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A Tool for Earth-System Modellers

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AWI, Climate Dynamics

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ALFRED-WEGENER-INSTITUT
HELMHOLTZ-ZENTRUM FÜR POLAR- UND MEERESFORSCHUNG

ESM Advanced Earth System Modelling Capacity

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RESEARCH FOR GRAND CHALLENGES

VS

BETTER SOFTWARE BETTER RESEARCH

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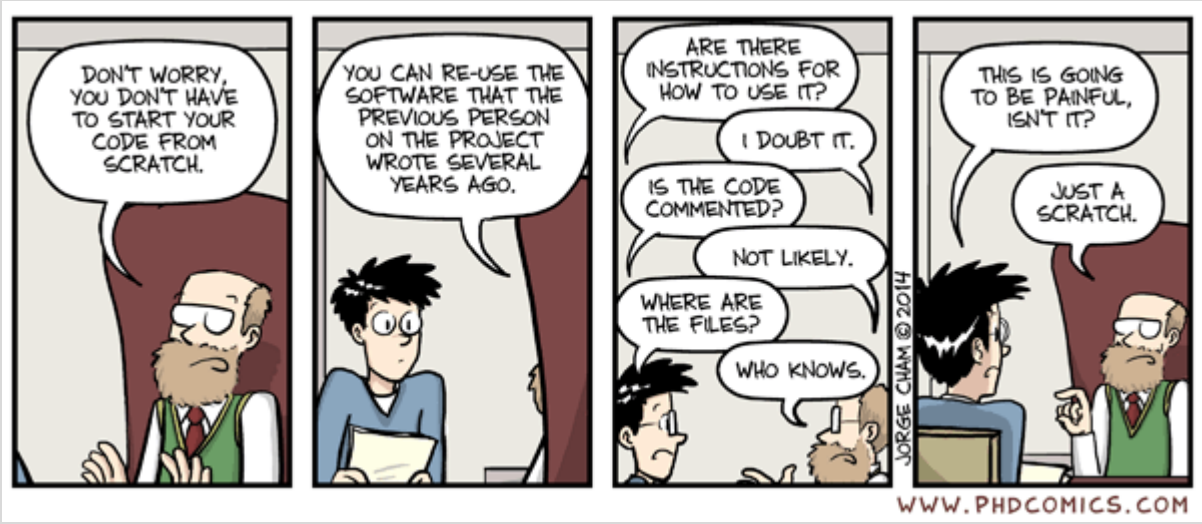


Carole Goble
https://ieeexplore.ieee.org/document/6886129

http://phdcomics.com/comics/archive/phd031214s.gif

OUTLINE

1. What are ESM-Tools? Motivation, General Structure, Comparison, Advantages
2. Components, Supported Systems
3. How we develop ESM-Tools
4. User Support & Information

1 What are ESM-Tools?

- Collection of scripts to download, compile, configure, and run different simulation models for the Earth system
- Standalone Atmosphere, Ocean, Geo-Biochemistry, Hydrology, Sea-Ice and Ice-sheet models as well as coupled systems
- Researchers should focus on science and less on technical details
- Provide a common infrastructure for
  - Models and coupled systems
  - HPC environment
  - Setup and run model experiments
  - Consistent file / directory structure

What ESM-Tools are / do

- A **unified** infrastructure for ESM modelling
- Build the models **without** knowing the details of the HPC system
- Provide **easy** to read/write **YAML** based configuration
- **Run** your simulation as easy as possible
- Generate a **log** documentation
- **Organize** files / directories (eg. input, forcing, output, log, executables, ...)
- **One interface:** standardize the modelling process for all of your models

What ESM-Tools are / do <u>not</u>

- A new model
- A new programming language or DSL
- Change the model code / build process

1 Why do we need ESM-Tools?

- **Target audience: Earth-System Modellers (Atmosphere, Ocean, Land-Surface, Earth, ...) working on HPC machines**
- **ESM are complex softwares that require technical knowledge**
- **Build is difficult:**
  - **Many different models & different build systems & different configurations**
  - **Different HPC and batch systems**
- **Setup & Run are difficult:**
  - **Complex configurations & Couplings**
  - **Requires and generates many files**
  - **Requires a consistent directory structure, CMORization**
  - **Automatization: Repeating the same simulation multiple times**
  - **Reproducibility**

Less technical demand → more time for science & research

Old Workflow

1. Obtain the model source code (usually a tar ball)
2. Build the model
    1. `configure`
    2. `make`
    3. **FAIL:** Read the HPC documentation and repeat (libraries, compilers, modules, ...)
3. Prepare the data folders (input, boundary conditions, output, ...)
4. Setup the namelist for the models
5. Submit your job to the HPC system
6. Resubmit / Iterative coupling
7. Move the data to the storage disk
8. Postprocessing of the results

Repeat the whole process for the next run or write a shell script for automatization.

