2020 Summer School on Effective HPC for Climate and Weather

Input/Output and Middleware

Luciana Pedro, Julian Kunkel

Department of Computer Science, University of Reading

18 June 2020

esiwace
CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER
AND CLIMATE IN EUROPE

Outline

1 NetCDF Files and C

2 NetCDF Utilities

3 Practising

Disclaimer: This material reflects only the author's view and the EU-Commission is not responsible for any use that may be made of the information it contains

Learning Objectives

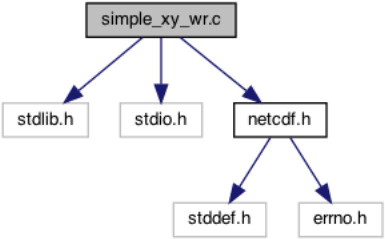
- Execute programs in C that read and write NetCDF files in a metadata-aware manner
- Analyze, manipulate and visualise NetCDF data

References

- The files and data used in this presentation were collected on the Unidata website.
    - `https://www.unidata.ucar.edu/`
- All files used here are available in the following Git Repository:
    - `https://github.com/ESiWACE/io-training`
- These files are also available with the NetCDF main installation, in the directory `examples`.
- For more information about how to install NetCDF in your personal computer, from scratch, check Section 4.

File Reference: simple_xy_wr.c

- This is an example program demonstrating a simple 2D write. It is intended to illustrate the use of the NetCDF C API.
  - https://www.unidata.ucar.edu/software/netcdf/docs/simple__xy__wr_8c.html
  - https://www.unidata.ucar.edu/software/netcdf/docs/simple__xy__wr_8c_source.html
- Dependency graph for simple_xy_wr:



File simple_xy_wr.c: Header and Constants Declaration

```
#include <stdlib.h>
#include <stdio.h>
#include <netcdf.h>

/* This is the name of the data file we will create. */
#define FILE_NAME "simple_xy.nc"

/* We are writing 2D data, a 6 x 12 grid. */
#define NDIMS 2
#define NX 6
#define NY 12

/* Handle errors by printing an error message and exiting with a
* non-zero status. */
#define ERRCODE 2
#define ERR(e) {printf("Error: %s\n", nc_strerror(e)); exit(ERRCODE);}
```

- Standard C libraries and main NetCDF library.
- Define the name for the NetCDF file.
- Define the total number of dimensions.
- Define each of the dimensions.
- Define error codes and messages.

File `simple_xy_wr.c`: Variables Declaration

```
...
...
...

int main()
{
  /* When we create NetCDF variables and dimensions, we get back an
   * ID for each one. */
  int ncid, x_dimid, y_dimid, varid;
  int dimids[NDIMS];

  /* This is the data array we will write. It will be filled with a
   * progression of numbers for this example. */
  int data_out[NX][NY];

  /* Loop indexes, and error handling. */
  int x, y, retval;

  ...
  ...
  ...
}
```

- Main program.
- Note that each variable represents an id.
  - `ncid`: id for the NetCDF file.
  - `x_dimid`: id for the x dimension.
  - `x_dimid`: id for the y dimension.
  - `dimids`: vector with all dimensions ids.
- Vector that will store the data.

File simple_xy_wr.c: Creating (loading!) Data

```
...

int main()
{
  ...

  /* Create some pretend data. If this wasn't an example program, we
   * would have some real data to write, for example, model
   * output. */
  for (x = 0; x < NX; x++)
     for (y = 0; y < NY; y++)
        data_out[x][y] = x * NY + y;

  ...
}
```

- Real data can be loaded using different databases and functions in C.
- In this example, the data is generated by a simple formula.

File simple_xy_wr.c: Creating the NetCDF file

```
...

int main()
{
  ...

  /* Always check the return code of every NetCDF function call. In
   * this example program, any retval which is not equal to NC_NOERR
   * (0) will cause the program to print an error message and exit
   * with a non-zero return code. */

  /* Create the file. The NC_CLOBBER parameter tells NetCDF to
   * overwrite this file, if it already exists.*/
  if ((retval = nc_create(FILE_NAME, NC_CLOBBER, &ncid)))
     ERR(retval);

  ...
}
```

- The function to create a NetCDF file is called `nc_create`.
- This function has three parameters:
  - The name of the file.
  - The mode to open the file.
  - It returns the id for the NetCDF file.

