Parallel I/O with NetCDF and HDF5

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September 21, 2015

What are NetCDF and HDF5?

Both are standardized file formats for scientific data, which are:

- Self-describing;
- Binary format;
- Many tools use these formats;
- Parallel access (NetCDF4 and HDF5).
- Format the same whether working in serial or in parallel.

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How do NetCDF and HDF5 differ?

- NetCDF is aimed at storing large multi-dimensional arrays, but simpler to use.
- HDF5 hold more general data, but is more complex to use;

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NetCDF

- Let's consider NetCDF first.
- A format as well as an Applications Program interface (API).
- MPI-IO was too low-level.
- Even for the vary common scientific use-cases.
- NetCDF gives you a higher level approach to writing and reading multi-dimensional arrays.

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Intro to the NetCDF Format

```
$ cd pario/netcdf
$ source setup
$ make 2darray-simple # or f2darray-simple
$ ./2darray-simple # or ./f2darray-simple
$ ncdump -h file.nc?
```

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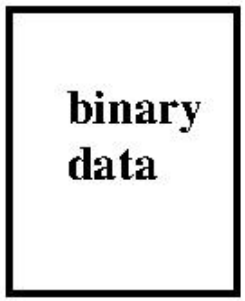
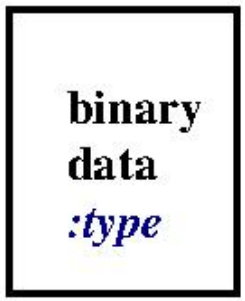
NetCDF Data Model

NetCDF Data Model



NetCDF Data Model



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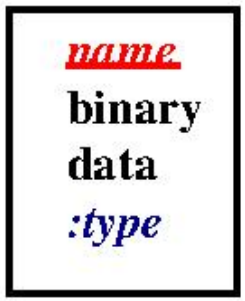

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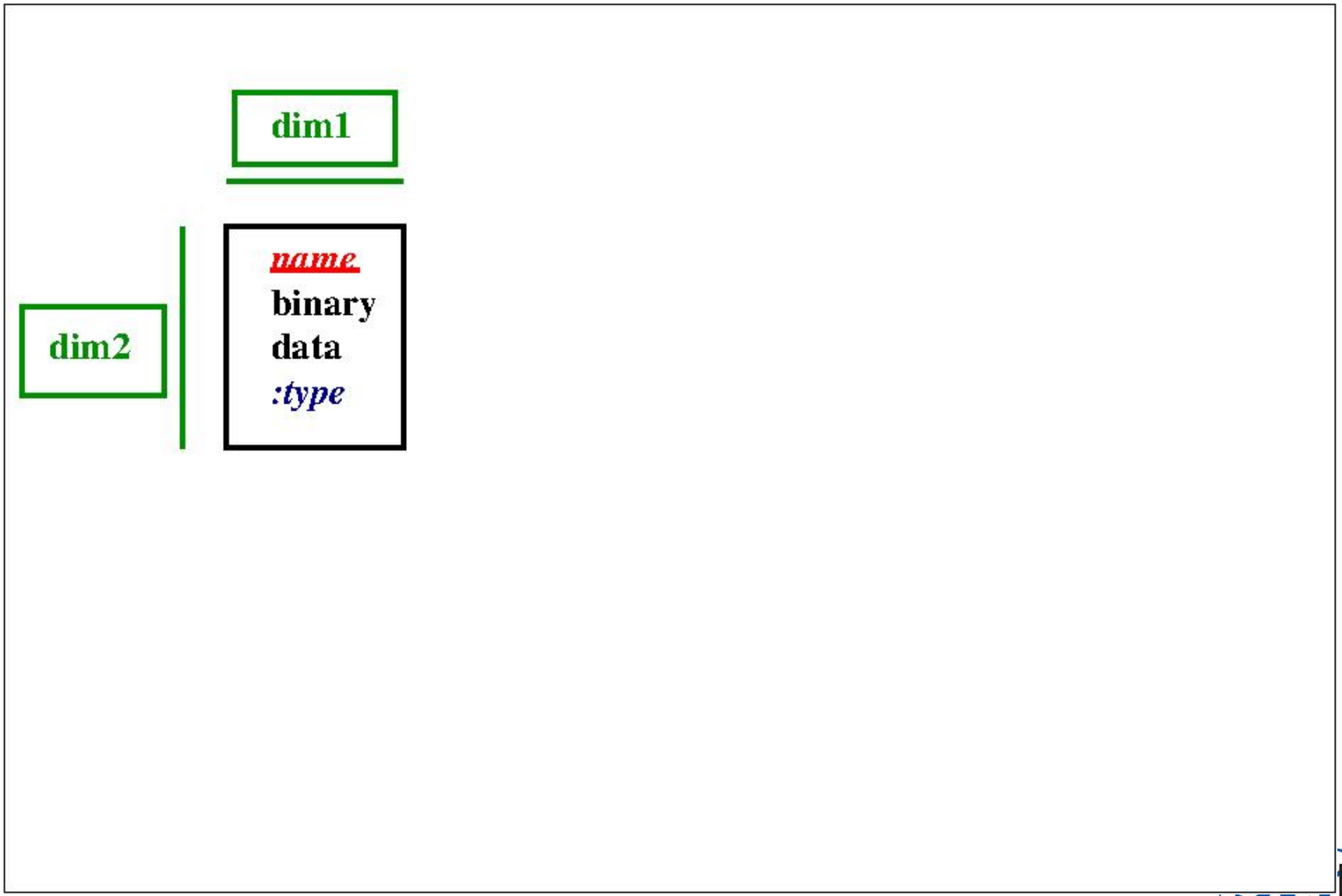

