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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.

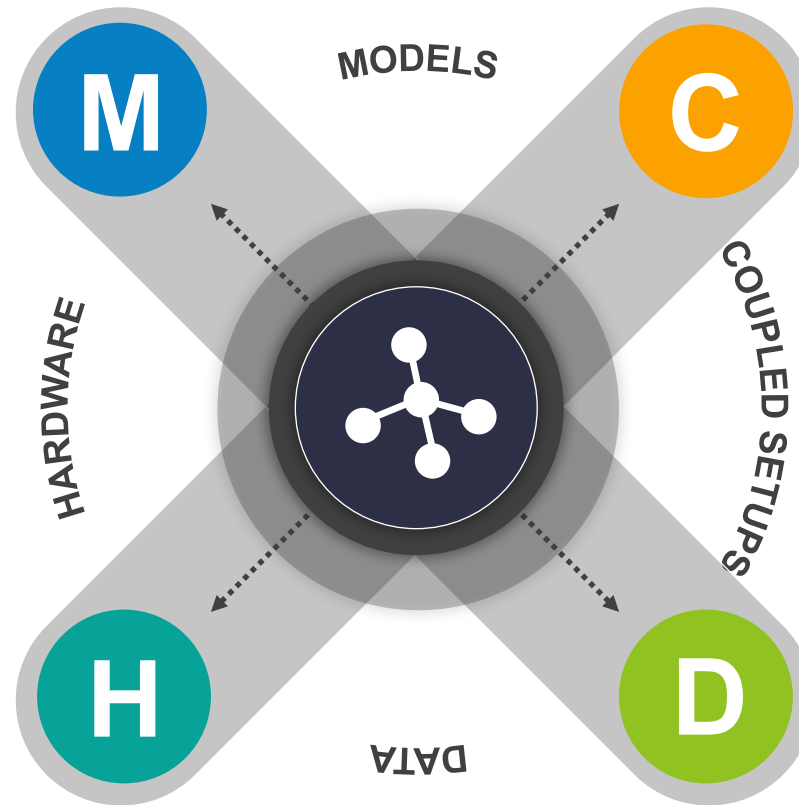
What are the ESM-Tools?

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

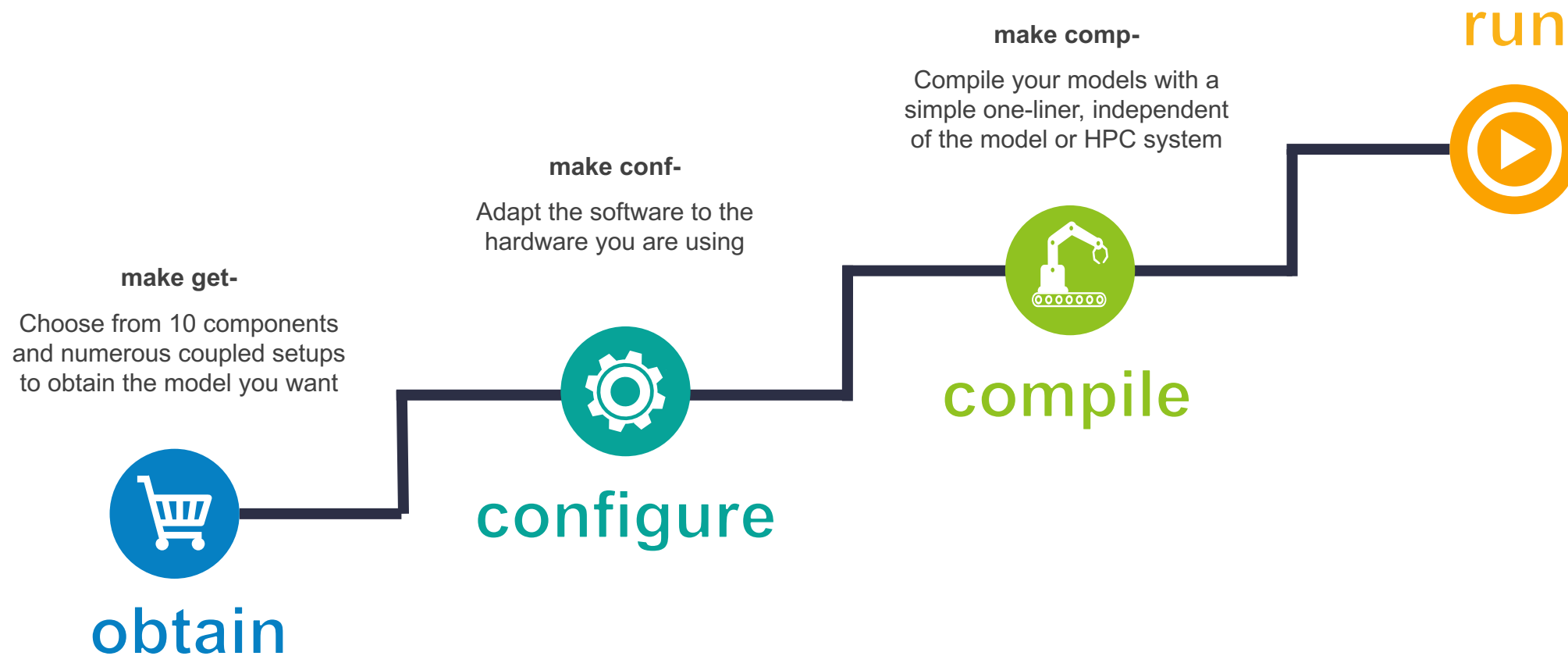
Out of the mentioned models, a variety of coupled systems can be combined. A graphical interface helps choosing the wanted components. Among the supported combinations are MPIESM, AWICM (1 and 2), FESOM-OIFS and FOCI-OIFS.

