
ESM Tools r6.25 UserManual

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

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INTRODUCTION

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

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

TEN STEPS TO A RUNNING MODEL

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

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

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

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

4. In the new folder `esm_tools`, run the installer:

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

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

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

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

You will be asked for your password to the repository of the model you are trying to install. If you don't have access to that repo yet, `esm_master` will not be able to install the model; you will have to contact the model developers to be granted access ([Supported Models](#)). Feel free to contact us if you don't know who the model developers are.

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

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

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

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

Notice that the examples exist with the endings `.yaml`.

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

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

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

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

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

10. Run the experiment:

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

That should really be it. Good luck!

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 documentation in `docs`. Also you will find the installer `install.sh` used to install the python packages.

3.2 Installing in an encapsulated environment

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

```
$ curl -sfl https://direnv.net/install.sh | bash # install direnv if not yet done - this_
↳ enables encapsulation and parallel use of different esm-tools versions
$ mkdir esm_tools_v6.1.10 #adjust version number as appropriate
$ cd esm_tools_v6.1.10/
  #create .envrc (e.g. via direnv edit .) and add information matching the result of the_
↳ cat command below
$ cat .envrc
  module load python3
  layout python
  module load gcc
$ pip install -U pip wheel
$ pip install esm-tools
```

3.3 Accessing components in DKRZ server

Some of the `esm_tools` components are hosted in the `gitlab.dkrz.de` servers. To be able to reach these components you will need:

1. A DKRZ account (<https://www.dkrz.de/up/my-dkrz/getting-started/account/DKRZ-user-account>).
2. Become a member of the group `esm_tools`. Either look for the group and request membership, or directly contact dirk.barbi@awi.de.
3. Request access from the corresponding author of the component. Feel free to contact us if you don't know who the model developers are or check the *Supported Models* section.

ESM TOOLS

4.1 Documentation

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

4.2 How to cite this software

To cite ESM-Tools, please use the following DOI: <https://zenodo.org/doi/10.5281/zenodo.3737927>. This DOI represents all versions of the software, and will always pointing to the latest version available on <https://zenodo.org>.

4.3 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:

albedo:

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

levante.dkrz.de:

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

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

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

juwels.fz-juelich.de:

```
$ module load Stages/2022
$ module load git
$ module load Python/3.9.6
```

aleph:

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

Note that some machines might raise an error `conflict netcdf_c` when loading `anaconda3`. In that case you will need to swap `netcdf_c` with `anaconda3`:

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

4.4 Installing

1. First, make sure you add the following lines to one of your login or profile files, i.e. `~/.bash_profile`, `~/.bashrc`, `~/.profile`, etc.:

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

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

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

5. Then, run the `install.sh`:

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

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

4.5 Upgrade ESM-Tools

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

```
$ esm_versions upgrade
```

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

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

```
$ esm_versions upgrade esm_parser
```

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

4.6 Uninstall ESM-Tools

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

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

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

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

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

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

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

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

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

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:	
<code>make</code>	-->	<code>esm_master</code>	(to get the list of <code>↵</code>
<code>↵available</code>			targets)
<code>make get-fesom-1.4</code>	-->	<code>esm_master get-fesom-1.4</code>	(download)
<code>make conf-...</code>	-->	<code>esm_master conf-...</code>	(configure)
<code>make comp-...</code>	-->	<code>esm_master comp-...</code>	(compile)
<code>make clean-...</code>	-->	<code>esm_master clean-...</code>	(clean)

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

<code>esm_master fesom</code>	(lists all available targets containing the string "fesom")
<code>esm_master install-...</code>	(shortcut for: get- , then conf- , then comp-)
<code>esm_master recomp-...</code>	(shortcut for: conf-, then clean-, then comp-)
<code>esm_master log-...</code>	(overview over last commits of the model, e.g. git log)
<code>esm_master status-...</code>	(changes in the model repository since last commit, e.g. git <code>↵</code>
<code>↵status</code>)	

If the user wants to define own shortcut commands, that can be done by editing `esm_tools/configs/esm_master/esm_master.yaml`. New wrappers for the version control software can be e.g. added in `esm_tools/configs/vcs/git.yaml`. Adding commands in these configuration files is sufficient that they show up in the list of targets.

The details about models, setups, etc. are now to be found in `esm_tools/configs/esm_master/setup2models.yaml`. This file is a structured list instead of a barely readable, and rapidly growing, makefile. If you want to change details of your model, or add new components, this is where it should be put. Please refer to the chapter *ESM Master* for further details.

5.2 ESM-Environment

A visible tool, like `esm-environment` used to be, doesn't exist anymore. The information about the environment needed for compiling / running a model is contained:

- in the machine yaml file (e.g. `esm_tools/configs/machines/oлие.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:
<code>./runscriptname -e experiment_id</code>	<code>esm_runscripts runscriptname -e experiment_id</code>

Instead of calling your runscript directly, it is now interpreted and executed by the wrapper `esm_runscripts`, the second executable to be added to your PATH when installing the Tools. Internally, `esm_runscripts` reads in the script file line by line and converts it into a python dictionary. It is therefore also possible to write the “runscripts” in the form of a yaml file itself, which can be imported by python much easier. The user is invited to try the yaml-style runscripts, some example can be found in `esm_tools/runscripts`.

Some of the variables which had to be set in the script when using the shell version are now deprecated, these include:

- `FUNCTION_PATH`
- `FPATH`
- `machine`

Also the last two lines of the normal runscript for the shell version of the tools, `load_all_functions` and `general_do_it_all`, don't do anything anymore, and can be safely removed. They don't hurt though.

(...to be continued...)

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 separated into python code (which is actually doing things, but doesn't have any model-, setup- or machine specific information), and yaml configurations (which are basically structured lists of all the information we have, including mesh resolutions, scenario simulation forcings,...). Anything really that you could possibly know about running a simulation belongs into the yaml configs that you can now find in `esm_runscripts/configs`, while ESM-Tools functionality is coded in the python packages.

5.5 Namelists

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

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.:

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

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

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

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

```
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):

```
choose_resolution:
  T63:
    levels: "L47"
    time_step: 450
    [ ... ]
  T31:
    levels: "L19"
    time_step: 450
    [ ... ]
  T127:
    levels: "L47"
    time_step: 200
    [ ... ]
```

- 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 other files provided that the file where it is defined is read for the given operation. The syntax for calling an already defined variable is:

```
"${name_of_the_variable}"
```

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

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

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

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

Example

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

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

Here we use *ini_parent_exp_id* to define part of the restart path *ini_restart_dir*. *general.ini_restart_dir* is going to be called from the *FESOM-REcoM* configuration file *configs/setups/fesom-recom/fesom-recom.yaml* to define the restart directory for *FESOM* *fesom.ini_restart_dir*:

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

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

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

```
a_new_variable: "${ollie.useMPI}"
```

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

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*:

```
variable_1: case_key_2

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

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

Example

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

```
resolution: CORE2

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

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

In the case in which `resolution: CORE2`, then `nx`, `mesh_dir` and `nproc` will take the values defined inside the `choose_resolution` for CORE2 (126858, `runscripts/fesom-recom/fesom-recom-ollie-restart-daily.yaml`, and 288 respectively), once resolved by the *esm_parser*, at the same **nesting level** of the `choose_resolution`.

Note: `choose_versions` inside configuration files is treated in a special way by the *esm_master*. To avoid conflicts in case an additional `choose_versions` is needed, include the compilation information inside a `compile_infos` section (including the `choose_versions` switch containing compilation information). Outside of this exception, it is possible to use as many `choose_<variable>` repetitions as needed.

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"
  "rrtmgs": "rrtmgs"
  "tslclim": "tslclim"
  "vgratclim": "vgratclim"
  "vltclim": "vltclim"

[ ... ]
```

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

```
[ ... ]
choose_scenario:
  [ ... ]
```

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

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

```
[ ... ]

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

This changes specified here will be combined with changes in other files (i.e. `echam.namelist_changes` in the coupled setups *AWICM* or *AWIESM* configuration files), not overwritten. However, *ECHAM*'s version 6.3.05p2-concurrent_radiation needs of further namelist changes written down in the same file inside a `choose_` block and for that we need to use the `add_` functionality:

```
[ ... ]

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

[ ... ]
```

6.2.4 Remove Elements from a List/Dictionary (`remove_`)

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

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

or:

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

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

```
remove_<model>.<dictionary>.<subkey1>.<subkey2>: [<element_to_remove1>, <element_to_remove2>, ... ]
```

6.2.5 Math and Calendar Operations

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

Arithmetic Operations

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

```
key: "$(( ${variable_1} operator ${variable_2} operator ... ${variable_n} ))"
```

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

```
runtime: $(( ${end_date} - ${time_step}seconds ))
```

time_step is a variable that is not given in date format, therefore, it is necessary to use *seconds* for *runtime* to be in date format. Another example is to subtract one day from the variable *end_date*:

```
$(( ${end_date} - 1days ))
```

The units available are:

Units supported by arithmetic 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!year}"
```

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.
sday	Day of the year, counting from Jan. 1.

6.2.6 Globbing

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

```
file_list: common_pathname*common_pathname
```

Note that this also works together with the [List Loops](#).

Example

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

```
[ ... ]

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

[ ... ]
```

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

6.2.7 Environment and Namelist Changes (`_changes`)

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

Environment Changes

Environment changes are used to make changes to the default environment defined in the machine files (`esm_tools/configs/machines/<name_of_the_machine>.yaml`). There are three types of environment changes:

Key	Description
<code>environment_changes</code>	Changes for both the compilation and the runtime environments.
<code>compiletime_environment_changes</code>	Changes in the environment applied only during compilation.
<code>runtime_environment_changes</code>	Changes in the environment applied only during runtime.

Two types of *yaml* elements can be nested inside an environment changes: `add_module_actions` and `add_export_vars`.

- Use `add_module_actions` to include one *module* command or a list of them. The shell command `module` is already invoked by *ESM-Tools*, therefore you only need to list the options (i.e. `load/unload <module_name>`).
- Use `add_export_vars` to export one or a list of environment variables. Shell command `export` is not needed here, just define the variable as `VAR_NAME: VAR_VALUE` or as a nested dictionary.

For more information about `esm_environment` package, please check [ESM Environment](#).

Example

`fesom.yaml`

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

```
[ ... ]

compiletime_environment_changes:
  add_export_vars:
    takenfrom:      fesom1
choose_computer.name:
  mistral:
    add_compiletime_environment_changes:
      add_module_actions:
        - "unload gcc"
        - "load gcc/4.8.2"
  blogin:
    add_compiletime_environment_changes:
      add_export_vars:
        - "NETCDF_DIR=/sw/dataformats/netcdf/intel.18/4.7.3/skl/"
        - "LD_LIBRARY_PATH=$NETCDF_DIR/lib/:$LD_LIBRARY_PATH"
        - "NETCDF_CXX_INCLUDE_DIRECTORIES=$NETCDF_DIR/include"
        - "NETCDF_CXX_LIBRARIES=$NETCDF_DIR/lib"
        - "takenfrom='fesom1'"

runtime_environment_changes:
  add_export_vars:
    AWI_FESOM_YAML:
      output_schedules:
        -
          vars: [restart]
          unit: ${restart_unit}
          first: ${restart_first}
```

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```

        rate: ${restart_rate}
    -
    [ ... ]

```

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

We also see here how `runtime_environment_changes` is used to add nested information about the output schedules for *FESOM* into an `AWI_FESOM_YAML` variable that will be exported to the runtime environment.

Changing Namelists

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

```

echam:
  namelist_changes:
    namelist.echam:
      runctl:
        l_orbvsop87: false
      radctl:
        co2vmr: 217e-6
        ch4vmr: 540e-9
        n2ovmr: 245e-9
        cecc: 0.017
        cobld: 23.8
        clonp: -0.008
        yr_perp: "remove_from_namelist"

```

In the example above, the `namelist.echam` file is changed in two specific chapters, first the section `runctl` parameter `l_orbvsop87` 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 (truncated):

```

&runctl
  l_orbvsop87 = .false.
/

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

```

Note that, although we set `l_orbvsop87` to be `false`, it is translated to the namelist as a fortran boolean (`.false.`). This occurs because *ESM-Tools* “understands” that it is writing a fortran namelist and transforms the `yaml` booleans into

fortran.

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

Coupling changes

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

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

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

6.2.8 List Loops

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

```
"[[list_to_loop_through-->ELEMENT_OF_THE_LIST]]"
```

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

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

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

Then, you need to declare the outdata_sources dictionary:

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

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

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