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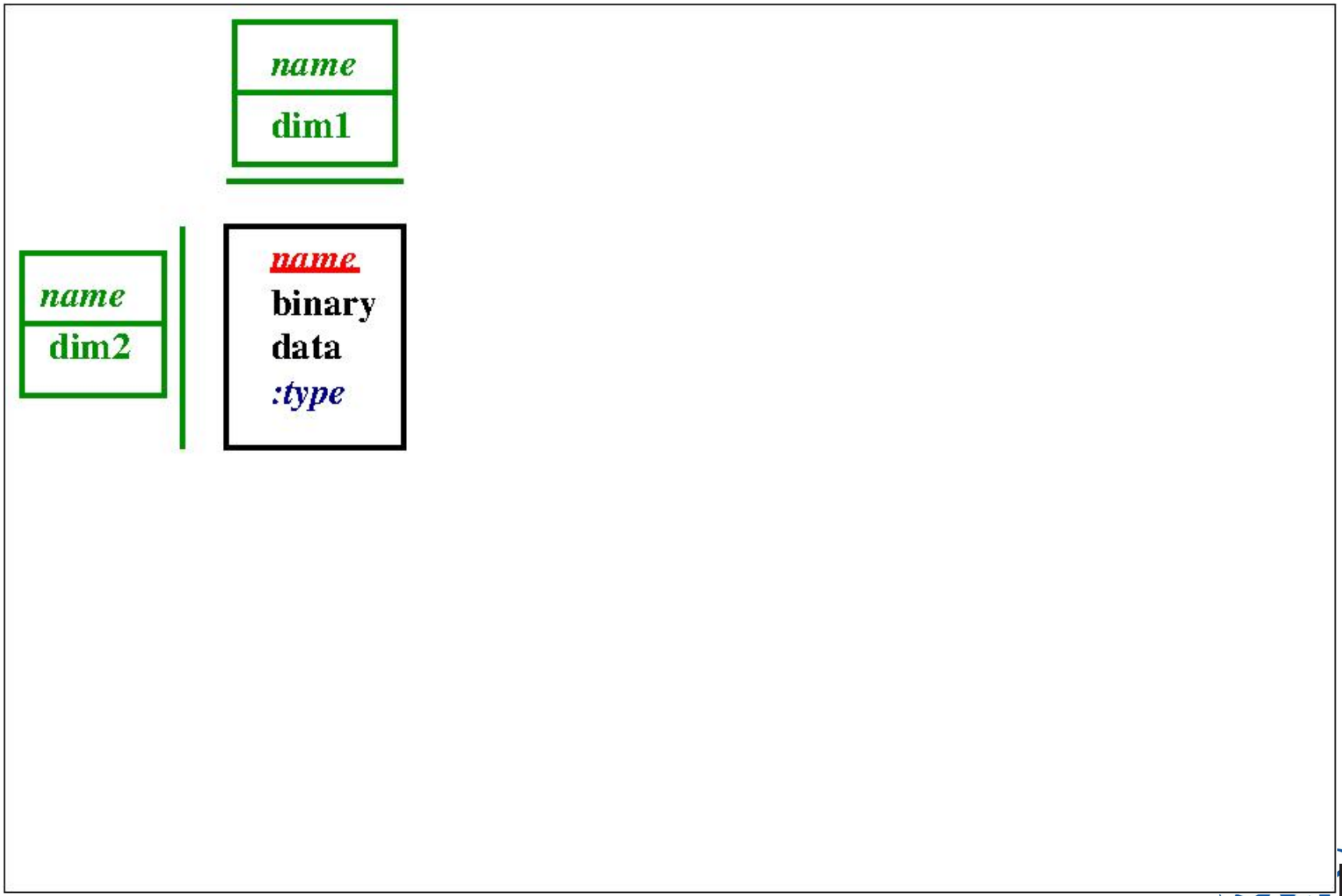

