How to compile the MOLOCH model and setup a domain on the ECMWF ATOS supercomputer

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- 1. Download the latest version of the Moloch (and ISAC's) model from the gitlab repository. It normally has the name globo-bolam-moloch-main.tar.gz
- 2. The suggested folders scheme is as in Figure 1
- 3. Load modules:
 - (a) module purge
 - (b) module load prgenv/intel
 - (c) module load intel
 - (d) module load ecmwf-toolbox
 - (e) module load netcdf4
 - (f) module list
- 4. Download from the github repository the radiation libray from ECMWF (latest version) and compile it in the suggested fols -Irtlder DA QUI
- 5. you need the following files:
 - moloch_v22.tar.gz, the model source files
 - rad_ecmwf.tar.gz, the radiation package from ECMWF
 - the compile-* files, which contain few commands to link libraries and compile sources with the appropriate compiler
- 6. the v22 folder contains the source code, namely common_routines.F90, moloch.F90, ppostmol.F90, premoloch.F90, prepar_grib2_coding_data.F90, read_grib2_data.F90, shf2grib2.F90, write_grib2_data.F90
- 7. go in the rad_ecmwf directory and compile radiation module (as edit by ISAC/CNR staff). Targeted instructions to compile rad_ecmwf library are available in the tar archive. Remember that this is the OLD version of ECMWF radiation scheme. More updated software is available since September 2023 from A. Buzzi (or someone else from ISAC/CNR); options for a standard Linux machine options.linux with gfortran are: FC=gfortran

FFLAGS = -c -w -fallow-invalid-boz -I ../module -fopt-info-vec-optimized

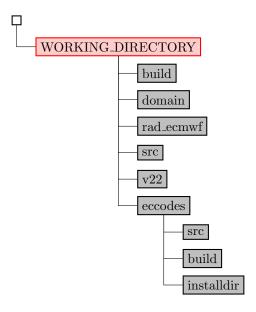


Figure 1: Suggested directory tree

- 8. go in the domain directory. You need the following files:
 - dimensions.inc: defines the dimensions of the grid based on the number of cores available
 - o geo.F90 and geo.inc: define the geographical position of the grid and the static fields
 - * premoloch.inp, moloch.inp, ppostmol.inp and grib_sample.inp: are namelists (see below)

Proceed as follows:

• dimensions.inc: it looks like

```
integer, parameter :: gnlon=450, gnlat=546, nlev=50, nlevg=7
integer, parameter :: nprocsx=8, nprocsy=16
```

Suppose you have P cores and you want to setup a domain with N_x and N_y grid points in the longitude and latitude direction, respectively. Then you have to:

- (a) factorize P as in $P = P_x \times P_y$ (8 and 16 in the example above)
- (b) divide N_x by P_x and consider the closest even number
- (c) add 2 to the result of the previous step and you get the value for gnlon
- o geo.inc: it looks like

```
! Grid parameters for {\tt geo.F90} and {\tt plot\_geo\_domain\_18.F90}
```

! (values must be consistent with those in prebolam.inp

where nlon and nlat are defined in dimensions.inc, dlat is the desired resolution (in degrees), for instance is approximately 0.025 for a grid spacing of 2500 m and dlon is obtained by applying the formula dlat/cos(lat0), where lat0 is a mean latitude of the model grid (latitude of the center fo the grid?). alon0 and alat0 must define the true coordinates of the bottom-left corner of the domain.

Once geo.inc is defined, compile geo.F90 with ifort, link the static global data, namely soil12.bin, orography120.bin and landuse120.bin, and run geo.exe, which should produce geo.bin

ATTENZIONE NON SI RIESCE A COMPILARE geo.F90 CON gfortran PERTANTO NON SI VA AVANTI...

- 9. go in the build directory where you need to have the compila-moloch file. In this file nothing has to be changed unless you want to use a more aggressive compilation flag (03). In this directory you further need the links the following files:
 - moloch.F90: available in the v22 directory
 - dimensions.inc: available in the domain directory
 - version: which should point to the v22 directory

Run compila-moloch which should produce moloch.exe.

Similar steps for compila-premoloch ¹, compila-ppostmol and compila-shf2grib2

A titolo d'esempio:

```
cp $SOURCE_DIR/compila-* .
cp $SOURCE_DIR/geo.F90 .
cp $SOURCE_DIR/dimensions.inc .
cp $SOURCE_DIR/geo.inc .
ln -svf $GEOG_DIR/GEOG_DATA/mol/* .
#vim dimensions.inc
#vim geo.inc
ifort geo.F90
./a.out
ln -svf $SOURCE_DIR/v22 version
cp version/moloch.F90 .
sh compila-moloch
module load ecmwf-toolbox
sh compila-premoloch
sh compila-ppostmol
sh compila-shf2grib2
```

dove vim dimensions.inc e vim geo.inc devono essere editati seguendo le regole per la griglia di MOLOCH.

¹if the eccodes is not loaded, load it first before compiling premoloch, then add the full pat of the library in the compila-premoloch