VS

ESM-Tools workflow

- **Obtain** and **build** the model code (from a repository)

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

- Prepare YAML based **runscript** (samples are available)
- [OPTIONAL] **Check** if your run would run successfully :

```
esm_runscripts my_awicm_runscript.yaml -e my_first_test -c
```

- [Checkt your log] **Submit** your job to the system

```
esm_runscripts my_awicm_runscript.yaml -e my_first_test
```

- **Postprocess** the results (esmviz, in progress)

Notes:

- `esm_master <operation>-<software>-<version>`
- AWICM = ECHAM + FESOM
- `esm_runscripts <runscript.yaml> -e <experiment_ID>`

Old Workflow

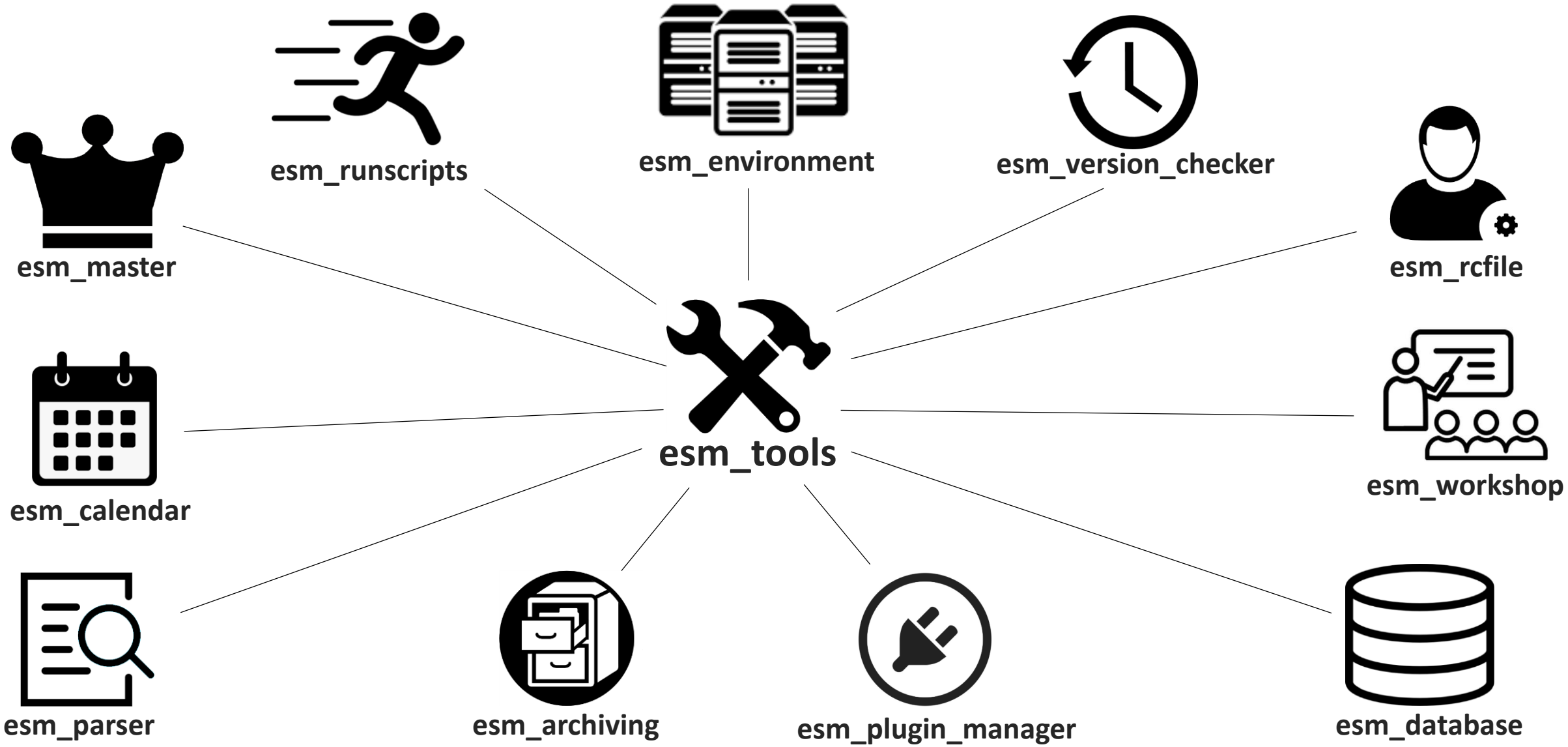
```
echam_prepare_forcing()
{
    # forcing

    if [[ "v$setup_name" = "vecham_standalone" ]]; then

        case $SCENARIO_echam in
            1850 | PI-CTRL*)
                add_to ${echam_INPUT_DIR}/${RES_echam}/${RES_echam}${OCERES_echam}_piControl-LR_sst_1880-2379.nc unit.20
                add_to ${echam_INPUT_DIR}/${RES_echam}/${RES_echam}${OCERES_echam}_piControl-LR_sic_1880-2379.nc unit.96
                ;;
            HIST )
...
...

for ((yr = YR0_echam + -2; yr <= YRN_echam + 2; ++yr)); do
