Advanced Parallel Programming

Alternative Parallel IO Libraries

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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

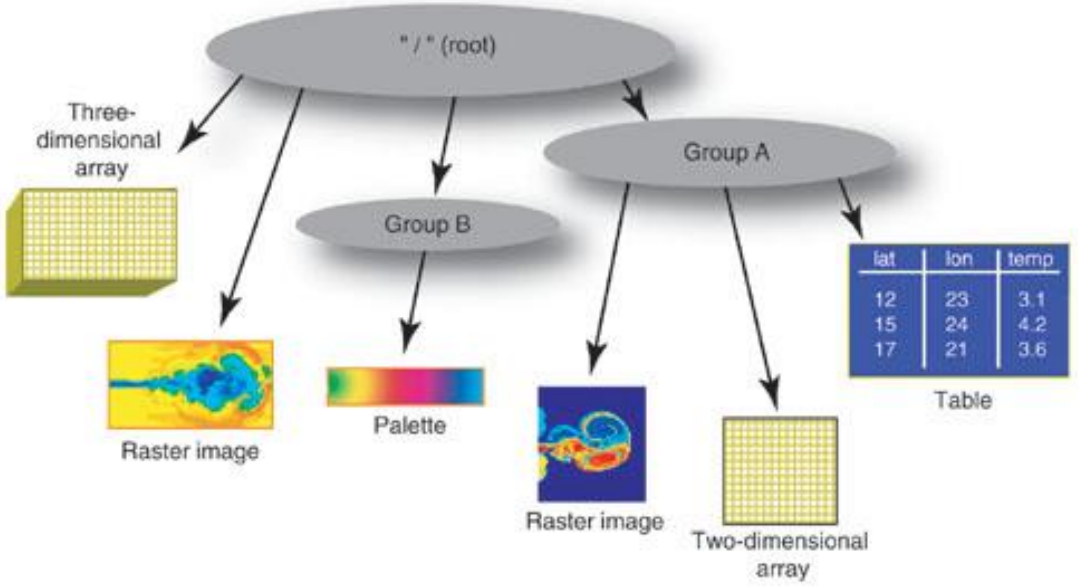
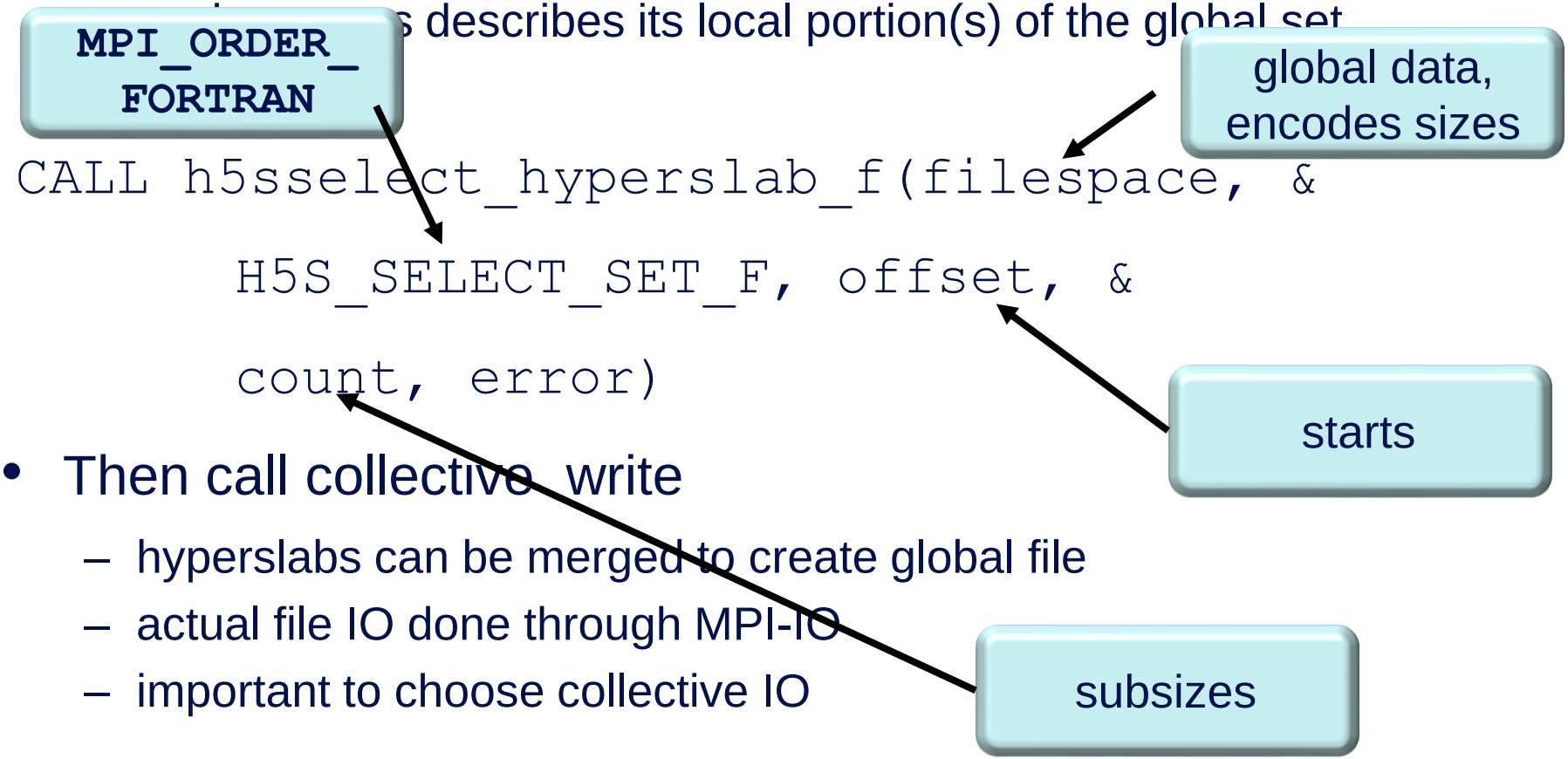