```
outdata_targets:
  "[[outputs-->OUTPUT]]": OUTPUT.fesom.${start_date!syear!smmonth}.${start_date!sday}.
  ↪nc
```

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 List Loops .
restart_in	Restart files to be copied from the experiment directory into the run directory (see Experiment Directory Structure), during the beginning of the <i>computing phase</i> (e.g. to copy restart files from the previous step into the new run folder).
restart_out	Restart files to be copied from the run directory into the experiment directory (see Experiment Directory Structure), during the <i>tidy and resubmit phase</i> (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 <code>targets</code> 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 (<code>file_name.extension_YYYYMMDD_YYYYMMDD</code>).
files	Links the general file tags (<i>key</i>) to the <i>source</i> elements defined in <i>sources</i> . files is optional. If not present, all <i>source</i> files are copied to the <i>target</i> directory, and the <i>source tags</i> need to be the same as the ones in <i>in_work</i> and <i>targets</i> . If present, only the <i>source</i> files included in <i>files</i> will be copied (see the <i>ECHAM</i> forcing files example below).
in_work	Files inside the <i>work</i> directory of a run (<code><base_dir>/<experiment_name>/run_date1_date2/work</code>) to be transferred to the <i>target</i> directory. This files copy to the <i>target</i> path even if they are not included inside the <i>files</i> 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 List Loops . 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 folders	sources	in_work	targets
bin			
config			
ignore			
forcing			
log			
outdata	<code><base_dir>/ <experiment_name>/ run_date1_date2/work</code>	<code><base_dir>/ <experiment_name>/ run_date1_date2/work</code>	<code><base_dir>/ <experiment_name>/ outdata/<model></code>
restart_in			
restart_out			

Example for ECHAM forcing files

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

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

  # sic
  "amipsic":
    "${forcing_dir}/amip/${resolution}_amipsic_@YEAR@.nc":
```

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```

        from: 1870
        to: 2016
        "pisc": "${forcing_dir}/${resolution}${ocean_resolution}_piControl-LR_sic_1880-
        ↪2379.nc"

    [ ... ]

```

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: pisc
      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`, `pisc`, `piaerocoarse`, `piaerofin`, `piaerofarir` and `piozone`, and they are tagged with new general *keys* (`sst`, `sic`, ...) that are common to all scenarios. The source files not included in `forcing_files` won't be used.

File movements

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

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

```

<model>:
  file_movements:
    <file_type>:
      <direction1>: <copy/link/move>
      <direction2>: <copy/link/move>

    [ ... ]

```

where the `file_type` is one among the *File Dictionary Types*, and the `direction` one of the following ones:

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

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

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

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

Movements specific to files are still compatible with the `file_type` option, and only the moves specifically defined for files in the `file_movements` will differ from those defined using the `file_type`.

6.2.10 Accessing Variables from the Previous Run (`prev_run`)

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

The syntax for that is as follows:

```
<your_var>: ${prev_run.<path>.<to>.<the>.<var>.<in>.<the>.<previous>.<run>}
```

For example, let's assume we want to access the `time_step` from the previous run of a *FESOM* simulation and store it in a variable called `prev_time_step`:

```
prev_time_step: ${prev_run.fesom.time_step}
```

Note: Only the single previous simulation loaded

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

Branchoff experiments with prev_run

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

```
prev_run_config_file: "/<basedir>/<expid>/config/<expid>_finished_config.yaml_<DATE>-
↳<DATE>"
```

6.2.11 Error-handling and warning syntax

This syntax allows for error-handling and raising of warnings from the configuration files (i.e. `yaml` files in `esm_tools/configs`). For including an error or a warning under a given condition (e.g. `choose_` block for a given selection) use the key words `error` or `warning` respectively (if more than one error/warning is present in the section of your file, use `add_error/warning` to combine them).

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

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

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

Example

```
recom:
  choose_scenario:
    HIST:
      [ ... ]
    PI-CTRL:
      [ ... ]
    "":
      add_warning:
        "wrong scenario type":
          message: "The scenario you specified (`${recom.scenario}`) is not
↳supported!"
          ask_user_to_continue: True
```

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

```
wrong scenario type WARNING
```

```
-----
```

```
Section: recom
```

```
Wrong scenario, scenario hist does not exist
```

```
? Do you want to continue (set general.ignore_config_warnings: False to avoid  
↪quesitoning)?
```


YAML FILE HIERARCHY

7.1 Hierarchy of YAML configuration files

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

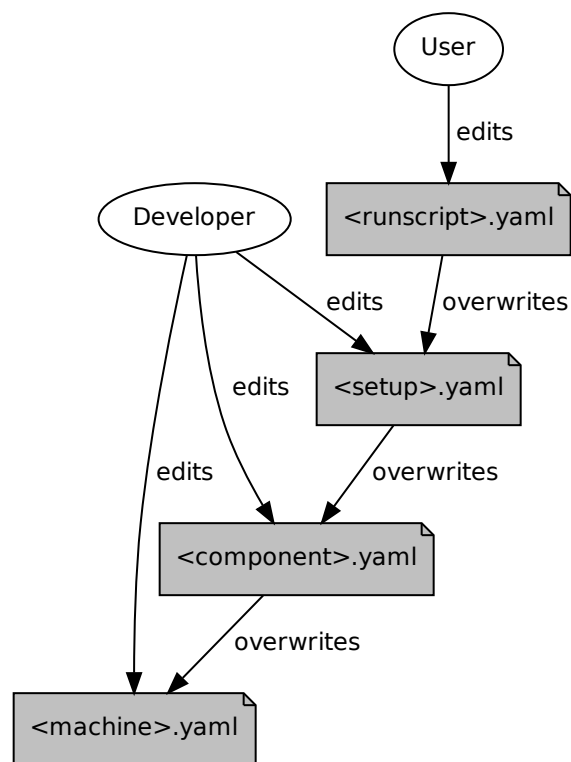


Fig. 1: ESM-Tools configuration files hierarchy

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 or 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/setup/<name>/<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 (<code>esm_tools/configs/components</code> for models and <code>esm_tools/configs/setups</code> for setups).
setup_name	Name of the coupled setup.
version	Version of the model/setup (one of the available options in the <code>available_versions</code> list).
available_versions	List 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 <code><component/setup_path>/bin</code> folder.
source_code_permissions	Set the file permissions for the source code using <code>chmod <source_code_permissions> -R <source_code_folder></code> .

8.1.2 Runtime variables

Key	Description
account	User account of the HPC system to be used to run the experiment.
model_dir	Absolute path of the model directory (where it was installed by <i>esm_master</i>).
setup_dir	Absolute path of the setup directory (where it was installed by <i>esm_master</i>).
executable	Name of the component executable file, as it shows in the <component/setup_path>/bin after compilation.
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_changes	Functionality to handle changes in the namelists from the yaml files (see Changing Namelists).
nproc	Number of processors to use for the model.
nproca/nprocb	Number of processors for different MPI tasks/ranks. Incompatible with nproc.
base_dir	Path to the directory that will contain the experiment folder (where the experiment will be run and data will be stored).
post_processing	Boolean to indicate whether to run postprocessing or not.
File Dictionaries	YAML dictionaries used to handle input, output, forcing, logging, binary and restart files (see File Dictionaries).
expid	ID of the experiment. This variable can also be defined when calling <i>esm_runscripts</i> with the <i>-e</i> flag.
ini_restart_expid	ID of the restarted experiment in case the current experiment has a different <i>expid</i> . For this variable to have an effect <i>lresume</i> needs to be <i>true</i> (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 <i>lresume</i> needs to be <i>true</i> (e.g. the experiment is a restart).
execution_command	Command for executing the component, including <i>\${executable}</i> and the necessary flags.
heterogeneous_parallelization	A boolean that controls whether the simulation needs to be run with or without heterogeneous parallelization. When <i>false</i> OpenMP is not used for any component, independently of the value of <i>omp_num_threads</i> defined in the components. When <i>true</i> , <i>open_num_threads</i> needs to be specified for each component using OpenMP. heterogeneous_parallelization variable needs to be defined inside the computer section of the runscrip t. See Heterogeneous Parallelization Run (MPI/OpenMP) for examples.
omp_num_threads	A variable to control the number of OpenMP threads used by a component during an heterogeneous parallelization run. This variable has to be defined inside the section of the components for which OpenMP needs to be used. This variable will be ignored if <i>computer.heterogeneous_parallelization</i> is not set to <i>true</i> .

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, nmonth, nday, nhour, nminute	Number of time unit per run. They can be combined (i.e. nyear: 1 and nmonth: 2 implies that each run will be 1 year and 2 months long).
parent_date	Ending date of the previous run.

8.1.4 Coupling variables

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

8.1.5 Other variables

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

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	Atmospheric component of the MPI-M earth system model: ECHAM6
License	Please make sure you have a license to use ECHAM. Otherwise downloading ECHAM will already fail. To use the repository on either gitlab.dkrz.de/modular_esm/echam6.git or gitlab.awi.de/paleodyn/models/echam6.git , please register for the MPI-ESM user forum at https://code.mpimet.mpg.de/projects/mpi-esm-license and send a screenshot of yourself logged in to the forum to either paul.gierz@awi.de , miguel.andres-martinez@awi.de , or na-dine.wieters@awi.de . Note also that you can otherwise ignore the instructions on that page, just the registration and login screen shot is the relevant part for obtaining the license.

9.4 ESM_INTERFACE

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

9.5 FESOM

Institute	Alfred Wegener Institute for Polar and Marine Research (AWI)
Description	Multiresolution sea ice-ocean model that solves the equations of motion on unstructured meshes
Authors	Dmitry Sidorenko (Dmitry.Sidorenko@awi.de), Nikolay V. Koldunov (nikolay.koldunov@awi.de)
Publications	Danilov et al. 2004: A finite-element ocean model: principles and evaluation Wang et al. 2014: The Finite Element Sea Ice-Ocean Model (FESOM) v.1.4: formulation of an ocean general circulation model.
License	www.fesom.de

9.6 FESOM_MESH_PART

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

9.7 HDMODEL

9.8 ICON

Institute	MPI-Met
Description	The ICON atmosphere model, major version 2
Authors	Marco Giorgetta (marco.giorgetta@mpimet.mpg.de), Peter Korn, Christian Reick, Reinhard Budich
Publications	ICON-A, the Atmosphere Component of the ICON Earth System Model: I. Model Description
License	Please make sure you have a license to use ICON. In case you are unsure, please contact redmine...

9.9 JSBACH

9.10 MEDUSA

Institute	University Liege
Description	MEDUSA is Model of Early Diagenesis in the Upper Sediment with Adatable complexity.
Authors	Guy Munhoven
Publications	Model of Early Diagenesis in the Upper Sediment with Adaptable complexity – MEDUSA (v. 2): a time-dependent biogeochemical sediment module for Earth system models, process analysis and teaching
License	Please make sure you have a licence to use MEDUSA. In case you are unsure, please contact Guy Munhoven (guy.munhoven@uliege.be)

9.11 MPIOM

Institute	MPI-Met
Description	The ocean-sea ice component of the MPI-ESM. MPIOM is a primitive equation model (C-Grid, z-coordinates, free surface) with the hydrostatic and Boussinesq assumptions made.
Authors	Till Maier-Reimer, Helmuth Haak, Johann Jungclaus
Publications	Characteristics of the ocean simulations in the Max Planck Institute Ocean Model (MPIOM) the ocean component of the MPI-Earth system model The Max-Planck-Institute global ocean/sea ice model with orthogonal curvilinear coordinates
License	Please make sure you have a licence to use MPIOM. In case you are unsure, please contact redmine...

9.12 NEMO

Organization	Nucleus for European Modelling of the Ocean
Institute	IPSL
Description	NEMO standing for Nucleus for European Modelling of the Ocean is a state-of-the-art 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...

9.13 NEMOBASEMODEL

9.14 OASIS3MCT

9.15 OpenIFS

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 OpenIFS. In case you are unsure, please contact redmine...

9.16 PISM

Institute	UAF and PIK
Description	The Parallel Ice Sheet Model (PISM) is an open source, parallel, high-resolution ice sheet model.
Authors	Ed Bueler, Jed Brown, Anders Levermann, Ricarda Winkelmann and many more (uaf-pism@alaska.edu)
Publications	Shallow shelf approximation as a “sliding law” in a thermomechanically coupled ice sheet model The Potsdam parallel ice sheet model (PISM-PIK) - Part 1: Model description
License	GPL 3.0

9.17 RECOM

Institute	Alfred Wegener Institute for Polar and Marine Research (AWI)
Description	REcoM (Regulated Ecosystem Model) is an ecosystem and biogeochemistry model.
Authors	Judith Hauck, Ozgur Gurses
Publications	Seasonally different carbon flux changes in the Southern Ocean in response to the southern annular mode Arctic Ocean biogeochemistry in the high resolution FESOM 1.4-REcoM2 model
License	https://recom.readthedocs.io/en/latest/index.html

9.18 RNFMAP

9.19 SAMPLE

9.20 SCOPE

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

9.21 TUX

Institute	
Description	
Authors	
Publications	` , _
License	GPL

9.22 VILMA


9.23 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...

9.24 YAC

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

9.25 YAXT

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

ESM TOOLS

The command line interface `esm_tools` also has a top-level program you can use to interact with several parts of our software.

10.1 Usage: Top level commands

To show all top-level commands:

```
$ esm_tools --help
Usage: esm_tools [OPTIONS] COMMAND [ARGS]...

