# 2020 Summer School on Effective HPC for Climate and Weather

# Input/Output and Middleware

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# Outline



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# Learning Objectives

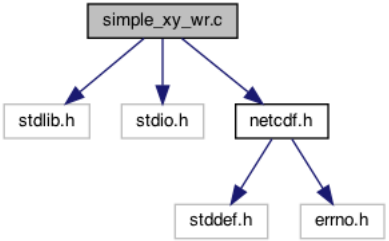
- Execute programs in C that read and write NetCDF files in a metadata-aware manner
- Analyze, manipulate and visualise NetCDF data
- Implement an application that utilizes parallel I/O to store and analyze data

# 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 6.

# 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);}

int main()
{
  ...
  ...
  ...
}
```

# 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;

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

# 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;

  ...
}
```

# 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);

  ...
}
```

# 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;

  ...
}
```

# File simple_xy_wr.c: Defining the 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);

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

  ...
}
```

# File simple_xy_wr.c: Writing data to 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);

  /* 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);

  ...
}
```

# File simple_xy_wr.c: Getting SUCCESS!

```
...

int main()
{
  ...

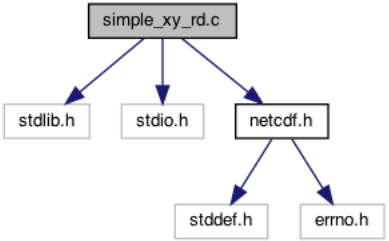
  printf("*** SUCCESS writing example file simple_xy.nc!\n");
  return 0;
}
```

# Compiling and running the file `simple_xy_wr.c`

- Create (copy!) and compile the file `simple_xy_wr.c`.
  - `gcc -I/home/username/local/include simple_xy_wr.c -o simple_xy_wr -L/home/username/local/lib -lnetcdf`
    - LR: What does that mean?!
- 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;