image taken from www.hdfgroup.org

Parallel HDF5 (Fortran)

- Approach much like MPI-IO
  - describe global dataset
  - [illegible]s describes its local portion(s) of the global set



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

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
  - ...

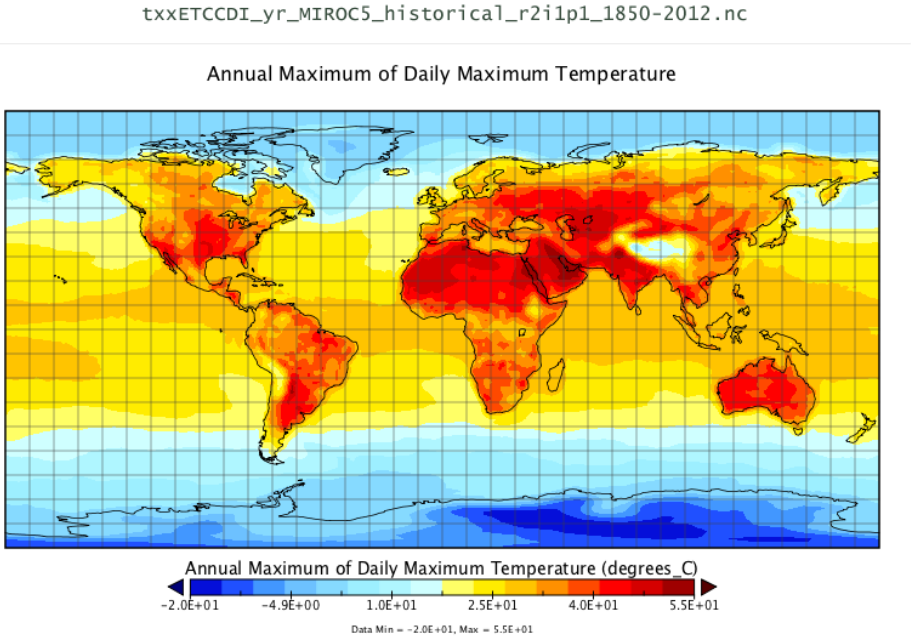
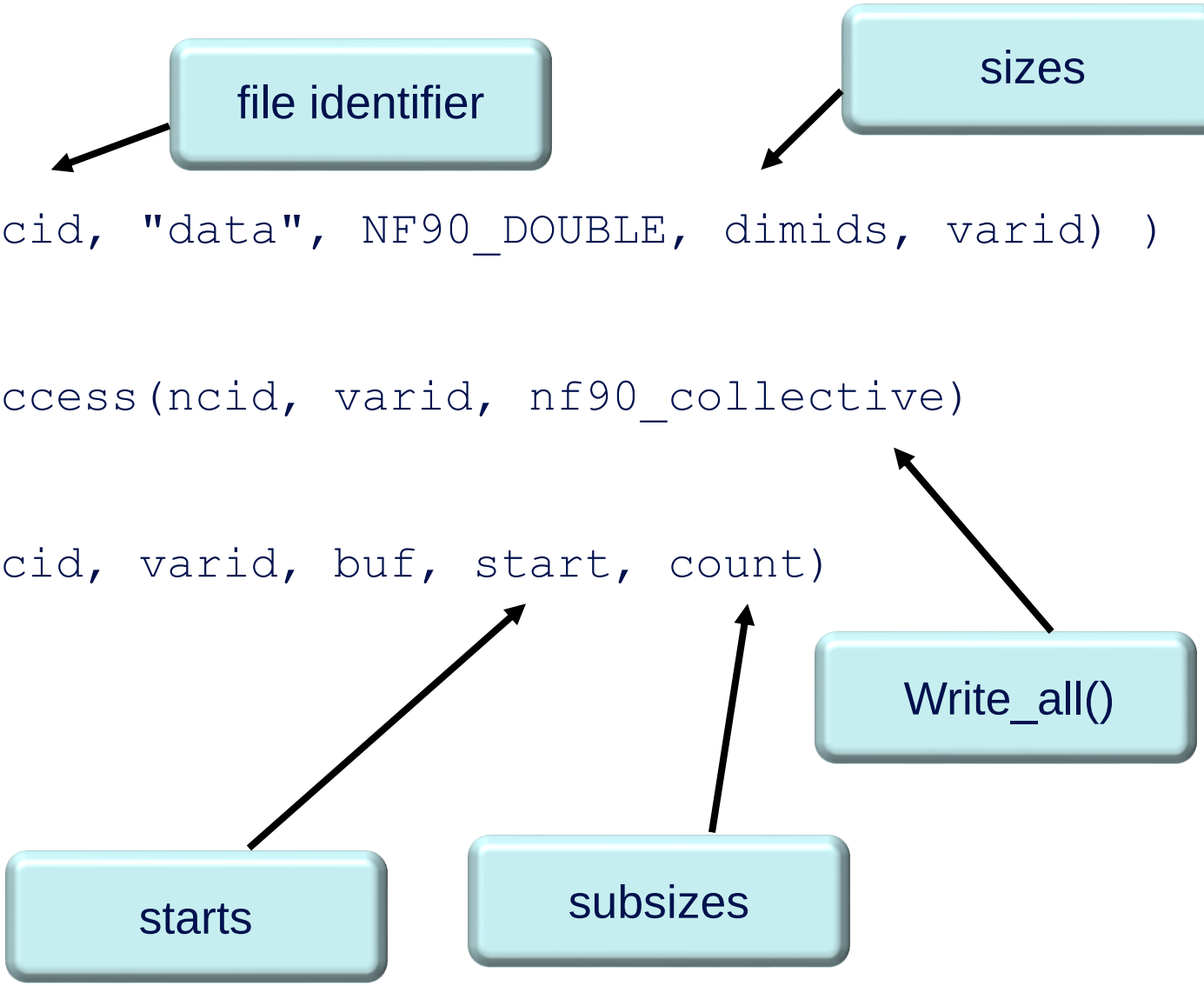


image taken from http://live.osgeo.org

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 om 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