Options:
  --version  Show the version and exit.
  --help     Show this message and exit.

Commands:
  create-new-config  Opens your $EDITOR and creates a new file for NAME
  test-state         Prints the state of the last tested experiments.
```

10.2 Usage: Getting the Version

You can get the version number you currently have with:

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

10.3 Usage: Checking current testing state

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

```
$ esm_tools test-state
```

10.4 Usage: Making a new component

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

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

...EDITOR OPENS....

Thank you! The new configuration has been saved. Please commit it (and get in touch with ↵
↵the
esm-tools team if you need help)!
```

You can also specify if you are creating a new `setup` or a new `component` with:

```
$ esm_tools create-new-config --type setup <MY_NEW_SETUP_NAME>
```

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

ESM MASTER

11.1 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
```

11.2 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`.

ESM-TOOLS VERSION

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

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

12.1 ESM-Versions (deprecated)

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

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

12.1.1 Usage

It doesn't matter from which folder you call `esm_versions`. You have two subcommands:

<code>esm_versions check</code>	gives you the version number of each installed esm python package
<code>esm_versions upgrade</code>	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.:

<code>esm_versions upgrade esm_parser</code>	upgrades only the package <code>esm_parser</code> to the newest version of the release branch
--	---

And yes, `esm_versions` can upgrade itself.

ESM RUNSCRIPTS

13.1 Usage

```
esm_runscripts [-h] [-d] [-v] [-e EXPID] [-c] [-P] [-j LAST_JOBTYPE]
                [-t TASK] [-p PID] [-x EXCLUDE] [-o ONLY]
                [-r RESUME_FROM] [-U] [-i INSPECT]
runscript
```

13.2 Arguments

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

13.3 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).

13.4 Job Phases

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

13.5 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
```

13.6 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>
```

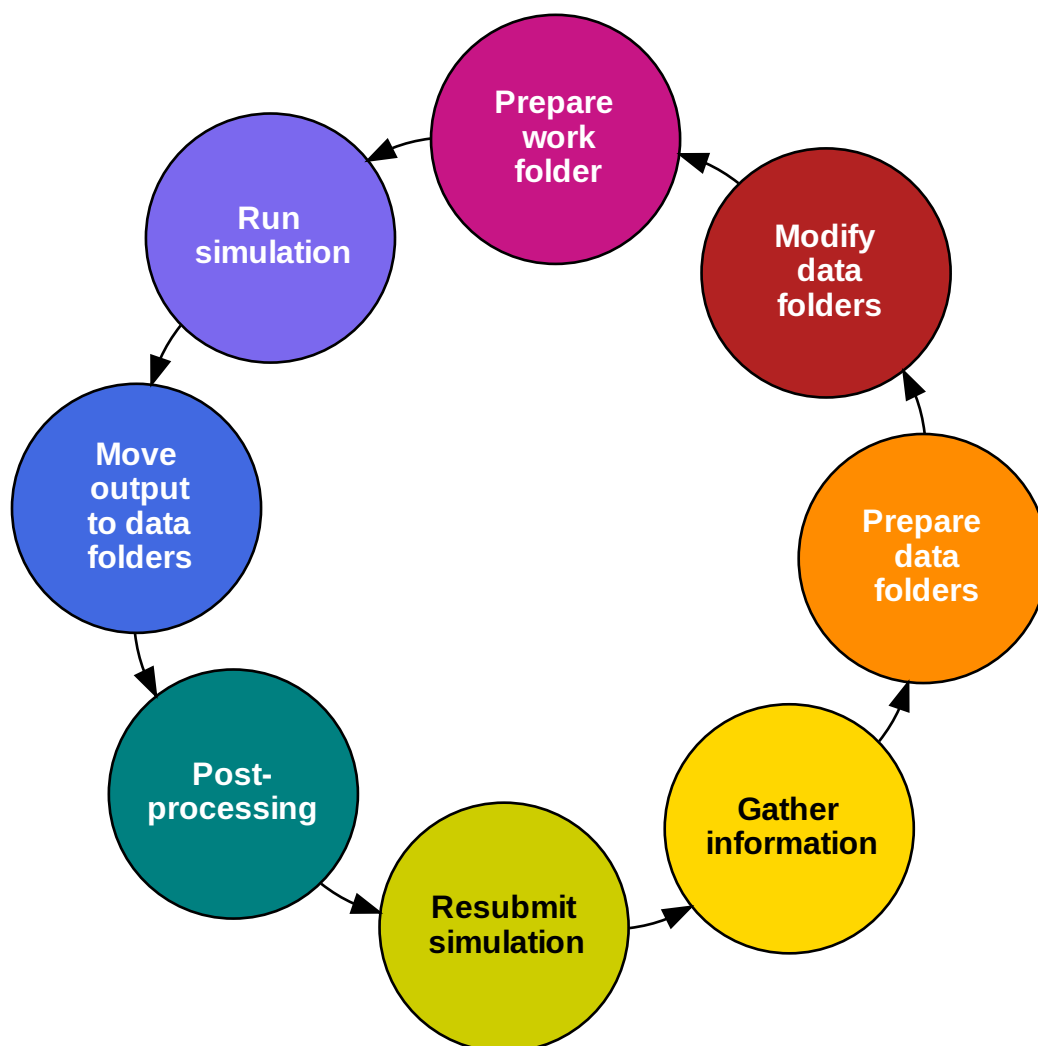


Fig. 1: ESM-Tools job phases

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.

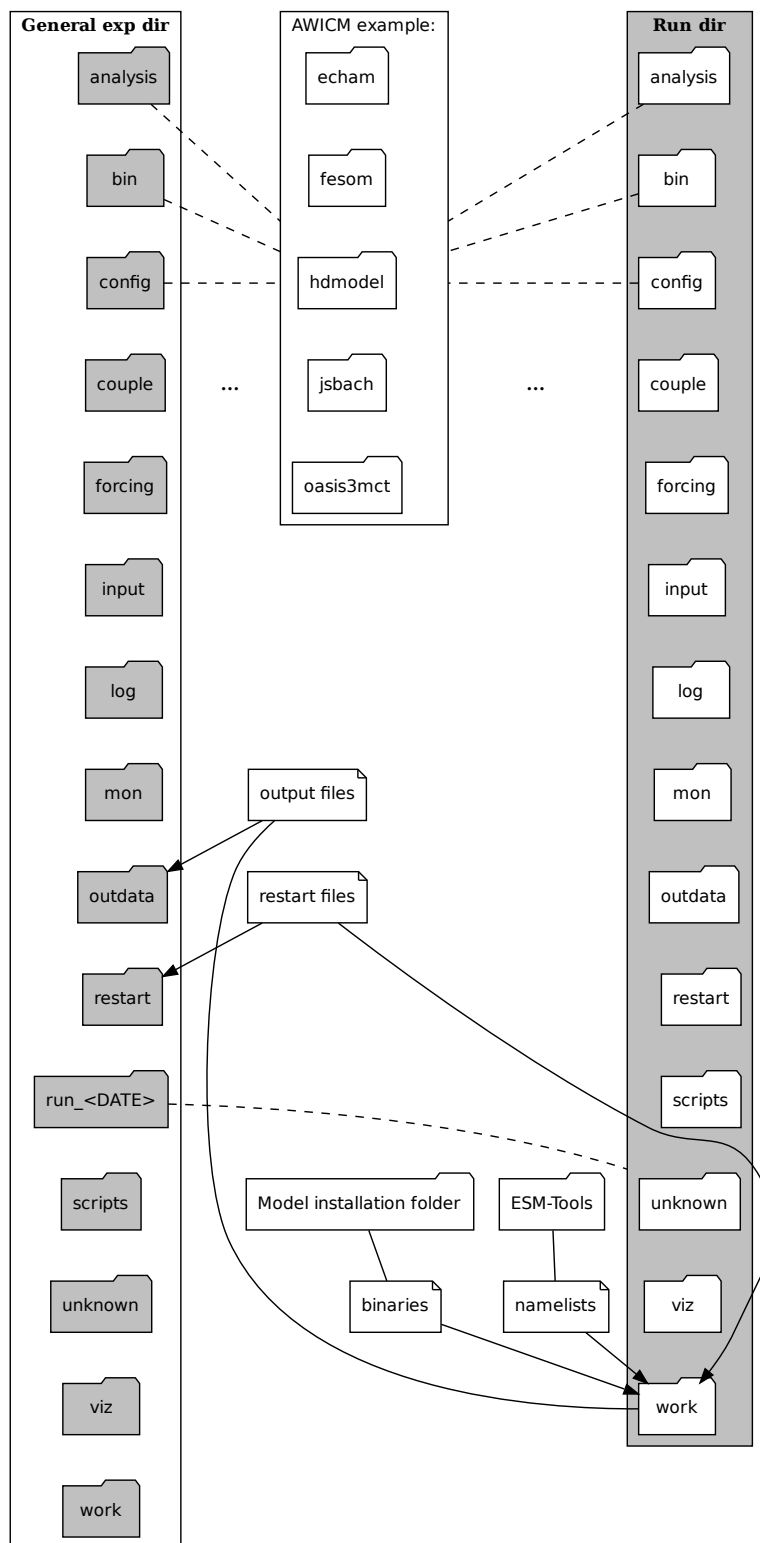


Fig. 2: Experiment directory structure

Subfolder	Files	Description
analysis	user's files	Results of user's "by-hand" analysis can be placed here.
bin	component binaries	Model binaries needed for the experiment.
config	<ul style="list-style-type: none"> • <experiment_ID>_finished_config.yaml • namelists • other configuration files 	<p>Configuration files for the experiment including namelists and other files specified in the component's configuration files (<PATH>/esm_tools/configs/<component>/<component>.yaml, see File Dictionaries). The file <experiment_ID>_finished_config.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.</p>
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 Dictionaries).
input	input files	Input files for the experiment. Only copied here when specified by the user in the runscript or in the configuration files (File Dictionaries).
log	<ul style="list-style-type: none"> • <experiment_ID>_<setup_name>.log • component log files 	<p>Experiment log files. The component specific log files are placed in their respective subfolder. The general log file <experiment_ID>_<setup_name>.log reports on the <i>ESM-Runscripts Job Phases</i> 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).</p>
mon	user's files	Monitoring scripts created by the user can be placed here.
outdata	outdata files	Outdata files are placed here. Outdata file names and copying instructions should be included in the configuration files of components (File Dictionaries).
restart	restart files	Restart files are placed here. Restart file names and copying instructions should be included in the configuration files of components (File Dictionaries).
run_YYYYMMDD	run files	Run folder containing all the files for a given run. Folders contained here have the same names as the ones contained in the general ex-

13.6. Experiment Directory Structure

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*).

13.7 Cleanup of run_ directories

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

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

Note: `clean_runs: (bool)` is incompatible with `clean_this_rundir` and `clean_runs: (int)` is incompatible with `clean_old_rundirs_except` (an error will be raised after the end of the first simulation). The functionality of `clean_runs` variable **alone will suffice most of the standard user requirements**. If finer tuning for the removal of `run_` directories is required you can use 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
```

13.8 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
```

13.9 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.

13.10 Running an experiment with a virtual environment

Running jobs can optionally be encapsulated into a virtual environment.

To use a virtual environment run `esm_runscripts` with the flag `--contained-run` or set `use_venv` within the `general` section of your runscript to `True`:

```
general:
  use_venv: True
```

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

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

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

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

```
/scratch/miguel/test/.venv_esmtools/lib/python3.10/site-packages/esm_tools
```

instead of:

```
/albedo/home/miguel/.local/lib/site-packages/esm_tools
```

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

```
general:
  install_esm_tools_branch: '<your_branch_name>'
```

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

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