File simple_xy_wr.c: Defining the Dimensions

```
...

int main()
{
  ...

  /* Define the dimensions. NetCDF will hand back an ID for each. */
  if ((retval = nc_def_dim(ncid, "x", NX, &x_dimid)))
     ERR(retval);
  if ((retval = nc_def_dim(ncid, "y", NY, &y_dimid)))
     ERR(retval);

  /* The dimids array is used to pass the IDs of the dimensions of
   * the variable. */
  dimids[0] = x_dimid;
  dimids[1] = y_dimid;

  ...
}
```

- The function to define new dimensions in a NetCDF file is called `nc_def_dim`.
- This function has four parameters:
  - The id of the NetCDF file.
  - The name of the dimension to be created.
  - The size of the dimension to be created.
  - It returns the id for created dimension.
- The vector `dimids` stores the ids for the created dimensions.

File simple_xy_wr.c: Defining a Variable

```
...

int main()
{
  ...

  /* Define the variable. The type of the variable in this case is
   * NC_INT (4-byte integer). */
  if ((retval = nc_def_var(ncid, "data", NC_INT, NDIMS,
                dimids, &varid)))
     ERR(retval);

  ...
}
```

- The function to define new variables in a NetCDF file is called `nc_def_var`.
- This function has six parameters:
  - The id of the NetCDF file.
  - The name of the variable to be created.
  - The type of the variable to be created.
  - The number of dimensions of the variable.
  - The vector that stores the ids for the dimensions.
  - It returns the id for created variable.

File simple_xy_wr.c: Defining a Variable

```
...

int main()
{
  ...

  /* End define mode. This tells NetCDF we are done defining
   * metadata. */
  if ((retval = nc_enddef(ncid)))
     ERR(retval);

  ...
}
```

- Classic NetCDF:
  - In **define mode**, dimensions, variables, and new attributes can be created but variable data cannot be read or written.
  - In **data mode**, data can be read or written and attributes can be changed, but new dimensions, variables, and attributes cannot be created.
- **NOTE:** NetCDF-4 does not distinguish between define and data modes.

File simple_xy_wr.c: Writing Data into the File

```
...

int main()
{
  ...

  /* Write the pretend data to the file. Although NetCDF supports
   * reading and writing subsets of data, in this case we write all
   * the data in one operation. */
  if ((retval = nc_put_var_int(ncid, varid, &data_out[0][0])))
     ERR(retval);

  ...
}
```

- The function to write the data in a variable is called `nc_put_var_*`. In this example, we have `nc_put_var_int`.
- This function has four parameters:
  - The id of the NetCDF file.
  - The id of the variable that will store the data.
  - (A pointer to) the data.

File simple_xy_wr.c: Writing Data into the File

```
...

int main()
{
  ...

  /* Close the file. This frees up any internal NetCDF resources
   * associated with the file, and flushes any buffers. */
  if ((retval = nc_close(ncid)))
     ERR(retval);

  ...
}
```

- The function to close a NetCDF file is called `nc_close`.
- This function has one parameter:
  - The id of the NetCDF file.

File `simple_xy_wr.c`: Getting SUCCESS!

```
...

int main()
{
  ...

  printf("*** SUCCESS writing example file simple_xy.nc!\n");
  return 0;
}
```

- If everything is done properly, we end the main program with a nice and encouraging message.
- Hopefully, also with a new NetCDF file!

Using nc-config

- The `nc-config` command-line utility assists with the setting of compiler and linker flags for building applications.

- `nc-config` is a simple script that reports the configuration flags used during the NetCDF build, as well as the installed version of the NetCDF C-based libraries.

- It has lots of options, listed by invoking `$(nc-config --all)`.

