Introduction

The **ICON modelling framework** is a joint project between the German Weather Service and the Max Planck Institute for Meteorology for developing a unified next-generation global numerical weather prediction and climate modelling system. The ICON model has been introduced into DWD's operational forecast system in January 2015.

This document provides technical details on how to build the model, as well as the description of basic steps required to run it. More information about ICON is available in the corresponding section of the project's public web page.

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Quick start

The process of building ICON consists of two parts: *configuring* the options and compiler flags, and *building* the source code with those options and flags.

The configuration step is normally done by running the ./configure script with command-line arguments, which, among other things, tell the script where to locate libraries and tools required for building. The list of arguments enabling a successful configuration might be quite long and difficult to compose, therefore, instead of running the generic ./configure script directly, users are recommended to execute a corresponding platform- or machine-specific *configuration wrapper* that sets the required compiler and linker flags as well as the recommended set of configure options. The wrappers can be found in the respective subdirectories of the ./config directory.

For example, if you need to build ICON on Mistral@DKRZ with OpenMP feature enabled using Intel compiler, you can run:

```
$ cd /path/to/icon
```

```
$ ./config/dkrz/mistral.intel --enable-openmp
```

Alternatively, you can create a directory and perform an *out-of-source* build:

\$ mkdir build && cd build

\$ /path/to/icon/config/dkrz/mistral.intel --enable-openmp

This way, you can build ICON in several different configurations, i.e. with different compilers and features, using the same copy of the source code.

NOTE: If there is no configure wrapper script for your platform or machine, refer to section Configuration for information on how to work with the ./configure script directly.

The building step is done by running **make** command with an optional argument specifying the number of jobs to run simultaneously. For example,

```
$ make -j8
```

The result of the building — the executable file of ICON — is saved to the ./bin subdirectory of the build directory.

NOTE: For more information on the building step, refer to section Building.

In case of an *in-source* build the *runscripts* can be generated by running:

```
$ ./make_runscripts
```

To run the model, switch to the **run** subdirectory of the build directory and submit the runscript of your choice, for example:

```
$ cd ./run && sbatch ./exp.atm_amip.run
```

NOTE: For more information on the runscript generation and running the model, refer to section Running.

Configuration

The configuration step is done by calling the configure script with arguments specifying the location of libraries and tools required for building, as well as options enabling or disabling particular features of the model. For example:

\$./configure CC=mpicc FC=mpif90 LIBS='-lnetcdff -lnetcdf -llapack -lblas' --disable-ocean --disable-co

NOTE: Users are recommended to get familiar with the full list of configuration options and their default values by running:

\$./configure --help

The configure script of ICON is implemented using Autoconf and its interface should be familiar to those who have experience with Autotools-based building systems.

The following sections provide information on some features and implementation details of the configuration process.

ICON dependencies

Fig. 1 shows a partial dependency graph of the model. A dependency can be either *mandatory* (i.e. the library is required regardless of the specified configure options) or *optional* (i.e. the library is required only if particular features of the model are enabled), and some of the dependencies are provided together with the source code of ICON as git submodules and referred to as *bundled* later in the text.

NOTE: The term *bundled library* does not apply to all packages listed in .gitmodules: some of them, e.g. JSBACH and ART, have circular dependencies with the ICON source code and therefore are treated as part of it.

ICON dependency graph

Fig. 1. ICON dependency graph

The list of libraries (packages) required for successful configuration and building depends on the selected options. To make the configuration process more transparent, the configure script does not accept paths to the installation directories of the packages, which would be used to extend the corresponding compiler flags. Instead, paths to the header and library files of the packages must be provided by the user as compiler and linker flags, i.e. in the FCFLAGS, CPPFLAGS, and LDFLAGS arguments. Moreover, the script does not try to guess the list of libraries to be used, therefore all the -1 linker flags need to be specified in the LIBS argument in the correct order. The recommended (topologically sorted) order for the LIBS argument is presented in Table 1, and the recommended order for the FCFLAGS, CPPFLAGS, CPPFLAGS, LDFLAGS is the reversed one.

Linking order	Package	Dependency condition1	Required flags1
1	SELF	with-external-self	FCFLAGS='-I/path/to/libself/include LDFLAGS='-L/path/to/libself/lib' LIBS='-lself'
2	ICON-TIXI (a modified version of TIXI)	enable-art with-external-tixi	FCFLAGS='-I/path/to/tixi/include' LDFLAGS='-L/path/to/tixi/lib' LIBS='-licon_tixi'
3	YAC	enable-coupling with-external-yac	FCFLAGS='-I/path/to/yac/include' LDFLAGS='-L/path/to/yac/lib' LIBS='-lyac'
4	XML2	enable-coupling2 or enable-art2	CPPFLAGS='-I/path/to/libxml2/includ LDFLAGS='-L/path/to/libxml2/lib' LIBS='-lxml2'
5	LAPACK (or analogue)	mandatory	LDFLAGS='-L/path/to/lapack/lib' LIBS='-llapack' (depends on the implementation)
6	BLAS (or analogue)	mandatory	LDFLAGS='-L/path/to/blas/lib' LIBS='-lblas' (depends on the implementation)
7	MTIME	with-external-mtime3	FCFLAGS='-I/path/to/mtime/include' CPPFLAGS='-I/path/to/mtime/include LDFLAGS='-L/path/to/mtime/lib' LIBS='-Imtime'
8	SERIALBOX2	enable-serialization	FCFLAGS='-I/path/to/serialbox2/inc LDFLAGS='-L/path/to/serialbox2/lib LIBS='-lSerialboxFortranShared'
9	CDI or CDI-PIO	with-external-cdi4	<pre>FCFLAGS='-I/path/to/libcdi/include LDFLAGS='-L/path/to/libcdi/lib' LIBS='-lcdi_f2003 -lcdi' (or LIBS='-lcdi_f2003 -lcdipio -lcdi')</pre>