```
general:
  install_<esm_package>_editable: true/false
```

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

ESM RUNSCRIPTS - USING THE WORKFLOW MANAGER

14.1 Introduction

Starting with Release 6.0, `esm_runscripts` allows to define additional phases for e.g. data processing, coupling. Such subjobs can be arranged into clusters, and the order of execution can be set in a flexible and short way from the runscript. This is applicable for both pre- and postprocessing, but especially useful for iterative coupling jobs, like e.g. coupling pism to vilma (see below). In this section we explain the basic concept, describe the keywords that have to be set in the runscript in order to make use of this feature, and give some examples on how to integrate pre- and postprocessing jobs and how to set up phases for iterative coupling.

14.2 Default phases of a general model simulation run

ESM-Tools uses the workflow manager itself to organize the default *workflow phases* of a simulation *run*. Since Release 6.0 the default workflow phases are the following:

```
newrun --> prepcompute --> compute --> observe_compute --> tidy (+ resubmit next run)
```

These standard phases are all separated and independant phases, each submitted (or started) by the previous phase in one of three ways (see below). Here is what each of the standard phases does:

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

It is important to understand that none of this has to be edited by the users. The above described workflow phases form the default set of phases. Changing anyone of these phases may lead `esm-tools` to fail.

14.3 Inspect workflow phases

To inspect the workflow and workflow phases that are defined by e.g. a chosen setup or in an already run simulation/experiment, you can run `esm_runscript` with the `-i` (`-inspect`) option. This can be done for two different cases:

- To inspect the workflow previous to running a certain experiment. For example, if you want to add a new workflow phase, and need to know which phases are already defined in a chosen setup or model configuration:

```
esm_runscripts runscript.yaml -i workflow
```

- To inspect a workflow from an experiment that has been carried out already or created during a check-run (`-c`):

```
esm_runscripts runscript.yaml -e <expid> -i workflow
```

It will display the workflow configuration showing the order of workflow phases and their attributes and possible dependencies. This output should help to find out the correct keywords to be set when integrating a new workflow phase.

Example output:

```
Workflow sequence (cluster [phases])
-----
prepcompute ['prepcompute'] -> compute ['compute'] -> tidy ['tidy'] -> prepcompute [
  ↳ 'prepcompute'] and my_own_new_cluster ['my_new_last_phase', 'my_second_new_phase']
```

14.4 Defining additional workflow phases

If it is necessary to complement the default workflow with simulation specific processing steps, this sequence of default workflow phases can be extended by adapting the runscript or any component specific configuration files. The workflow manager will evaluate these additional phases and integrate them into the default sequence of the workflow. In order to integrate the additional phases correctly, these phases have to be defined by providing the following information. In the following, we will explain how an additional phase can be defined by describing the necessary keywords and what kind of restrictions need to be taken into account.

In order to integrate a user defined phase into the default workflow, the following information need to be provided:

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

In general, a workflow can be defined in the runscript or in any component configuration file. But there are some restrictions to

- The name of each phase needs to be unique. Otherwise, an exception error will be raised.
- The names of the default phases are not allowed to be used for any new phases. This will also cause an exception error during runtime.

- Settings in the runscript will overwrite settings in other config files. (See also *Hierarchy of YAML configuration files*.)

14.4.1 Keywords to define a new workflow phase

To define a new phase, the following keywords and mappings (key/value pairs) are available. (Keywords that are indicated with < > need to be adapted by the user.)

Keyword	Mandatory	(Default) values	Function
workflow	yes	–	Chapter headline in a runscript or configuration section, indicating that an alterations to the standard workflow will be defined here.
phases	yes	user defined string	Section within the workflow chapter that contains new additional workflow phases.
<new_phase_name>		user defined string	Section within the new_phases section for each new phase. The name of the new phase needs to be unique. See also further explanation here Defining additional workflow phases
run_after: <value> or run_before: <value>	no	default: last phase in (default) workflow (e.g. tidy)	Key/value entry in each <new_phase_name> section. This mapping defines the (default or user) phase of the workflow after or before the new phase should be executed. Only one of the two should be specified.
submit_to_batch_system: <value>	no	false , true	Key/value entry in each <new_phase_name> section. This mapping defines if the (default or user) phase is submitted to batch system or not.
run_on_queue: <value>	no	None	Key/value entry in each <new_phase_name> section. This mapping defines to which queue (name) the job of the new phase should be submitted to.
batch_or_shell: <value>	no	shell , batch	Key/value entry in each <new_phase_name> section. This mapping defines if the (default or user) phase is submitted as batch job or as shell script. This attribute will be overwritten depending on submit_to_batch_system
cluster: <value>	no	Phase name	Key/value entry in each <new_phase_name> section. Phases that have the same entry in cluster will be run from the same batch script.
order_in_cluster: <value>	no	sequential , concurrent	Key/value entry in each <new_phase_name> section. This mapping defines how phases in the same <cluster> should be run. Concurrent or serial.
script: <value>	yes	None	Key/value entry in each <new_phase_name> section. This mapping defines the name of the script that is going to be executed during the new workflow phase.
script_dir: <value>	yes	None	Key/value entry in each <new_phase_name> section. This mapping defines the path to the script set by the variable <script> .
call_function: <value>	no	None	Key/value entry in each <new_phase_name> section. This mapping defines the function within the script defined in variable <script> should be executed.
env_preparation: <value>	no	None	Key/value entry in each <new_phase_name> section. This mapping defines e.g. a Python script/function that prepares a dictionary with environment variables.
nproc: <value>	no	1	Key/value entry in each <new_phase_name> section. This mapping defines the number of CPUs a phase should run with (if run via sbatch).
run_only: <value>	no	None	Key/value entry in each <new_phase_name> section. This mapping defines when the phase should be run. E.g. run only at the beginning of a <i>chunk</i> (set of runs).
skip_chunk_number: <value>	no	None	Key/value entry in each <new_phase_name> section. This mapping defines how many chunks should be skipped before the phase will be executed.
trigger_next_run: <value>	no	false , true	If phase should trigger next run

14.4.2 Syntax example

The following code snippet shows the general syntax for defining a new workflow phase.

```
workflow:
  phases:
    <new_phase_name>:
      run_after: <value>
      submit_to_batch_system: <value>
      run_on_queue: <value>
      cluster: <value>
      order_in_cluster: <value>
      script: <value>
      call_function: <value>
      env_preparation: <value>
      nproc: <value>
      run_only: <value>
      skip_chunk_number: <value>
      trigger_next_run: <value>
```

14.5 Workflow defaults

A minimal example of defining a new workflow phase is given in Example 1. This will integrate a new phase with the following default assumptions:

- The new phase will be run after the last phase of the default workflow.
- The script given for this phase is run as a subprocess (not a batch run).
- The next run of the overall experiment will be (still) triggered by the last phase of the default workflow and not the new phase.

14.6 Examples for the definition of new workflow phases

14.6.1 Example 1: Adding an additional postprocessing subjob

In the case of a simple postprocessing task (here for model Echam), that could be run as the last task of each run, independantly from restarting the experiment, the corresponding minimal code snippet in a runscript could look like this:

```
echam:
  [...other information...]

workflow:
  phases:
    my_postprocessing:
      script_dir: <value>
      script: <values>
```

14.6.2 Example 2: Adding an additional preprocessing subjob

A preprocessing job basically is configured the same way as a postprocessing job, but the `run_before` keyword is needed now, to define when the new phase should be run:

```
echam:
  [...other information...]

  workflow:
    phases:
      my_preprocessing:
        run_before: precompute
        script_dir: <value>
        script: <values>
```

14.6.3 Example 3: Adding a new phase as the last task in a run

To integrate a new phase that should be run as the last task in every run but before the next run starts, use the following example:

```
echam:
  [...other information...]

  workflow:
    phases:
      my_new_last_phase:
        script_dir: <value>
        script: <values>
        trigger_next_run: True
```

14.6.4 Example 4: Adding multiple user phases that can be run concurrently in a workflow cluster

It is possible to define multiple new phases that should start at the same but can be run independently from each other. This can be done by assigning these phases to the same workflow cluster and run them concurrently over the batch system:

```
echam:
  [...other information...]

  workflow:
    phases:
      my_new_last_phase:
        script_dir: <value>
        script: <values>
        submit_to_batch_system: True
        run_on_queue: <value>
        cluster: my_own_new_cluster

      my_second_new_phase:
        script_dir: <value>
```

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```

script: <values>
submit_to_batch_system: True
run_on_queue: <value>
cluster: my_own_new_cluster

```

14.6.5 Example 5: Adding an iterative coupling job

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

```

echam:
  [...other information...]

  workflow:
    subjobs:
      couple_in:
        nproc: 1
        run_before: prepcompute
        script: coupling_ice2echam.functions
        script_dir: ${general.script_dir}/echam
        call_function: ice2echam
        env_preparation: env_echam.py
        run_only: first_run_in_chunk
        skip_chunk_number: 1

      couple_out:
        nproc: 1
        run_after: tidy
        script: coupling_echam2ice.functions
        script_dir: ${general.script_dir}/echam
        call_function: echam2ice
        env_preparation: env_echam.py
        run_only: last_run_in_chunk
        trigger_next_run: True

fesom:
  [...other information...]

  workflow:
    subjobs:
      couple_in:
        nproc: 1
        run_before: prepcompute
        script: coupling_ice2fesom.functions
        script_dir: ${general.script_dir}/fesom
        call_function: ice2fesom
        env_preparation: env_fesom.py
        run_only: first_run_in_chunk

```

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```
        skip_chunk_number: 1

couple_out:
  nproc: 1
  run_after: tidy
  script: coupling_fesom2ice.functions
  script_dir: ${general.script_dir}/fesom
  call_function: fesom2ice
  env_preparation: env_fesom.py
  run_only: last_run_in_chunk
  trigger_next_run: True
```

ESM ENVIRONMENT

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

For the correct definition of an environment for an HPC a *yaml* file for that system needs to be included inside the `esm_tools` package inside the `configs/machines/` folder (e.g. `ollie.yaml`). This file should contain all the required preset variables for that system and the environment variables `module_actions` and `export_vars`.

15.1 Environment variables

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

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

This variable also allows for sourcing files by adding a member to the list such as `source <file_to_be_sourced>`.

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

```
export_vars:
  A_VAR_TO_BE_EXPORTED: the_value
```

The previous example will result in the following export in the script produced by `esm_master` or `esm_runscripts`:

```
export A_VAR_TO_BE_EXPORTED=the_value
```

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

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

The resulting script will contain the following exports:

```
export A_VAR_TO_BE_EXPORTED=the_value
export A_VAR_TO_BE_EXPORTED=$A_VAR_TO_BE_EXPORTED:another_value
```

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

15.2 Modification of the environment through the model/setup files

As previously mentioned, the default environment for a HPC system is defined inside its machine file (in `esm_tools/machines/<machine_name>.yaml`). However, it is possible to modify this environment through the model and/or coupled setup files (or even inside the runscrip) to adjust to the model/setup requirements. For this purpose, the variables `environment_changes`, `compiletime_environment_changes` and `runtime_environment_changes` can be used.

environment_changes (dict) Allows for modifications of the machine `module_actions` and `export_vars`, both during compilation and runtime.

compiletime_environment_changes (dict) Allows for modifications of the machine `module_actions` and `export_vars`, only applied during compilation time.

runtime_environment_changes (dict) Allows for modifications of the machine `module_actions` and `export_vars`, only applied during run time.

The syntax for this dictionary is the same as that defined in Environment variables, but using `add_` in front of the environment variables (`add_module_actions` and `add_export_vars`). Furthermore, the environment variables can be nested inside `choose_` blocks:

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

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

15.3 Coupled setup environment control

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

15.3.1 Component-by-component

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

Warning: Handling `environment_changes` in this fashion implies that compilation scripts can potentially end up containing different environments.

15.3.2 General environment for setups

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

ESM-TESTS

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

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

16.1 Glossary

actual vs check test An *actual test* is a test where the model has been compiled and run in one of the supported HPCs.

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

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

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

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

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

16.2 Usage

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

- *Arguments*
- Runscripts via the usual `esm_parser` syntax (e.g. `choose_computer.name`)
- *Model control file* (`config.yaml`)
- *Local test configuration* (`test_config.yaml`)

The commands syntax is as follows:

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

16.3 Arguments

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

16.4 Last-state

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

16.5 Check test status

As a user, you can check the last-state status (the online one of the `esm_tests_info` repo, release branch) by running:

```
esm_tools test-state
```

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

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

```
esm_tests -t
```

16.6 Model control file (config.yaml)

File location: `esm_tools/src/esm_tests/resources/runscripts/<model>/config.yaml` **Versioned:** Yes, distributed with `esm_tests_info`

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

Within this file you can control:

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

The file should contain this structure:

