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ESM-Tools

Infrastructure for Earth System Modelling

ESM User Workshop May 2019

Agenda

01

What are the ESM-Tools?

A unified infrastructure for ESM modelling

02

Who benefits?

The Tools are designed to simplify the work of modelers, model developers, software supporters and HPC admins.

03

How are the ESM-Tools developed?

Developed within the ESM project, the Tools have more than 30 authors from 6 institutes. Main development is done at AWI.

04

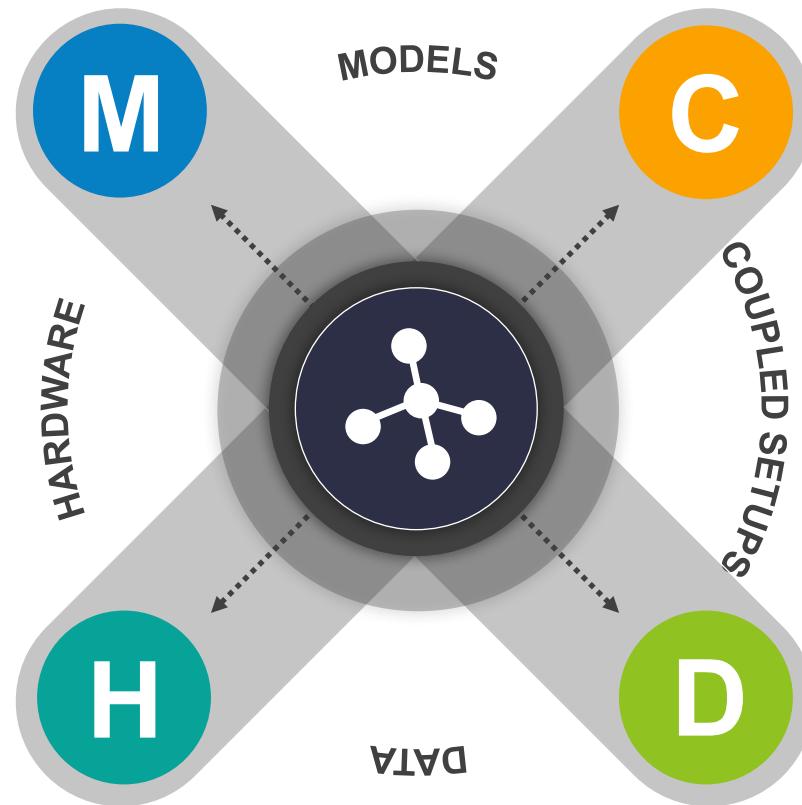
How can I get the ESM-Tools?

ESM-Tools can be obtained for free, it is open source under GPL.

What are the ESM-Tools?

Models

The Tools provide an easy and standardized way to obtain, configure and compile model components. As of May 2019, we support 10 independent components, including 4 ocean, 2 atmosphere, 1 ice sheet, 1 BGC, 1 GIA model and a coupler, all organized under version control.



Hardware

Currently the Tools are running on 6 HPC systems, holding the machine specifications in a central place that can be used by the models during compile and run time, leaving more time for the user to focus on scientific questions.