    if [ $yr -le 1849 ] ; then
        eval add_to ${echam_INPUT_DIR}/${RES_echam}/ozone/$ozonefile_1850 ozon$yr

    elif [ $yr -le 2014 ] ; then
        eval add_to ${echam_INPUT_DIR}/${RES_echam}/ozone/$ozonefile_hist ozon$yr

    else
        eval add_to ${echam_INPUT_DIR}/${RES_echam}/ozone/$ozonefile_scen ozon$yr
    fi

    if [ $yr -le 1849 ] ; then
        add_to ${echam_INPUT_DIR}/${RES_echam}/volcano_aerosols/strat_aerosol_ir_${RES_echam}_1850.nc
strat_aerosol_ir_${yr}.nc
        add_to ${echam_INPUT_DIR}/${RES_echam}/volcano_aerosols/strat_aerosol_sw_${RES_echam}_1850.nc
strat_aerosol_sw_${yr}.nc

    elif [ $yr -le 2024 ] ; then
        add_to ${echam_INPUT_DIR}/${RES_echam}/volcano_aerosols/strat_aerosol_ir_${RES_echam}_${yr}.nc
strat_aerosol_ir_${yr}.nc
        add_to ${echam_INPUT_DIR}/${RES_echam}/volcano_aerosols/strat_aerosol_sw_${RES_echam}_${yr}.nc
strat_aerosol_sw_${yr}.nc

    elif [ $yr -gt 2024 ] ; then
        add_to ${echam_INPUT_DIR}/${RES_echam}/volcano_aerosols/strat_aerosol_ir_${RES_echam}_2024.nc
strat_aerosol_ir_${yr}.nc
        add_to ${echam_INPUT_DIR}/${RES_echam}/volcano_aerosols/strat_aerosol_sw_${RES_echam}_2024.nc
strat_aerosol_sw_${yr}.nc

...
```

