

HOW TO

install libraries to compile/run Eco3M in the mini-CLUSTER (IEO)

Step-by-step guide to setting up an environment where you use the **Intel ifort compiler** for fortran with MPI and have support for **HDF5**, **NetCDF**, and **PnetCDF** libraries.

This setup uses **conda** for managing dependencies but Intel compilers and PnetCDF are not available via conda, therefore they need to be installed separately.

Conda is not available in the cluster, you can install miniconda following these instructions:
/home/alvarez/EVA/Eco3M-MAR_MENOR/instructions_conda.txt

1. Install Intel OneAPI:

The Intel oneAPI toolkit includes ifort, icc, icpc, and Intel MPI. Go to the Intel OneAPI page (<https://www.intel.com/content/www/us/en/developer/tools/oneapi/toolkits.html#gs.fk8h75>) and download the "Base Toolkit" and "HPC Toolkit", for Linux and the Offline Installer.

Follow Intel's official installation guide:

<https://www.intel.com/content/www/us/en/docs/oneapi/installation-guide-linux/2024-2/install-with-command-line.html#GUID-56B16998-1363-40F5-A6D5-6A3D5B877F37>

which, if you do not have root permission, summarizes in doing:

```
sh ./l_BaseKit_p_2024.2.1.100_offline.sh -a --silent --eula accept
sh ./l_HPCKit_p_2024.2.1.79_offline.sh -a --silent --eula accept
```

Find the files here: /home/alvarez/EVA/Eco3M-MAR_MENOR/intel-oneAPI

After installation, find where `/intel/oneapi/` was installed (if you installed as user, it will be at `$HOME`) and source the `setvars.sh` script by doing:

```
source ~/intel/oneapi/setvars.sh
```

This script sets up the environment for Intel compilers and MPI.

Add the line to your `.bashrc` file in case you want to set the variables every time you enter the cluster.

2. Create the Conda Environment:

Create a new conda environment using the `.yml` file available in the repository (https://github.com/ealvarez-s/Eco3M-MAR_MENOR.git).

```
cd /home/alvarez/EVA/Eco3M-MAR_MENOR/
conda env create -f environment.yml
conda activate belich-legos
```

Find the files here: /home/alvarez/EVA/Eco3M-MAR_MENOR

3. Set Compilers and MPI Environment Variables:

With the conda environment active! ensure that mpifort uses the Intel ifort compiler and Intel MPI. You'll need to configure your environment variables as follows:

```
export CC=gcc
export CXX=g++
export FC=ifort
export MPICC=mpiicc
export MPICXX=mpiicpc
export MPIFC=mpiifort

export I_MPI_CC=gcc
export I_MPI_CXX=g++
export I_MPI_FC=ifort
```

To ensure that mpifort will use ifort, find the *mpifort* script within the conda environment and change the FC variable (*this step can be done after installing pnetcdf*):

```
~/miniconda3/envs/belich-/bin/mpifort
#FC="x86_64-conda-linux-gnu-gfortran"
FC="ifort"
```

4. Install PnetCDF:

You need to build and install PnetCDF from the source, as it is not available directly through conda channels. Download PnetCDF by doing:

```
wget https://parallel-netcdf.github.io/Release/pnetcdf-1.12.3.tar.gz
tar -xvf pnetcdf-1.12.3.tar.gz
cd pnetcdf-1.12.3
```

Find the files here: /home/alvarez/EVA/Eco3M-MAR_MENOR/pnetcdf-1.12.3

Before running `./configure`, ensure any previous failed configuration attempt is completely removed. Just in case, run:

```
make clean
rm -rf config.log
rm -rf autom4te.cache
```

And make sure you are installing PnetCDF within the conda environment.

Configure PnetCDF with Intel compilers and MPI by doing:

```
./configure --prefix=$CONDA_PREFIX CC=gcc CXX=g++ FC=ifort MPICC=mpiicc
MPIFC=mpiifort
```

If the configure step fails, use these flags for a debug and more verbose version:

```
CFLAGS="-O2" --enable-debug
```

Build and install it, by doing:

```
make
make install
```

If installation is successful, it will tell you the LIB and NETINC paths. They should be the same for **netcdf**, but just in case double check by running:

```
nc-config -all
```

Those paths need to go to the `makefile.inc` in:

```
~/EVA/Eco3M-MAR_MENOR/SYMPHONIE_368/UDIR/BGC_MAR_MENOR2/makefile.inc
```

Example:

```
NETINC=-I/home/alvarez/miniconda3/envs/belich-legos/include  
LIB=-L/home/alvarez/miniconda3/envs/belich-legos/lib -lnetcdff -lnetcdf -  
lpnetcdf
```

Other tips in the `makefile.inc`:

to avoid messages about the intel MPI version, use `-diag-disable=10448` as compiling flag.
F90 can be set to `mpifort` or `mpiifort`.

To compile:

```
conda activate belich-legos (make sure the environment is active!)  
cd ~/EVA/Eco3M-MAR_MENOR/SYMPHONIE_368/UDIR/BGC_MAR_MENOR2  
make
```

This will create the executable in:

```
~/EVA/Eco3M-MAR_MENOR/SYMPHONIE_368/RDIR/BGC_MAR_MENOR2/S26.exe
```