Coupled Setups

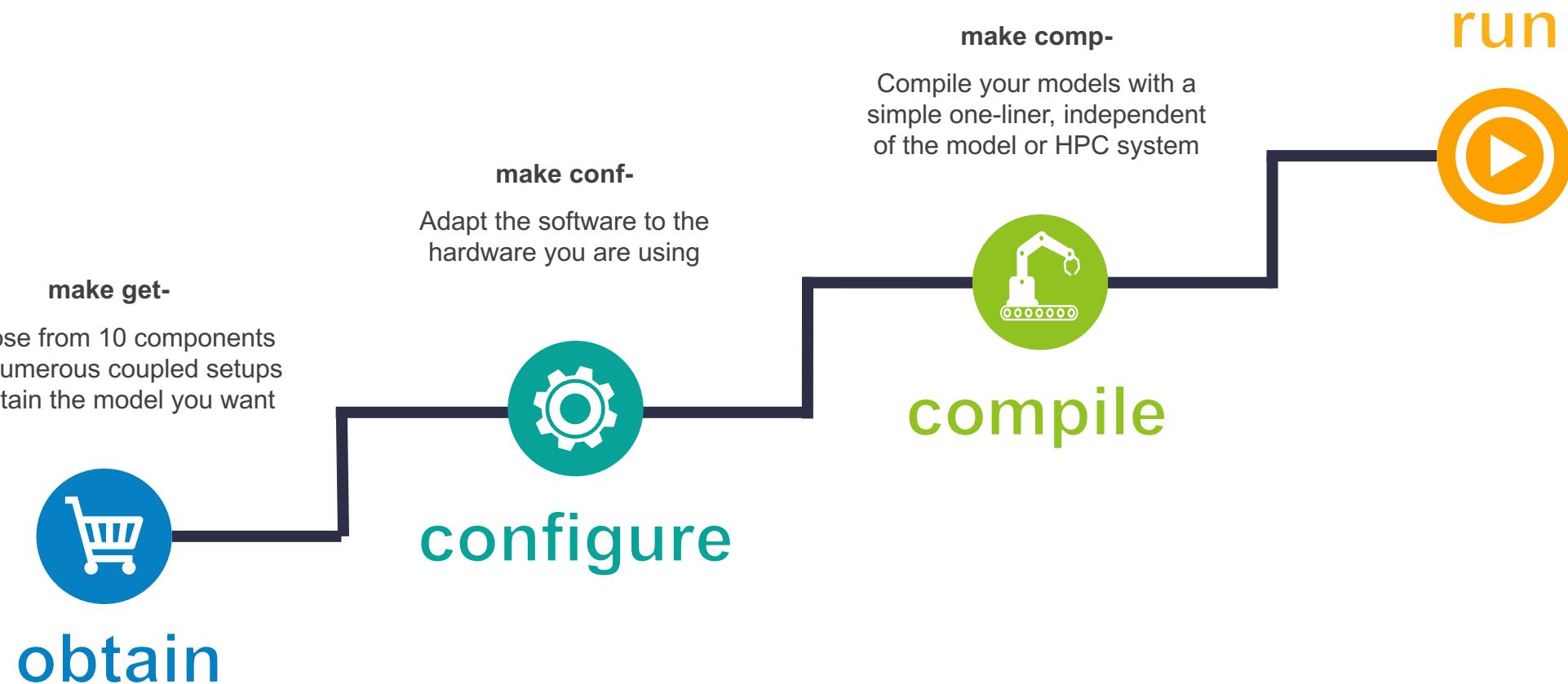
Out of the mentioned models, a variety of coupled systems can be combined. A graphical interface helps choosing the wanted components. Among the supported combinations are MPIESM, AWICM (1 and 2), FESOM-OIFS and FOCI-OIFS.

Data

The life cycle of model data has become increasingly important. The tools try to help – by referring to standardized input data pools, managing model output and restarts, and functionality for tar-balling and archiving data. CMOR support is planned.

Obtaining models

esm-master



Running Simulations

esm-runscripts

Small runscripts

Focus on your simulation, defaults are pre-defined. Typically around 40 lines, similar for all models.



Input / Forcing Data

The Tools organize the data, recognizing standard data pools on the machines.