Table 1. Topologically sorted list of the ICON dependency graph

Linking order	Package	Dependency condition1	Required flags1
10	ECCODES or GRIB-API	enable-grib2 without-external-cdi	CPPFLAGS='-I/path/to/eccodes/includ 5LDFLAGS='-L/path/to/eccodes/lib' LIBS='-leccodes' (or LIBS='-lgrib_api')
11	YAXT	enable-yaxt with-external-yaxt orenable-cdi-pio with-external-yaxt6	FCFLAGS='-I/path/to/yaxt/include' LDFLAGS='-L/path/to/yaxt/lib' LIBS='-lyaxt'
12	SCT	enable-sct with-external-sct	FCFLAGS='-I/path/to/sct/include' LDFLAGS='-L/path/to/sct/lib' LIBS='-lsct'
13	RTTOV (a modified version of RTTOV)	enable-rttov	<pre>FCFLAGS='-I/path/to/rttov/include' LDFLAGS='-L/path/to/rttov/lib' LIBS='-lradiance -lrttov10.2'</pre>
14	ECRAD	enable-ecrad with-external-ecrad	<pre>FCFLAGS='-I/path/to/ecrad/include' LDFLAGS='-L/path/to/ecrad/lib' LIBS='-lradiation -lifsrrtm -lutilities -lifsaux'</pre>
15	RTE+RRTMGP	enable-rte-rrtmgp with-external-rte-rr	FCFLAGS='-I/path/to/rte-rrtmgp/inc: tmgpLAGS='-L/path/to/rte-rrtmgp/lib LIBS='-lrrtmgp -lrte'
16	NetCDF-Fortran	mandatory	FCFLAGS='-I/path/to/netcdf-fortran, LDFLAGS='-L/path/to/netcdf-fortran, LIBS='-lnetcdff'
17	NetCDF-C	without-external-cdi orenable-coupling7	CPPFLAGS='-I/path/to/netcdf/include LDFLAGS='-L/path/to/netcdf/lib' LIBS='-lnetcdf'
18	HDF5	enable-sct without-external-sct	CPPFLAGS='-I/path/to/hdf5/include' LDFLAGS='-L/path/to/hdf5/lib' LIBS='-lhdf5'
19	AEC or SZIP	static linking	LDFLAGS='-L/path/to/aec/lib' LIBS='-laec' (or LIBS='-lsz')
20	MPI (Fortran interface)	enable-mpi or enable-yaxt without-external-yax orenable-coupling without-external-yac	<pre>FC='/path/to/mpi/bin/mpif90' or tFCFLAGS='-I/path/to/mpi/include' LDFLAGS='-L/path/to/mpi/lib' 8 LIBS='-Impifort -Impi' (depends on the implementation)</pre>

Linking order	Package	Dependency condition1	Required flags1		
21	MPI (C interface)	enable-mpi enable-coupling	CC=/path/to/mpi/bin/mpicc		
		without-external-ya			
		orenable-yaxt	LDFLAGS='-L/path/to/mpi/lib'		
			xtLIBS='-lmpi' (depends		
		orenable-mpi	on the implementation)		
		enable-sct	- ,		
	without-external-sct				
22	CUB	enable-gpu with-external-cub	NVCFLAGS=-I/path/to/cub9		
23	CUDA	enable-gpu	LDFLAGS=-L/path/to/cuda/lib LIBS=-lcudart10		
24	STDC++	enable-gpu	LDFLAGS=-L/path/to/gcc/used/by/nvo LIBS=-lstdc++		

- 1. The dependency conditions and required flags are specified assuming that the shared versions of the libraries containing RPATH entries pointing to their dependencies are used.
- 2. There are no shared versions of YAC and ICON-TIXI libraries, which would enable implicit linking to XML2 library, therefore, the latter needs to be linked explicitly regardless of whether external or the bundled versions of YAC and ICON-TIXI are used.
- 3. When the coupling is enabled (--enable-coupling) and an external version of YAC (--with-external-yac) is used, the usage of an external MTIME library (--with-external-mtime) is mandatory (must be the library that YAC has been built with).
- 4. Currently, the bundled version of CDI does not provide CDI-PIO features, therefore the usage of an external version of CDI (--with-external-cdi) is the only option when the parallel I/O features (--enable-cdi-pio) are required.
- 5. Another possible case when a special treatment for ECCODES/GRIB-API library might not be expected but is required is when the bundled version of YAXT (--enable-yaxt --without-external-yaxt) and an external version of CDI (--with-external-cdi) are used. The configure script of YAXT runs a check that links an executable using libtool and then runs it. Since neither ECCODES nor GRIB-API is a libtool library (i.e. there are no .la files for them), the resulting executable does not have the required RPATH entry for it, which results into a false negative result of the check, which fails the configuration with a misleading message. To circumvent this problem, the path to the ECCODES/GRIB-API library must be passed to the linker before running the configure script of ICON, e.g. by means of the LD_LIBRARY_PATH environment variable.
- 6. When the usage of the parallel features of CDI is enabled (--enable-cdi-pio) and an external version of CDI (--with-external-cdi) is used, the usage of an external YAXT library (--with-external-yaxt) is mandatory (must be the library that CDI has been built with).
- 7. There is no shared version of YAC library, which could link NetCDF-C library implicitly, therefore the latter needs to be linked explicitly, regardless of whether an external or the bundled version of YAC is used.
- 8. Both mpif.h and mpi.mod interfaces are required for the bundled version of YAC.
- 9. CUB is a header-only library and does not need additional linker flags.
- 10. Currently, the only Fortran compiler that supports all features required to build the GPU version of ICON is PGI, which specifies linker flags enabling CUDA automatically.

Bundled libraries

As it was mentioned in the previous section, some of the libraries are bundled together with the ICON source code. However, users can download and install those libraries before configuring ICON and use them

instead. This is controlled by the --with-external-<package> arguments of the configure script of ICON. The arguments accept either yes or no. If the usage of an external version of a library is requested (i.e. --with-external-<package>=yes), the compiler and linker flags, i.e. FCFLAGS, CPPFLAGS, LDFLAGS and LIBS, are supposed to be extended accordingly (see Table 1). The configure script of ICON fails if the flags are not set correctly or enable a version of the library that is known to be incompatible with ICON.

