

Advanced Parallel Programming

Alternative Parallel IO Libraries

ARCHER Training Courses

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Overview

- Issues with MPI-IO
- HDF5
- NetCDF
- Availability on ARCHER
- Summary

MPI-IO Issues

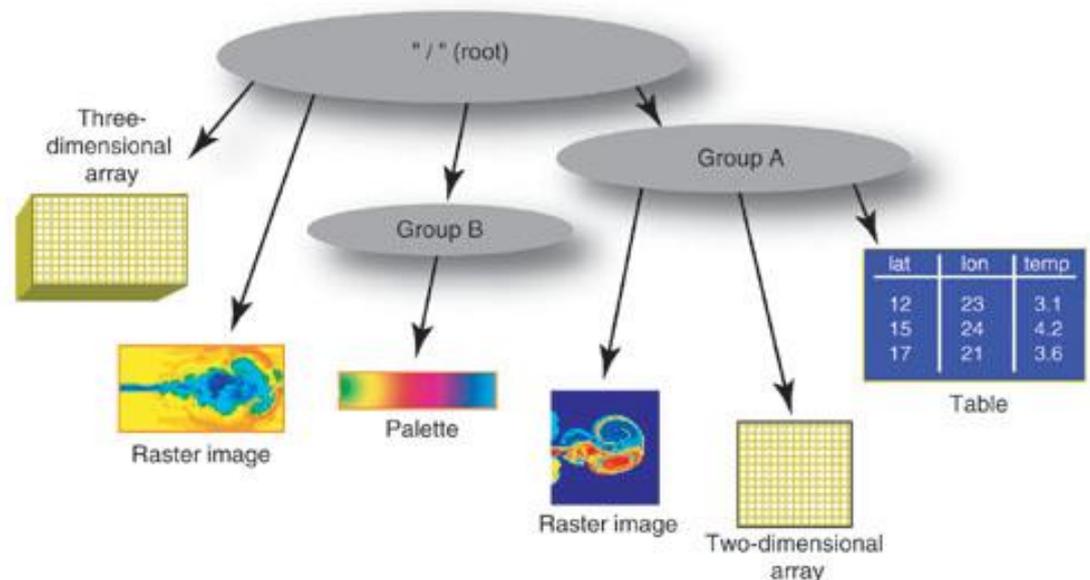
- Files are raw bytes
 - no header information
 - storage is architecture-specific (e.g. big / little-endian floating-point)
- Difficult to cope with in other codes downstream
 - user must write their own post-processing tools
 - c.f. cioview / fioview with “metadata” encoded in file name!
- But ...
 - it can be very fast!

Solution

- For functionality
 - define higher-level formats
 - include metadata, e.g. “this is a 4x5x7 array of doubles”
 - enables standard data converters, browsers, viewers etc.
- For performance
 - layer on top of MPI-IO
- Many real applications use higher-level formats
 - understanding MPI-IO will enable you to get performance as well

HDF5

- “**Hierarchical Data Format (HDF)** is a set of file formats (**HDF4, HDF5**) designed to store and organize large amounts of data.” (Wikipedia)
 - data arranged like a Unix file system
 - self-describing
 - hierarchical
 - can use MPI-IO



Parallel HDF5 (Fortran)

- Approach much like MPI-IO

- describe global dataset

MPI_ORDER_
FORTTRAN

... describes its local portion(s) of the g

global data,
encodes sizes

```
CALL h5sselect_hyperslab_f(filespace, &  
    H5S_SELECT_SET_F, offset, &  
    count, error)
```

starts

- Then call collective write

- hyperslabs can be merged to create global file
- actual file IO done through MPI-IO
- important to choose collective IO

subsizes

NetCDF: Network Common Data Form

- “a set of software libraries and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data..” (Wikipedia)