Runtime Functionality

A lot of nice stuff – restarts, monitoring, iterative coupling,



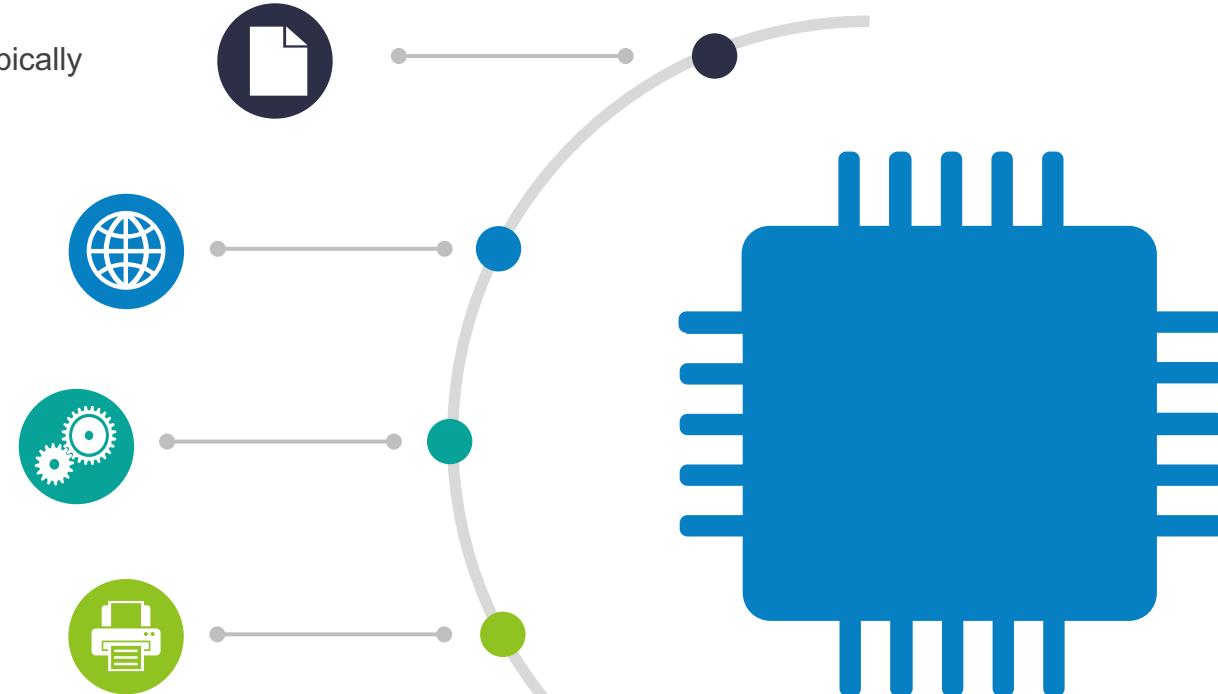
Output Data

Model Output is automatically sorted and postprocessed, even tarred and archived.

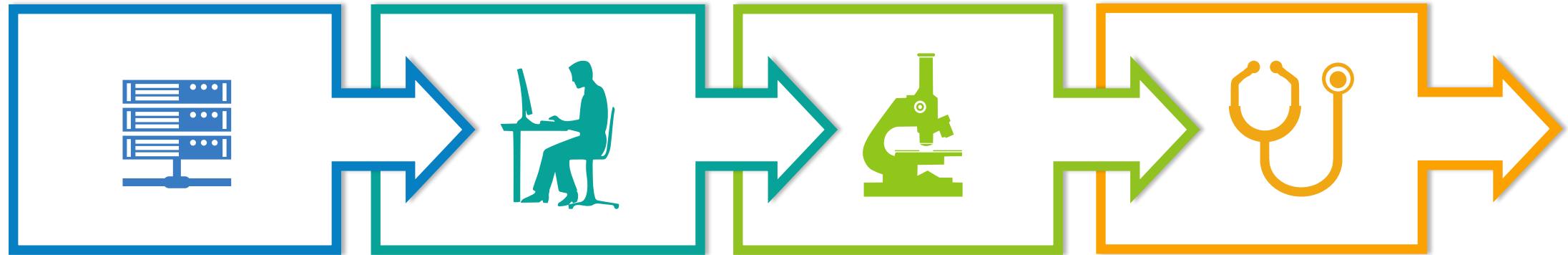


Reproducibility / Documentation

Simulation folders contain (almost) everything, and a ton of log files provide all the information to re-run or continue a simulation.



Who benefits from the Tools?