By default, the bundled versions of the libraries are used. In this case, the configure script of ICON runs the configure scripts of the libraries and extends the compiler and linker flags automatically. The arguments that are passed to the configure scripts of the bundled libraries are composed based on the arguments provided to the configure script of ICON as follows: - by default, the arguments are passed unchanged, which means that if you need to give an additional argument to the configure script of a bundled library, you can specify it when calling the configure script of ICON, even though, the argument is not listed in its help message; - arguments that potentially break the configuration and building of ICON are filtered out, for example, it is important that the bundled libraries are linked statically, therefore the argument **--enable-shared** is never passed to the configure scripts that support it; - the list of arguments is extended with ones that enforce consistent building, for example, the configure scripts of the libraries receive additional arguments **--disable-shared** and **--enable-static** (see calls to the **ACX_CONFIG_SUBDIR** macro in configure.ac for the full lists of argument modifications done by the configure script of ICON for each particular library); - compiler flags are modified as described in section Compiler flags.

NOTE: Oftentimes, error and warning messages that a printed at configure time are emitted not by the configure script of ICON but by the configure scripts of the bundled libraries. Each of the scripts generates its own config.log file, which can help in better understanding of the reported issue. The log files are put to the corresponding subdirectories of the ./externals directory residing in the root build directory of ICON.

Compilers and tools

Compilers and tools to be used for building are read by the configure script of ICON from the following environment variables: - FC — Fortran compiler command; - CC — C compiler command; - NVCC — NVIDIA CUDA Compiler command (used only when the GPU support is enabled); - PYTHON — Python interpreter command (used for source dependency tracking and some of the preprocessing steps); - PERL — Perl interpreter command (used for source provenance collection); - CLAW — CLAW compiler (source preprocessor) command (see section Preprocessing for more details); - FPP — Fortran preprocessor command (used when explicit Fortran preprocessing is enabled, see section Preprocessing for more details), must treat the first positional command-line argument as the path to the input source file and print the result to the standard output stream; - SB2PP — Serialbox2 preprocessor command (used when the Serialbox2 serialization is enabled, see section Preprocessing for more details); - MPI_LAUNCH — interactive (synchronous) MPI launcher command (used by the bundled libraries for configure-time checks).

If the variables are set, the configure script will check whether their values meet the requirements, otherwise the script will try to guess suitable values for them. Thus, if you want to make sure that a particular command for a particular operation is used, you need to specify the corresponding variable explicitly. For example, the usage of NAG compiler is enforced with the following additional command-line argument of the configure script:

\$./configure FC=nagfor <other arguments>

Compiler flags

The configure script supports several groups of compiler flags. Each group is associated with one of the following environment variables: - FCFLAGS — Fortran compiler flags to be used at the configuration and building stages when compiling and linking ICON and the bundled libraries (the list of flags might be extended by the configure scripts, e.g. to enable required compiler features, however, in contrast to standard Autoconfbased scripts, the configure script of ICON does not set FCFLAGS to -g -02 by default); - ICON_FCFLAGS — Fortran compiler flags to be appended to FCFLAGS at the building stage when compiling and linking ICON: - ICON OCEAN FCFLAGS — Fortran compiler flags to be appended to FCFLAGS at the building stage when compiling the ocean component of ICON, i.e. the Fortran source files residing in subdirectories of the src/hamocc, src/ocean, and src/sea ice directories (defaults to ICON FCFLAGS, which can be overridden by setting the variable to an empty value: ICON_OCEAN_FCFLAGS=); - ICON_BUNDLED_FCFLAGS - Fortran compiler flags to be appended to FCFLAGS when configuring the bundled libraries (defaults to ICON FCFLAGS, which can be overridden by setting the variable to an empty value: ICON BUNDLED FCFLAGS=); - CFLAGS -C compiler flags to be used at the configuration and building stages when compiling ICON, as well as compiling and linking the bundled libraries (the list of flags might be extended by the configure scripts, e.g. to enable required compiler features, however, in contrast to standard Autoconf-based scripts, the configure script of ICON does not set CFLAGS to -g -02 by default); - CPPFLAGS — C preprocessor flags to be used at the configuration **and** building stages when compiling ICON, as well as compiling **and** linking the bundled libraries; - ICON_CFLAGS — C compiler flags to be appended to CFLAGS at the building stage when compiling ICON; - ICON_BUNDLED_CFLAGS — C compiler flags to be appended to CFLAGS when configuring the bundled libraries (defaults to ICON_CFLAGS, which can be overridden by setting the variable to an empty value: ICON_BUNDLED_CFLAGS=); - NVCFLAGS — NVIDIA CUDA Compiler flags to be used at the configuration and building stages when compiling ICON (the list of flags might be extended by the configure script, e.g. to enable required compiler features); - CLAWFLAGS — extra CLAW compiler flags to be used at the building stage together with the flags that are composed automatically based on the configure options (e.g. Fortran compiler flags specifying search paths (-I<path>) and macros (-D<macro=value>) found in FCFLAGS are passed to the CLAW preprocessor); - LDFLAGS — common Fortran and C compiler flags to be used at the configuration and building stages when linking ICON and the bundled libraries; - LIBS — a list of libraries (see Table 1 for the recommended order) to be passed to the linker by the Fortran compiler when linking ICON and to the configure scripts of the bundled libraries (which might use both Fortran and C compiler for linking).

NOTE: It is recommended to specify the environment variables that influence the configuration as command line arguments of the configure script in the form VAR=VALUE, for example:

\$./configure FCFLAGS='-02 -g' <other arguments>

The general recommendation to follow when composing the flags is: 1. Flags specifying search paths for header and module files, i.e. the -I<path> flags, should be specified as FCFLAGS and CPPFLAGS, depending on whether they need to be passed to Fortran or C compiler, respectively. 2. By default, other flags, e.g. the optimization ones, that are meant for Fortran and C compilers should be appended to FCFLAGS and CFLAGS, respectively. 3. Fortran and C compiler flags that need to be used when compiling and linking ICON but at the same time can break the configuration (a flag is to restrictive for the configure checks to pass, e.g. -fimplicit-none for Gfortran) or the functionality of the bundled libraries (e.g. the optimization level required for ICON is too high and leads to errors in the functionality of the bundled libraries) can be put to ICON_FCFLAGS and ICON_CFLAGS, respectively. 4. Special optimization flags for the ocean component of ICON can be put to ICON_GCEAN_FCFLAGS. 5. Fortran and C compiler flags that need to be used when compiling and linking the bundled libraries but at the same time conflict with the flags required for ICON (e.g. you want to compile ICON with -O3 flag but the bundled libraies need to be compiled with -O2) can be specified as ICON_BUNDLED_FCFLAGS and ICON_BUNDLED_CFLAGS, respectively.