```
comp:
  actual:
    files:
      - "file/path" # Typically the binaries
    check: {}
run:
  actual:
    errors:
      - "error message to mark the test as not successful # Typically
↪ "MISSING FILES"
    files: # Typically restart files and outdata files
      - "path/to/file1"
      - "globbing/path/*/to*files"
    check: {}
computers:
  - <computer1>
  - <computer2>
```

In the files sections, **globbing is supported**.

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

Each file name can be followed by the syntax `in/except [<model_version1>, <model_version2>, ...]` to only check for that file in that set of model versions, or to exclude (except) that file from being check for a set of model versions.

Example

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

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(continued from previous page)

- blogin
- levante

16.7 Local test configuration (test_config.yaml)

File location: `esm_tools/src/esm_tests/test_config.yaml` **Versioned:** No, user specific, git-ignored

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

```
<model1>:
  - <runscript1_name>.yaml
  - <runscript2_name>.yaml
  - [ ... ]
<model2>: all
[ ... ]
```

The `model` sections need to be named after the folders in `esm_tools/src/esm_tests/resources/runscripts`. If you want to run all the supported runscripts for a model in this platform, make the `model` section have the value `all`. If you want to select a set of **supported runscripts** make the `model` be a list of runscripts (this runscripts need to be in `esm_tools/src/esm_tests/resources/runscripts/<model>/`). If you want to run all the supported runscripts for all supported models in this platform, but still keep this file around (i.e. commented most of the contents), make the file content be an empty dictionary (`{}`).

Example

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

16.8 ESM-Tests cookbook

16.8.1 How to include a new model/runscript

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

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


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


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

1. In the corresponding *Model control file* (`esm_tools/src/esm_tests/resources/runscripts/<model>/config.yaml`), add the name of the platform to the `computers` list
2. In the runscripts (`esm_tools/src/esm_tests/resources/runscripts/<model>/<runscript>.yaml`), add the necessary case to the `choose_computer.name` to specify pool directories, forcing files, `nproc`, etc.

16.8.3 How to approve changes on a GitHub Pull-Request







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




**Some checks were not successful**

12 successful and 3 failing checks

[Hide all checks](#)

✓		esm-tools no Docker / Python 3.9 sample (push)	Successful in 1m	Details
✗		esm_tests / ollie / ollie1 (pull_request)	Failing after 6m	Details
✗		esm_tests / levante / levante1 (pull_request)	Failing after 5m	Details
✓		esm_tests / juwels / jwlogin01.juwels (pull_request)	Successful in 2m	Details
✓		esm_tests / aleph / elogin1 (pull_request)	Successful in 2m	Details
✗		esm_tests / blogin / blogin1 (pull_request)	Failing after 3m	Details

**This pull request is still a work in progress**

Draft pull requests cannot be merged.

[Ready for review](#)

Merge pull request

▼

You can also [open this in GitHub Desktop](#) or view [command line instructions](#).

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

```

52  ▶ COMPILING (5.9%) vilma-pism-1.0v1d
57  ▶ COMPILING (11.8%) fesom-recom-1.4
62  ▶ COMPILING (17.6%) fesom-2.0
66  ▶ COMPILING (23.5%) fesom-2.1
70  ▶ COMPILING (29.4%) echam-6.3.04p1
74  ▶ COMPILING (35.3%) awiesm-2.1
80  ▶ COMPILING (41.2%) awiesm-2.1
86  ▶ COMPILING (47.1%) awiesm-2.1-wiso
92  ▶ COMPILING (52.9%) awiesm-2.1
98  ▶ COMPILING (58.8%) awiesm-2.1
104 ▶ COMPILING (64.7%) awiesm-2.1
110 ▶ COMPILING (70.6%) awiesm-2.1-recom
116 ▶ COMPILING (76.5%) awicm-CMIP6
122 ▶ COMPILING (82.4%) awicm-2.0
128 ▶ COMPILING (88.2%) awicm3-v3.0
135 ▶ COMPILING (94.1%) awicm3-frontiers-xios
143 ▶ COMPILING (100.0%) awicm3-v3.1
151 ▶ SUBMITTING (5.9%) vilma-pism/vilmald_1ky-pism_ly
152 ▶ SUBMITTING (11.8%) fesom-recom/fesom-recom1.4-initial-daily
161 ▶ SUBMITTING (17.6%) fesom/fesom2.0-initial-monthly
169 ▶ SUBMITTING (23.5%) fesom/fesom2.1-initial-monthly
179 ▶ SUBMITTING (29.4%) echam/echam6.3.04p1-initial-monthly
230 ▶ SUBMITTING (35.3%) awiesm/awiesm-2.1_icebergs
372 ▶ SUBMITTING (41.2%) awiesm/pico
514 ▶ SUBMITTING (47.1%) awiesm/PI_ctrl_awiesm-2.1-wiso
662 ▶ SUBMITTING (52.9%) awiesm/bootstrap
805 ▶ SUBMITTING (58.8%) awiesm/pi
947 ▶ SUBMITTING (64.7%) awiesm/pi-wiso
1095 ▶ SUBMITTING (70.6%) awiesm/all_awiesm-2.1-recom
1238 ▶ SUBMITTING (76.5%) awicm/awicm1-CMIP6-initial-monthly
1295 ▶ SUBMITTING (82.4%) awicm/awicm2-initial-monthly
1352 ▶ SUBMITTING (88.2%) awicm3/awicm3-v3.0-TC0159L91-CORE2_initial
1364 ▶ SUBMITTING (94.1%) awicm3/awicm3-frontiers-xios-TC0159L91-CORE2_initial
1376 ▶ SUBMITTING (100.0%) awicm3/awicm3-v3.1-TC095L91-CORE2_initial

```

```

1026 ▼ SUBMITTING (52.9%) awiesm/all_awiesm-2.1-recom
1027 'run/awiesm/all_awiesm-2.1-recom/run_20010101-20010101/scripts/all_awiesm-2.1-recom_compute_20010101-20010101.run' files are identical
1028
1029 Differences in run/awiesm/all_awiesm-2.1-recom/run_20010101-20010101/config/all_awiesm-2.1-recom_finished_config.yaml:
1030 -----
1031 +++
1032 @@ -356,7 +356,7 @@
1033     grid: atmo
1034     w3_atm:
1035         grid: atmo
1036 -   dataset: r0007
1037 +   dataset: r0008
1038   debug_info:
1039     loaded_from_file:
1040     - <HOME_DIR>/esm_tools/configs/components/echam/echam.yaml
1041 @@ -489,7 +489,7 @@
1042     - need_year_after
1043     - need_2years_before
1044     - need_2years_after
1045 -   forcing_dir: /pool/data/ECHAM6/input/r0007/T63
1046 +   forcing_dir: /pool/data/ECHAM6/input/r0008/T63

```

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

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

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

ESM MOTD

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

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

This check occurs every time the user uses `esm_runscripts`.

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

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

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"]`.

18.1 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 runsript, inside the `computer` section:

Key	Description
<code>mail_type</code> , <code>mail_user</code>	Define these two variables to get updates about your slurm-job through email.
<code>single_proc_submit_flag</code>	By default defined as <code>--ntasks-per-node=1</code>
<code>additional_flags</code>	To add any additional flag that is not predefined in <i>ESM-Tools</i>

18.1.1 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"
```

18.1.2 Adding more than one flag

Alternatively, you can include a list of additional flags:

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

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

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

Feature available since version: `esm_runscripts v4.2.1`

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

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

To overcome this problem, you can apply a small change to the factor “by which stratospheric horizontal diffusion 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, separated 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.

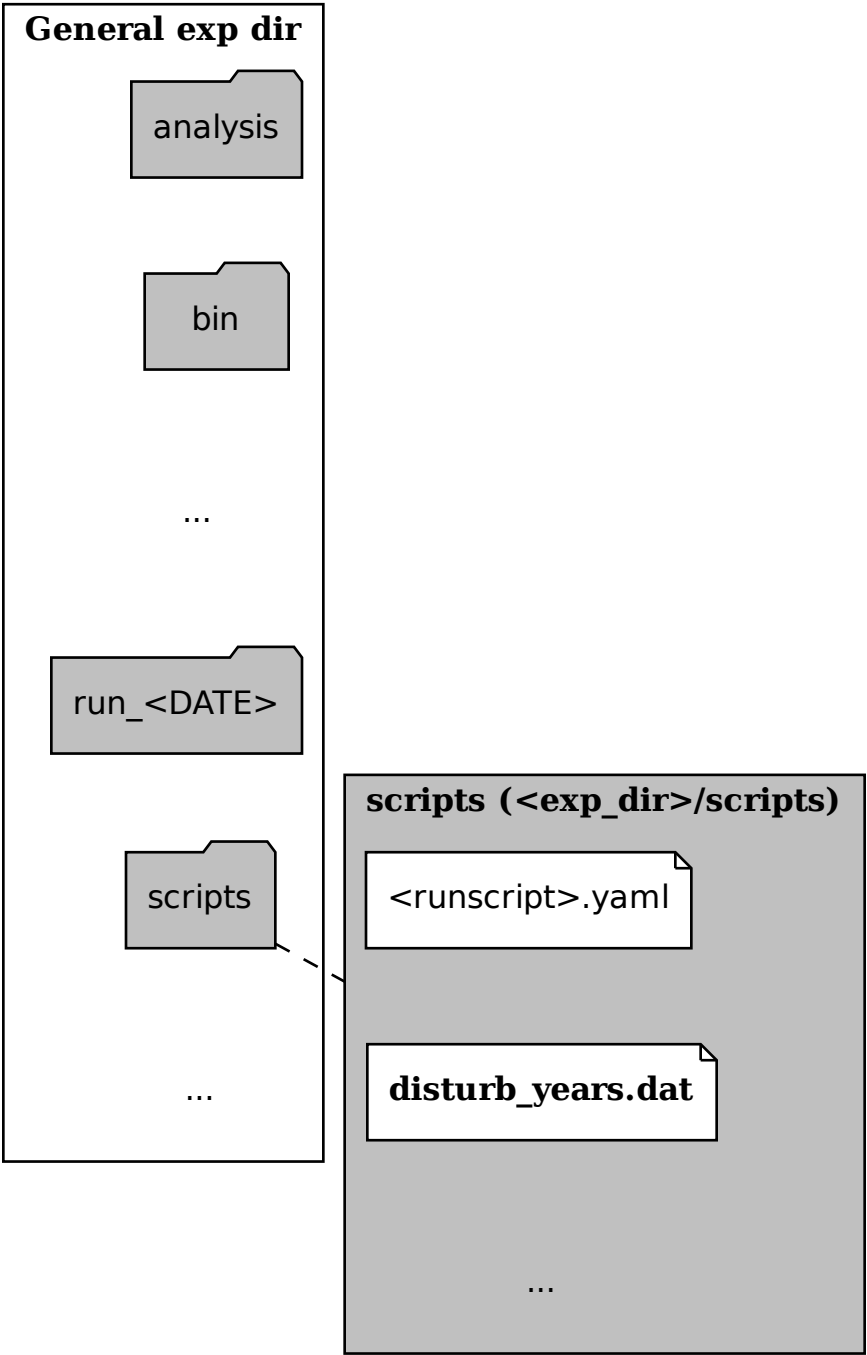


Fig. 1: disturb_years.dat location

18.2.1 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
```

18.2.2 See also

- [ECHAM6 User Handbook](#), Table 2.4, `dynctl`
- [Relevant source code](#)

18.3 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>`

18.3.1 Example

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

Snippet

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

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

Full Runscript

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

```

general:
  setup_name: "awiesm"
  compute_time: "02:30:00"
  initial_date: "2000-01-01"
  final_date: "2002-12-31"
  base_dir: "/work/ab0246/a270077/For_Christian/experiments/"
  nmonth: 0
  nyear: 1
  account: "ab0246"

echam:
  restart_unit: "years"
  nprocar: 0
  nprocbr: 0
  namelist_changes:
    namelist.echam:
      radctl:
        co2vmr: 1137.e-6
      parctl:
        nprocar: 0
        nprocbr: 0
      runctl:
        default_output: True

awiesm:
  version: "2.1"
  postprocessing: true
  scenario: "PALEO"
  model_dir: "/work/ab0246/a270077/For_Christian/model_codes/awiesm-2.1/"

fesom:
  version: "2.0"
  res: "CORE2"
  pool_dir: "/pool/data/AWICM/FESOM2"
  mesh_dir: "/work/ba1066/a270061/mesh_CORE2_finaltopo_mean/"
  restart_rate: 1
  restart_unit: "y"
  restart_first: 1
  lresume: 0
  namelist_changes:
    namelist.config:
      paths:
        ClimateDataPath: "/work/ba0989/a270077/AWIESM_2_1_LR_concurrent_rad/
↪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"

```

18.3.2 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](#)).

18.3.3 Unusual Namelists

Some times, you have strange namelists of the form:

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

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

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

18.3.4 See also

- [Default namelists on GitHub](#)
- [Changing Namelists](#)
- [What Is YAML?](#)

18.4 Heterogeneous Parallelization Run (MPI/OpenMP)

Feature available since version: 5.1

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

1. Add `heterogenous_parallelization: true` in the `computer` section of your runscript. If the `computer` section does not exist create one.
2. Add `omp_num_threads: <number>` to the sections of the components you'd like to have OpenMP parallelization.

18.4.1 Example

AWICM3

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

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

18.4.2 See also

- *Runtime variables*

18.5 How to setup runscrip

This recipe describes how to setup a runscrip for the following different kinds of experiments. Besides the variables described in *ESM-Tools Variables*, add the following variables to your runscrip, 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 redat**: An experiment that restarts from a previous experiment with a different experiment id and if this experiment should be continued with a diiferent 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>
```

18.5.1 See also

- [ESM-Tools Variables](#)
- [What Is YAML?](#)

18.6 Implement a New Model

Feature available since version: 4.2

Note: since version 6.20.2 a template is available in `esm_tools/configs/templates/component_template.yaml`

1. Upload your model into a repository such as *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>/<model>.yaml
```

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

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

6. Complete the following information about your model:

```
# YOUR_MODEL YAML CONFIGURATION FILE
#

model: your_model_name
type: type_of_your_model      # atmosphere, ocean, etc.
version: "the_default_version_of_your_model"
```

7. Include the names of the different versions in the `available_versions` section and the compiling information for the default version:

```
[...]