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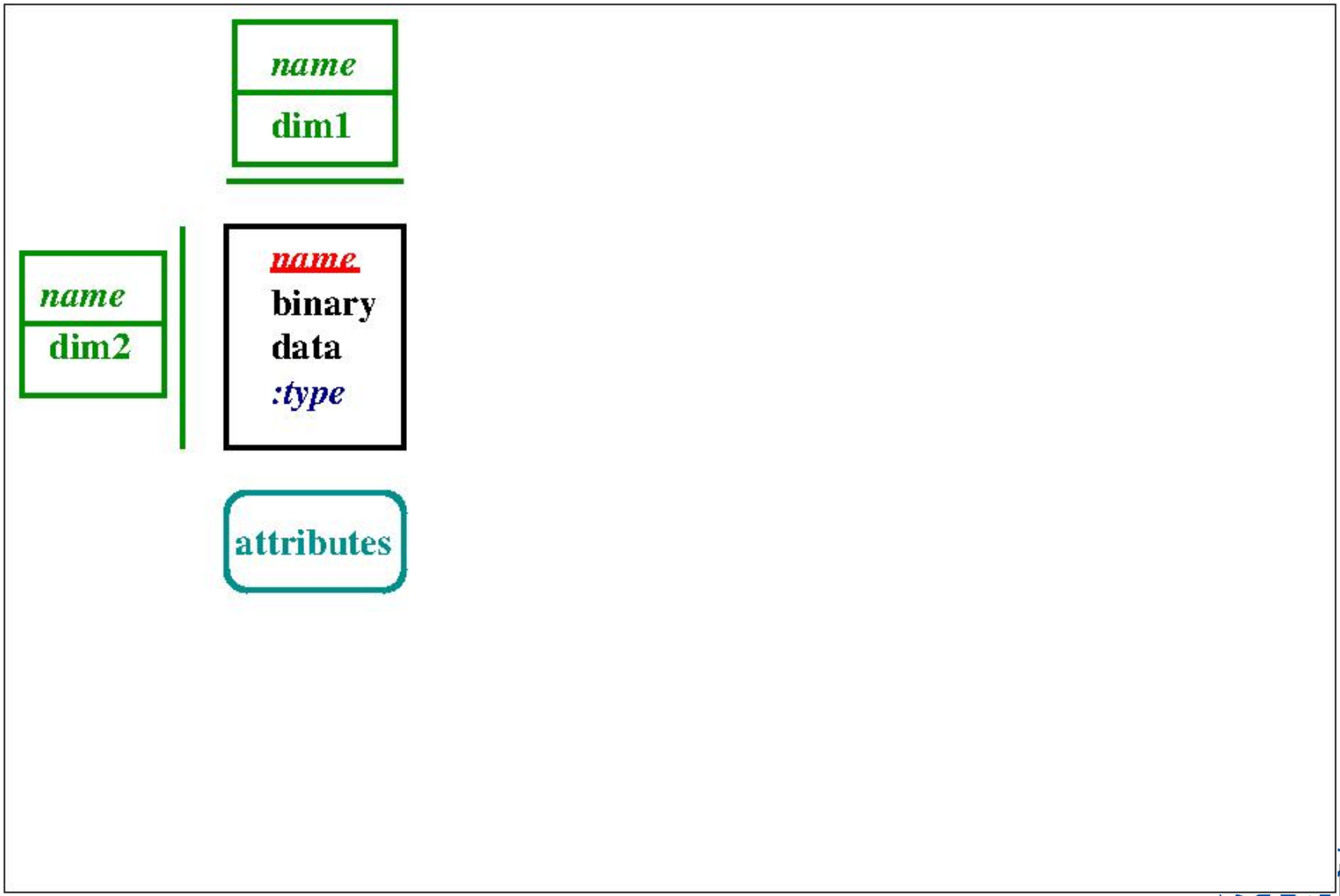
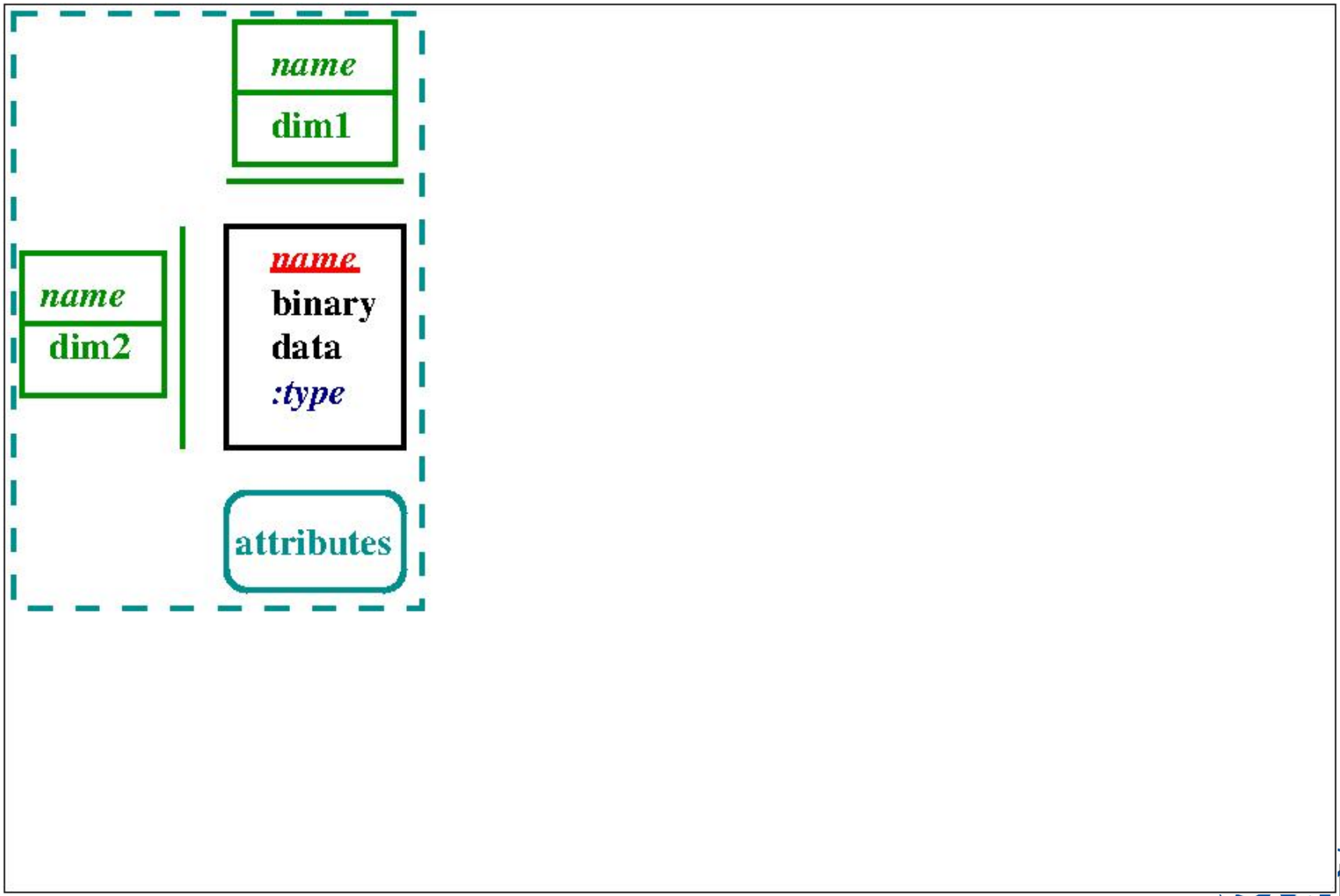


