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Materials Science and Technology

2022.06.30 Ivanova Kseniya

How to install, compile, configure and run ICON

See Icon wiki page and tutorial here :

ICONIconModel - MODELS - C2SM Wiki (ethz.ch)

ICON Model Tutorial 2020 (dwd.de)

Icon grid can be downloaded here : ICON — Grid File Server (mpg.de)

DWD icontools are a repository on the C2SM github: https://github.com/C2SM/icontools

First, one clone Icon repository recursively (with all externals submodels, such as , for example, icon-art) from gitHub using SSH protocol:

```
git clone git@github.com:C2SM/icon.git
```

Execute

```
git submodule update --init
```

ICON needs to be configured before compilation. There is a configure-script for each compiler and/or machines located in config folder in the downloaded locally ICON source code. On daint I configure by running the following in the terminal in the icon source code folder:

```
./config/cscs/daint.cpu.pgi-20.1.1-eccodes
```

Often I got problems with eccodes root, you have to be sure that inside the configure file the provided link exists. For example, if in configure file you provide the following

ECCODES_ROOT='/project/g110/spack-install/daint/ec-codes/2.19.0/pgi/6btxe4laukde6xhzonqnnczpz6tech7b'

Check that the directory

'/project/g110/spack-install/daint/eccodes/2.19.0/pgi/6btxe4laukde6xhzonqnnczpz6tech7b/share/ec-codes/samples'

really exists and containing file GRIB2.tmpl.

Question: what is the difference between "01" configuration and "02" configuration for daint.pgi ?

Answer: this is the optimization level of the compiler

Optimization Levels - GNAT User's Guide (gnu.org)

02 Full optimization; generates highly optimized code and has the slowest compilation time

01 Moderate optimization; optimizes reasonably well but does not degrade compilation time significantly

After configuring, **Makefile** will be created. Compile with

```
make -j8
```

The **exe** file will be created in the /bin directory in the icon source code folder.

After that, if all steps were successful, you have to run requirenments file

python -m pip install -r requirements.txt

and finally you can run icon or icon-art through processing chain using the following command with preparing data

python run_chain.py icon-art-BRM 2018-12-21 0 24 -f -j prepare_data icon

or without preparing data :

python run_chain.py icon-art-BRM 2018-12-21 0 24 -f -j icon

All namelists one can find in the run file icon_runjob.cfg . One can change the output namelist as you wish (grib2 output format or netCDF, both are possible) and add/remove output variables as you wish in (**ml_varlist**).

Grib2 output:

In order to write grb output, in configure file we need additional flag

EXTRA_CONFIG_ARGS+=' --disable-mpi-checks --enable-grib2 --without-external-cdi --enable-art'

This flag is also enable ART model from externals.

Here are some modificatios I did to run Icon with processing chain:

I commented in prepare_data.py

the following lines in order to avoid problems with lateral boundary conditions :

```
  # tools.copy_file(cfg.lateral_boundary_grid,
        #            cfg.lateral_boundary_grid_scratch,
          #          output_log=True)
```

I also changed a bit the file config.py in /users/kivanova/processing-chain/cases/icon-art-BRM :

-created additional input root with meteoswiss data grid , dictionary etc

```
input_root2 = '/users/kivanova/icon1.config'
input_root = '/store/empa/em05/input_iconart_processing_chain_example/'
```

Icontool directory I used from Michael Steiner

```
icontools_dir = '/scratch/snx3000/msteiner/spack-stages/daint/spack-stage-icontools-master-t524rnfa5sfyn4rbvarypyzwae4jg46d/spack-src/icontools'
```

Also, I used the following :

```
radiation_grid_filename = os.path.join(input_root2,
                                       "ICON-1E_DOM01.parent.nc")
dynamics_grid_filename = os.path.join(input_root2, "ICON-1E_DOM01.nc")
map_file_latbc = os.path.join(input_root_grid, "map_file.latbc")
extpar_filename = os.path.join(
    input_root2, "external_parameter_mch_ICON_1E_R19B08_DOM1.nc")
lateral_boundary_grid = "/scratch/snx3000/kivanova/processing_chain/icon-art-BRM/2018122100_0_24/icon/input/grid/lateral_boundary.grid.grid.nc"
```