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

executable: your_model_command

setup_dir: "${model_dir}"
bin_dir: "${setup_dir}/name_of_the_binary"
```

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

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

Single file

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"
```

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

Multiple version files

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

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

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

```
branch: "develop"
```

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

`fesom.yaml`

```
[ ... ]

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

[ ... ]
```

`fesom-2.0.yaml`

```
[ ... ]

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

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```

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

[ ... ]

```

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

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

```
$ esm_master
```

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

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

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

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

18.6.1 See also

- [ESM-Tools Variables](#)
- [Switches \(choose_\)](#)
- [What Is YAML?](#)

18.7 Implement a New Coupled Setup

Feature available since version: 4.2

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

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 *yml* file inside the coupling folder with the same name:

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

- c. Include the following information in each coupling file:

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

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

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

```
#####
↪#####
##### NAME_VERSION YAML CONFIGURATION FILE #####
↪#####
#####
↪#####

general:
  model: your_setup
  version: "your_setup_version"

  coupled_setup: True

  include_models:          # List of models, couplers and componentes of the_
↪setup.                    # Do not include the version number
                           - component_1
                           - component_2
                           - [ ... ]
```

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

7. Include the names of the different versions in the `available_versions` section:

```
general:

  [ ... ]

  available_versions:
    - "1.0.0"
    - "1.0.1"
```

The `available_versions` key is needed for *esm_master* to list the versions of your setup.

8. In the `<setup>.yaml`, use a `choose_` switch (see [Switches \(choose_\)](#)) to assign the coupling files (created in step 3) to their corresponding setup versions:

```
general:

  [ ... ]

  choose_version:
    "1.0.0":
      couplings:
        - "model1-1.0+model2-1.0"
    "1.0.1":
      couplings:
        - "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>/<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*).

18.7.1 Example

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

fesom-1.4+echam-6.3.04p1.yaml

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

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

awicm.yaml

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

```
#####
##### AWICM 1 YAML CONFIGURATION FILE #####
#####

general:
  model: awicm
  #model_dir: ${esm_master_dir}/awicm-${version}

  coupled_setup: True

  include_models:
```

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```

- 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

```

18.7.2 See also

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

18.8 Implement a New HPC Machine

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

- <PATH>/esm_tools/configs/machines/all_machines.yaml
- <PATH>/esm_tools/configs/machines/<new_machine>.yaml

1. Add an additional entry for the new machine.

Use your favourite text editor and open the file <PATH>/esm_tools/configs/machines/all_machines.yaml:

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

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

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

2. Create a new machine file.

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

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

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

```
$ cp <PATH>/esm_tools/configs/templates/machine_template.yaml <PATH>/esm_tools/
↳configs/machines/<new_machine>.yaml
$ <your_text_editor> <PATH>/esm_tools/configs/machines/<new_machine>.yaml
```

You can also reproduce the two steps above simply by running the following esm_tools command:

```
$ esm_tools create-new-config <PATH>/esm_tools/configs/machines/<new_machine>.yaml -
↳t machine
```

This will copy the machine_template.yaml in the target location and open the file in your default editor.

18.8.1 See also

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

18.9 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 choosing 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.

18.9.1 Source Path Already Defined in a Config File

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

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

Example

ECHAM

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

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

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
```

18.9.2 Modify the Source of a File

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

1. Include the source path under a *key* inside `forcing_sources` or `input_sources` in your runscript:

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

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

```
<forcing/input>_sources:
  <key_for_your_source>: <first_part_of_the_path>@YEAR@<second_part_of_the_
  ↳path>
```

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```

from: <first_year>
to: <last_year>

```

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

```

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

```

18.9.3 Copy the file in the work folder and/or rename it

To copy the files from the forcing/input folders into the work folder (<base_dir>/<exp_id>/run_<DATE>/work) or rename them:

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

```

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

```

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

```

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

```

Example

ECHAM

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

esm_tools/config/component/echam/echam.datasets.yaml

```

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

```

esm_tools/config/component/echam/echam.yaml

```

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

```

If `scenario: "PI-CTRL"` then the source selected will be `${forcing_dir}/${resolution}${ocean_resolution}_piControl-LR_sst_1880-2379.nc` and the name of the file copied to the experiment forcing folder will be `${resolution}${ocean_resolution}_piControl-LR_sst_1880-2379.nc`. However, *ECHAM* needs this file in the same folder as the binary (the work folder) under the name `unit.20`. To copy and rename this file into the work folder the following lines are used in the `echam.yaml` configuration file:

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

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

18.9.4 See also

- *What Is YAML?*
- *File Dictionaries*

18.10 Exclude a Forcing/Input File

Feature available since version: 4.2

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

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

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

18.10.1 Example

ECHAM

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

```
remove_forcing_files:
  - sst
```

18.10.2 See also

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

18.11 Using your own namelist

Feature available since version: 4.2

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

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

1. Search for the `config_sources` variable inside the configuration file of the model you are trying to run, and then, identify the “key” containing the path to the default namelist.
2. In your runscript, indented in the corresponding model section, add an `add_config_sources` section, containing a variable whose “key” is the one of step 1, and the value is the path of the new namelist.
3. Bare in mind, that namelists are first loaded by *ESM-Tools*, and then modified by the default `namelist_changes` in the configuration files. If you want to ignore all those changes for the your new namelist you’ll need to add `remove_namelist_changes: [<name_of_your_namelist>]`.

In dot notation both steps will look like: `<model_name>.<add_config_sources>.<key_of_the_namelist>:<path_of_your_namelist>` `<model_name>.<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.

18.11.1 Example

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

ECHAM

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

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

In this case the “key” is `"namelist.echam"` and the “value” is `"${namelist_dir}/namelist.echam"`. Let’s assume your namelist is in the directory `/home/ollie/<usr>/my_namelists`. Following step 2, you will need to include the following in your runscript:

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

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

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

  remove_namelist_changes: [namelist.echam]
```

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

```
choose_lresume:
  False:
    restart_in_modifications:
      "[[streams-->STREAM]]":
        - "vdate <--set_global_attr-- ${start_date!syear!smoth!
↪sday}"
          # - fdate "<--set_dim--" ${year_before_date}
          # - ndate "<--set_dim--" ${steps_in_year_before}

  True:
    # pseudo_start_date: $(( ${start_date} - ${time_step} ))
    add_namelist_changes:
      namelist.echam:
        runctl:
          dt_start: "remove_from_namelist"
```

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

FESOM

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

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

In this case the “key” is `ice` and the “value” is `${namelist_dir}/namelist.ice`. Let’s assume your namelist is in the directory `/home/ollie/<usr>/my_namelists`. Following step 2, you will need to include the following in your runscript:

```
fesom:
  add_config_sources:
```

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```
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.

18.11.2 See also

- [Default namelists on GitHub](#)
- [Append to an Existing List \(add_\)](#)
- [Changing Namelists](#)
- [What Is YAML?](#)

18.12 How to branch-off FESOM from old spinup restart files

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

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

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

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

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

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

```
ncrename -d T,time <copy_of_restart_spinup_file>.nc
```

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

18.12.1 See also

- [cookbook:How to run a branch-off experiment](#)

GLOSSARY

chunk A chunk is a set of runs.

experiment The whole simulation.

phase A phase is a part of a workflow that is executed during a run.

run A run is the period until a restart is performed.

workflow A workflow is a series of phases that are executed during a run.

FREQUENTLY ASKED QUESTIONS

20.1 Installation

- 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/>.
- 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.

20.2 ESM Runscripts

- Q:** I get the error: `load_all_functions: not found [No such file or directory]` when calling my runscript like this:

```
$ ./my_run_script.sh -e some_expid
```

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

```
$ esm_runscripts my_run_script.sh -e some_expid
```

All the command line options still apply. By the way, “`load_all_function`” doesn't hurt to have in the runscript, but can safely be removed.

- 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.
- 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.

20.3 ESM Master

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

A: You can add a choose-block in the models yaml-file (`esm_tools/configs/model_name.yaml`), e.g.:

```
choose_version:
  40r1:
    environment_changes:
      add_export_vars:
        - 'MY_VAR="something"'
      add_module_actions:
        - load my_own_module

  43r3:
    environment_changes:
      add_export_vars:
        - 'MY_VAR="something_else"'
```

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

A: Add your configuration in the file `configs/esm_master/setups2models.yaml`

20.4 Frequent Errors

1. **Q:** When I try to install *ESM-Tools* or use `esm_versions` I get the following error:

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

or something on the following lines:

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

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```
UnicodeDecodeError: 'ascii' codec can't decode byte 0xf0 in position 1468: ordinal not
↳ in range(128)
```

```
-----
ERROR: Command errored out with exit status 1: python setup.py egg_info Check the logs.
↳ for full command output.
```

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

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

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

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

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:

21.1 `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`).

21.2 `esm_master.git`

This repository contains the python files that give the `esm_master` executable in the subfolder `esm_master`.

21.3 `esm_runscripts.git`

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

21.4 `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.

21.5 esm_calendar.git

ESM TOOLS CODE DOCUMENTATION

22.1 esm_archiving package

Top-level package for ESM Archiving.

`esm_archiving.archive_mistral(tfile, rtfile=None)`

Puts the `tfile` to the tape archive using `tape_command`

Parameters

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

Return type `None`

`esm_archiving.check_tar_lists(tar_lists)`

`esm_archiving.delete_original_data(tfile, force=False)`

Erases data which is found in the tar file.

Parameters

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

Return type `None`

`esm_archiving.determine_datestamp_location(files)`

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

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

Returns A slice object giving the location of the datestamp

Return type `slice`

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

`esm_archiving.determine_potential_datestamp_locations(filepattern)`

For a filepattern, gives back index of potential date locations

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

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

Return type list

`esm_archiving.find_indices_of(char, in_string)`

Finds indicies of a specific character in a string

Parameters

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

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

`esm_archiving.get_files_for_date_range(filepattern, start_date, stop_date, frequency,
date_format='%Y%m%d')`

Creates a list of files for specified start/stop dates

Parameters

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

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

Return type list

Example

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

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

Return type dict

`esm_archiving.group_indexes(index_list)`

Splits indexes into tuples of monotonically ascending values.

Parameters **list** – The list to split up

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

Return type list

Example

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

`esm_archiving.log_tarfile_contents(tfile)`

Generates a log of the tarball contents

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

Return type None

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

`esm_archiving.pack_tarfile(flist, wdir, outname)`

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

Parameters

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

Returns The output file name

Return type str

`esm_archiving.purify_expid_in(model_files, expid, restore=False)`

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

Parameters

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

Returns Dictionary containing keys for each model, values for file patterns

Return type dict

`esm_archiving.sort_files_to_tarlists(model_files, start_date, end_date, config)`

`esm_archiving.split_list_due_to_size_limit(in_list, slimit)`

`esm_archiving.stamp_filepattern(filepattern, force_return=False)`

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

Parameters

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

Returns New filepattern, with >>>DATE<<<

Return type str

`esm_archiving.stamp_files(model_files)`

Given a standard file dictionary (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 dictionary 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.