NetCDF Data Model



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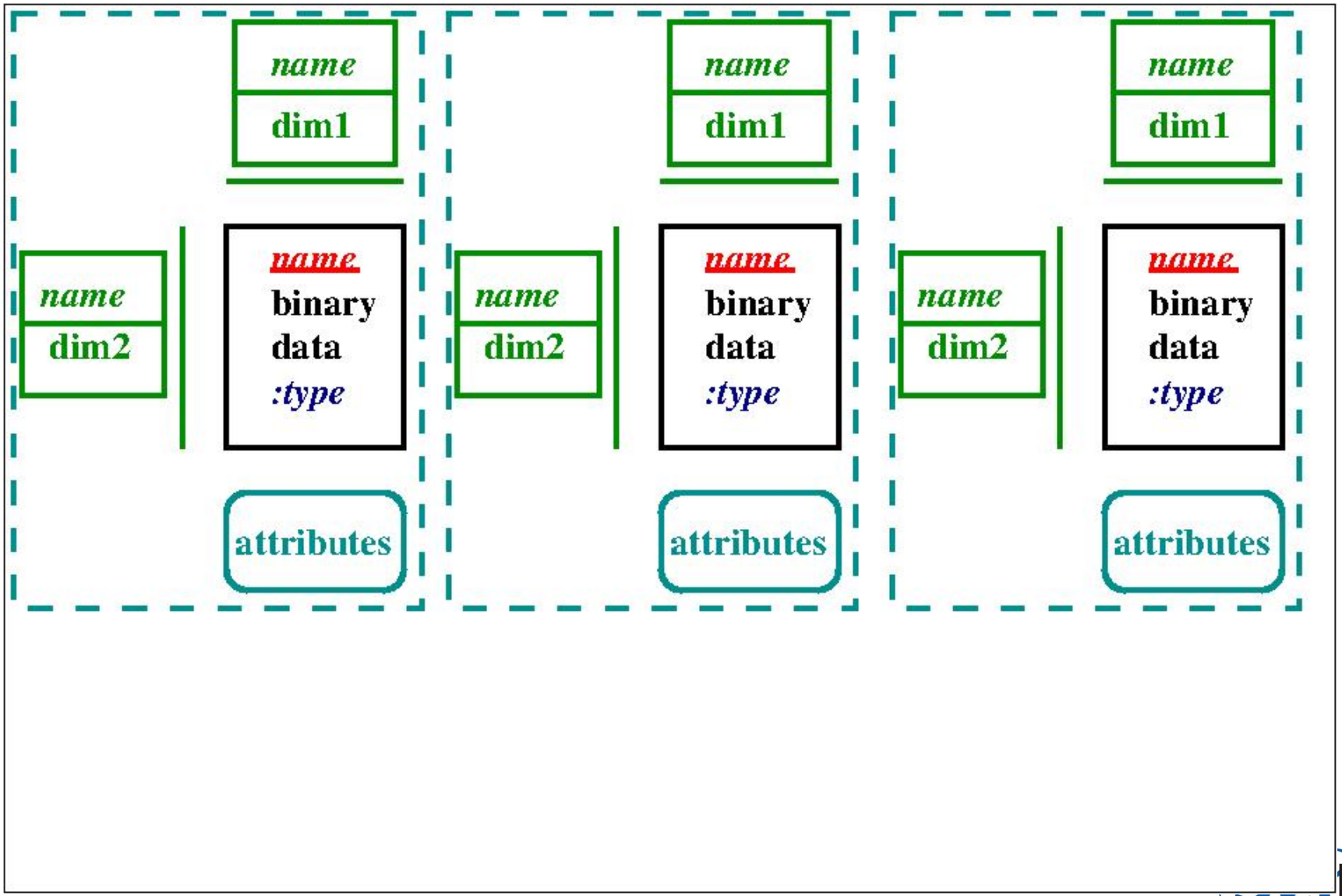