And

```
# ART settings----------------------------------------------------------------
input_root_tracers = os.path.join(input_root, 'XML')
chemtracer_xml_filename = os.path.join(input_root_tracers,
                                       'tracers_BRM_pntsrc.xml')
```

```
pntSrc_xml_filename = os.path.join(input_root_tracers, 'pntSrc_BRM.xml')
art_input_folder = os.path.join(input_root, 'ART')

# SIMULATION
================================================================
# ICON ----------------------------------------------------------
# Executable
icon_bin ="/scratch/snx3000/kivanova/icon_src/bin/icon"
#os.path.join(exe_dir, "icon-kit-art_20211018")

# Namelists and slurm runscript templates
icon_runjob = os.path.join(case_dir, 'icon_runjob.cfg')
```

XML files one can find here :

/store/empa/em05/input_iconart_processing_chain_example/XML

In tracers_BRM_pntsrc.xml I changed the units :

mol mol-1 to kg kg-1

The tags "mol_weight" and "unit" are not required for passive tracers. And if they are provided, they have no influence on the tracer or output.

All tracers are treated as mass mixing ratios in the model. Passive tracers are also written out as MMR in the output. These 2 tags are used for chemical tracers in a conversion-routine such that the output is then in VMR, but passive tracers are skipped in this conversion-routine and are written out as MMR.

At the beginning of icon run script icon_runjob.cfg after SBATCH lines I added radiation input files coping it one by one

```
# Link radiation input files
# ------------------------------------------------------------------------
ln -sf {cfg.art_input_folder}/runctrl_examples/photo_ctrl/* .
ln -sf {cfg.art_input_folder}/runctrl_examples/init_ctrl/* .
ln -sf /users/kivanova/icon1.config/ecrad_data/*
ln -sf /users/kivanova/icon1.config/ecrad_data/socrates_droplet_scattering_rrtm.nc
```

ln -sf /users/kivanova/icon1.config/ecrad_data/fu_ice_scattering_rrtm.nc

ln -sf /users/kivanova/icon1.config/ecrad_data/mcica_gamma.nc

ln -sf /users/kivanova/icon1.config/ecrad_data/RADRRTM

ln -sf /users/kivanova/icon1.config/ecrad_data/RADSRTM

ln -sf /users/kivanova/icon1.config/ecrad_data/slingo_droplet_scattering_rrtm.nc

ln -sf /users/kivanova/icon1.config/ecrad_data/yi_ice_scattering_rrtm.nc

ln -sf /users/kivanova/icon1.config/ecrad_data/baran_ice_scattering_rrtm.nc

ln -sf /users/kivanova/icon1.config/ecrad_data/es_droplet_scattering_rrtm.nc

Fieldextra

In fieldextra it is mandatory to remap variable hsurf since we use tag grid from this variable

&Process in_field = "HSURF", use_tag="GRID" /

&Process

in_file = "_tmp_u<DDHH>0000"

out_file = "IconPntSr<DDHH>0000", out_type = "GRIB2"

in_regrid_target = "GRID"

tstart = 0, tstop = 24, tincr = 1

/

I also changed the levels to 80, as in Meteoswiss

levmax = 80

and in icon_runjob.cfg in /users/kivanova/processing-chain/cases/icon-art-BRM

num_lev = 80 ! number of full levels (atm.) for each domain

To run new date with icon art we have to change XML file pntSrc_BRM.xml,config.py in processing chain (output_dir = os.path.join(work_root, casename, '2018041500_0_24', 'icon', 'output') and lateral_boundary_grid = "/scratch/snx3000/kivanova/processing_chain/icon-art-BRM/2018041500_0_24/icon/input/grid/lateral_boundary.grid.grid.nc"), in icon_runjob.cfg name of outputfiles

for Flexpart files we have to change AVAILABLE, COMMAND.