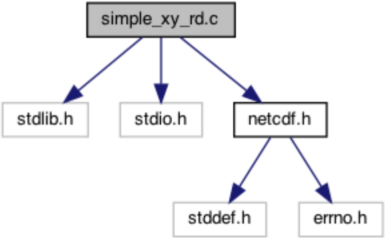
- Here we will use `nc-config` to compile and link a C application:
  - `gcc myapp.c -o myapp $(nc-config --libs --cflags)`

Compiling and Running the File simple_xy_wr.c

- Create (copy!) and compile the file `simple_xy_wr.c`.
  - `gcc simple_xy_wr.c -o simple_xy_wr $(nc-config --libs --cflags)`
- Run the file `simple_xy_wr`.
  - `./simple_xy_wr`
  - `*** SUCCESS writing example file simple_xy.nc!`
- Check that the file `simple_xy.nc` is in your directory.

File Reference: `simple_xy_rd.c`

- This is a simple example which reads a small dummy array that was written by `simple_xy_wr.c`.
  - `https://www.unidata.ucar.edu/software/netcdf/docs/simple__xy__rd_8c.html`
  - `https://www.unidata.ucar.edu/software/netcdf/docs/simple__xy__rd_8c_source.html`
- Dependency graph for `simple_xy_rd`:



File simple_xy_rd.c

```
int main()
{
   /* Open the file. NC_NOWRITE tells NetCDF we want read-only access
    * to the file.*/
   if ((retval = nc_open(FILE_NAME, NC_NOWRITE, &ncid)))
      ERR(retval);

   /* Get the varid of the data variable, based on its name. */
   if ((retval = nc_inq_varid(ncid, "data", &varid)))
      ERR(retval);

   /* Read the data. */
   if ((retval = nc_get_var_int(ncid, varid, &data_in[0][0])))
      ERR(retval);

   /* Check the data. */
   for (x = 0; x < NX; x++)
      for (y = 0; y < NY; y++)
         if (data_in[x][y] != x * NY + y)
            return ERRCODE;

   /* Close the file, freeing all resources. */
   if ((retval = nc_close(ncid)))
      ERR(retval);
}
```

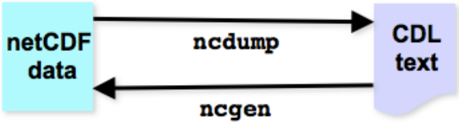
- The function to open a NetCDF file is called `nc_open`. It is similar to the function `nc_create` and it has the same parameters.
- The function `nc_inq_varid` is called to find the id of a variable. It has three parameters:
  - The id of the NetCDF file.
  - The name of the variable.
  - It returns the id for the variable.
- The function `nc_get_var_*` is called to read data of a variable. In this example, we have `nc_get_var_int`. It has three parameters:
  - The id of the NetCDF file.
  - The id of the variable.
  - It returns the data stored in the variable.

Reading the File `simple_xy.nc`

- Check that the file `simple_xy.nc` is in your directory.
- Create (copy!), compile and run the file `simple_xy_rd.c`.
  - `gcc simple_xy_rd.c -o simple_xy_rd $(nc-config --libs --cflags)`
- Run the file `simple_xy_rd`.
  - `./simple_xy_rd`
  - `*** SUCCESS reading example file simple_xy.nc!`

ncdump and ncgen

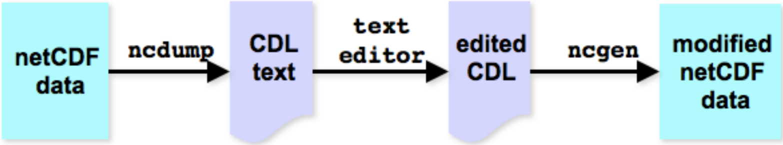
- ncdump and ncgen are inverses:



- Used together, ncdump and ncgen can accomplish simple NetCDF manipulations with little or no programming.