22.1.1 Subpackages

esm_archiving.external package

Submodules

esm_archiving.external.pyftp module

class esm_archiving.external.pyftp.**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 transferring the file

exists(*path*)

check if a path exists

files(*path=None*)

gather files at the given path

is_connected()

check if the connection is still active

isdir(*pathname*)

Returns true if pathname refers to an existing directory

isfile(*pathname*)

Returns true if pathname refers to an existing file

islink(*pathname*)

listdir(*path=None*)

list directory contents

listing(*path=None*)

list directory contents

listing2(*path=None*)

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

makedirs(*path*)

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

mkdir(*path*)

mlsd(*path*)

pwd()

present working directory

quit()

reconnect()

reconnects to the ftp server

remove(*filename*)

removedirs(*path*)

rename(*from_name*, *to_name*)

rmdir(*path*)

remove directory

size(*pathname*)

Returns size of path in bytes

stat(*pathname*)

Returns stat of the path

static upload(*source*, *destination*)

uses pftp binary for transferring 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)`

22.1.2 Submodules

22.1.3 esm_archiving.cli module

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

`esm_archive`

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

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

`Console script for esm_archiving.`

`Options:`

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<code>--version</code>	Show the version and exit.
<code>--write_local_config</code>	Write a local configuration YAML file in the current working directory
<code>--write_config</code>	Write a global configuration YAML file in <code>~/.config/esm_archiving/</code>
<code>--help</code>	Show this message and exit.
Commands:	
<code>create</code>	
<code>upload</code>	

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

Creating tarballs

Use `esm_archive create` to generate tar files from an experiment:

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

The arguments `start_date` and `end_date` should take the form `YYYY-MM-DD`. A complete example would be:

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

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

Please be aware that there are size limits in place on DKRZ's tape server. Any tar files **larger than 500 Gb will be truncated**. 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 the 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>

22.1.4 esm_archiving.config module

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

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

By default, `esm_archive` looks in the following locations:

1. Current working directory
2. **Any files in the XDG Standard:** <https://specifications.freedesktop.org/basedir-spec/basedir-spec-latest.html>

If nothing is found, the program reverts to the hard-coded defaults, found in `esm_archiving/esm_archiving/config.py`

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

Generating a configuration

You can use the command line switches `--write_local_config` and `--write_config` to generate configuration files either in the current working directory, or in the global directory for your user account defined by the XDG standard (typically `~/.config/esm_archiving`):

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

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

`esm_archiving.config.load_config()`

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

Returns A representation of the configuration used for archiving.

Return type dict

`esm_archiving.config.write_config_yaml(path=None)`

22.1.5 esm_archiving.esm_archiving module

This is the esm_archiving module.

exception esm_archiving.esm_archiving.DatestampLocationError

Bases: Exception

esm_archiving.esm_archiving.archive_mistral(*tfile*, *rtfile=None*)

Puts the *tfile* to the tape archive using *tape_command*

Parameters

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

Return type None

esm_archiving.esm_archiving.check_tar_lists(*tar_lists*)

esm_archiving.esm_archiving.delete_original_data(*tfile*, *force=False*)

Erases data which is found in the tar file.

Parameters

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

Return type None

esm_archiving.esm_archiving.determine_datestamp_location(*files*)

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

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

Returns A slice object giving the location of the datestamp

Return type slice

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

esm_archiving.esm_archiving.determine_potential_datestamp_locations(*filepattern*)

For a filepattern, gives back index of potential date locations

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

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

Return type list

esm_archiving.esm_archiving.find_indices_of(*char*, *in_string*)

Finds indices of a specific character in a string

Parameters

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

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

```
esm_archiving.esm_archiving.get_files_for_date_range(filepattern, start_date, stop_date, frequency,  
                                                    date_format='%Y%m%d')
```

Creates a list of files for specified start/stop dates

Parameters

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

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

Return type list

Example

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

```
esm_archiving.esm_archiving.get_list_from_filepattern(filepattern)
```

```
esm_archiving.esm_archiving.group_files(top, filetype)
```

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

Parameters

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

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

Return type dict

`esm_archiving.esm_archiving.group_indexes(index_list)`

Splits indexes into tuples of monotonically ascending values.

Parameters **list** – The list to split up

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

Return type list

Example

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

`esm_archiving.esm_archiving.log_tarfile_contents(tfile)`

Generates a log of the tarball contents

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

Return type None

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

`esm_archiving.esm_archiving.pack_tarfile(flist, wdir, outname)`

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

Parameters

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

Returns The output file name

Return type str

`esm_archiving.esm_archiving.purify_expid_in(model_files, expid, restore=False)`

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

Parameters

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

Returns Dictionary containing keys for each model, values for file patterns

Return type dict

`esm_archiving.esm_archiving.query_yes_no(question, default='yes')`

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

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

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

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

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

Parameters

- **question** (*str*) – The question you’d like to ask the user
- **default** (*str*) – The presumed answer for question. Defaults to “yes”.

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

Return type bool

`esm_archiving.esm_archiving.run_command(command)`

Runs command and directly prints output to screen.

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

Returns **rc** – The return code of the subprocess.

Return type int

`esm_archiving.esm_archiving.sort_files_to_tarlists(model_files, start_date, end_date, config)`

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

`esm_archiving.esm_archiving.stamp_filepattern(filepattern, force_return=False)`

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

Parameters

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

Returns New filepattern, with >>>DATE<<<

Return type str

`esm_archiving.esm_archiving.stamp_files(model_files)`

Given a standard 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.

22.2 esm_calendar package

Top-level package for ESM Calendar.

22.2.1 Submodules

22.2.2 esm_calendar.esm_calendar module

Module Docstring,...?

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

Bases: object

Class to contain various types of calendars.

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

Supported calendar types: 0

no leap years

1 proleptic gregorian calendar (default)

n equal months of n days

timeunits

A list of accepted time units.

Type list of str

monthnames

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

Type list of str

isleapyear(*year*)

Returns a boolean testing if the given year is a leapyear

day_in_year(*year*)

Returns the total number of days in a given year

day_in_month(*year, month*)

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

day_in_month(*year, month*)

Finds the number of days in a given month

Parameters

- **year** (*int*) – The year to check
- **month** (*int or str*) – The month number or short name.

Returns The number of days in this month, considering leapyears if needed.**Return type** int**Raises** **TypeError** – Raised when you give an incorrect type for month**day_in_year**(*year*)

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

Parameters **year** (*int*) – The year to check**Returns** The total number of days for this specific calendar type**Return type** int**isleapyear**(*year*)

Checks if a year is a leapyear

Parameters **year** (*int*) – The year to check**Returns** True if the given year is a leapyear**Return type** bool**monthnames** = ['Jan', 'Feb', 'Mar', 'Apr', 'May', 'Jun', 'Jul', 'Aug', 'Sep', 'Oct', 'Nov', 'Dec']**timeunits** = ['years', 'months', 'days', 'hours', 'minutes', 'seconds']**class** **esm_calendar.esm_calendar.Date**(*indate, calendar=esm_calendar(calendar_type=1)*)

Bases: object

A class to contain dates, also compatible 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)

Beautifully returns a Date object as a string.

Parameters

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

Note:

How to use the ``form`` argument The following forms are accepted: + SELF: uses the format which was given when constructing the date + 0: A Date formatted as YYYY

In [5]: test.format(form=1) Out[5]: '1850-01-01_00:00:00'

In [6]: test.format(form=2) Out[6]: '1850-01-01T00:00:00'

In [7]: test.format(form=3) Out[7]: '1850-01-01 00:00:00'

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

classmethod from_list(*_list*)

Creates a new Date from a list

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

Returns *date* – A new date of year month day, hour minute, second

Return type *Date`*

classmethod fromlist(*_list*)

Creates a new Date from a list

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

Returns *date* – A new date of year month day, hour minute, second

Return type *Date`*

makesense(*ndate*)

Puts overflowed time back into the correct unit.

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

output(*form*='SELF')**property sday****property sday****property shour****property sminute****property smonth****property ssecond****sub_date(*other*)****sub_tuple(*to_sub*)**

Adds another date to from one.

Parameters *to_sub* (*Date`*) – The other date to sub from this one.

Returns *new_date* – A new date object with the subtracted dates

Return type *Date`*

property syear

time_between(*date*, *outformat*='seconds')

Computes the time between two dates

Parameters *date* (*date`*) – The date to compare against.

Return type

??

class `esm_calendar.esm_calendar.Dateformat`(*form=1*, *printhours=True*, *printminutes=True*,
printseconds=True)

Bases: object

datesep = [' ', '-', '-', '-', ' ', ' ', ' ', '-', ' ', ' ', ' ', '/']

dtsep = ['_', '-', 'T', ' ', ' ', ' ', '-', '-', ' ', '-', ' ']

timesep = [' ', ':', ':', ':', ' ', ':', ':', ' ', ' ', ' ', ':']

`esm_calendar.esm_calendar.date_range`(*start_date*, *stop_date*, *frequency*)

`esm_calendar.esm_calendar.find_remaining_hours`(*seconds*)

Finds the remaining full minutes of a given number of seconds

Parameters *seconds* (*int*) – The number of seconds to allocate

Returns The leftover seconds once new minutes have been filled.

Return type int

`esm_calendar.esm_calendar.find_remaining_minutes`(*seconds*)

Finds the remaining full minutes of a given number of seconds

Parameters *seconds* (*int*) – The number of seconds to allocate

Returns The leftover seconds once new minutes have been filled.

Return type int

22.3 esm_cleanup package

Cleanup tool for ESM-Tools simulations

22.3.1 Submodules

22.3.2 esm_cleanup.cli module

`esm_cleanup.cli.evaluate_arguments`()

The arg parser for interactive use

`esm_cleanup.cli.main`()

`esm_cleanup.cli.main_loop`(*folder*)

22.3.3 `esm_cleanup.esm_cleanup` module

```
esm_cleanup.esm_cleanup.add_size_information(toplevel, item)
esm_cleanup.esm_cleanup.ask_for_action(folder)
esm_cleanup.esm_cleanup.assert_question(question)
esm_cleanup.esm_cleanup.check_if_folder_exists(folder)
esm_cleanup.esm_cleanup.dir_size(somepath)
esm_cleanup.esm_cleanup.file_size(somepath)
esm_cleanup.esm_cleanup.format_size(total_size)
esm_cleanup.esm_cleanup.inspect_size(thisfile)
esm_cleanup.esm_cleanup.is_experiment_folder(checkpath)
esm_cleanup.esm_cleanup.pick_experiment_folder(folder)
esm_cleanup.esm_cleanup.pick_subfolder(folder)
esm_cleanup.esm_cleanup.print_disclaimer()
esm_cleanup.esm_cleanup.print_folder_content(checkpath, saved_space)
esm_cleanup.esm_cleanup.read_in_yaml_file(filename)
esm_cleanup.esm_cleanup.remove_post_subfolders(folder, saved_space)
esm_cleanup.esm_cleanup.remove_run_subfolders(folder, saved_space)
esm_cleanup.esm_cleanup.remove_size_information(name_with_file)
esm_cleanup.esm_cleanup.remove_some_files(folder, saved_space)
esm_cleanup.esm_cleanup.remove_subfolder(folder, saved_space)
```

22.4 `esm_database` package

Top-level package for ESM Database.

22.4.1 Submodules

22.4.2 `esm_database.cli` module

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

```
esm_database.cli.main()

esm_database.cli.parse_shargs()
    The arg parser for interactive use
```

22.4.3 esm_database.esm_database module

```
class esm_database.esm_database.DisplayDatabase(tablename=None)
    Bases: object
    ask_column()
    ask_dataset()
    decision_maker()
    edit_dataset()
    output_writer()
    remove_datasets()
    select_stuff()
```

22.4.4 esm_database.getch module

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

22.4.5 esm_database.location_database module

```
class esm_database.location_database.database_location(**kwargs)
    Bases: sqlalchemy.orm.decl_api.Base
    class_in
    id
    location
    table_name
    static topline()

esm_database.location_database.register(table_name, given_location, class_in)
```

22.5 esm_environment package

22.5.1 Submodules

22.5.2 esm_environment.esm_environment module

22.6 esm_master package

Top-level package for ESM Master.