Dynamic libraries

For each -L<path> flag found in the LDFLAGS and LIBS variables, the configure script of ICON generates an additional linker flag that puts the <path> on the list of runtime library search paths of the ICON executable. This allows for automatic location of the required libraries by the *dynamic linker* at the runtime. The flags are appended to LDFLAGS at the build time and their actual form depends on the Fortran compiler in use. By default, the flags are composed using the template -Wl,-rpath -Wl,<path> with currently the only exception for NAG compiler, which accepts the flags in the form -Wl,-Wl,,-rpath -Wl,-Vl,,<path>. If the -rpath flags generated by the configure script break the building or you perform a completely static linking, you can disable the feature by calling the configure script with an additional argument --disable-rpaths.

NOTE: The GNU Linker (GNU ld) implements a feature called new-dtags. If this feature is

enabled (usually by default), the linker treats the -rpath path> flag differently: besides setting the DT_RPATH attribute of the output shared library file to the <path>, it also sets the DT_RUNPATH attribute of the file to the same value. This alters the way the dynamic linker locates the required dynamic libraries at the runtime: if the dynamic linker finds a DT_RUNPATH attribute, it ignores the value of the DT RPATH attribute, with the effect that the LD LIBRARY PATH environmane variable is checked first and the paths in the DT RUNPATH attribute are only searched afterwards. Moreover, the dynamic linker does not search DT RUNPATH locations for transitive dependencies. unlike DT RPATH. Therefore, it is important to keep in mind that: 1. The ICON executable is not agnostic to the environment if it has been linked with the new-dtags feature enabled: the LD_LIBRARY_PATH environment variable can override the rpath entries set by the linker. The feature can be disabled by appending the -Wl,--disable-new-dtags flags to the LDFLAGS variable. 2. If an immediate ICON dependency, e.g. libnetcdf.so, has at least one DT_RUNPATH entry but none of them points to a directory containing one of the libraries required by that dependency, e.g. libsz.so, the dynamic linker will not be able to locate the latter at the runtime even if the ICON executable has been linked without the new-dtags feature and an -W1,-rpath flag pointing to the right location, e.g. -Wl, --disable-new-dtags -Wl, -rpath -Wl, /path/to/libsz. A possible workaround for this is to make the secondary dependency of ICON a primary one by overlinking (i.e. linking to a library, which is not used by the executable directly) to it, e.g. by adding the -lsz to the LIBS variable. This way, the dependency will become a non-transitive one and the dynamic linker will be able to locate it using either DT RUNPATH or DT RPATH entries of the ICON executable.

For more details, refer to the man pages of the linker (man ld) and the dynamic linker (man ld.so).

NOTE: Some of the bundled libraries employ Libtool, which is known to be **not** fully compatible with some compilers. For example, the flags -Wl,-Wl,,-rpath -Wl,-Wl,,<path>, which are valid for NAG compiler, are incorrectly transformed by Libtool into -Wl,-Wl -Wl,,"" -Wl,-rpath -Wl,-Wl -Wl,-Wl -Wl,'" -Wl,<path>. A possible solution for this problem is to add the flags in the form understood by NAG compiler not to LDFLAGS but to ICON_FCFLAGS and make sure that the bundled libraries, especially the Libtool-based ones, will not receive them: ICON_BUNDLED_FCFLAGS=.

NOTE: The generated -rpath flags are applied only at the building stage and for the ICON executable only. However, some of the checks performed by the configure script of ICON and the configure scripts of the bundled libraries imply running executables linked with the flags listed in the LIBS variable. To prevent those checks from false negative results, which oftentimes are reported with misleading messages, the dynamic linker needs to be able to locate all the libraries referenced in the LIBS variable. A way to achive that is to list paths to the libraries in the LD_LIBRARY_PATH variable and export it, i.e. run export LD_LIBRARY_PATH="<path1>:<path2>:..." before running the configure script.

Configuration and building environments

It is important that both the configuration and the building stages are performed in the same environment, i.e. the environment variables that might influence the way the compilers and the linker work are set to the same values when running the configure script and when running the make command for building (see also section Initialization of the building environment). For example, NAG compiler will not work if the environment variable NAG_KUSARI_FILE is not set properly. Keeping track of all the steps required to reinitialize the environment for the building stage, e.g. when the configuration stage has already been done but in another terminal session, might be challenging, especially in HPC environments offering multiple compilers and libraries.

One way to make sure that the configuration and the building environments are consistent is to set the BUILD_ENV argument of the configure script to a set of shell commands that initialize the environment variables with the required values. If the BUILD_ENV variable is not empty, the configure script will run

the commands it contains before running any checks. Additionally, the commands will be saved to the Makefile, so they will be executed each time the make command is launched for building. The shell script that is provided as value of the BUILD_ENV argument must be a one-liner ending with a semicolon (;) symbol, for example:

\$./configure BUILD_ENV='. /etc/profile.d/modules.sh; module purge; module load intel;' <other argument

Also, a proper implementation of the BUILD_ENV script allows for switching between multiple build directories (see section Out-of-source configuration (building)) without having to re-initialize the environment accordingly.

Configuration wrappers

Real case configuration commands might be rather long and complex. For example, below, you can find an example of the configuration command for Mistral@DKRZ:

```
$ ./configure \
  AR=xiar \
  BUILD_ENV=". /sw/rhel6-x64/etc/profile.mistral; \
             . ./config/dkrz/module_switcher; \
             switch for module gcc/6.4.0 intel/17.0.6 openmpi/2.0.2p1 hpcx-intel14;" \
  CC=mpicc ∖
  CFLAGS='-gdwarf-4 -03 -qno-opt-dynamic-align -ftz -march=native -g' \
  CPPFLAGS="-I/sw/rhel6-x64/hdf5/hdf5-1.8.18-parallel-openmpi2-intel14/include \
            -I/sw/rhel6-x64/netcdf/netcdf_c-4.4.0-parallel-openmpi2-intel14/include \
            -I/sw/rhel6-x64/grib_api/grib_api-1.15.0-gcc48/include \
            -I/usr/include/libxml2" \
  FC=mpif90 ∖
  FCFLAGS="-I/sw/rhel6-x64/netcdf/netcdf_fortran-4.4.3-parallel-openmpi2-intel14/include \
           -gdwarf-4 -g -march=native -pc64 -fp-model source" \
  ICON_FCFLAGS='-O2 -assume realloc_lhs -ftz' \
  ICON_OCEAN_FCFLAGS='-O3 -assume norealloc_lhs -reentrancy threaded -qopt-report-file=stdout -qopt-rep
  LDFLAGS="-L/sw/rhel6-x64/hdf5/hdf5-1.8.18-parallel-openmpi2-intel14/lib \
           -L/sw/rhel6-x64/netcdf/netcdf_c-4.4.0-parallel-openmpi2-intel14/lib \
           -L/sw/rhel6-x64/netcdf/netcdf_fortran-4.4.3-parallel-openmpi2-intel14/lib \
           -L/sw/rhel6-x64/grib_api/grib_api-1.15.0-gcc48/lib \
           -mkl=sequential" \
  LIBS='-Wl,--as-needed -lxml2 -lgrib_api -lnetcdff -lnetcdf -lhdf5' \
  MPI LAUNCH=mpiexec \
  --enable-intel-consistency \
  --enable-vectorized-lrtm \
  --enable-parallel-netcdf
```