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Plot Icon unstructured mesh

To plot Icon unstructured, one can use **Paraview with Reader plagin CDIReader**

(available on ddm06 and on Daint), **psyplot with python**

```
import psyplot.project as psy
fN = '/project/ivme/MCH-1/icon-art-BRM/icon_output/ICON-ART-OEM_AllVarUnstr_DOM01_00130000.nc'
ncf = nc.Dataset(fN)
print(ncf)
print(ncf.variables.keys())
ds = xr.open_dataset(fN)
print(ds)
print(ds.t_2m.CDI_grid_type)
psy.rcParams['plotter.maps.xgrid'] = False
psy.rcParams['plotter.maps.ygrid'] = False
mpl.rcParams['figure.figsize'] = [10., 8.]
BRM = psy.plot.mapplot(fN, name="testtr12", load=True, maskleq=0,
                       levels=[80],
       clabel="%(long_name)s",
    title='%(time)s', cmap='Blues',
      post="import cartopy.feature as cf; self.ax.add_feature(cf.BORDERS, color='red')",
    post_timing="replot",
    enable_post=True)
BRM.update(projection="moll")
BRM.show()
```

Or PolyCollection with python

```
from   matplotlib.collections import PolyCollection
```

Icontools, problems:

Interpolation method 3 (RBF) with scaling factor 0.01 produce errors after running icon-art with processing-chain (100hPA level is not found).