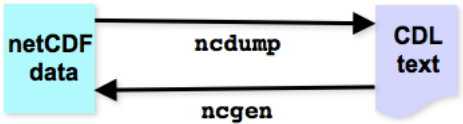
   /* Close the file, freeing all resources. */
   if ((retval = nc_close(ncid)))
      ERR(retval);
}
```

# 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 -I/home/username/local/include simple_xy_rd.c -o simple_xy_rd -L/home/username/local/lib -lnetcdf`
- Run the file `simple_xy_rd`.
  - `./simple_xy_rd`
  - `*** SUCCESS reading example file simple_xy.nc!`

# ncdump and ncgen

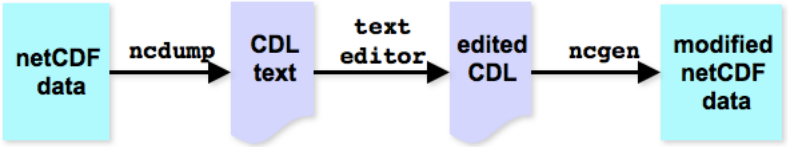
- ncdump and ncgen are inverses:




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

# Editing a NetCDF File

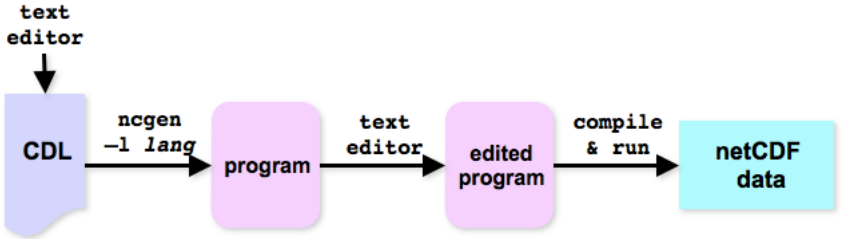
- To edit metadata or data in a netCDF file:




  - 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`
  - LR: Only works like that in my laptop:
  - `/home/lucy/netcdf/netcdf-c-4.7.4/ncdump/ncdump simple_xy.nc`
  - LR: It should be just ncdump file, but esdm is on my way and I don't know how to make another link.

# 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
  - `/home/lucy/netcdf/netcdf-c-4.7.4/ncdump/ncdump simple_xy.nc > simple_xy_t`
  - `more simple_xy_test.cdl`
  - `/home/lucy/netcdf/netcdf-c-4.7.4/ncgen/ncgen -b simple_xy_test.cdl`
  - `cmp simple_xy_test.nc simple_xy.nc`
  - LR: Fix ncdump!

# Creating the C File

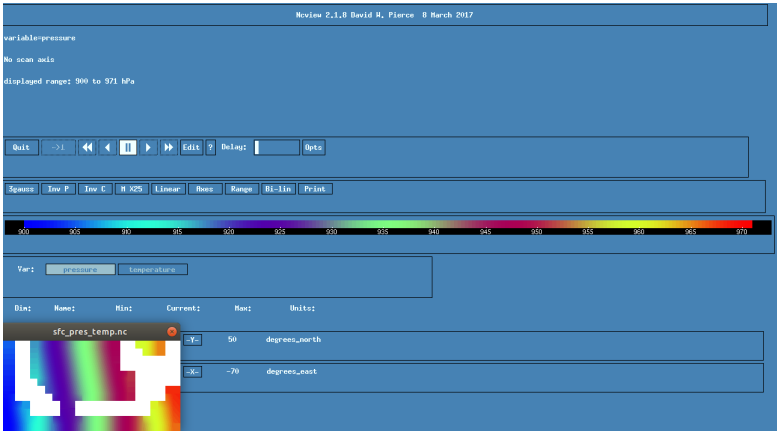
- Create a C file using `ncgen` and the CDL output
  - `/home/lucy/netcdf/netcdf-c-4.7.4/ncgen/ncgen -lc simple_xy_test.cdl > sim`
  - `more simple_xy_test.c`
  - What is the difference between the files `simple_xy_test.c` and `simple_xy_wr.c`?
  - LR: Fix ncgen!
    - `cmp simple_xy_test.c simple_xy_wr.c`
    - `meld simple_xy_test.c simple_xy_wr.c`

# Starting all over again!

- `gcc -I/home/username/local/include simple_xy_test.c -o simple_xy_test -L/home/username/local/lib -lnetcdf`
- `mv simple_xy_test.nc simple_xy_test2.nc`
- `./simple_xy_test`
- `cmp simple_xy_test.nc simple_xy_test2.nc`

# ncview

- LR: Installation is fine.
- LR: What does it do?



# NetCDF Operators (NCO)LR: Is there time to explore?

- NCO is a package of command line operators that manipulates generic netCDF data and supports some CF conventions. The NCO utilities are:

| | |
|---|---|
| ncap2 | arithmetic processor |
| ncatted | attribute editor |
| ncbo | binary operator |
| ncdiff | differencer |
| ncea | ensemble averager |
| ncecat | ensemble concatenator |
| ncflint | file interpolator |

| | |
|---|---|
| ncks | kitchen sink (extract, cut, paste, print data) |
| ncpdq | permute dimensions quickly |
| ncra | running averager |
| ncrcat | record concatenator |
| ncrename | renamer |
| ncwa | weighted averager |

- NCO utilities have as a goal being as generic as possible, imposing no limitations on data dimensionality, size, or type. All established national and international climate modelling centers now install and maintain NCO for their users for data post-processing, hyper-slabbing, and serving.

# Parallel I/O

Implement an application that utilises parallel I/O to store and analyse data

# 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`
- File `sfc_pres_temp_wr`
  - 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_wr`
  - 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`

# Summary of Actions

- Inspect the read and write 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`.

# Building NetCDF from Scratch

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

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

# Installing curl

- apt-get install libcurl4-openssl-dev

# 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

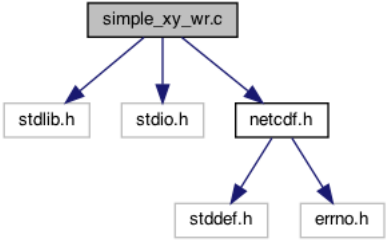
- Link the NetCDF library
  - export `LD_LIBRARY_PATH=/home/username/local/lib/`
  - `sudo ldconfig`
- Create a new directory (for instance, /home/username/example) and create the file from the given source using an editor of your choice.

# 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:



# Compiling and running the file `simple_xy_wr.c`

- Create (copy!) and compile the file `simple_xy_wr.c`.
  - `gcc -I/home/username/local/include simple_xy_wr.c -o simple_xy_wr -L/home/username/local/lib -lnetcdf`
- Run the file `simple_xy_wr`.
  - `./simple_xy_wr`
  - `*** SUCCESS writing example file simple_xy.nc!`
- Check that the file `cmp test.nc simple_xy.nc` is in your directory.

# Using ncdump

Inspect the output file `simple_xy.nc` using `ncdump`

- `ncdump simple_xy.nc`
- LR: Only works like that in my laptop:
- `/home/lucy/netcdf/netcdf-c-4.7.4/ncdump/ncdump simple_xy.nc`
- LR: It should be just ncdump file, but esdm is on my way and I don't know how to make another link

# 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
  - ```
    /home/lucy/netcdf/netcdf-c-4.7.4/ncdump/ncdump simple_xy.nc > test.cdl
    ```
  - ```
    more test.cdl
    ```
  - ```
    /home/lucy/netcdf/netcdf-c-4.7.4/ncgen/ncgen -b test.cdl
    ```
  - ```
    cmp test.nc simple_xy.nc
    ```
  - LR: Fix ncdump!

# Creating the C File

- Create a C file using ncgen and the CDL output
  - ```
    /home/lucy/netcdf/netcdf-c-4.7.4/ncgen/ncgen -lc simple_xy_test.cdl > sim
    ```
  - `more simple_xy_test.c`
  - `cmp simple_xy_test.c simple_xy_wr.c`
  - LR: Fix ncgen!
    ```