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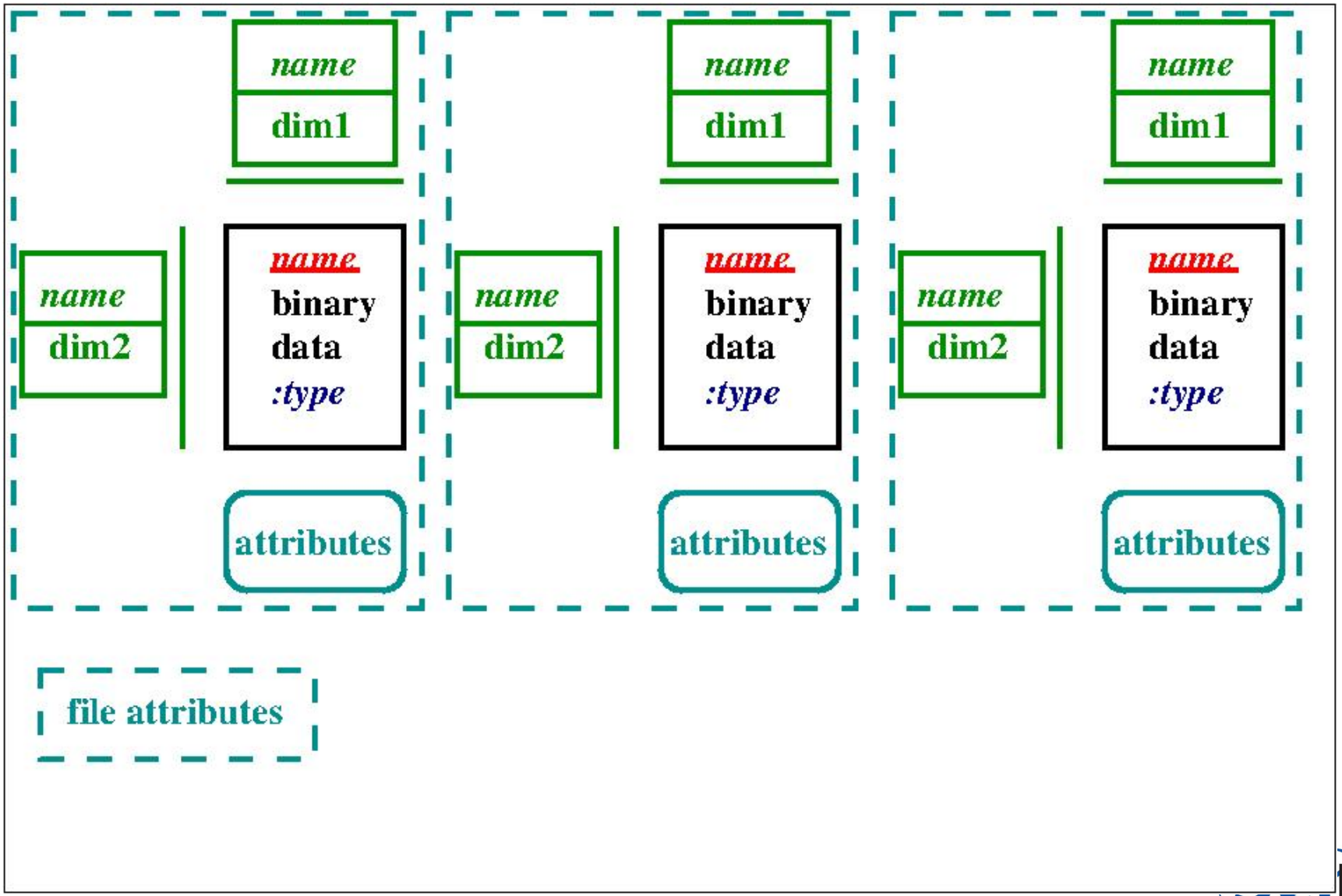
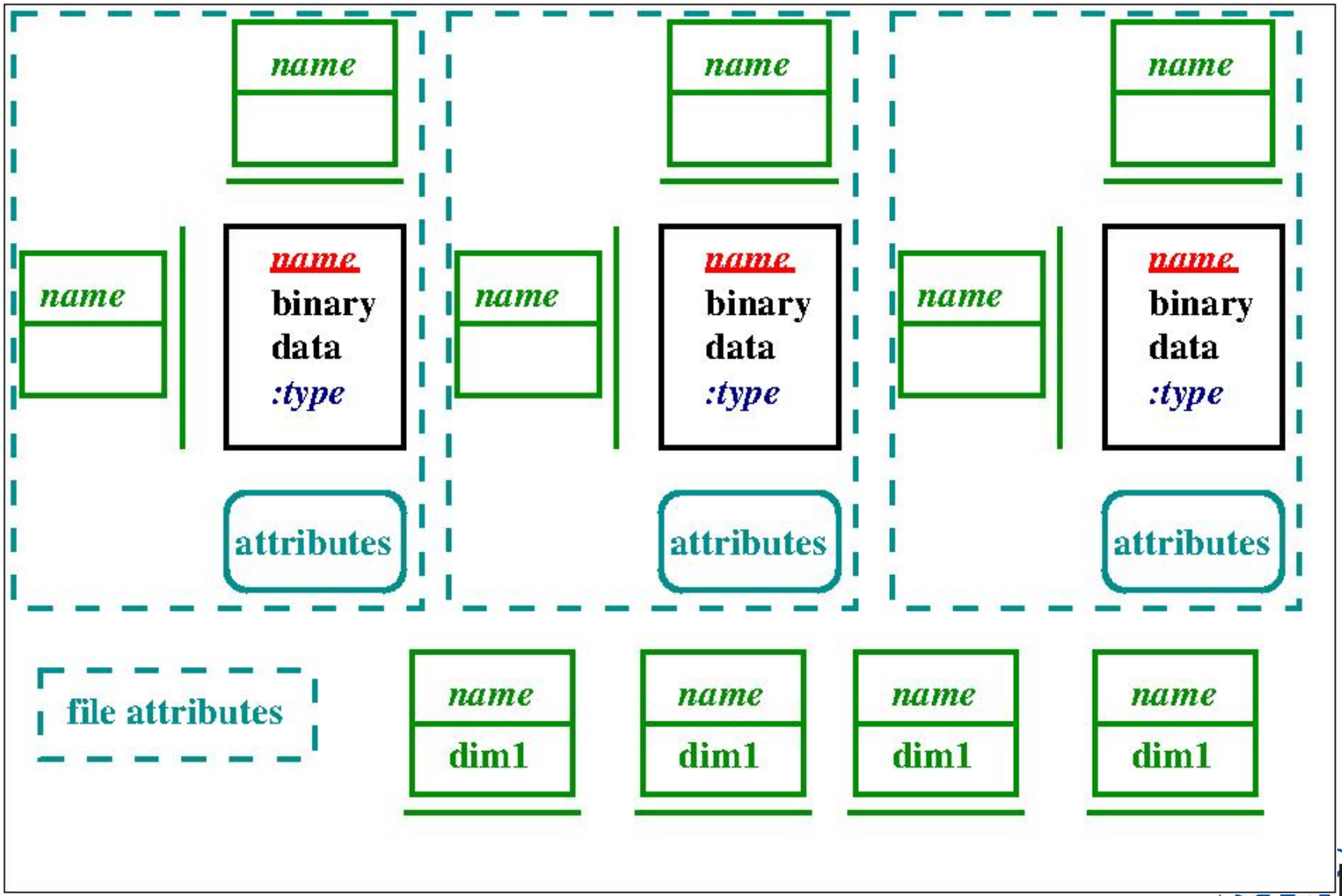