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-runscrip

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

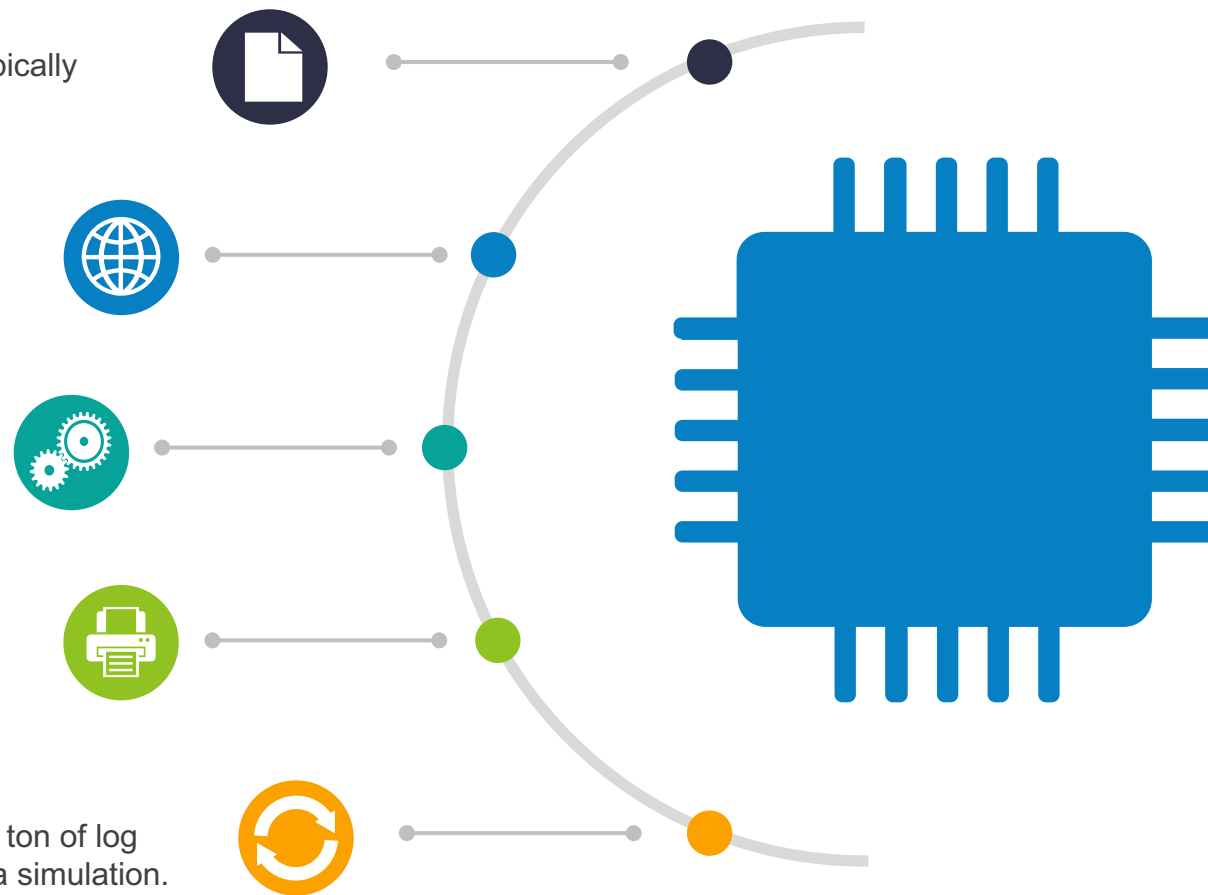
A lot of nice stuff – restarts, monitoring, iterative coupling,