1st

System Admins

Standardized Compile and Runtime Environments means fewer needed software packages. Deploy optimal machine settings or new modules easily.

3rd

Modellers

Run your simulations in an easy and unified way, independent of the model and hardware. Have lots of functions with a few lines of runscript.

2nd

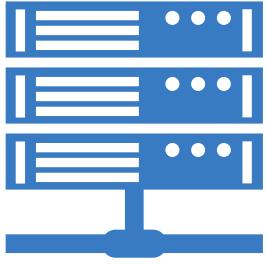
Model developers

Organize your developments, deploy them on different machines. Co-work with other institutes on the same code.

4th

Model supporters

Solve problems once, not over and over again. Deploy bugfixes / new hardware configurations quickly to all users. Same experiment layout also means less context switching.



System Admins

- A group of users all use the same configuration file – solve problems once, and deploy the solution quickly.
- Provide an “optimal” standard configuration to your users.
- Get less requests for additional tools / packages or incompatible combinations.
- Get a reduced '.sad' – runscript only containing the information needed by the batch system. (WIP)

```
#module unload python && module load python3

module load cmake
module load udnutils

module unload intel.compiler intel.mpi && module load intel.compiler intel.mpi
module unload netcdf
module load centoslibs cdo nco netcdf/4.4.0_intel

export PATH=/work/oillie/jhegewal/sw/cmake/bin:$PATH

export FC="mpiifort -mkl" CC=mpiicc CXX=mpiicpc

export ZLIBROOT=/usr

export MPIROOT=${I_MPI_ROOT}/intel64
export MPIFC='mpiifort'
export MPICC='mpiicc'

export NETCDFROOT=${NETCDF_DIR}
export NETCDFFROOT=${NETCDF_DIR}
export NETCDF_Fortran_INCLUDE_DIRECTORIES=${NETCDF_DIR}/include

export HDF5ROOT=/usr//

export LAPACK_LIB='-lmkl_intel_lp64 -lmkl_core -mkl=sequential -lpthread -lm -ldl'

export CC='mpiicc'
export CXX='mpiicpc'
```

Model Developers

```
Available compile options:  
comp-amip  
comp-awicm-CMIP6  
comp-awicm-1.1  
comp-awicm-1.0  
comp-awicm-2.0  
comp-awicm-3.0  
comp-awicm-test  
comp-echam-6.3.04p1  
comp-echam-6.3.02p4  
comp-fesom-1.4  
comp-fesom-1.4-recom  
comp-fesom-1.4-recom-modular  
comp-fesom-2.0  
comp-fesom-2.0-mesh-part  
comp-fesom-2.0-recom-modular  
comp-mpiesm-1.2.01p1  
comp-mpiesm-1.2.01  
comp-mpiesm-1.2.00p4  
comp-nemo-3.6  
comp-oasis3-mct  
comp-oifs-40r1  
comp-oifsamip  
comp-recom-lib  
comp-rnfmap  
comp-xios-2.0_r982
```

Concentrate more on your model, and less on the technical side

The ESM-Tools provide standard configurations for a number of HPC systems. Chances are good that you can compile and run your development on these out of the box.

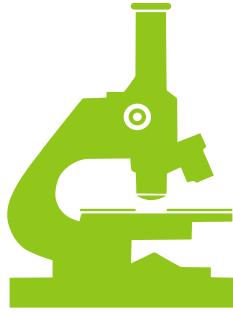
Get your developments to the users

New standard versions of your codes can be distributed with esm-master.

Runscripts with a ton of functions for a new model - without coding

All you need in a runscript is already there. You can just go and use it.