# Starting all over again!

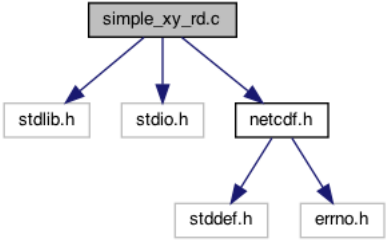
- 
```
gcc -I/home/username/local/include simple_xy_test.c -o simple_xy_test -L
```
- `mv simple_xy_test.nc simple_xy_test2.nc`
- `./simple_xy_test`
- `cmp simple_xy_test.nc simple_xy_test2.nc`

# File Reference: simple_xy_rd.c

This is a simple example which reads a small dummy array, which was written by simple_xy_wr.c. It is intended to illustrate the use of the netCDF C API.

- 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_wr:

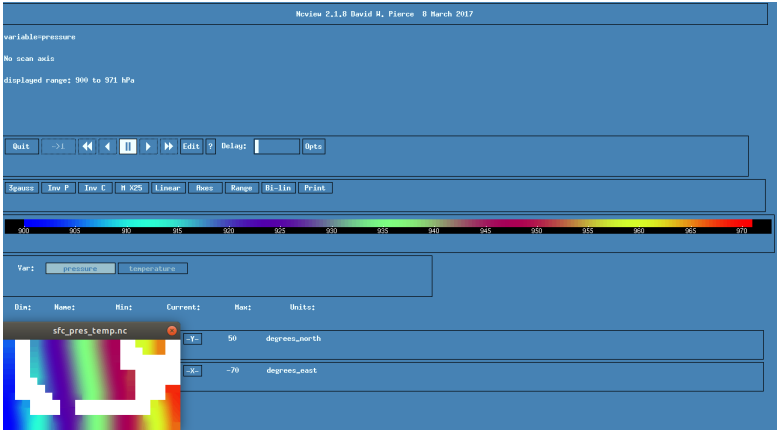


# Reading the file `simple_xy.nc`

- Check that the file `simple_xy.nc` is in your directory.
- Create (copy!), compile and run the file `simple_xy_rd.c`
  - `gcc -I/home/username/local/include simple_xy_rd.c -o simple_xy_rd -L/home/username/local/lib -lnetcdf`
- Run the file `simple_xy_rd`
  - `./simple_xy_rd`
  - `*** SUCCESS reading example file simple_xy.nc!`

# ncview

- Installation is fine.
- What does it do?



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**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