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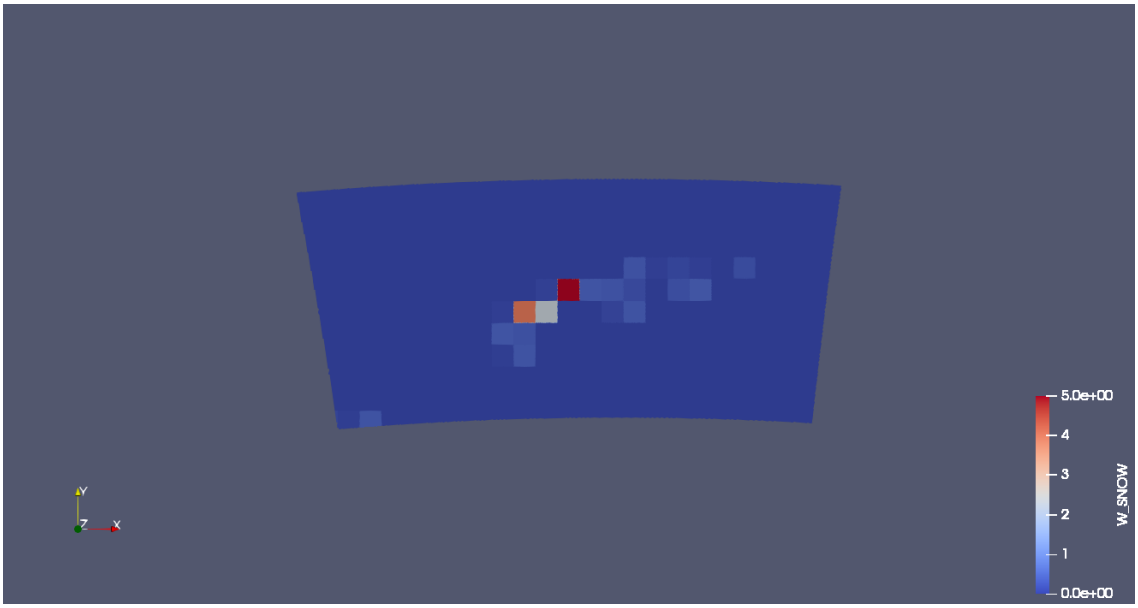
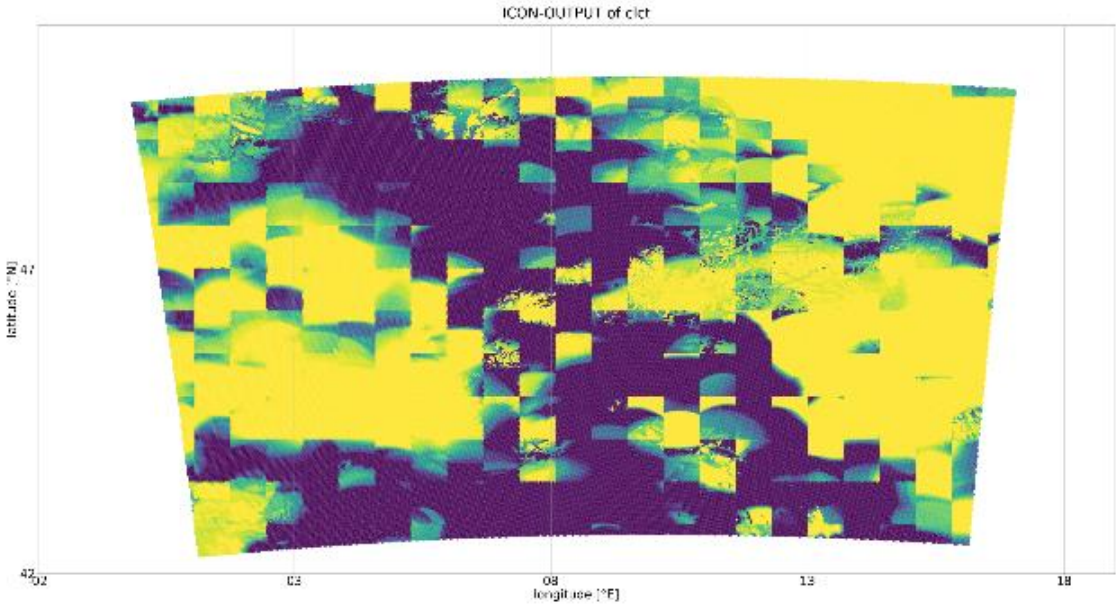
Before running Icon, we have to prepare initial conditions, i.e. remap it. Before we were doing it with Icontools, which is produced the strange chess-like pattern for almost all ic variables, we also had unrealistic w_snow variable, this snow was not melting with time and that influenced on surface fluxes in Flexpart simulations. That is why we replaced the icontools by CDO for remappinf step for IC and BCs.

Below one can see the illustration of chess-like problems in IC and unrealistic values of W_snow.



Chess-like pattern in IC remapped with Icontools:



Icon and Icontools with spack

To install icontools with spack we need to run just 3 command (it didn't work for me on Daint with icon from CSCS, but it worked for David Oschner with Icon from DWD):

```
module load cray-python

source /project/g110/spack/user/daint/spack/share/spack/setup-env.sh
```

spack install -v icontools@c2sm-master%gcc slave=daint

to install icon with spack we need git clone icon source code and run the following command

```
touch file_for_spack
spack dev-build -u build icon@dev-build%nvhpc \
          icon_target=cpu \
          +art +eccodes\
          config_dir=/users/kivanova/icon
```

```
rm file_for_spack
touch file_for_spack
spack dev-build -u build icon@dev-build%pgi \
          icon_target=cpu \
          +art +eccodes\
          config_dir=/users/kivanova/icon

rm file_for_spack
```

Icontools -> CDO for preprocessing step

Before running Icon, we have to prepare initial conditions, i.e. remap it. Before we were doing it with Icontools, which is produced the strange chess-like pattern for almost all ic variables, we also had unrealistic w_snow variable, this snow was not melting with time and that influenced on surface fluxes in Flexpart simulations. That is why we replaced the icontools by CDO for remappinf step for IC and BCs.