Obviously, repeatedly composing such a command is exhausting and error-prone. Therefore, each team involved in the development of ICON is encouraged to implement and maintain *configuration wrappers*, which would simplify the configuration stage for their users. The wrappers should be put in a subdirectory with a relevant name of the ./config directory. Although there are no hard requirements on how the scripts should be implemented, we recommend to consider the following features:

- Pass the command-line arguments of the wrapper script to the configure script, so that the users are able to override the default values of the configure options, for example: console \$
 ./config/dkrz/mistral.intel --enable-openmp Also, account for the case of calling the wrapper with the --help argument.
- 2. Account for out-of-source building:
 - the wrapper script should be able to locate the configure script when called from a directory other than the source root directory, for example: bash SCRIPT_DIR=\$(cd "\$(dirname "\$0")";

pwd) ICON_DIR=\$(cd "\${SCRIPT_DIR}/../.."; pwd) "\${ICON_DIR}/configure"
<a list of predefined arguments> "\$@"

- the wrapper script should prepare the current working directory for the following runscript generation (see section Running for more details).
- 3. Prepend the LIBS variable with -Wl,--as-needed flag so that the actual list of the libraries the ICON executable depends on would include only those required for the particular configuration of the model (see the man pages of the linker for more details: man ld).
- 4. Allow for running the make check command (see section Building of the bundled libraries for more details) by extending the LD_LIBRARY_PATH environmane variable in the BUILD_ENV script, instead of doing so in the wrapper script itself.

Out-of-source configuration (building)

The building system of ICON supports so-called *out-of-source* builds. This means that you can build ICON in a directory other than the *source* root directory. The main advantage of this is that you can easily switch between several different configurations (each in its own *build* directory) of the model, while working on the same source code. Hence, it is possible to introduce changes into the source code and test them with different compilers, flags and options without having to re-configure the model or copy the updated source files to other directories.

The configure script (also when called via a configuration wrapper) prepares the *current working directory* for the following building. The particular case of the current working directory being the source root directory is called *in-source* configuration.

NOTE: It is not allowed to mix in-source and out-of-source builds: the source directory must be cleaned from the files generated as a result of a prior in-source configuration and building before an out-of-source configuration can take place.

The following example shows how ICON can be configured on Mistral@DKRZ in two different directories using Intel and GCC compiler toolchains (assuming that the source root directory of ICON is /path/to/icon-srcdir):

```
$ mkdir intel && cd intel
$ /path/to/icon-srcdir/config/dkrz/mistral.intel
$ cd ..
$ mkdir gcc && cd gcc
$ /path/to/icon-srcdir/config/dkrz/mistral.gcc
$ cd..
```

As a result of the previous commands, you will have two directories intel and gcc prepared for the following building of ICON using Intel and GCC compilers, respectively.

Building

The building stage is done with GNU make upon successful completion of the configuration stage. The oldest supported version of make is **3.81**, however, it has significant limitations and it is recommended to use version **4.1** or later.

The building step is done by running **make** command with an optional argument specifying the number of jobs to run simultaneously. For example:

\$ make -j8

NOTE: Users are recommended to get familiar with the list of basic *targets*, i.e. supported subcommands, by running:

\$ make help

The *makefiles* of ICON, i.e. the instructions for **make** on how to build the model, are generated at the final step of the configuration stage based on the template files. Unlike most of the Autotools-based packages, the makefile templates of ICON are **not** generated automatically with Automake but implemented manually. The main reasons for that are, first, avoid the need to maintain an explicit list of source files, and, second, keep the makefiles human-readable and, therefore, human-hackable, which is often required for productive model development.

By default, make reads the instructions from a file called Makefile, which in the case of ICON is generated based on the Makefile.in template and is mainly responsible for the initialization of the building environment. The initialization is performed by the shell script provided to the configure script as the BUILD_ENV argument (see section Configuration and building environments). The script is saved in the Makefile. Each time make is executed in the root of the ICON build directory, it reads the Makefile, runs the initialization script and recursively executes itself in the same directory but with another input makefile called icon.mk. The latter is generated based on the icon.mk.in template and contains the instructions on how to perform the following building steps required to generate the ICON executable.

NOTE: All modifications of the makefiles and other files that are automatically generated at the configuration stage can be reverted by calling the ./config.status script residing in the build directory.

The following sections provide information on some features and implementation details of the building process.

NOTE: By default, make produces very minimalistic output to the standard output stream. This allows for better recogniction of the warnings messages emitted by the compilers and other tools. This can be altered either at the configuration stage by calling the configure script with an additional option --disable-silent-rules or at the building stage by calling make with an additional command-line argument V, which can be set either to 1 (enable verbose output) or to 0 (disable verbose output). For example, if you want to see the exact commands executed by make, you can run:

\$ make V=1 <other arguments>

Source file collection

The list of source files that need to be compiled to produce the ICON executable is generated dynamically each time the make command is executed. This is done using find command (both GNU and BSD versions are supported) with the assumption that the source files have the following filename extensions:

- .f90 Fortran source files, regardless of whether they contain Fortran preprocessor directives;
- .inc Fortran header files included with the Fortran preprocessor **#include** directives, e.g. **#include** "filename.inc";
- .incf Fortran header files included with the Fortran INCLUDE statements, e.g. include 'filename.incf' (these files are not allowed to have Fortran preprocessor directives);
- .c C source files;
- .cu CUDA source files.

