2020 Summer School on Effective HPC for Climate and Weather

Input/Output and Middleware

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

Outline

1 NetCDF Files and C

2 NetCDF Utilities

3 Parallel I/O

4 Practising

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Learning Objectives

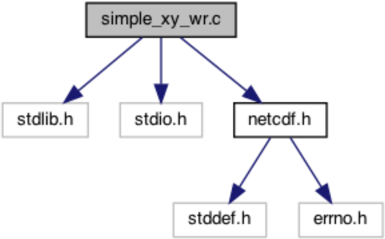
- Execute programs in C that read and write NetCDF files in a metadata-aware manner
- Analyze, manipulate and visualise NetCDF data
- Implement an application that utilizes parallel I/O to store and analyze data

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 5.

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 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);

  /* 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 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);

  /* 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`.

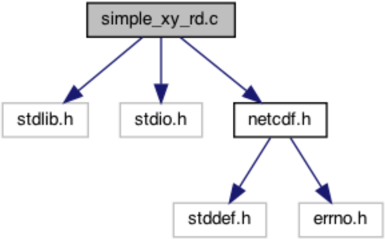
  -
    ```
    gcc simple_xy_wr.c -o simple_xy_wr $(nc-config --libs --cflags)
    ```
- Run the file `simple_xy_wr`.

  -
    ```
    ./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);
}
```

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.

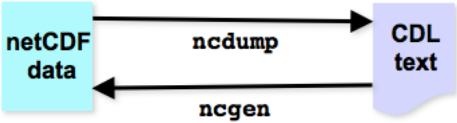
  -
    ```
    gcc simple_xy_rd.c -o simple_xy_rd $(nc-config --libs --cflags)
    ```
- Run the file simple_xy_rd.

  -
    ```
    ./simple_xy_rd
    ```

  -
    ```
    *** SUCCESS reading example file simple_xy.nc!
    ```

ncdump and ncgen

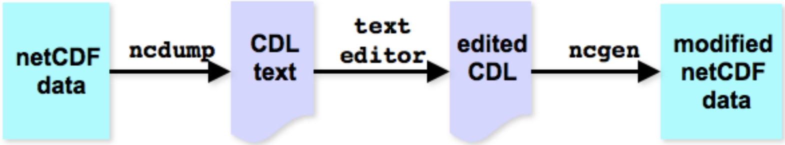
- ncdump and ncgen are inverses:



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

Editing a NetCDF File

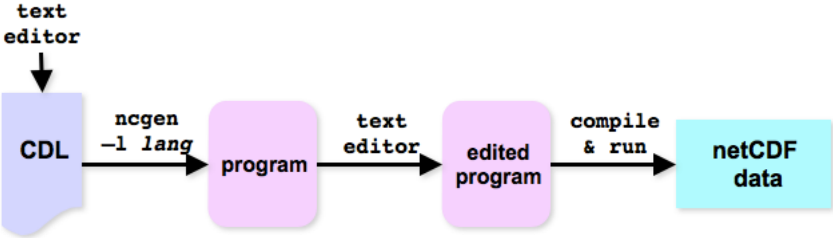
- To edit metadata or data in a netCDF file:



- 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

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 $(nc-config --libs --cflags)
  -o simple_xy_test -L/home/username/local/lib -lnetcdf
  ```

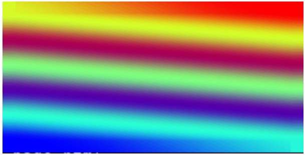
-
  ```
  mv simple_xy_test.nc simple_xy_test2.nc
  ```

-
  ```
  ./simple_xy_test
  ```

-
  ```
  cmp simple_xy_test.nc simple_xy_test2.nc
  ```

Using ncview

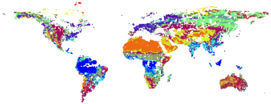
- `ncview simple_xy.nc`



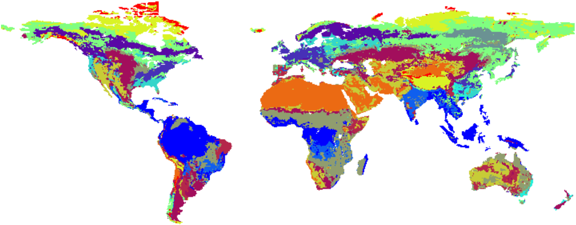
```
netcdf simple_xy {
dimensions:
x = 6 ;
y = 12 ;
variables:
int data(x, y) ;
data:

 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 ;
}
```

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

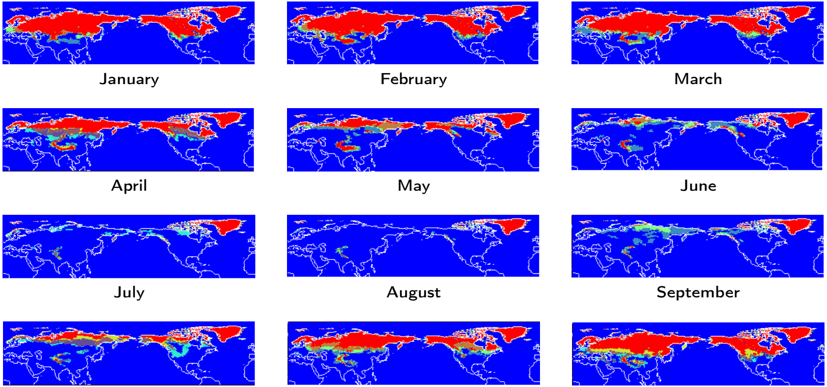


File vegtype_0.5.nc

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`.

Parallel I/O Example – MPI-IO

```
#include <stdio.h>
#include <mpi.h>
int main(int argc, char *argv[])
{
 MPI_File fh;
 int buf[1000], rank;
 MPI_Init(0,0);
 MPI_Comm_rank(MPI_COMM_WORLD, &rank);
 MPI_File_open(MPI_COMM_WORLD, "test.out",
 MPI_MODE_CREATE|MPI_MODE_WRONLY,
 MPI_INFO_NULL, &fh);
 if (rank == 0)
 MPI_File_write(fh, buf, 1000, MPI_INT, MPI_STATUS_IGNORE);
 MPI_File_close(&fh);
 MPI_Finalize();
 return 0;
}
```

Parallel I/O Example – NetCDF4 – Part I

```
/* Initialize MPI. */
    MPI_Init(&argc,&argv);
    MPI_Comm_size(MPI_COMM_WORLD, &mpi_size);
    MPI_Comm_rank(MPI_COMM_WORLD, &mpi_rank);
    MPI_Get_processor_name(mpi_name, &mpi_namelen);

    if (mpi_rank == 1)
       printf("\n*** tst_parallel testing very basic parallel access.\n");

    /* Create a parallel netcdf-4 file. */
    if ((res = nc_create_par(FILE, NC_NETCDF4|NC_MPIIO, comm,
     info, &ncid))) ERR;

    /* Create two dimensions. */
    if ((res = nc_def_dim(ncid, "d1", DIMSIZE, dimids))) ERR;
    if ((res = nc_def_dim(ncid, "d2", DIMSIZE, &dimids[1]))) ERR;

    /* Create one var. */
    if ((res = nc_def_var(ncid, "v1", NC_INT, NDIMS, dimids, &v1id))) ERR;

    if ((res = nc_enddef(ncid))) ERR;
```

Parallel I/O Example – NetCDF4 – Part II

```
/* Set up slab for this process. */
start[0] = mpi_rank * DIMSIZE/mpi_size;
start[1] = 0;
count[0] = DIMSIZE/mpi_size;
count[1] = DIMSIZE;

/* Create phoney data. We're going to write a 24x24 array of ints,
   in 4 sets of 144. */
for (i=mpi_rank*QTR_DATA; i < (mpi_rank+1)*QTR_DATA; i++)
   data[i] = mpi_rank;

/*if ((res = nc_var_par_access(ncid, v1id, NC_COLLECTIVE)))
  ERR;*/
if ((res = nc_var_par_access(ncid, v1id, NC_INDEPENDENT))) ERR;

/* Write slabs of phoney data. */
if ((res = nc_put_vara_int(ncid, v1id, start, count,
   &data[mpi_rank*QTR_DATA]))) ERR;

/* Close the netcdf file. */
if ((res = nc_close(ncid))) ERR;

/* Shut down MPI. */
MPI_Finalize();

return 0;
```

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`.

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

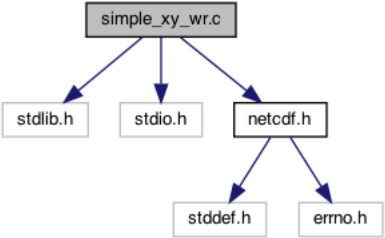
- Link the NetCDF library
  - export `LD_LIBRARY_PATH=/home/username/local/lib/`
  - `sudo ldconfig`
- Create a new directory (for instance, /home/username/example) and create the file from the given source using an editor of your choice.

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 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 `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`

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 > test.cdl`
    - `more test.cdl`
    - `ncgen -b test.cdl`
    - `cmp 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`
  - `cmp simple_xy_test.c simple_xy_wr.c`

Starting all over again!

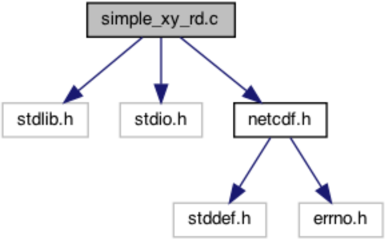
-
  ```
  gcc simple_xy_test.c -o simple_xy_test $(nc-config --libs --cflags)
  ```
-
  ```
  mv simple_xy_test.nc simple_xy_test2.nc
  ```
-
  ```
  ./simple_xy_test
  ```
-
  ```
  cmp simple_xy_test.nc simple_xy_test2.nc
  ```

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 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!`

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esiwace

CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER
AND CLIMATE IN EUROPE

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