Below one can the script for remappimg ICs with CDO:

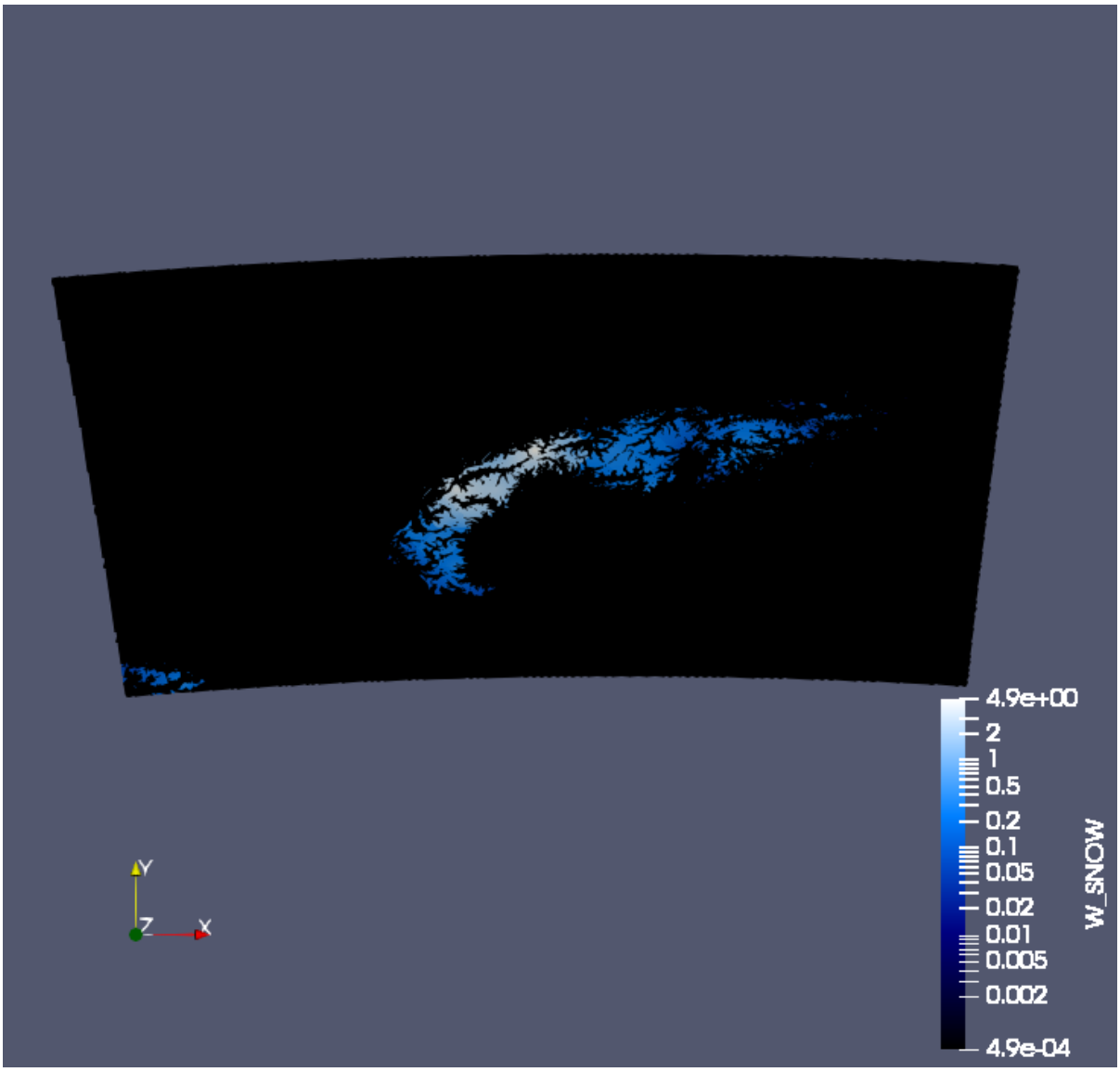
```
datafilename={cfg.input_root_meteo}/{cfg.meteo_prefix}{cfg.inidate_yyyymmddhh}{cfg.meteo_suffix}
datafile="${{datafilename##*/}}"  # get filename without path
outdatafile=${{datafile%.*}}      # get filename without suffix


cdo -t ecmwf -f nc copy {cfg.input_root_meteo}/${{datafile}} tmp1.nc
cdo setpartabn,/users/kivanova/new_lbc_processing_chain/cases/icon-art-BRM-CDOic/mypartab,convert tmp1.nc tmp2.nc

cdo selname,LSM tmp2.nc input_FR_LAND.nc
ncrename -h -v LSM,FR_LAND input_FR_LAND.nc
ls -l {cfg.extpar_filename_scratch}
cdo selname,FR_LAND {cfg.extpar_filename_scratch} output_FR_LAND.nc
ncecat -O -u time output_FR_LAND.nc output_FR_LAND.nc # add time dimension otherwise ICON stops
ncks -h -A -v time input_FR_LAND.nc output_FR_LAND.nc # give time a value to avoid CDO warnings
cdo -L setctomiss,0. -ltc,0.5  input_FR_LAND.nc input_ocean_area.nc
cdo -L setctomiss,0. -gec,0.5 input_FR_LAND.nc input_land_area.nc
cdo -L setctomiss,0. -ltc,1. output_FR_LAND.nc output_ocean_area.nc
cdo -L setctomiss,0. -gtc,0. output_FR_LAND.nc output_land_area.nc
cdo -L setrtoc2,0.5,1.0,1,0 output_FR_LAND.nc output_lsm.nc
#rm input_FR_LAND.nc output_FR_LAND.nc

# create file with ICON grid information for CDO
cdo -s selgrid,2 {cfg.dynamics_grid_filename} triangular-grid.nc

# remap land area only variables (ocean points are assumed to be undefined in the input data)
cdo setmisstodis -selname,SMIL1,SMIL2,SMIL3,SMIL4,STL1,STL2,STL3,STL4,W_SNOW,T_SNOW tmp2.nc tmpl1.nc
cdo remapdis,triangular-grid.nc tmpl1.nc tmpl2.nc
# cdo -s div tmpl2.nc output_land_area.nc tmp_output_l.nc
mv tmpl2.nc tmp_output_l.nc
rm tmpl*.nc

## remap land and ocean area differently for variables
# ocean part
cdo -s selname,SKT tmp2.nc tmp_input_ls.nc
cdo -s div tmp_input_ls.nc input_ocean_area.nc  tmpls1.nc