The list of source files is a result of recursive search for files that have the aforementioned extenions and reside in the src and support subdirectories of the source root directory of ICON. Additionaly, depending on the whether the corresponding components of the model were enabled at the configuration stage, the list is extended with files Fortran source files from the ./externals/jsbach and ./externals/art subdirectories.

NOTE: In general, you can extend the source base of ICON just by adding the source files to the src subdirectory of the source root directory of ICON.

Preprocessing

Depending on the configuration, Fortran source and header files undergo one or more of the following preprocessing precedures. 1. Fortran source files residing in the ./externals/jsbach/src are preprocessed with the dsl4jsb.py script. This is done only if the JSBACH component has been enabled at the configuration stage (--enable-jsbach). Otherwise, the source files of the component are completely ignored. The result of this procedure is stored to the ./pp/jsb subdirectory of the root build directory. 2. Depending on whether the CLAW preprocessing (--enable-claw) is enabled, the result of the previous step (currently, only JSBACH files are optionally preprocessed at this step) are preprocessed with the CLAW compiler. The result of this procedure is stored to the ./pp/claw subdirectory. > NOTE: Unlike the rest of the preprocessing steps, the instructions for CLAW preprocessing are moved to a separate makefile called claw.mk, which is generated based on the claw.mk.in template. This is done to employ the .NOTPARALLEL feature of GNU make, which is required to meet the limitation of the CLAW compiler manifested in the fact that the files must be processed serially. 3. Depending on whether the *explicit Fortran preprocessing* is enabled (--enable-explicit-fpp), the results of the actual previous preprocessing step, together with Fortran source and header files of ICON (including the ART component, if enabled) that have not been preprocessed yet, are treated as follows: - .f90 files are preprocessed with the standard Fortran preprocessor; - .inc files are withdrown from further preprocessing since their contents are supposed to be injected into the output of the Fortran preprocessor when processing .f90 files that include them; - .incf files that do not reside in the common include directory are copied as-is to the corresponding subdirectories of the output directory, so they can be later found by the Fortran compiler without additional search path flags (.incf files that are stored in the common directory do not need to be copied because the compiler is always called with the -I/path/to/icon-srcdir/src/include search path flag and therefore is able to locate them).

The result of this procedure is stored to the `./pp/fpp` subdirectory.

- 4. If the *Serialbox2 serialization* is enabled (--enable-serialization), the results of the actual previous preprocessing step, as well as Fortran source and header files of ICON (including the ART component, if enabled) that have not been preprocessed yet, are treated as follows:
 - .f90 files are preprocessed with the corresponding script of the Serialbox2 toolkit;
 - .inc files, if not withdrown at the previous step, are preprocessed with the same script as for .f90 files and an additional search path flag -I/path/to/icon-builddir/pp/sb2/src/include is prepended to the list of Fortran compiler flags, so the compiler would later prefer the **preprocessed** versions of the files over the original ones residing in the common include directory;
 - .incf that do not reside in the common include directory are copied as-is to the corresponding subdirectories of the output directory (for the same reason as in the case of the explicit Fortran preprocessing) The result of this procedure is stored to the ./pp/sb2 subdirectory.

NOTE: The explicit Fortran preprocessing is enabled automatically when the Serialbox2 serialization is enabled. You can override this by disabling the preprocessing with the --disable-explicit-fpp option.

The output directories of the preprocessing steps have the same layout as the directories containing their input files and the output files have the same basenames as the corresponding intput files. For example if the original source file of JSBACH /icon-srcdir/externals/jsbach/src/base/mo_jsb_base.f90 is preprocessed by each of the preprocessing steps, the corresponding output files are saved as follows: - /icon-build/pp/jsb/src/base/mo_jsb_base.f90 — JSBACH preprocessing output; - /icon-build/pp/jsb/src/base/mo_jsb_base.f90 — CLAW preprocessing output; - /icon-build/pp/jsb/src/base/mo_jsb_base.f90 — explicit Fortran preprocessing output; - /icon-build/pp/jsb/src/base/mo_jsb_base.f90 — explicit Fortran preprocessing output; - /icon-build/pp/sb2/pp/fpp/pp/claw/pp/jsb/src/base/mo_jsb_base.f90 — Serialbox2 preprocessing output.

NOTE: In contrast to the original source files residing in the source directory, output files of the preprocessing steps are treated by **make** by their absolute paths. This is done to avoid potential ambiguity between the preprocessed files residing in the current build directory and the preprocessed files in the source directory generated as a result of a prior in-source configuration and building.

NOTE: Source files are additionally preprocessed with the corresponding standard language-specific (i.e. Fortran, C, CUDA) preprocessors as part of the compilation process. In contrast to the procedures described in this section, the compilation-time preprocessing is non-optional and run by the compilers *implicitly*.

Source dependency tracking

Before the compilation can take place, it is required to identify the exact list of source files that need to be compiled in order to produce the ICON executable. The actual content of the list depends not only on how the code is configured, possible modifications of the source code made since the last call of make need to be taken into account too. Moreover, in the case of Fortran source files, the compilation order becomes important since a source file declaring a Fortran module must be compiled before any other source file using that module. Both tasks are accomplished as follows.

Once the preprocessing is finished, all source files of ICON (as well as JSBACH and ART, if enabled) or their **final** preprocessed versions are processed with the dependency generator. The tool parses each source file, detects which header and module files are required for its succesful compilation, and stores this information in the form of a makefile. The makefiles a then read by **make** and the dependency listing script. The former makes sure that the source files are compiled in the right order, the latter identifies the list of source files that need to be compiled.

NOTE: The dependency listing script recognizes only the basic makefile syntax. For example, it does not support variables and functions.

The dependency generator recognizes preprocessor **#include**, **#if** and the associated directives as well as Fortran INCLUDE, USE and MODULE statements. If the usage of a module or a header file is surrounded with the **#ifdef SOME_MACRO** and **#endif** directives, it will be put on the list of files required for the compilation only if the macro SOME_MACRO is defined. The list of macro definitions enabling various features of the model is generated at the configuration stage in the form of compiler flags, e.g. -DSOME_MACRO -DSOME_OTHER_MACRO, which are appended to FCFLAGS. This way, some Fortran modules do not need to be generated in particular configurations of the model and, therefore, the source files declaring them are not compiled.

