Compilation of WRF on HPC

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Introduction

- HPC is not only hardware but also best practices with software and efficient use of resources.
- Synonymous with parallel processing.
- Procedure :
  - configure
  - compile
  - Run
- How many faced problem early in configure phase ?

Build WRF on HPC (not only)

- WRF depends on `NetCDF` (and its dependencies), requires although not necessary parallel `NetCDF`, `NetCDF4` features, compression.
- Typically one has to setup the environment modules necessary to fulfill these requirements :
- modules : Compiler(s), MPI, netcdf, hdf5, szip (necessary for hdf5), jasper
- On ARIS with intel compilers, IntelMPI : gnu/8 intel/18 intelmpi/2018 netcdf/4.4.1/intel hdf5/1.8.17/intel szip jasper
- ./configure, select the right option (depends on version, with 4.6.1, option 20 (dmpar, Intel, SNB)
- First failure

Build WRF on HPC (not only)

- Message from configure

```
NETCDF4 IO features are requested, but this
installation of NetCDF
/apps/libraries/netcdf/4.4.1/intel
DOES NOT support these IO features.

Please make sure NETCDF version is 4.1.3 or
later and was built with --enable-netcdf4

OR set NETCDF_classic variable
   bash/ksh : export NETCDF_classic=1
        csh : setenv NETCDF_classic 1

Then re-run this configure script

!!! configure.wrf has been REMOVED !!!
```

Build WRF on HPC (not only)

- It says : Need netcdf > 4.1.3 while we use 4.4.1, needs netcdf4, suggest to export vars for `NETCDF_classic` $\Longrightarrow$ no parallel, no compression $\Longrightarrow$ parallel issues and large files.
- Those who are familiar with netcdf, can see with nc-config that netcdf in use **IS** nc4 enabled :
  `nc-config --has-nc4` gives `yes`
- Next steps : Ask support to install netcdf with these features (while available), or just help.
- Indication that the configure system netcdf features detection is problematic.

Build WRF on HPC (not only)

- What to look :
- In WRF-4.x.y tree there is a directory `tools`. There configure checks for features of netcdf. In `nc4_test.log` you see the reason : Many undefined references to MPI calls, i.e. tries to link with MPI enabled library without MPI compiler or supplying MPI libraries.

Build WRF on HPC (not only)

- What to do to fix it permanently i.e. valid for another future configure:
  - in `arch/configure.defaults`, section with SNB (in the case of option 20 in configure of 4.6.1), change

```
SFC             =       ifort
SCC             =       icc
CCOMP           =       icc
DM_FC           =       mpif90 -f90=$(SFC)
DM_CC           =       mpicc -cc=$(SCC)
```

with

```
SFC             =       mpiifort
SCC             =       mpiicc
CCOMP           =       mpiicc
DM_FC           =       mpiifor
DM_CC           =       mpiicc
```

Build WRF on HPC (not only)

- configure again, select option 20,

```
....
NetCDF version: 4.4.1
Enabled NetCDF-4/HDF-5: yes
NetCDF built with PnetCDF: no

******************************************************************************
This build of WRF will use NETCDF4 with HDF5 compression
******************************************************************************
```

- So simple ? Problem solved. Let's try to compile : `./compile -j 4 em_real`, wait few hours.....

```
--->                  Executables successfully built                  <---
```

- Executables created.
- With 4.6.1 a lot of things improved, with previous versions more modifications are needed - see WPS notes.

Build WRF on HPC (not only)

- Let’s go to WPS (not yet improved.)

```
export WRF_DIR=`pwd`
cd ../WPS-4.6.0
```

- configure again, select option 20, `./configure`, select option 23 to be consistent with previous build of WRF, compile.

Build WRF on HPC (not only)

- ```
  Configuration successful. To build the WPS, type: compile
  ------------------------------------------------------------------------

  Testing for NetCDF, C and Fortran compiler

  This installation NetCDF is 64-bit
  C compiler is 64-bit
  Fortran compiler is 64-bit

  Your versions of Fortran and NETCDF are not consistent.
  ```
- New inconsistency, different.
  ```

Build WRF on HPC (not only)

- Now we are aware, in arch/configure.defaults in the corresponding section change

```
SFC                     = ifort
SCC                     = icc
DM_FC                   = mpif90
DM_CC                   = mpicc
```

to

```
SFC                     = mpiifort
SCC                     = mpiicc
DM_FC                   = mpiifort
DM_CC                   = mpiicc
```

- Problem Remains.

Build WRF on HPC (not only)

- in `configure`, lin 434 of v4.6.0, it tries for netcdf only with `-lnetcdf` and no dependencies.
- Add after `-lnetcdf` :

```
-L${HDF5ROOT}/lib -L${SZIPROOT}/lib -lnetcdf \
-lhdf5_hl -lhdf5 -lcurl -lsz -lz
```

- `./configure`, `./compile`, Again fails, a lot of undefined H5 calls, suggest that extra necessary libs are not used in link.

Build WRF on HPC (not only)

- In arch/preample, `WRF_LIB` variable add after `-lnetcdf`,
  `-L$(HDF5ROOT)/lib -L$(SZIPROOT)/lib -lhdf5_hl\`
  `-lhdf5 -ldl -lm -lcurl -lsz -lz`
  Note parentheses instead curly brackets in notation.
- In previous versions, more points to change.
- If you need to use GRIB2 format files, more libraries are needed (jpegturbo etc.) and adjustments.
- In variants like `WRF_CHEM`, `WRF_DA` more libraries and adjustments are necessary.
- Up to now, only success in compilation covered, optimizations in next session.

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