Modellers

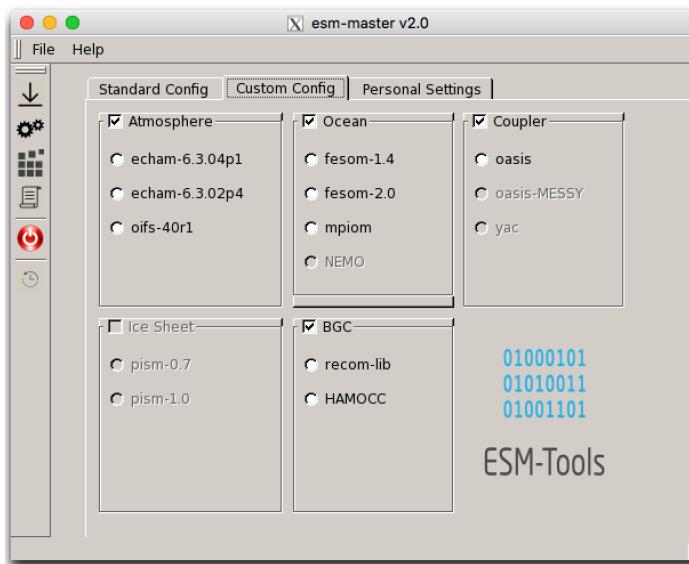
Start running simulations quickly. With a steep learning curve.

New colleague, about to work with an unknown model? Maybe even new to programming, shell scripting, HPC?

Changing to a new model (system), maybe for intercomparison, or exchanging one implementation of a model with a different one?

Changing to a different HPC system?

Getting lost in too many simulations, and needing an automatic way to "document" them?



**Easy access to a
huge variety of
model
components and
coupled setups**

Short (but do-it-all) runscripts, almost independent of the model and hardware you use

```

export FUNCTION_PATH=${WORK}/esm-master/esm-runscripts/functions/all
export FPATH=${FUNCTION_PATH}:$FPATH

machine_name="ollie"
setup_name="fesom_standalone"
#check=1

compute_time="05:00:00"
#####
#Xsrun I know what I am doing

INITIAL_DATE_fesom_standalone=2008-01-01           # Initial exp. date
FINAL_DATE_fesom_standalone=2010-01-01             # Final date of the experiment

RES_fesom=CORE2

MODEL_DIR_fesom_standalone=${WORK}/esm-master/fesom_standalone/
BIN_DIR_fesom=${MODEL_DIR_fesom_standalone}/fesom_cpl/
EXE_fesom=fesom.x

BASE_DIR=${WORK}/esm-experiments/

POOL_DIR_fesom_standalone=/work/ollie/pool/FESOM/

MESH_DIR_fesom=/work/ollie/pool/FESOM/meshes_default/core/

NYEAR_fesom_standalone=1          # Number of years per run

#####

```



Model Support



One environment configuration

If anything goes wrong with the environment, you know where to look.

One runscript

Effectively people can use the same runscript for a variety of models, so no need to work through a new one each time. Plus ESM-Tools support.

Automatic testing

You can know about problems before your users do, and also where it might come from.

Deploy solutions

Once a problem is fixed, the solution can be picked up by all users directly.

ESM-Tools distribution

Supported machines:

AWI: ollie
JSC: juwels, jureca
HLRN: blogin, glogin
DKRZ: mistral

Bonn

Uni Bonn : MESSY / EMACS

Oberpfaffenhofen

DLR : MESSY / EMACS

Bremerhaven

AWI : ESM-Tools, FESOM, REcoM,
AWICM, PISM

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Kiel

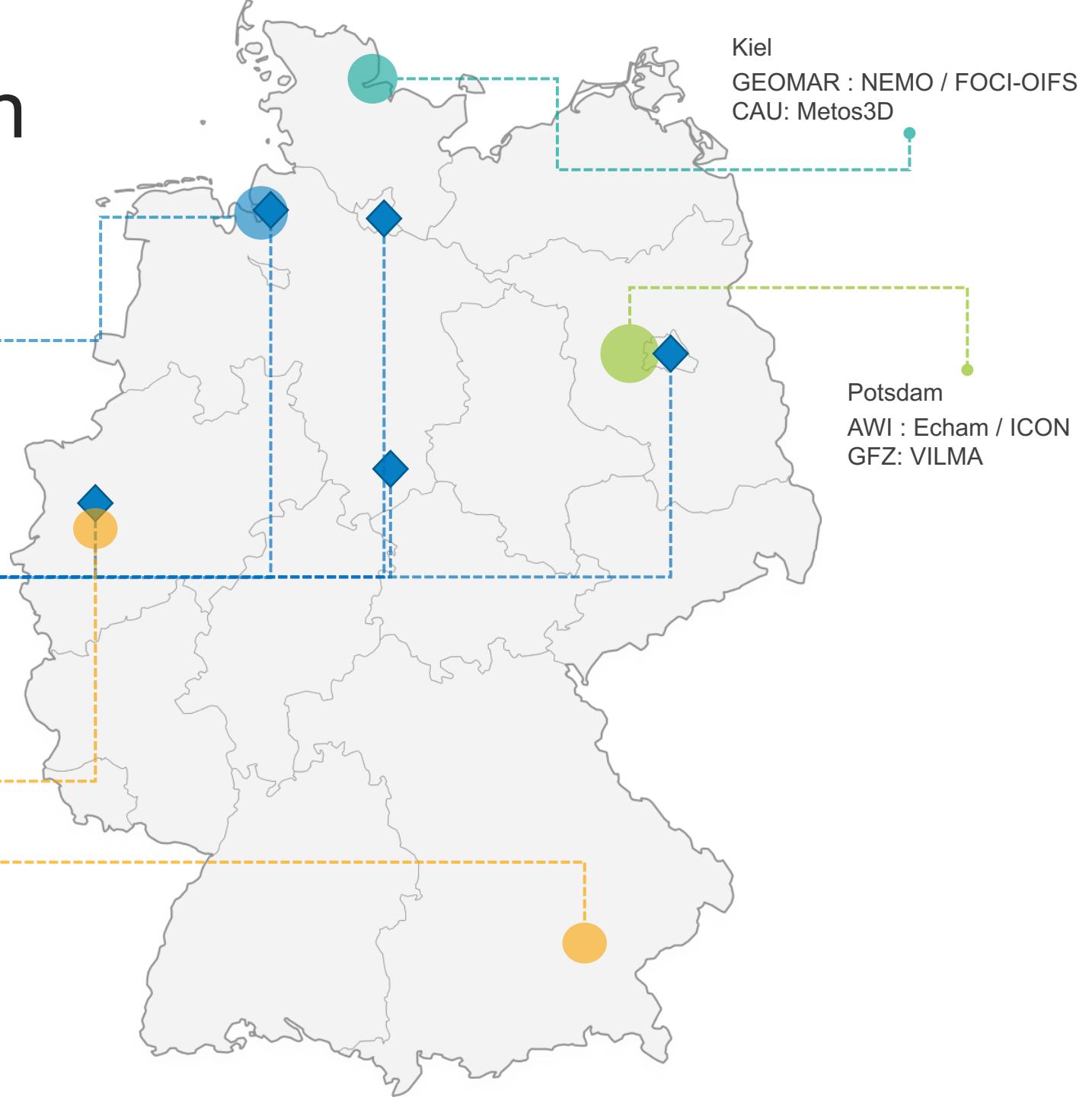
GEOMAR : NEMO / FOCI-OIFS
CAU: Metos3D

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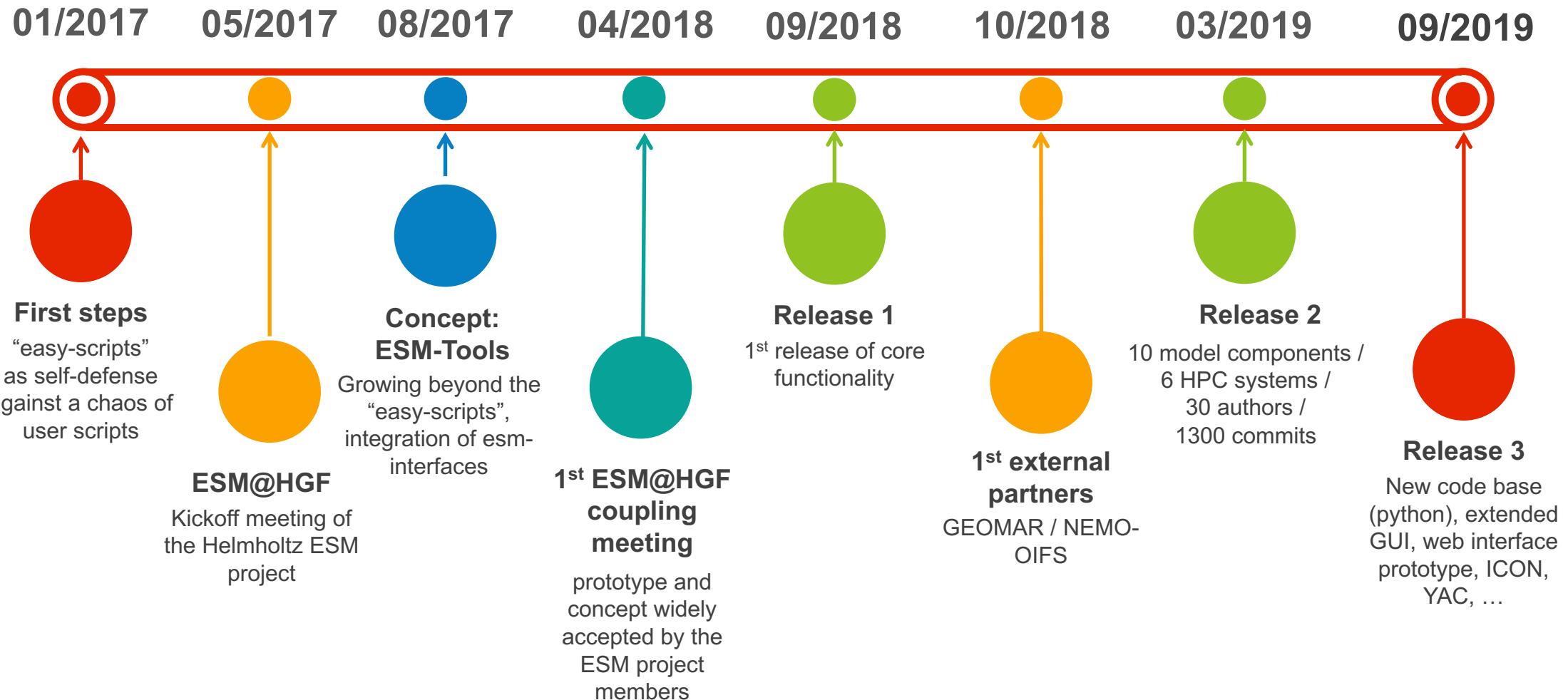
Potsdam

AWI : Echam / ICON
GFZ: VILMA

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Timeline



Development strategy

ESM-Tools TEAM@AWI

Nadine Wieters, Dirk Barbi, Luisa Cristini
(Paul Gierz)
New colleague (position is open for applications) starting in summer '19.



Model Users

Reporting problems using the issue tracking system of gitlab helps us to provide quick solutions.

Model Developers

All component models are available in VCS repositories, most of them in modular_esm. Frequent communication ensures that the versions are up-to-date. Regular tagging.

System Admins and Supporters

Contribute changes in the machine settings and bugfixes back to the Tools to deploy them.

How can I get the ESM-Tools?