NOTE: There are two types of source dependencies that cannot be detected by the dependency generator. Undetectable dependencies of the first type are related to C/Fortran interoperability: if a Fortran source file contains a declaration of a binding to a function defined in a C source file, the dependency of the respective object files must be reflected in the recipe for target c_binding.d of the icon.mk.in template. The second type of undetectable dependencies is associated with Fortran external procedures: if a Fortran source file contains a call to an external procedure, i.e. a function or a subroutine that is not part of any Fortran module, the dependency of the respective object files must be specified in the recipe for target extra_f90.d of the icon.mk.in template.

The dependency listing script reads the dependency makefiles, builds a source dependency graph and traverses it starting with the vertex associated with the src/drivers/icon.o object file. Each vertex of the graph accessible from the starting one is printed to the output. The output is then filtered by make in order to generate the list of object files required for the ICON executable. This is the main purpose of the listing script. Additionaly, the tool can run code consistency checks described in the following subsection.

Code consistency checks

Each failed code consistency check run by the dependency listing script is reported to the standard error stream. The identified problems are expressed in terms of files and makefile dependencies and, therefore, require additional explanation provided in this subsection. Normally, the codebase is kept consistent and users do not see the messages described below until they introduce a modification to the source code that breaks the consistency. Currently, the dependency listing script checks the source dependency graph for the following problems:

1. Two or more Fortran source files declare modules with the same name.

This type of inconsistency is reported as follows: deplist.py: WARNING: 'mod/some_module.mod.proxy' has more than one immediate prerequisite matching pattern '*.o': some/dir/some_file.o some/other/dir/some_other_file.o This means that the module some_module is declared twice. The first declaration is found in the file some/dir/some_file.f90 and the second declaration is found in some/other/dir/some_other_file.f90.

2. Two or more Fortran modules circularly depend on each other.

This type of inconsistency is reported as follows: deplist.py: WARNING: the dependency graph has a cycle: src/drivers/icon.o ... mod/some_module.mod.proxy some/dir/some_file.o mod/some_module_1.mod.proxy <- start of cycle some/other/dir/some_file mod/some_module_2.mod.proxy some/other/dir2/some_file_2.o mod/some_module_1.mod.proxy <- end of cycle This reads as that the module some_module_1 (declared in some/dir/some_file_1.f90) uses module some_module_2 (declared in some/other/dir/some_file_2.f90), which in turn uses some_module_1. Usually, this means that the compilation of some/dir/some_file_1.f90 will fail.

3. A Fortran module is used but not declared.

This problem is reported by the dependency listing script with the following message: deplist.py: WARNING: 'mod/missing_module.mod.proxy' does not have an immediate prerequisite matching any of the patterns: '*.o' This means that the module missing_module is used in one of the source files but there is no Fortran source file in the ICON codebase that declares it.

NOTE: Missing Fortran modules are additionaly reported by **make** with the message:

Cannot find Fortran source file providing module 'missing_module'.

However, it might be the case that the module is not actually missing but just not part of the ICON codebase, e.g. mpi, sct, yaxt, etc. Such modules are external to ICON and need to be explicitly specified as such in the file depgen.f90.config residing in the current build directory. The file is generated at configuration time based on a template file residing in the source directory. Therefore, in order to make the modifications persistent, you need to introduce them in the file depgen.f90.config.in.

Compilation cascade prevention

It is important, especially for the development process, that the modifications of the source code done after the initial compilation trigger as few recompilations as possible. One of the basic features of **make** is to keep track of the file modification timestamps. Based on the information from the makefiles generated by the dependency generator, the tool triggers recompilation of a source file only if the file itself or a header file it includes, or a Fortran module file it uses has been modified since the last execution. Unfortunately, most of the Fortran compilers (with an exception of Gfortran) update the module files even if their relevant contents do not change, i.e. the modification timestamp of a module file gets updated even if the declaration of the associated Fortran module in the source file remains the same. This leads to so-called *compilation cascades*.

Partially, this issue is circumvented in the building system of ICON as follows. 1. If a Fortran source file filename.f90 uses a module modulename, the corresponding dependency makefile filename.f90.d (created by the dependency generator) gets an entry declaring the dependency of the respective object file on a module *proxy* file: make filename.o: mod/modulename.mod.proxy 2. When the compilation of the file declaring the module modulename takes place for the first time, the original module file mod/modulename.mod generated by the compiler is backed up under the name mod/modulename.mod.proxy. 3. When make checks whether the object file filename.o needs to be updated (i.e. the source file filename.f90 needs to be recompiled), it compares the potentially updated original module file mod/modulename.mod with the proxy file mod/modulename.mod.proxy and triggers the recompilation only if they are *significantly different*. The latter fact is determined in two steps: first, the files a compared for binary identity with the cmp command, second, if the first check shows the difference, the contents of the files are compared with the fortmodcmp.py script, which employs compiler-specific heuristics. 4. Each time the proxy file mod/modulename.mod.proxy

is detected to be significantly different from the original module file mod/modulename.mod, it is replaced with a new copy of the latter.

The described mechanism helps to avoid compilation cascades in many cases. However, the structure of the module files generated by most of the compilers is usually not documented, which makes the comparison of the module files difficult. Thus, the redundant recompilations are not guaranteed to be eliminated entirely.

Building of the bundled libraries

The building of the bundled libraries is based on the makefiles generated by their configure scripts. The makefiles are put to the corresponding subdirectories of the ./externals directory residing in the root build directory of ICON. The libraries are built before the compilation of any Fortran source file of ICON takes place. This is done to make sure that the interface Fortran modules of the libraries are available in advance.

NOTE: Some of the bundled libraries, e.g. CUB, do not require configuration and building and, therefore, are not handled at this building step.

Once called in the build directory of ICON, make recursively runs itself in the build directories of the bundled libraries. The list of targets passed to the instances of make running in the directories of the bundled libraries depends on the list of targets specifed by the user when calling make in the build directory of ICON. The targets all, mostlyclean, clean, distclean, or check are preserved and passed over. All other targets are filtered out.