NetCDF Data Model



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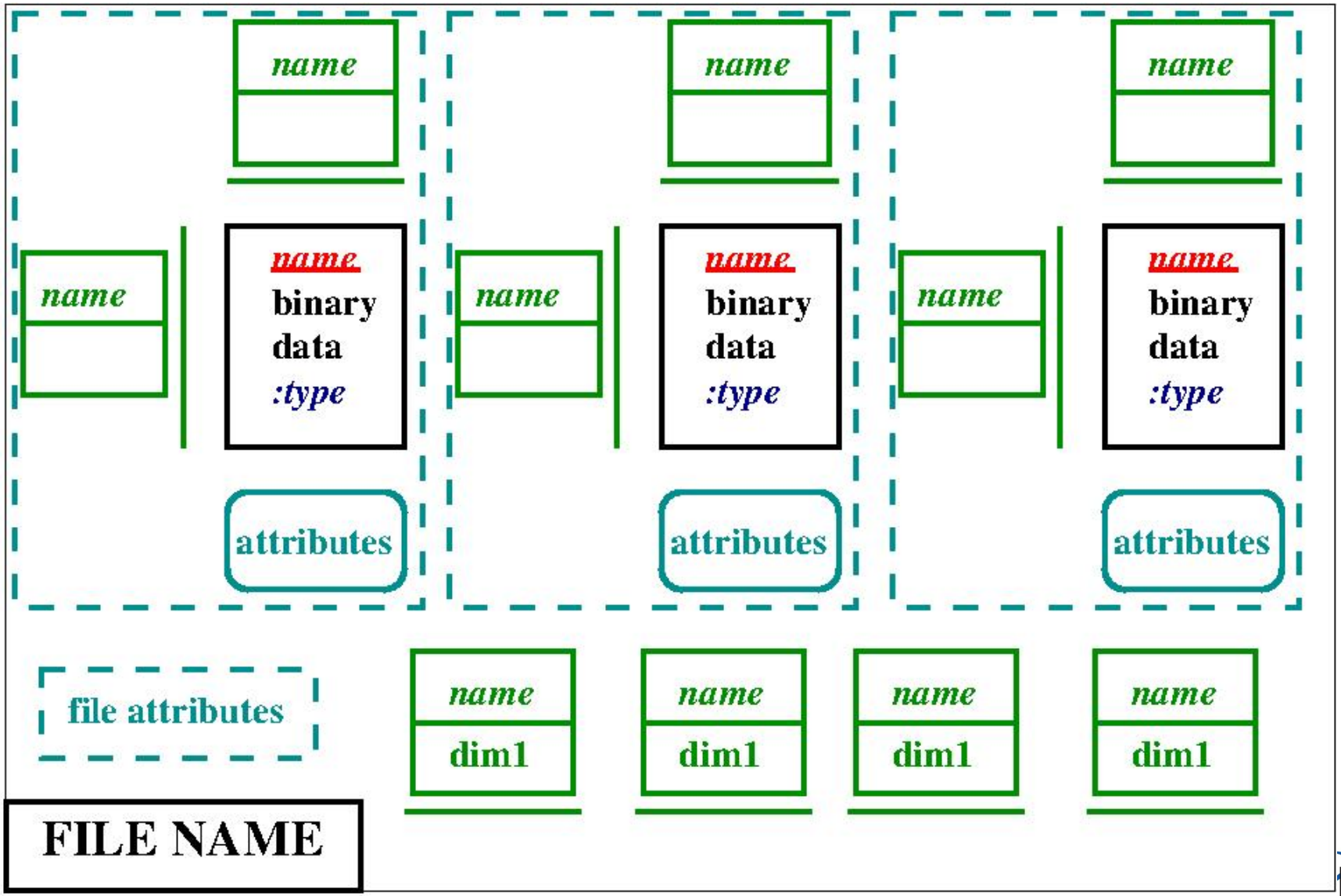

NetCDF API

What's an API, anyways?

- Defines function prototypes:
  - What's their input?
  - What's their output?
  - What are they supposed to do?
- Constants:
  - Encode options
  - Encode errors
- Types
  - NetCDF just uses `int` for c types.
  - The types of the data encoded in integer options.

NetCDF's main APIs are for Fortran and C.

There are interfaces for C++, python, R, ruby, ...

Sample Code

```
$ cp -r /scinet/course/pario15 .
$ cd pario15/netcdf
$ source setup
$ make netcdftest
$ ./netcdftest
...
```

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...
```

```
$ ncdump -h test.nc
netcdf netcdftest {
dimensions:
        X = 48 ;
        Y = 48 ;
variables:
        int M(X,Y) ;
}
```

Sample Code

```
$ cp -r /scinet/course/pario15 .
$ cd pario15/netcdf
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```

```
$ ./ncview test.nc
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```
$ ./ncview test.nc
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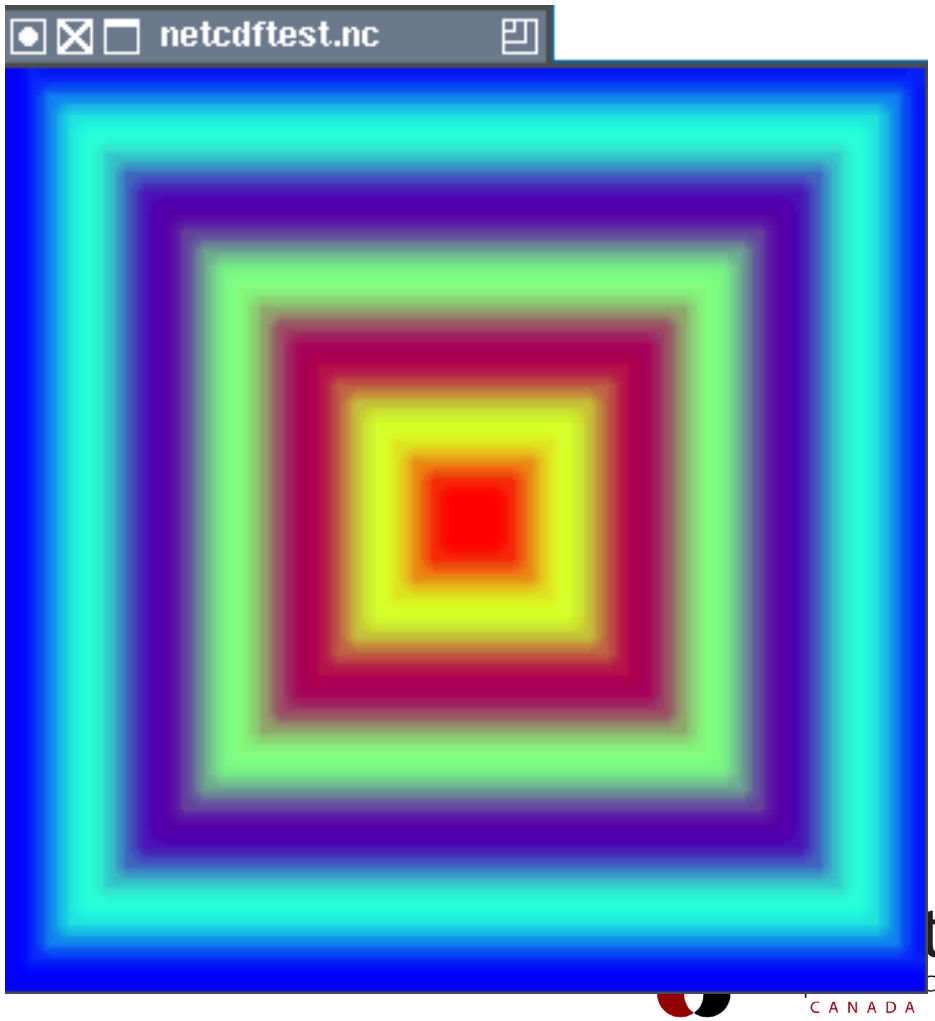

netcdftest.c