Editing a NetCDF File

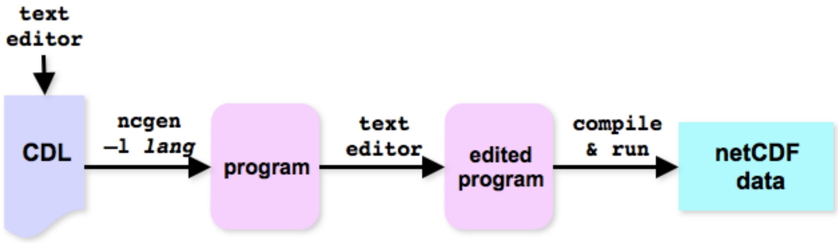
- To edit metadata or data in a NetCDF file:



  - Use `ncdump` to convert NetCDF file to CDL.
  - Use a text editor to make desired change to CDL.
  - Use `ncgen` to turn modified CDL back into NetCDF file.
  - **Note:** This option is not practical for huge NetCDF files or if one intend to modify lots of files. For that, need to write a program using NetCDF library.

Creating a NetCDF File

- To create a new NetCDF file with lots of metadata:



- Use a text editor to write a CDL file with lots of metadata but little or no data.
- Use `ncgen` to generate corresponding C or Fortran program for writing NetCDF.
- Insert appropriate NetCDF **var_put** calls for writing data.
- Compile and run program to create NetCDF file.
- Use `ncdump` to verify result.

Using ncdump

- Inspect the file `simple_xy.nc` using `ncdump`:
  - `ncdump simple_xy.nc`
- Inspect the metadata of the file `simple_xy.nc` using `ncdump`:
  - `ncdump -h simple_xy.nc`
- Check other options for `ncdump` with:
  - `ncdump --help`

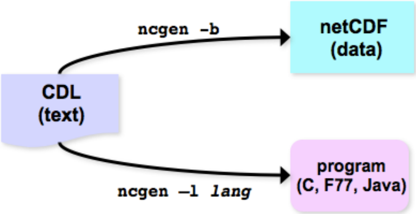
NetCDF CDL Format

```
netcdf simple_xy {
dimensions:
x = 6 ;
y = 12 ;
variables:
int data(x, y) ;
data:

 data =
  0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11,
  12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23,
  24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35,
  36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47,
  48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59,
  60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71 ;
}
```

Using ncgen

- Create a NetCDF file using ncgen and the CDL output
  - `ncdump simple_xy.nc > simple_xy_test.cdl`
  - `more simple_xy_test.cdl`
  - `ncgen -b simple_xy_test.cdl`
  - `cmp simple_xy_test.nc simple_xy.nc`



Creating the C File

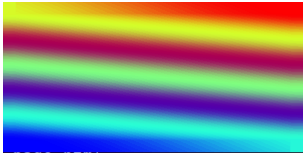
- Create a C file using `ncgen` and the CDL output
  - `ncgen -lc simple_xy_test.cdl > simple_xy_test.c`
  - `more simple_xy_test.c`
  - What is the difference between the files `simple_xy_test.c` and `simple_xy_wr.c`?
    - `cmp simple_xy_test.c simple_xy_wr.c`
    - `meld simple_xy_test.c simple_xy_wr.c`

Starting All Over Again!

```
gcc simple_xy_test.c -o simple_xy_test $(nc-config --libs --cflags)
mv simple_xy_test.nc simple_xy_test2.nc
./simple_xy_test
cmp simple_xy_test.nc simple_xy_test2.nc
```

Using ncview

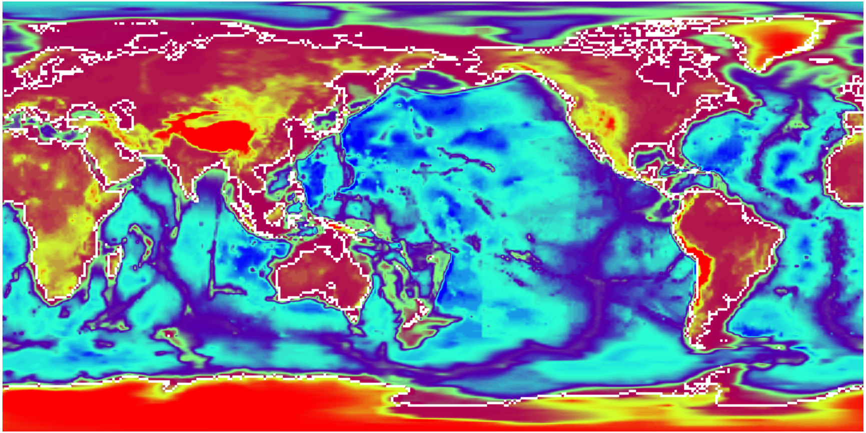
- `ncview simple_xy.nc`



```
netcdf simple_xy {
dimensions:
x = 6 ;
y = 12 ;
variables:
int data(x, y) ;
data:

 data =
  0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11,
  12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23,
  24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35,
  36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47,
  48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59,
  60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71 ;
}
```