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.

2nd

Model developers

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

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.

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' – runsript only containing the information needed by the batch system. (WIP)

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

module load cmake
module load udunits

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/ollie/jhegewal/sw/cmake/bin:$PATH

export FC="mpiifort -mk1" CC=mpiicc CXX=mpicpc

export ZLIBROOT=/usr

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

export NETCDFROOT=${NETCDF_DIR}
export NETCDFROOT=${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='mpicpc'
```

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

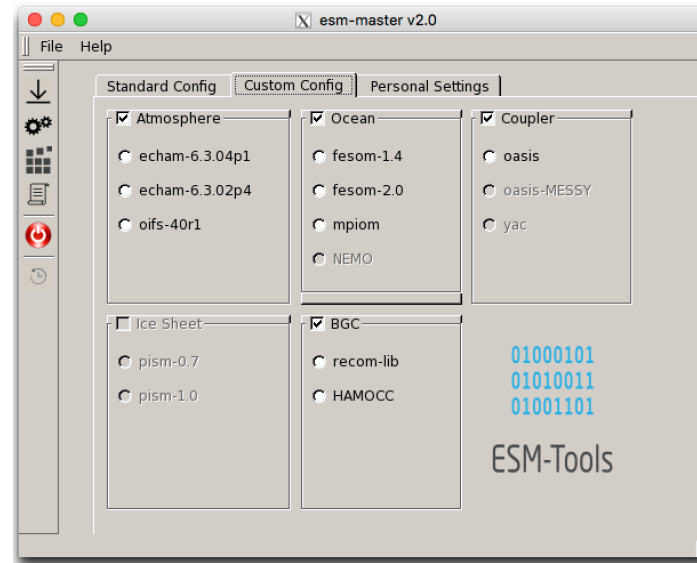
Start running simulations quickly. With a steep learning curve.

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=${WORK}/esm-master/esm-runcscripts/functions/all
export FPATH=${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_cp1/
EXE_fesom=fesom.x

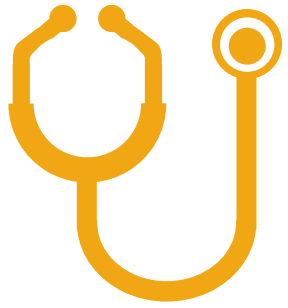
BASE_DIR=${WORK}/esm-experiments/

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

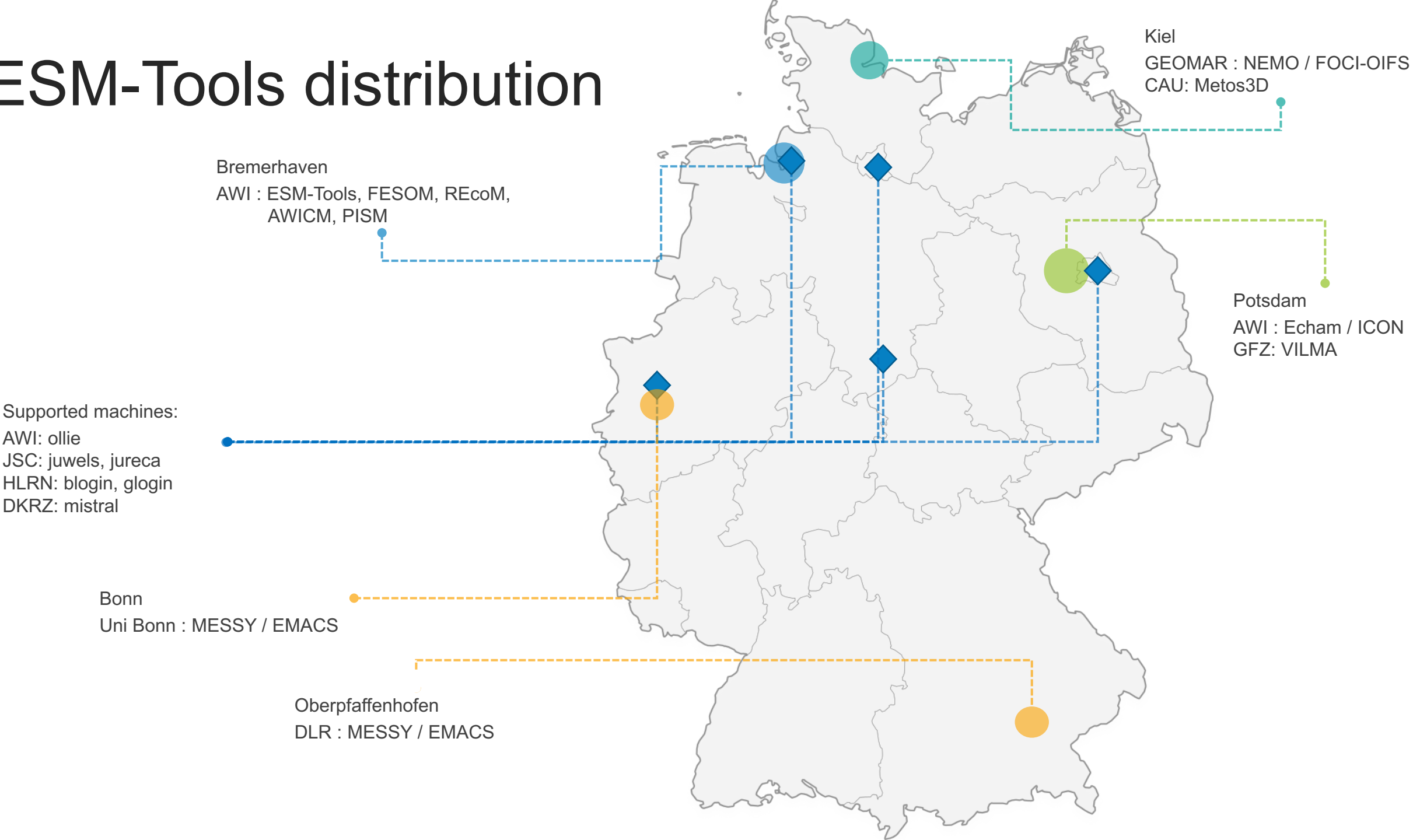
You can know about problems before your users do, and also where it might come from.



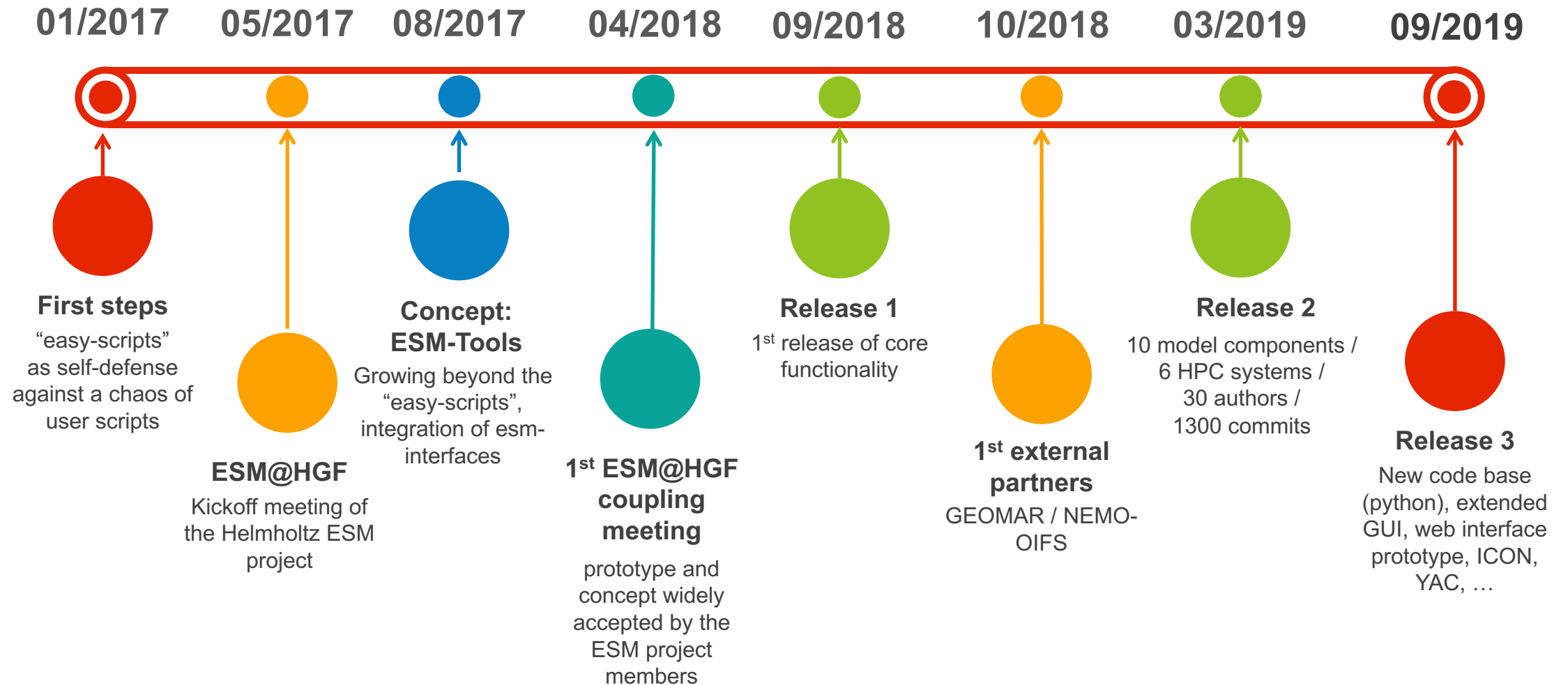
Deploy solutions

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

