez (miguel.andres-martinez@awi.de).

Parameters config (dict) – Dictionary containing the simulation/compilation information

Raises User Note/Error – If the same variable is found in two or more different component environments. Asks the user how to proceed.

```
esm_runscripts.prepare.resolve_some_choose_blocks(config)
esm_runscripts.prepare.run_job(config)
esm_runscripts.prepare.set_leapyear(config)
esm_runscripts.prepare.set_logfile(config)
esm_runscripts.prepare.set_most_dates(config)
esm_runscripts.prepare.set_overall_calendar(config)
esm_runscripts.prepare.set_parent_info(config)
esm_runscripts.prepare.set_prev_date(config)
esm_runscripts.prepare.set_prev_date(config)
```

17.9.17 esm runscripts.sim objects module

Documentation goes here

Performs steps for tidying up a simulation after a job has finished and submission of following jobs.

This method uses two lists, all_files_to_copy and all_listed_filetypes to sort finished data from the current run folder back to the main experiment folder and submit new compute and post-process jobs. Files for log, mon, outdata, and restart_out are gathered. The program waits until the job completes or an error is found (See ~self.wait_and_observe). Then, if necessary, the coupler cleans up it's files (unless it's a standalone run), and the files in the lists are copied from the work folder to the current run folder. A check for unknown files is performed (see ~self.check_for_unknown_files), files are moved from the the current run folder to the main experiment folder, and new compute and post process jobs are started.

Warning: The date is changed during this routine! Be careful where you put any calls that may depend on date information!

Note: This method is also responsible for calling the next compute job as well as the post processing job!

viz (kill_after_submit=True)

Starts the Viz job.

Parameters kill_after_submit (bool) – Default True. If set, the entire Python instance is killed with sys.exit().

17.9.18 esm_runscripts.slurm module

Contains functions for dealing with SLURM-based batch systems

class esm_runscripts.slurm.Slurm(config)

Bases: object

Deals with SLURM, allowing you to check if a job is submitted, get the current job ID, generate a srun hostfile, get the current job state, and check if a job is still running.

filename

The filename for srun commands, defaults to hostfile_srun

Type str

path

Full path to this file, defaults to this run scripts dir / filename

Type str

Parameters config (dict) – The run configuration, needed to determine where the script directory for this particular run is.

calc_requirements(config)

Calculates requirements and writes them to self.path.

static check_if_submitted()

Determines if a job is submitted in the currently running shell by checking for SLURM_JOB_ID in the environment

Returns

Return type bool

static get_job_state(jobid)

Returns the jobstate full name. See man squeue, section JOB STATE CODES for more details.

Parameters jobid - str or int. The SLURM job id as displayed in, e.g. squeue

Returns The short job state.

Return type str

static get_jobid()

Gets the current SLURM JOB ID

Returns

Return type str or None

static job_is_still_running(jobid)

Returns a boolean if the job is still running

17.9.19 esm runscripts.tidy module

```
class esm_runscripts.tidy.RunFolders(config)
    Bases: list
```

Logs the run_directories in <experiment_id>/log/run_folders.log, updating it with new folders. The resulting object is a list of run_ paths that exist or existed during the run time (even if they got deleted). This is useful for indexing operations such as <object_name>[::<interval>] used when removing run folders. ... rubric:: Notes

It keeps the folder names sorted so there is no need of sorting out of the object, and it also prevents the existence of duplicates.

load()

Loads the existing paths of the run_folders.

save()

Saves all folder names.

update()

Updates the folders read from the log file with the currently existing folders, removes duplicates, sorts them and save them into the log file.

```
esm_runscripts.tidy.all_done(config)
esm_runscripts.tidy.assemble_error_list(config)
esm_runscripts.tidy.check_for_errors(config)
esm_runscripts.tidy.clean_run_dir(config)
```

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
```

Parameters path (str) – Path or directory to remove

```
esm_runscripts.tidy.run_job(config)
esm_runscripts.tidy.signal_tidy_completion(config)
esm_runscripts.tidy.size_bytes_to_human(num, suffix='B')
esm_runscripts.tidy.size_human_to_bytes(s, suffix='B')
esm_runscripts.tidy.start_post_job(config)
esm_runscripts.tidy.start_various_jobtypes_after_compute(config)
esm_runscripts.tidy.throw_away_some_infiles(config)
esm_runscripts.tidy.tidy_coupler(config)
esm_runscripts.tidy.wait_and_observe(config)
esm_runscripts.tidy.wait_and_observe(config)
```

17.9.20 esm runscripts.virtual env builder module

```
esm_runscripts.virtual_env_builder.find_package (pkg)
esm_runscripts.virtual_env_builder.get_base_prefix_compat()
    Get base/real prefix, or sys.prefix if there is none.
esm_runscripts.virtual_env_builder.in_virtualenv()
esm_runscripts.virtual_env_builder.venv_bootstrap(config)
    Bootstraps your run into a virtual environment
```

17.9.21 esm runscripts.yac module

17.10 esm_version_checker package

esm_version_checker - Mini package to check versions of diverse esm_tools software

17.10.1 Submodules

17.10.2 esm version checker.cli module

Console script for esm_version_checker.

```
class esm_version_checker.cli.GlobalVars
    Bases: object
```

A struct-like class for holding the global variables. GlobalVars instance should only be updated by the main function and should be 'read-only' by the other functions

from_github

top-level command-line option flag for connecting to the GitHub repo

Type bool

```
esm_tools_github_url
```

repository URL of the ESM-Tools

Type str

```
esm tools installed
         each key is the specidif ESM-Tools package and value is bool
             Type dict
     esm_tools_github_url = 'https://github.com/esm-tools/'
     esm tools installed = {}
     from_github = False
esm_version_checker.cli.check_importable_tools()
esm_version_checker.cli.dist_is_editable(dist)
     Is distribution an editable install?
esm_version_checker.cli.editable_dist_location(dist)
     Determines where an editable dist is installed
esm_version_checker.cli.get_esm_package_attributes(tool)
     Gets the attributes of the ESM-Tools package
         Parameters tool (str) – name of the ESM-Tools package
         Returns attr_dict – dictionary of attributes.
         Return type dict
esm_version_checker.cli.get_esm_packages()
     Gets the list of the installed ESM-Tools packages either locally or from the GitHub repository
         Returns esm_tools_modules – list of strings where each item corresponds to a ESM-Tools package
             name
         Return type list
esm_version_checker.cli.global_options_decorator(func)
     decorator function for the global option
esm_version_checker.cli.pip_install(package)
esm_version_checker.cli.pip_or_pull (tool, version=None)
esm_version_checker.cli.pip_uninstall(package)
esm_version_checker.cli.pip_upgrade(package, version=None)
esm_version_checker.cli.report_single_package (package, version, file_path, branch, de-
                                                        scribe)
     Nice output similar to the tree command in Linux
esm_version_checker.cli.user_owns(binary)
     True or False if user owns binary
```

CHAPTER

EIGHTEEN

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:

18.1 Types of Contributions

18.1.1 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.

18.1.2 Fix Bugs

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

18.1.3 Implement Features

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

18.1.4 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.

18.1.5 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:)

18.2 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*).

18.2.1 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.

18.2.2 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 <code>esm_master</code> 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*.

18.3 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.

18.4 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

NINETEEN

CREDITS

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validate only subtask() (esm master.task.Task
        method), 99
```