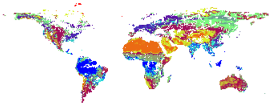
Using ncview – A Global Example



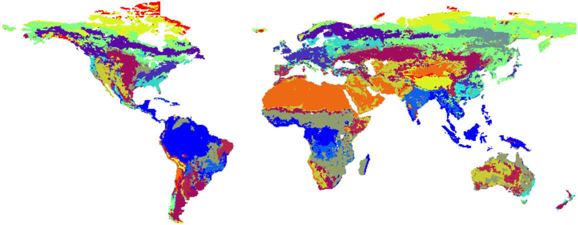
File `elevations.nc`

Global Potential Vegetation Dataset

- File vegtype_5min.nc – NetCDF 5 min data
- File vegtype_0.5.nc – NetCDF data aggregated to a 0.5 deg resolution



File vegtype_5min.nc

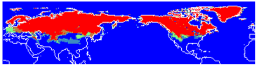


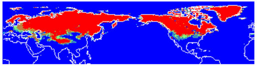
File vegtype_0.5.nc

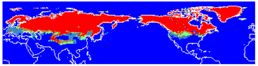
Files available at http://nelson.wisc.edu/sage/data-and-models/global-potential-vegetation/index.php

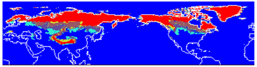
Northern Hemisphere EASE-Grid Weekly Snow Cover

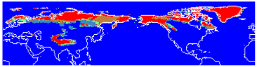
- File `snowcover.mon.mean.nc`

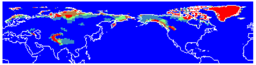

January

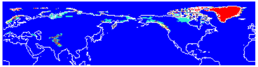

February

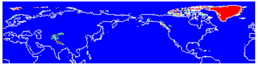

March

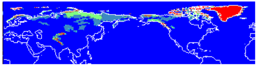

April

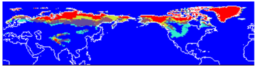

May

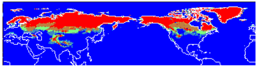

June

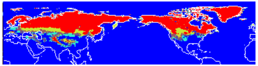

July


August


September


October


November


December

File available at `https://psl.noaa.gov/data/gridded/data.snowcover.html`.

Other NetCDF Utilities

- Many other useful netCDF utilities developed by third parties are available:
  - NCAR Command Language (NCL)
    - `https://www.unidata.ucar.edu/software/netcdf/software.html#NCL`
  - NCO (NetCDF operators)
    - `https://www.unidata.ucar.edu/software/netcdf/software.html#NCO`
  - CDO (Climate Data Operators)
    - `https://www.unidata.ucar.edu/software/netcdf/software.html#CDO`
- For additional utility software, consult:
  - Unidata's Software for Manipulating or Displaying NetCDF Data
    - `http://www.unidata.ucar.edu/netcdf/software.html`

Files for Practising

- File `simple_xy_nc4`
  - Write/Read the `simple_xy` file with some of the features of NetCDF-4.
  - https://www.unidata.ucar.edu/software/netcdf/docs/simple__xy__nc4__wr_8c.html
  - https://www.unidata.ucar.edu/software/netcdf/docs/simple__xy__nc4__rd_8c.html
- File `simple_nc4`
  - Write/Read a file demonstrating some of the features of NetCDF-4.
  - https://www.unidata.ucar.edu/software/netcdf/docs/simple__nc4__wr_8c.html
  - https://www.unidata.ucar.edu/software/netcdf/docs/simple__nc4__rd_8c.html