ESM-Tools distribution



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 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.



Model Users

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

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.awi.de/esm-tools>)



Contact us:

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

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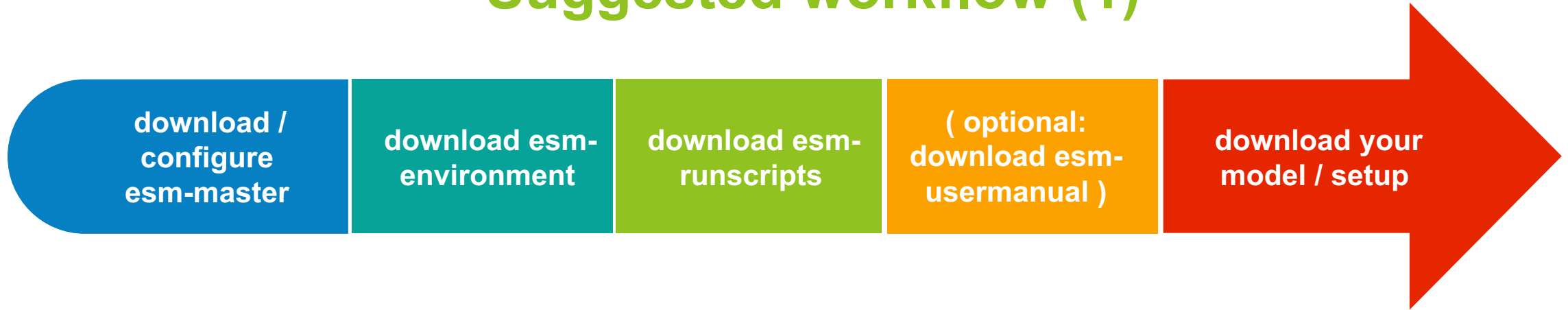
ESM-Tools



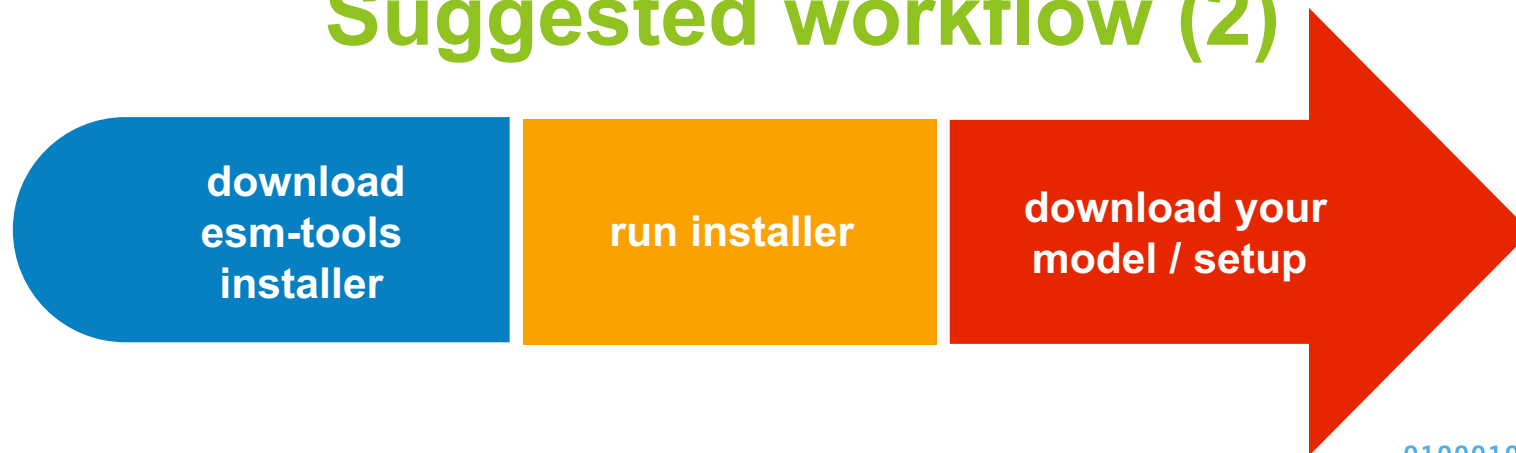
Get the Tools

Getting the esm-tools

Suggested workflow (1)



Suggested workflow (2)



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)
```

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>)

Download esm-runscripsts

In the esm-master folder, type:

```
make get-esm-runscripsts
```

(Same as:

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

```
cd esm-runscripsts/functions
```

```
./set_links
```

```
cd ../../ )
```

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

Shortcut 1:

After downloading and configuring esm-master, type:

make get-esm-tools

(Same as:

make get-esm-environment

make get-esm-runscripts

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-runscreens 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>

How can I get Information / Documentation?

www.esm-tools.net

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



Contact us:

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