VS

ESM-Tools workflow

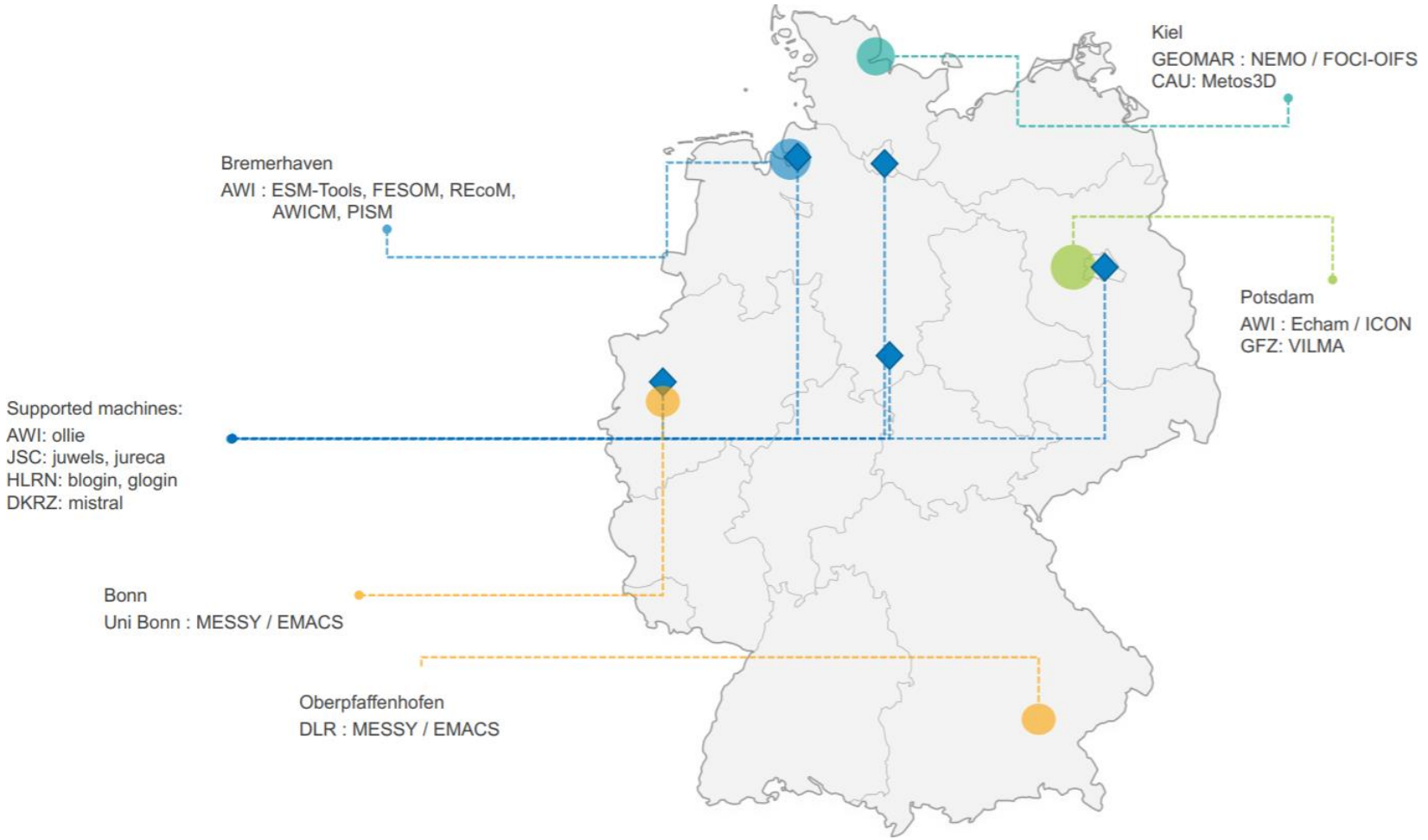
```yaml
general:
    setup_name: "awicm"
    compute_time: "00:15:00"
    initial_date: "2000-01-01"
    final_date:   "2000-02-29"
    base_dir: "/work/ollie/dbarbi/esm_yaml_tests/"
    nmonth: 1
    nyear: 0

awicm:
    version: "CMIP6"
    postprocessing: false
    scenario: "PI-CTRL"
    model_dir: "/work/ollie/dbarbi/modelcodes/awicm-CMIP6/"

fesom:
    pool_dir: "/work/ollie/pool/FESOM/"
    mesh_dir: "/work/ollie/pool/FESOM/meshes_default/core/"
    restart_rate: 1
    restart_unit: "m"
    restart_first: 1
    further_reading:
        - "fesom_output_control.yaml"
```

2 Components of the ESM-Tools



❷ Supported Models & Couplings, Partners

Coupled Systems	Components
FOCI	VILMA
FOCI-OIFS	ICON
FESOM-REcoM	NEMO
AWIESM	REcoM
OIFSCL	AMIP
AWICM	debm
AWICM3	FESOM
OIFSAMIP	scope
AWICMCR	xios
MPIESM	Echam
	YAC
	fesom_mesh_part
	oasis3mct
	rnfmap
	MPIOM
	PISM
	nemobasemodel
	OIFS



2 Summary: Why you should use ESM-Tools?

For Users

- (extended) YAML syntax is easy to read
- Sample runscripts are already available
- Well maintained
- Issues on GitHub (and we will take care of them)
- Updated regularly
- Portable & Tested
- Documentation (sphinx, readthedocs)
- Workshops

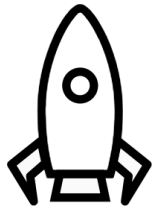
For Developers

- python powered
- Easier to read / write (compared to 

)
- OOP, High level data structures
- Easier to debug (via pdb, ipdb)
- Configuration files are «inherited»
- Hosted on GitHub & robust branching model
- Open-source development is encouraged
- [In progress] CI/CD, DevOps, Automated tests

❸ How we develop ESM-Tools?

Core development team + external developers (total >30 people)



Release

- **Default branch**
- **Latest stable release**
- **Full user support**
- **Update only at next planned release date**
- **Bugfixes will be merged at any time**

Develop branch(es)

- **Branch to collect new features and bugfixes for next release**
- **Testing**
- **Work in progress**
- **Will be merged into release at next planned release date**

Hotfix

- **Urgent bugfixes**

Contributions are encouraged: `fork → clone → branch & push (to your fork) → pull requests`

4 Future Goals & Information

- More users & HPC systems
- More models
- More features (eg. online monitoring & visualization, GUI, CI/CD, ...)
- 

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Preprints

Abstract | Discussion | Metrics

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11 Aug 2020

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ESM-Tools Version 4.0: A modular infrastructure for stand-alone and coupled Earth System Modelling (ESM)

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4 Contact

https://www.esm-tools.net

https://esm-tools.readthedocs.io

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Thank you very much for your attention!