Files for Practising

- File `sfc_pres_temp`
  - This is an example program which writes/reads surface pressure and temperatures.
  - `https://www.unidata.ucar.edu/software/netcdf/docs/sfc__pres__temp__wr_8c.html`
  - `https://www.unidata.ucar.edu/software/netcdf/docs/sfc__pres__temp__rd_8c.html`
- File `pres_temp_4D`
  - This is an example program which writes/reads 4D pressure and temperatures.
  - `https://www.unidata.ucar.edu/software/netcdf/docs/pres__temp__4D__wr_8c.html`
  - `https://www.unidata.ucar.edu/software/netcdf/docs/pres__temp__4D__rd_8c.html`

Files for Practising

Global Potential Vegetation Dataset

- File vegtype_5min.nc – NetCDF 5 min data
- File vegtype_0.5.nc – NetCDF data aggregated to a 0.5 deg resolution
- Files available at:
  - http://nelson.wisc.edu/sage/data-and-models/global-potential-vegetation/index.php

Northern Hemisphere EASE-Grid Weekly Snow Cover

- File snowcover.mon.mean.nc – Monthly Mean
- File snowcover.mon.ltm.nc – Monthly Long Term Mean
- Files available at:
  - https://psl.noaa.gov/data/gridded/data.snowcover.html

Summary of Actions

- Inspect the write and read files in C code.
- Compile and run the write/read C files.
- Inspect the output NetCDF file (.nc) using `ncdump`.
- Create a CDL file for the NetCDF file.
- Recreate the NetCDF file using `ncgen` and the CDL file.
- Recreate the C file using `ncgen` and the CDL file.
- Visualize the data in the NetCDF file with `ncview`.
- Change dimensions, variables, and attributes and rebuild the previous steps.

Appendix

Building NetCDF from Scratch

- The usual way of building NetCDF requires the HDF5, zlib, curl and m4 libraries.
- Files for the libraries can be found in:

```
ftp://ftp.unidata.ucar.edu/pub/netcdf/netcdf-4
```

- The following slides presents the steps for installing NetCDF in Ubuntu 18.04 and 20.04 for a user named **username**. Adapt the path to your own user.

Installing curl and m4

- apt-get install libcurl4-openssl-dev
- apt-get install m4

Installing zlib

- wget `ftp://ftp.unidata.ucar.edu/pub/netcdf/netcdf-4/zlib-1.2.8.tar.gz`
  - Newest version to later use `ncview`
  - wget `https://sourceforge.net/projects/libpng/files/zlib/1.2.9/zlib-1.2.9.tar.gz`
- tar -xvzf zlib-1.2.8.tar.gz
- cd zlib-1.2.8
- mkdir /home/username/local/
- ./configure --prefix=/home/username/local/
- make check install

Installing HDF5

- wget ftp://ftp.unidata.ucar.edu/pub/netcdf/netcdf-4/hdf5-1.8.13.tar.gz
- tar -xvzf hdf5-1.8.13.tar.gz
- cd hdf5-1.8.13
- ./configure --with-zlib=/home/username/local/ --prefix=/home/username/local/
- make
- make check
- make install
  - make check install
  - If not done separately, it might not work!

Installing NetCDF

- Check the latest version at `https://www.unidata.ucar.edu/downloads/netcdf/`
- wget `ftp://ftp.unidata.ucar.edu/pub/netcdf/netcdf-c-4.7.4.tar.gz`
- tar -xvzf netcdf-c-4.7.4.tar.gz
- cd netcdf-c-4.7.4
- CPPFLAGS=-I/home/username/local/include LDFLAGS=-L/home/username/local/lib ./configure --prefix=/home/username/local
- make check install

Finishing the Set Up

- Link the NetCDF library
  - export `LD_LIBRARY_PATH=/home/username/local/lib/`
  - `sudo ldconfig`

The ESiWACE1/2 projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No **675191** and No **823988**

esiwace

CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER
AND CLIMATE IN EUROPE

Disclaimer: This material reflects only the author's view and the EU-Commission is not responsible for any use that may be made of the information it contains