cdo -s setmisstodis tmpls1.nc tmpls2.nc
cdo -s remapdis,triangular-grid.nc tmpls2.nc tmpls3.nc
cdo -s div tmpls3.nc output_ocean_area.nc tmp_ocean_part.nc
# rm tmpls*.nc output_ocean_area.nc input_ocean_area.nc

# land part
cdo -s div tmp_input_ls.nc input_land_area.nc  tmpls1.nc
cdo -s setmisstodis tmpls1.nc tmpls2.nc
cdo -s remapdis,triangular-grid.nc tmpls2.nc tmpls3.nc
cdo -s div tmpls3.nc output_land_area.nc tmp_land_part.nc
# rm tmpls*.nc output_land_area.nc input_land_area.nc

# merge remapped land and ocean part
cdo -s ifthenelse output_lsm.nc tmp_land_part.nc  tmp_ocean_part.nc tmp_output_ls.nc
```

```
# remap the rest
ncks -h -O -x -v T_SNOW,STL1,STL2,STL3,STL4,SMIL1,SMIL2,SMIL3,SMIL4,SKT,LSM tmp2.nc tmp_input_rest.nc
cdo -s remapdis,triangular-grid.nc tmp_input_rest.nc ifs_ini.nc


# remap the snow
ncks -h -O -x -v W_SNOW tmp2.nc tmp_input_snow.nc
cdo -s remapdis,triangular-grid.nc tmp_input_snow.nc ifs_ini.nc



# merge remapped files plus land sea mask from EXTPAR
ncks -h -A tmp_output_l.nc ifs_ini.nc
ncks -h -A tmp_output_ls.nc ifs_ini.nc
ncks -h -A output_lsm.nc  ifs_ini.nc
rm -f tmp_output_l.nc tmp_output_ls.nc tmp_input_ls.nc tmp_input_rest.nc output_lsm.nc


# attribute modifications
ncatted -h -a coordinates,FR_LAND,o,c,"clon clat" ifs_ini.nc

# renamings
ncrename -h -v FR_LAND,LSM ifs_ini.nc
ncrename -h -d cell,ncells ifs_ini.nc
ncrename -h -d nv,vertices ifs_ini.nc

cdo expr,"PS=exp(LNPS)" ifs_ini.nc PS.nc
cdo merge PS.nc ifs_ini.nc out_test1.nc
cdo selvar,W_SNOW out_test1.nc wsnow.nc
cdo selvar,topography_c {cfg.extpar_filename_scratch} topo.nc
cdo merge wsnow.nc topo.nc merged.nc
# cdo setrtoc,-1.e99,9999,0 out_wsnow0.nc {cfg.icon_input_icbc}/${{outdatafile}}.nc
ncap2 -s 'where(topography_c<=2000) W_SNOW=0' merged.nc wsnow_topo.nc
cdo selvar,W_SNOW wsnow_topo.nc right_wsnow.nc
cdo replace out_test1.nc right_wsnow.nc {cfg.icon_input_icbc}/${{outdatafile}}.nc
```