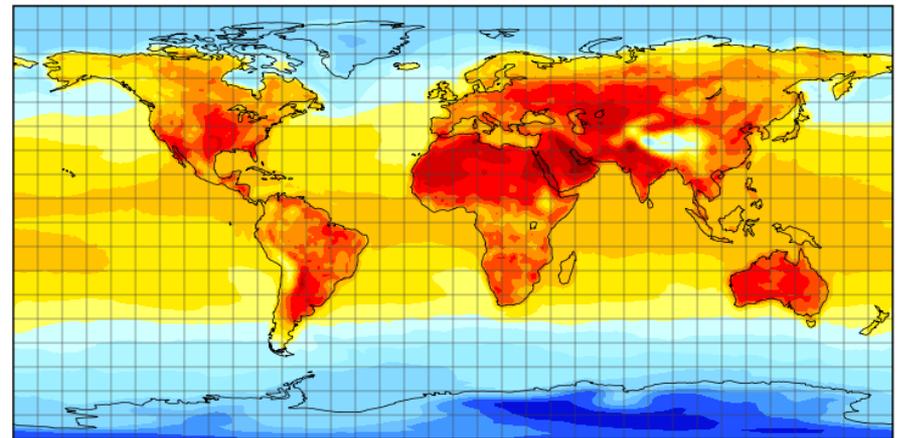
- more restricted than HDF5
- common in certain communities
 - climate research
 - oceanography
 - GIS ...

- Rich set of tools
 - data manipulation
 - visualisation

- ...

txxETCCDI_yr_MIROC5_historical_r2i1p1_1850-2012.nc

Annual Maximum of Daily Maximum Temperature



Annual Maximum of Daily Maximum Temperature (degrees_C)
-2.0E+01 -4.9E+00 1.0E+01 2.5E+01 4.0E+01 5.5E+01
Data Min = -2.0E+01, Max = 5.5E+01

image taken from <http://live.osgeo.org>

Parallel NetCDF (Fortran)



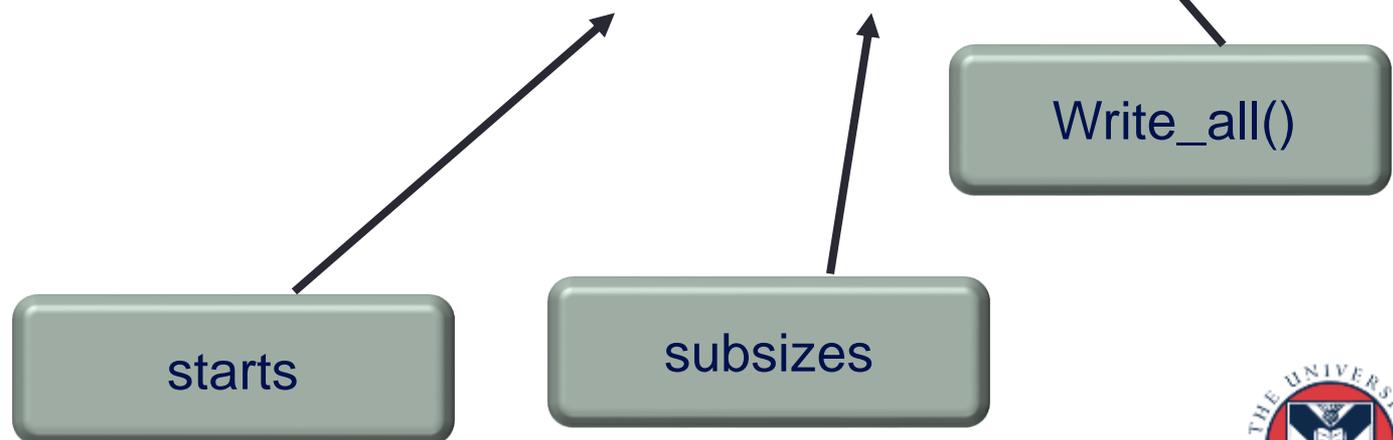
```
nf90_def_var(ncid, "data", NF90_DOUBLE, dimids,  
varid) )
```

...

```
nf90_var_par_access(ncid, varid, nf90_collective)
```

...

```
nf90_put_var(ncid, varid, buf, start, count)
```



ARCHER details

- HDF5

- `user@archer:~> module load cray-hdf5-parallel`
- interfaces to Cray MPI-IO

- NetCDF

- `user@archer:~> module load cray-netcdf-hdf5parallel`
- interfaces to HDF5 ...
- ... which interfaces to Cray MPI-IO

Summary

- MPI-IO may seem a little low-level
 - but is building block of parallel IO on ARCHER
- Higher-level formats layer on top of MPI-IO
 - to benefit from performance work by Cray, Lustre etc.
- Common formats are HDF5 and NetCDF
 - both supported on ARCHER
- Understanding MPI-IO performance is key to getting good performance for HDF5 and NetCDF