```c
#include <stdio.h>
#include <stdlib.h>
#include <netcdf.h>
#define MIN(x,y) ((x)<(y)?(x):(y))
int main(void) {
 const int N = 48;
 int ncid, varid, status, dimid[2], *data;
 printf("Testing i/o in netcdf4\n");
 data = malloc(sizeof(int)*N*N);
 for (int i = 0; i < N*N; i++)
    data[i] = MIN(N/2-abs((i%N)-N/2), N/2-abs((i/N)-N/2));
 status = nc_create("test.nc", NC_CLOBBER|NC_NETCDF4, &ncid);
 status = nc_def_dim(ncid, "X", N, &dimid[0]);
 status = nc_def_dim(ncid, "Y", N, &dimid[1]);
 status = nc_def_var(ncid, "M", NC_INT, 2, dimid, &varid);
 status = nc_enddef(ncid);
 status = nc_put_var_int(ncid, varid, data);
 status = nc_close(ncid);
 free(data);
 printf("Done.\n"); }
```

fnetcdftest.f90

```
program fnetcdftest
 use netcdf
 integer, parameter :: N=48
 integer :: i, j, ncid, varid, status, dimidx, dimidy
 integer, dimension(:,:), allocatable :: data
 print *, "Testing i/o in netcdf4"
 allocate(data(N,N));
 do i=1,N; do j=1,N
   data(i,j) = min(N/2-abs(i-N/2), N/2-abs(j-N/2))
 enddo; enddo
 status = nf90_create("test.nc",IOR(NF90_NETCDF4,NF90_CLOBBER),ncid)
 status = nf90_def_dim(ncid,"X",N,dimidx)
 status = nf90_def_dim(ncid,"Y",N,dimidy)
 status = nf90_def_var(ncid,"M",NF90_INT,(/dimidx,dimidy/),varid)
 status = nf90_enddef(ncid)
 status = nf90_put_var(ncid, varid, data)
 status = nf90_close(ncid)
 deallocate(data)
 print *, "Done."
end program fnetcdftest
```

Writing a NetCDF File

To write a NetCDF file, we go through the following steps:

- Create the file
- Define dimensions
- Define variables
- End definitions
- Write variables
- Close file

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Reading a NetCDF File

To read in (part of) a NetCDF file, we go through the following steps:

- Open the file
- Get dimension ids
- Get dimension lengths
- Get variable ids
- Read variables
- Close file

Example Reading NetCDF File (C)

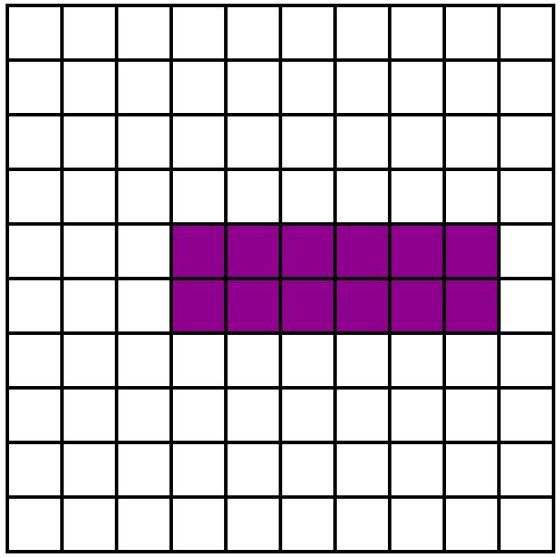
```c
#include "netcdf.h"
#define MAX(x,y) ((x)>(y)?(x):(y))
int main(void){
  int fileid, varid, status, dimid[2], maximum=0, *data;
  size_t nx, ny;
  char name[256];
  printf("Testing read in of a netcdf4 file\n");
  status = nc_open("test.nc", NC_NOWRITE, &fileid);
  status = nc_inq_dimid(fileid, "X", &dimid[0]);
  status = nc_inq_dimid(fileid, "Y", &dimid[1]);
  status = nc_inq_dim(fileid, dimid[0], name, &nx);
  status = nc_inq_dim(fileid, dimid[1], name, &ny);
  data = malloc(nx*ny*sizeof(int));
  status = nc_inq_varid(fileid, "M", &varid);
  status = nc_get_var(fileid, varid, data);
  status = nc_close(fileid);
  for (int i=0; i<nx*ny; i++)
     maximum = maximum<data[i]?data[i]:maximum;
  printf("Max. value = %d\n", maximum);
  free(data);  printf ("Done.\n");  }
```

Example Reading NetCDF File (Fortran)