The described mechanism imposes the following requirements on the makefiles of the bundled libraries: - the default targets of the makefiles (i.e. targets that are triggered when no targets are specified on the commandline) must be called **all** and are supposed to generate all files (libraries, module files, etc.) required for ICON; - the makefiles must implement at least dummy rules for targets **mostlyclean**, **clean**, and **distclean**, ideally, following the heuristic adopted in Automake; - the makefiles must implement at least a dummy rule for target **check**, which ideally triggers self-tests of the library.

NOTE: Many of the bundled libraries have a collection of tests, which can be triggered by running make check command from the root build directory of ICON. The tests cant help to identify potential runtime problems at an early stage and make sure that the core functionality of a library works as expected in the given software environment.

Source provenance collection

Source provenance information is collected at the building stage and injected in the ICON executable. This information is saved at runtime in the output files of the model, so that the latter could be matched with the exact version of ICON that was used to produce them. The information is collected automatically with the help of the pvcs.pl script. The script generated a source file version.c containing the url of the git repository, the name of the git branch, and the hash of the git commit. The source file is then treated by make as part of the ICON codebase.

Running

The executable of ICON is usually not launched directly. The common practice is to implement or generate a *runscript*, which sets up a working directory, populates it with all required input files (grid files, namelists, etc.), runs the model, and postprocesses its output. This section does not cover the details of how to set up an experiment but ruther provides superficial information on how to generate runscripts using standard templates.

The building system of ICON is currently fully detached from the runscript generation mechanism. Therefore, the latter requires additional configuration steps before it can be used.

NOTE: Normally, the additional configuration steps enabling the runscript generation mechanism are performed by the configuration wrappers.

The generation of the runscripts is done with the make_runscripts shell script, which does not yet support the case of out-of-source builds. In particular, this means that the script itself, together with some other input files, needs to be copied from the source directory to the build directory of ICON. The following example shows how this can be done using the rsync tool:

```
$ cd /path/to/icon-builddir
$ rsync -uavz /path/to/icon-srcdir/run . --exclude='*in' --exclude='.*'
$ rsync -uavz /path/to/icon-srcdir/externals . --exclude='.git' \
    --exclude='*.f90' --exclude='*.F90' --exclude='*.c' --exclude='*.h' \
    --exclude='*.Po' --exclude='tests' --exclude='rrtmgp*.nc' --exclude='*.mod' \
    --exclude='*.o'
$ rsync -uavz /path/to/icon-srcdir/make_runscripts .
$ ln -sf /path/to/icon-srcdir/data
```

\$ ln -sf /path/to/icon-srcdir/vertical_coord_tables

Once the runscript generation mechanism is initialized following the instructions above, you can switch to the root build directory of ICON and run the make_runscripts script:

```
$ cd /path/to/icon-builddir
$ ./make runscripts
```

NOTE: By default, the generator creates runscripts for multiple experiments. The users can also chose to generate a single runscript for the experiment of their choice, for example:

\$./make_runscripts -s atm_amip

The generated runscripts are saved to the ./run subdirectory of the build directory. The headers of the runscripts containing arguments for the HPC workload manager, e.g. SLURM, might require additional manual adjustments regarding CPU time accounting, node allocation, etc.

NOTE: Alternatively, the users can employ the low-level tool for runscript generation offering a more fine-grained control over certain parameters. For example, the wall clock limit and the number of allocated node can be injected into the runscript as follows:

```
$ cd ./run && ln -sf ./checksuite.ocean_internal/omip/exp.ocean_omip_long exp.ocean_omip_long
$ ./make_target_runscript in_script=exp.ocean_omip_long in_script=exec.iconrun \
EXPNAME=ocean_omip_long cpu_time=08:00:00 no_of_nodes=20
```

Once created and adjusted, the runscript can be submitted for execution. For example:

```
$ cd ./run && sbatch ./exp.atm_amip.run
```

Out-of-build runs

The configuration and building of ICON require significant amount of time, which heavily depends on the performance of the file system. Therefore, the users are recommended to consider a scenario in which they build the model on a fast local disk partition of a *login* node of an HPC cluster and then transfer the executable and all data required for their experiment to a slow This way, they can effectively reduce the time-toshared partition available on *compute* nodes. solution. The transfer of the data can be done with the help of the move_to_prefix.sh script as follows: 1. Create a copy of the ICON source directory on the fast partition, e.g. by cloning \$ git clone --recursive git@gitlab.dkrz.de:icon/icon.git the git repository: console /path/to/fast/partition/icon-srcdir 2. Create a build directory on the fast partition, switch to it, and run the configure script or a configuration wrappers with an *additional* argument --prefix pointing to the shared (but slow) partition: console \$ mkdir /path/to/fast/partition/icon-builddir \$ cd /path/to/fast/partition/icon-builddir \$ /path/to/fast/partition/icon-srcdir/configure --prefix=/path/to/shared/partition/icon-rundir <other arguments> 3. Build the model: console \$ make -j8 4. Transfer the executable together with required data to the shared partition: console \$ /path/to/fast/partition/icon-srcdir/utils/move_to_prefix.sh 5. Switch to the shared partition

and generate the runscripts: console \$ cd /path/to/shared/partition/icon-rundir \$./make_runscripts 6. Switch to the ./run subdirectory and submit the runscript of your choice, for example: console \$ cd ./run && sbatch ./exp.atm_amip.run

FAQ

1. I run the configure script without any arguments and it fails. What should I do?

First, you are recommended to check whether there is a suitable configuration wrapper in the ./config directory that you could use instead of running the configure script directly.

If that is not the case, you need at least to specify the LIBS variable telling the configure script which libraries to link the executables to. The content of the list depends on the configure options you specify (see Table 1), for example:

\$./configure --disable-mpi --disable-coupling LIBS='-lnetcdff -lnetcdf -llapack -lblas'

If the libraries reside in nonstandard directories, you might also need to specify the FCFLAGS, CPPFLAGS, and LDFLAGS variables to tell the script which directories need to be searched for header and library files (see section Configuration for more details).

2. How can I reproduce the configuration of the model used in a Buildbot test?

Scripts run by Buildbot for configuration and building of the model reside in the ./config/buildbot directory. You can run them manually on the corresponding machine.

3. I get an error message from the configure script starting with "configure: error: unable to find sources of...". What does this mean?

Most probably, you forgot to initialize and/or update git submodules. You can do that by switching to the *source* root directory of ICON and running the following command:

\$ git submodule update --init