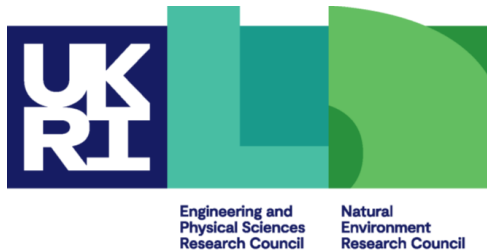


Advanced Message-Passing Programming

Alternative Parallel IO Libraries



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Overview

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

MPI-IO Issues

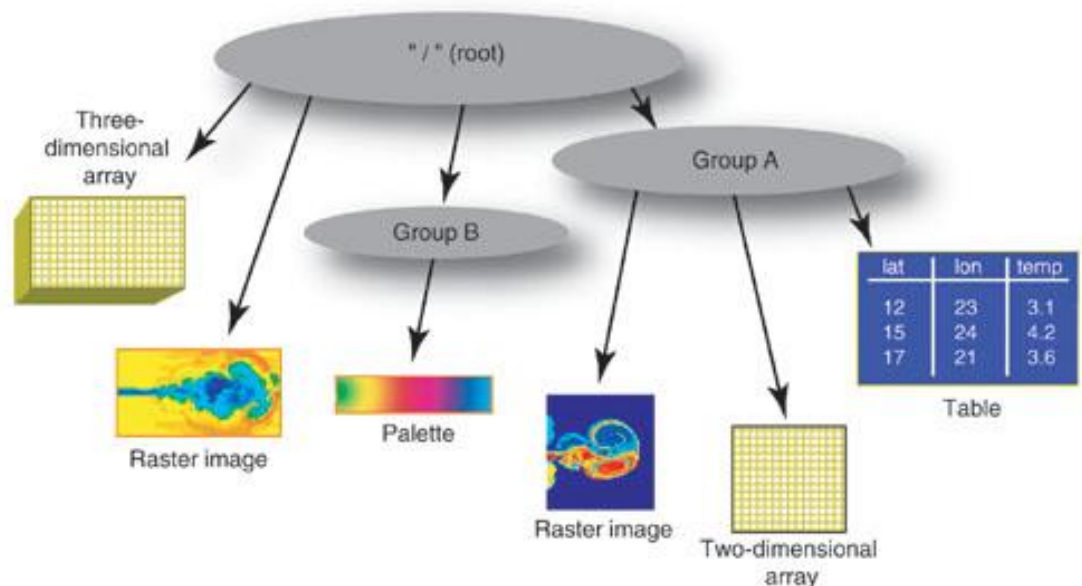
- Files are raw bytes
 - no header information
 - storage is architecture-specific (e.g. big / little-endian floating-point)
- Difficult to deal with in other codes downstream
 - user must write their own post-processing tools
- But ...
 - it can be very fast!

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

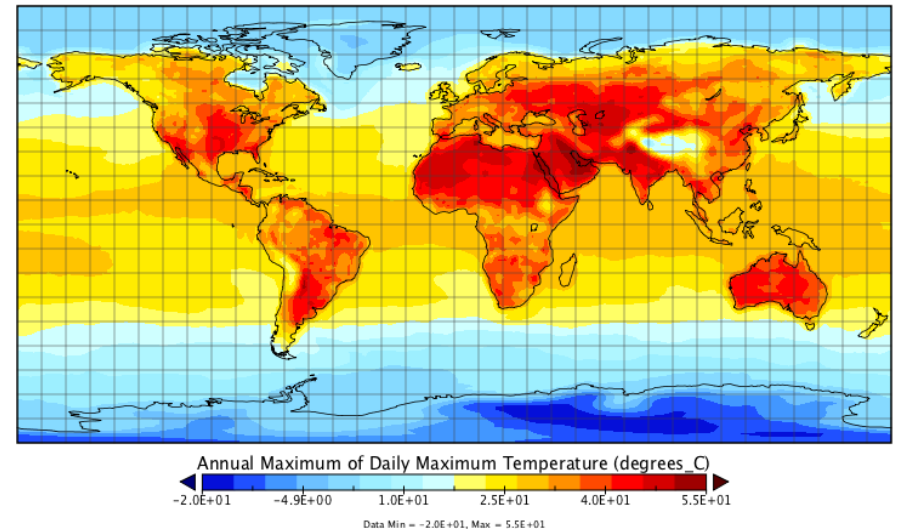


image taken from <http://live.osgeo.org>

Parallel NetCDF (Fortran)

file identifier

sizes

```
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)
```

Write_all()

starts

subsizes

ADIOS2

- A recent IO parallel library <https://adios2.readthedocs.io/>
 - can output using native MPI-IO or HDF5
 - also supports its own formats, e.g. BP5 (binary-pack v5)
- Same overall approach
 - each process defines what portion(s) of global data it owns
 - call read/write routines
- Much more configurable at runtime via “config.xml”
 - e.g. no need to recompile to switch MPI-IO to BP5
- Not yet part of benchio but colleagues have seen potential benefits from BP5 format in other codes
 - writes multiple files under the hood (with associated metadata)
 - may get round the limits of MPI-IO which has a single shared file

Summary

- MPI-IO may seem a little low-level
 - but is fundamental building block of parallel IO on most systems
- Higher-level formats layer on top of MPI-IO
 - to benefit from performance work by vendors, Lustre etc.
- Common formats are HDF5 and NetCDF
 - both supported on ARCHER2
 - you might also want to look at the newer ADIOS2 library
- Understanding MPI-IO performance is key to getting good performance for HDF5 and NetCDF