Below one can see the script to remap BCs with CDO.

```
export ECCODES_DEFINITION_PATH=/project/g110/spack-install/daint/eccodes/2.19.0/pgi/g5wilnyap5zgpzwfuamx6g47zrki2uk4/share/eccodes/definitions
echo $ECCODES_DEFINITION_PATH

export BINARY_DIR=/project/g110/spack-install/daint/icontools/c2sm-master/gcc/eg76zscn2fwv3fkglbmas63pnqe6dywx/bin

ln -sf /users/kivanova/new_lbc_processing_chain/cases/icon-art-BRM-CDOic/mypartab

#------------------------------------------------------------------------
# Extract boundary data
#------------------------------------------------------------------------
#------------------------------------------------------------------------
cdo selgrid,2 {cfg.lateral_boundary_grid} triangular-grid_lbc.nc
# loop over file list:

echo "DATAFILELIST is {datafile_list_rest}"
for datafilename in {datafile_list_rest} ; do
    datafile="${{datafilename##*/}}"  # get filename without path
    outdatafile=${{datafile%.*}}      # get filename without suffix
  
  cdo -t ecmwf -f nc copy {cfg.input_root_meteo}/${{datafile}} tmp1_lbc.nc
  cdo setpartabn,/users/kivanova/new_lbc_processing_chain/cases/icon-art-BRM-CDOic/mypartab,convert tmp1_lbc.nc tmp2_lbc.nc
  cdo -s remapdis,triangular-grid_lbc.nc -selname,T,U,V,W,LNPS,QV,QI,QR,QC,QS tmp2_lbc.nc {cfg.icon_input_icbc}/${{outdatafile}}_lbc.nc
  cdo merge {cfg.icon_input_icbc}/${{outdatafile}}_lbc.nc GEOSP.nc mergedlbc.nc
  mv mergedlbc.nc {cfg.icon_input_icbc}/${{outdatafile}}_lbc.nc
  ncrename -d cell,ncells {cfg.icon_input_icbc}/${{outdatafile}}_lbc.nc
  ncrename -d nv,vertices {cfg.icon_input_icbc}/${{outdatafile}}_lbc.nc

done

#------------------------------------------------------------------------
# clean-up

rm -f nml.log

#------------------------------------------------------------------------
exit
```

W_snow



LNPS initial condition remapped with CDO