```
program fnetcdfread
  use netcdf
  integer, parameter :: N=48
  integer :: maximum, fileid, varid, status, dimidx, dimidy, nx, ny
  integer, dimension(:,:), allocatable :: data
  print *, "Testing read in of netcdf4 file"
  status = nf90_open("test.nc", NF90_NOWRITE, fileid)
  status = nf90_inq_dimid(fileid, "X", dimidx)
  status = nf90_inq_dimid(fileid, "Y", dimidy)
  status = nf90_inquire_dimension(fileid, dimidx, len=nx)
  status = nf90_inquire_dimension(fileid, dimidy, len=ny)
  allocate(data(nx,ny));
  status = nf90_inq_varid(fileid, 'M', varid)
  status = nf90_get_var(fileid, varid, data)
  status = nf90_close(fileid)
  maximum = maxval(data)
  print *, "Max. value =", maximum
  deallocate(data)
  print *, "Done."
end program fnetcdfread
```

Accessing subregions in a file

- `nc_put_var_type` or `nf90_put_var` puts in the whole array.
- Subarrays can be specified with starts and counts.



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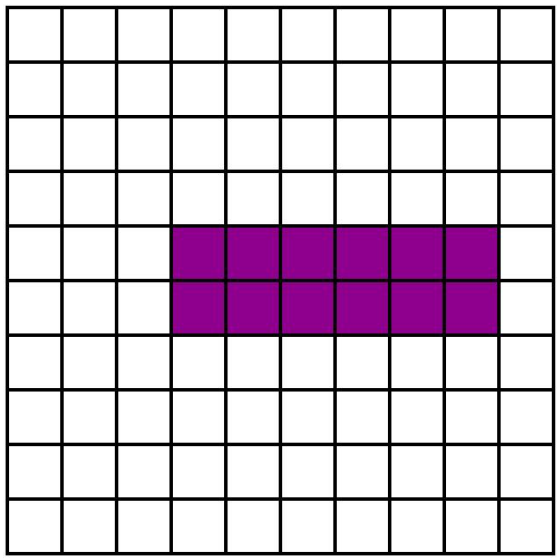

C

```
start[0] = 3;
start[1] = 4;
count[0] = 6;
count[1] = 2;
nc_put_vara_int(fileid,varid,
                start,count,data);
```

Fortran

```
start(1) = 4
start(2) = 5
count(1) = 6
count(2) = 2
nf90_put_var(fileid,varid,data,
       START=start,COUNT=count)
```

Further notes on (serial) NetCDF

- NetCDF adapts to the storage convention of C and Fortran as appropriate.
- Can have 'unlimited' size (e.g. can grow).
- Can add attributes: do this!

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Parallel I/O with NetCDF

- NetCDF4 builds on top of HFD5, which can use MPI-IO.
- NetCDF4's parallel IO uses the subregions construction.
- Must use in conjunction with MPI (no threaded parallel I/O).
- Can be as simple as changing the creation/opening of the file.
- And using the subregions in `put` and `get`.

Parallel I/O with NetCDF (C)

```
nc_create_par(filename,mode,MPI_COMM,MPI_INFO,fileid);
nc_open_par(filename,mode,MPI_COMM,MPI_INFO,fileid);
nc_var_par_access(fileid,varid,NC_COLLECTIVE);
nc_put_vara_type(...)
nc_get_vara_type(...)
```

Parallel I/O with NetCDF (Fortran)

```
nf90_create_par(filename,mode,MPI_COMM,MPI_INFO,fileid);
nf90_open_par(filename,mode,MPI_COMM,MPI_INFO,fileid);
nf90_var_par_access(fileid,varid,NC_COLLECTIVE);
nf90_put_var(...,START=,COUNT=)
nf90_get_var(...,START=,COUNT=)
```

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Parallel I/O Example with NetCDF (1)

```
#include <netcdf_par.h>
int main(int argc, char **argv) {
  const int N = 48;
  int size, rank, fileid, varid, dimid[2], *localdata;
  size_t start[2], count[2];
  MPI_Init(&argc,&argv);
  MPI_Comm_size(MPI_COMM_WORLD, &size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  if (rank==0) printf("Testing parallel i/o in netcdf4\n");
  start[0] = (rank*N)/size;  count[0] = N/size;
  start[1] = 0;              count[1] = N;
  localdata = malloc(sizeof(int)*count[0]*count[1]);
  for (int i = 0; i < count[0]*count[1]; i++)
     localdata[i] = MIN(N/2-abs(start[1]+(i%count[1])-N/2),
                        N/2-abs(start[0]+(i/count[1])-N/2));
  nc_create_par("netcdfpartest.nc", NC_NETCDF4|NC_MPIIO,
     MPI_COMM_WORLD, MPI_INFO_NULL, &fileid);
  nc_def_dim(fileid, "X", N, &dimid[0]);
  nc_def_dim(fileid, "Y", N, &dimid[1]);
```

Parallel I/O Example with NetCDF (2)

```
  nc_def_var(fileid, "M", NC_INT, 2, dimid, &varid);
  nc_enddef(fileid);
  nc_var_par_access(fileid, varid, NC_COLLECTIVE);
  nc_put_vara_int(fileid, varid, start, count, localdata);
  nc_close(fileid);
  MPI_Finalize();
  free(localdata);
  if (rank==0) printf("Done.\n");
}
```

NetCDF References

- C Interface:
  http://www.unidata.ucar.edu/software/netcdf/docs/netcdf-c/
- Fortran Interface:
  http://www.unidata.ucar.edu/software/netcdf/docs/netcdf-f90/

HDF5

- HDF=Hierarchical Data Format
- Can be seen as a generalization of NetCDF.
- HDF5 allows for parallel IO, using MPI-IO under the hood.

- But HDF5 allows for a lot more than NetCDF:
  - Object-oriented description of datasets, groups, attributes, types, data spaces and property lists.
  - File content can be arranges in a Unix-like file system
  - Groups can contains structures that hold data sets, other groups, etc.
  - Optional compression.
- But: have to do more work when reading and writing HDF5 files.

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Use other slide deck for rest of HDF5

Old slides still valid!

Conclusions

- Quite a few options for doing parallel I/O.
- MPI-IO underlies most of these.
- NetCDF and HDF5 allow you to store metadata, structure your data, and make it portable: recommended!
- Apart from performance gains, also makes your output independent of the number of preocesses that produces it.
- Pay attention to disk I/O! Bandwidth and IOPs are limited, and shared with other users.
- Still keep other common I/O best practices in mind: Fewer files, binary formats, store only what you need to keep, write in big chunks.

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