[**https://gitlab.dkrz.de/esm-tools**](https://gitlab.dkrz.de/esm-tools)
[**\(https://gitlab.awi.de/esm-tools\)**](https://gitlab.awi.de/esm-tools)



Contact us:

info@esm-tools.net
0471/4831-1561 /
www.esm-tools.net
twitter.com/ToolsESM

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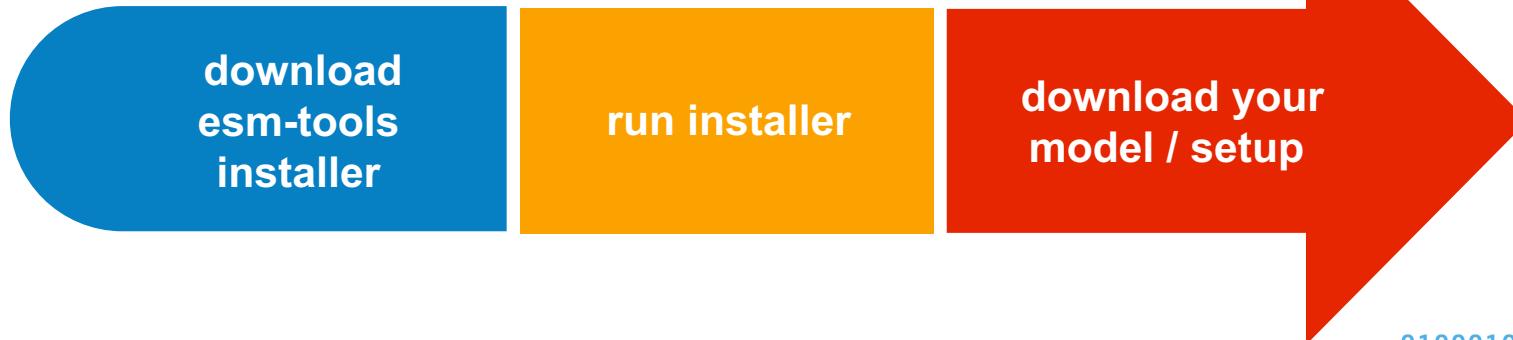
Get the Tools

Getting the esm-tools

Suggested workflow (1)



Suggested workflow (2)



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ESM-Tools

Download esm-master

git clone <https://gitlab.dkrz.de/esm-tools/esm-master.git>
(git clone <https://gitlab.awi.de/esm-tools/esm-master.git>)

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Configure esm-master

In the esm-master folder, type
make

and answer the questions that pop up. The configuration is written to a file called

esm-master.conf

which can be edited by hand. If it is messed up, remove it, or run

make conf-esm-master

Download esm-environment

In the **esm-master** folder, type:

make get-esm-environment

(Same as:

git clone <https://gitlab.dkrz.de/esm-tools/esm-environment.git>)

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ESM-Tools

Download esm-runscripts

In the **esm-master** folder, type:

make get-esm-runscripts

(Same as:

git clone https://gitlab.dkrz.de/esm-tools/esm-runscripts.git

cd esm-runscripts/functions

./set_links

cd ../../

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ESM-Tools

Download esm-usermanual

In the **esm-master** folder, type:

make get-esm-usermanual

(Same as:

git clone https://gitlab.dkrz.de/esm-tools/esm-usermanual.git)

Or:

Download the pdf from www.esm-tools.net

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ESM-Tools

Shortcut 1:

After downloading and configuring esm-master, type:

make get-esm-tools

(Same as:

make get-esm-environment

make get-esm-runscrips

make get-esm-usermanual)

Shortcut 2:

Download and run the esm-tools installer:

```
git clone https://gitlab.dkrz.de/esm-tools/esm-tools.git  
cd esm-tools  
.install.sh
```

In this case, esm-master still needs to be configured!

Three ways to get the Tools

	01	<pre>git clone https://gitlab.dkrz.de/esm-tools.de/esm-master.git cd esm-master; make make get-esm-environment make get-esm-runscripts make get-esm-usermanual</pre>
	02	<pre>git clone https://gitlab.dkrz.de/esm-tools.de/esm-master.git cd esm-master; make make get-esm-tools</pre>
	03	<pre>git clone https://gitlab.dkrz.de/esm-tools.de/esm-tools.git cd esm-tools ../install.sh</pre>

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ESM-Tools

How can I get Information / Documentation?

www.esm-tools.net

<https://gitlab.dkrz.de/esm-tools>



Contact us:

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