22.6.1 Submodules

22.6.2 `esm_master.cli` module

22.6.3 `esm_master.compile_info` module

22.6.4 `esm_master.database` module

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

22.6.5 `esm_master.database_actions` module

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

22.6.6 `esm_master.esm_master` module

22.6.7 `esm_master.general_stuff` module

22.6.8 `esm_master.software_package` module

```
esm_master.software_package.replace_var(var, tag, value)

class esm_master.software_package.software_package(raw, setup_info, vcs, general, no_infos=False)
    Bases: object
    complete_targets(setup_info)
    fill_in_infos(setup_info, vcs, general)
    get_command_list(setup_info, vcs, general)
    get_comp_type(setup_info)
    get_coupling_changes(setup_info)
    get_repo_info(setup_info, vcs)
    get_subpackages(setup_info, vcs, general)
```

```
get_targets(setup_info, vcs)
output()
```

22.6.9 esm_master.task module

22.7 esm_motd package

22.7.1 Submodules

22.7.2 esm_motd.esm_motd module

22.8 esm_parser package

22.8.1 Submodules

22.8.2 esm_parser.esm_parser module

22.8.3 esm_parser.yaml_to_dict module

exception `esm_parser.yaml_to_dict.EsmConfigFileError(fpath, yaml_error)`

Bases: Exception

Exception for yaml file containing tabs or other syntax issues.

An exception used when `yaml.load()` throws a `yaml.scanner.ScannerError`. This error occurs mainly when there are tabs inside a yaml file or when the syntax is incorrect. If tabs are found, this exception returns a user-friendly message indicating where the tabs are located in the yaml file.

Parameters `fpath` (*str*) – Path to the yaml file

`esm_parser.yaml_to_dict.check_changes_duplicates(yamldict_all, fpath)`

Checks for duplicates and conflicting `_changes` and `add_`:

1. Finds variables containing `_changes` (but excluding `add_`) and checks if they are compatible with the same `_changes` inside the same file. If they are not compatible returns an error where the conflicting variable paths are specified. More than one `_changes` type in a file are allowed but they need to be part of the same `_choose` and not be accessible simultaneously in any situation.
2. Checks if there is any variable containing `add_` in the main sections of a file and labels it as incompatible if the same variable is found inside a `choose_` block. `add_<variable>``s` are compatible as long as they are inside ```choose_` blocks, but if you want to include something as a default, please just do it inside the `<variable>`.

Warning: `add_<variable>``s` are not checked for incompatibility when they are included inside ```choose_` blocks. Merging of these `add_<variable>``s` is done using ```deep_update`, meaning that the merge is arbitrary (i.e. if two `choose_` blocks are modifying the same variable using `add_`, the final value would be decided arbitrarily). It is up to the developer/user to make good use of `add_``s` inside ```choose_` blocks.

Parameters

- **yamldict_all** (*dict*) – Dictionary read from the yaml file
- **fpath** (*str*) – Path to the yaml file

`esm_parser.yaml_to_dict.check_duplicates(src)`

Checks that there are no duplicates in a yaml file, and if there are returns an error stating which key is repeated and in which file the duplication occurs.

Parameters **src** (*object*) – Source file object

Raises **ConstructorError** – If duplicated keys are found, returns an error

`esm_parser.yaml_to_dict.check_for_empty_components(yaml_load, fpath)`

`esm_parser.yaml_to_dict.create_env_loader(tag='!ENV', loader=<class 'yaml.loader.SafeLoader'>)`

`esm_parser.yaml_to_dict.find_last_choose(var_path)`

Locates the last `choose_` on a string containing the path to a variable separated by “;”, and returns the path to the `choose_` (also separated by “;”) and the case that follows the `choose_`.

Parameters **var_path** (*str*) – String containing the path to the last `choose_` separated by “;”.

Returns

- **path2choose** (*str*) – Path to the last `choose_`.
- **case** (*str*) – Case after the `choose_`.

`esm_parser.yaml_to_dict.yaml_file_to_dict(filepath)`

Given a yaml file, returns a corresponding dictionary.

If you do not give an extension, tries again after appending one. It raises an `EsmConfigFileError` exception if yaml files contain tabs.

Parameters **filepath** (*str*) – Where to get the YAML file from

Returns A dictionary representation of the yaml file.

Return type dict

Raises

- **EsmConfigFileError** – Raised when YAML file contains tabs or other syntax issues.
- **FileNotFoundError** – Raised when the YAML file cannot be found and all extensions have been tried.

22.9 esm_plugin_manager package

22.9.1 Submodules

22.9.2 esm_plugin_manager.cli module

22.9.3 esm_plugin_manager.esm_plugin_manager module

22.10 esm_profile package

Top-level package for ESM Profile.

22.10.1 Submodules

22.10.2 `esm_profile.esm_profile` module

`esm_profile.esm_profile.timing(f)`

22.11 esm_runscripts package

22.11.1 Submodules

22.11.2 esm_runscripts.assembler module

22.11.3 esm_runscripts.batch_system module

22.11.4 esm_runscripts.chunky_parts module

22.11.5 esm_runscripts.cli module

22.11.6 esm_runscripts.compute module

22.11.7 esm_runscripts.config_initialization module

22.11.8 esm_runscripts.coupler module

22.11.9 esm_runscripts.database module

22.11.10 esm_runscripts.database_actions module

22.11.11 esm_runscripts.dataprocess module

22.11.12 esm_runscripts.event_handlers module

22.11.13 esm_runscripts.filelists module

22.11.14 esm_runscripts.helpers module

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22.11.26 esm_runscripts.prepcompute module

module, please refer to the handbook for user documentation as well as API documentation for the various sub-modules of the project.

Accessing Configuration

To access a particular configuration, you can use:

```
>>> from esm_tools import read_config_file
>>> ollie_config = read_config_file("machines/ollie")
```

Important note here is that the configuration file **has not yet been parsed**, so it's just the dictionary representation of the YAML.

`esm_tools.EDITABLE_INSTALL = False`

Shows if the installation is installed in editable mode or not.

Type bool

`esm_tools.caller_wrapper(func)`

`esm_tools.copy_config_folder(dest_path)`

`esm_tools.copy_namelist_folder(dest_path)`

`esm_tools.copy_runscript_folder(dest_path)`

`esm_tools.get_config_as_str(config)`

`esm_tools.get_config_filepath(config="")`

`esm_tools.get_namelist_filepath(namelist="")`

`esm_tools.get_runscript_filepath(runscript="")`

`esm_tools.list_config_dir(dirpath)`

`esm_tools.read_config_file(config)`

Reads a configuration file, which should be separated by “/”. For example, “machines/ollie” will retrieve the (unparsed) configuration of the Ollie supercomputer.

Parameters `config` (*str*) – Configuration to get, e.g. machines/ollie.yaml, or echam/echam. You may omit the “.yaml” ending if you want, it will be appended automatically if not already there.

Returns A dictionary representation of the config.

Return type dict

`esm_tools.read_namelist_file(nml)`

Reads a namelist file from a path, separated by “/”. Similar to `read_config_file`

Parameters `nml` (*str*) – The namelist to load

Returns A string of the namelist file

Return type str

22.13.2 Submodules

22.13.3 `esm_tools.cli` module

22.14 `esm_utilities` package

Top-level package for ESM Utilities.

22.14.1 Submodules

22.14.2 `esm_utilities.cli` module

Console script for `esm_utilities`.

22.14.3 `esm_utilities.esm_utilities` module

Main module.

22.14.4 `esm_utilities.utils` module

`esm_utilities.utils.check_valid_version(versionrange, version="")`

Returns True if the version provided matches the condition of `versionrange`.

Parameters

- **version** (*str*) – String specifying the version number with the format `X.Y.Z`.
- **versionrange** (*str*) – Condition for the version range, expressed as a comparison operator followed by a version number in the format `X.Y.Z`.

Returns `True`, `False` – True if the condition is met, False if not.

Return type `bool`

`esm_utilities.utils.logfile_stats(logfile_to_read)`

CONTRIBUTING

Contributions are welcome, and they are greatly appreciated! Every little bit helps, and credit will always be given. You can contribute in many ways:

23.1 Types of Contributions

23.1.1 Report Bugs

Report bugs at https://github.com/esm-tools/esm_tools/issues.

If you are reporting a bug, please include:

- Your operating system name and version.
- Any details about your local setup that might be helpful in troubleshooting.
- Detailed steps to reproduce the bug.

23.1.2 Fix Bugs

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

23.1.3 Implement Features

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

23.1.4 Write Documentation

ESM Tools could always use more documentation, whether as part of the official ESM Tools docs, in docstrings, or even on the web in blog posts, articles, and such.

23.1.5 Submit Feedback

The best way to send feedback is to file an issue at https://github.com/esm-tools/esm_tools/issues.

If you are proposing a feature:

- Explain in detail how it would work.
- Keep the scope as narrow as possible, to make it easier to implement.
- Remember that this is a volunteer-driven project, and that contributions are welcome :)

23.2 Get Started!

Ready to contribute? Here's how to set up *esm-tools* packages for local development (see *Python Packages* for a list of available packages). Note that the procedure of contributing to the *esm_tools* package (see *Contribution to esm_tools Package*) is different from the one to contribute to the other packages (*Contribution to Other Packages*).

23.2.1 Contribution to esm_tools Package

1. Fork the *esm_tools* repo on GitHub.
2. Clone your fork locally:

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

(or whatever subproject you want to contribute to).

3. By default, `git clone` will give you the release branch of the project. You might want to consider checking out the development branch, which might not always be as stable, but usually more up-to-date than the release branch:

```
$ git checkout develop
```

4. Create a branch for local development:

```
$ git checkout -b name-of-your-bugfix-or-feature
```

Now you can make your changes locally.

5. When you're done making changes, check that your changes pass `flake8`:

```
$ flake8 esm_tools
```

6. Commit your changes and push your branch to GitHub:

```
$ git add .  
$ git commit -m "Your detailed description of your changes."  
$ git push origin name-of-your-bugfix-or-feature
```

7. Submit a pull request through the GitHub website.

23.2.2 Contribution to Other Packages

1. Follow steps 1-4 in *Contribution to esm_tools Package* for the desired package, cloning your fork locally with:

```
$ git clone https://github.com/esm-tools/<PACKAGE>.git
```

2. Proceed to do a development install of the package in the package's folder:

```
$ cd <package's_folder>
$ pip install -e .
```

3. From now on when binaries are called, they will refer to the source code you are working on, located in your local package's folder. For example, if you are editing the package *esm_master* located in `~/esm_master` and you run `$ esm_master install-fesom-2.0` you'll be using the edited files in `~/esm_master` to install FESOM 2.0.
4. Follow steps 5-7 in *Contribution to esm_tools Package*.

Get Back to the Standard Distribution

Once finished with the contribution, you might want to get back to the standard non-editable mode version of the package in the release branch. To do that please follow these steps:

1. Uninstall all *ESM-Tools* packages (*Uninstall ESM-Tools*). This will not remove the folder where you installed the package in editable mode, just delete the links to that folder.
2. Navigate to the `esm_tools` folder and run the `./install.sh` script.
3. Check that your package is now installed in the folder `~/local/lib/python3.<version>/site-packages/`.

Note: If the package is still shows the path to the editable-mode folder, try running `pip install --use-feature=in-tree-build .` from `esm_tools`.

23.3 Pull Request Guidelines

Before you submit a pull request, check that it meets these guidelines:

1. The pull request should include tests.
2. If the pull request adds functionality, the docs should be updated. Put your new functionality into a function with a docstring, and add the feature to the list in `README.rst`.
3. The pull request should work for Python 3.5, 3.6, 3.7 and 3.8, and for PyPy. Check https://travis-ci.com/dbarbi/esm_tools/pull_requests and make sure that the tests pass for all supported Python versions.

23.4 Deploying

A reminder for the maintainers on how to deploy. Make sure all your changes are committed (including an entry in HISTORY.rst). Then run:

```
$ bumpversion patch # possible: major / minor / patch
$ git push
$ git push --tags
```

24.1 Development Lead

- Dirk Barbi <dirk.barbi@awi.de>
- Paul Gierz <paul.gierz@awi.de>
- Nadine Wieters <nadine.wieters@awi.de>
- Miguel Andrés-Martínez <miguel.andres-martinez@awi.de>
- Deniz Ural <deniz.ural@awi.de>

24.2 Project Management

- Luisa Cristini <luisa.cristini@awi.de>

24.3 Contributors

- Sara Khosravi <sara.khosravi@awi.de>
- Fatemeh Chegini <fatemeh.chegini@mpimet.mpg.de>
- Joakim Kjellsson <jkjellsson@geomar.de>
- Sebastian Wahl <swahl@geomar.de>
- ...

24.4 Beta Testers

- Tido Semmler <tido.semmler@awi.de>
- Christopher Danek <christopher.danek@awi.de>
- ...

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