Parallel netCDF:
A High-Performance Scientific I/O Interface

Jianwei Li

ECE Department, Northwestern University

(jianwei@ece.northwestern.edu)

W. Liao, A. Choudhary (Northwestern University)

R. Ross, R. Thakur, W. Gropp, R. Latham, A. Siegel (Argonne National Laboratory)

B. Gallagher (University of Chicago)

M. Zingale (University of California, Santa Cruz)

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Outline

- Overview of netCDF & our motivation
- NetCDF file format & current serial interface
- Access netCDF files in parallel applications
- Parallel netCDF design & implementation
- Parallel netCDF vs Parallel HDF5
- Performance evaluation
- Summary & future work
- Software and documentation resources

Introduction

- netCDF (network Common Data Form)
  - Initially by Unidata Program Center in Boulder, Colorado.
  - Provide a common data access method for various scientific apps.
- File format & programming interface
  - Portable, platform independent and self-describing file format
  - Libraries for array-oriented data access in C, FORTRAN, etc.
- A broad community of netCDF users
  - Easy to learn and use
  - A de facto data access standard for much of the climate community
  - atmospheric app., ocean modeling, fusion simulations, medical images, satellite/radar images
  - Huge amount of existing netCDF datasets, and processing tools
- Well supported by Unidata
- Parallel interface support from NWU/ANL

Why Parallel I/O?

- Most scientific applications are in parallel
- Increasing requirement on data amount
- I/O bottleneck
- Scalability needs parallel I/O
- Programming convenience with parallel I/O
- Significant I/O performance improvement with appropriate parallel I/O techniques
- Well studied and supported

NetCDF File Format

header:

definition of the netCDF dataset

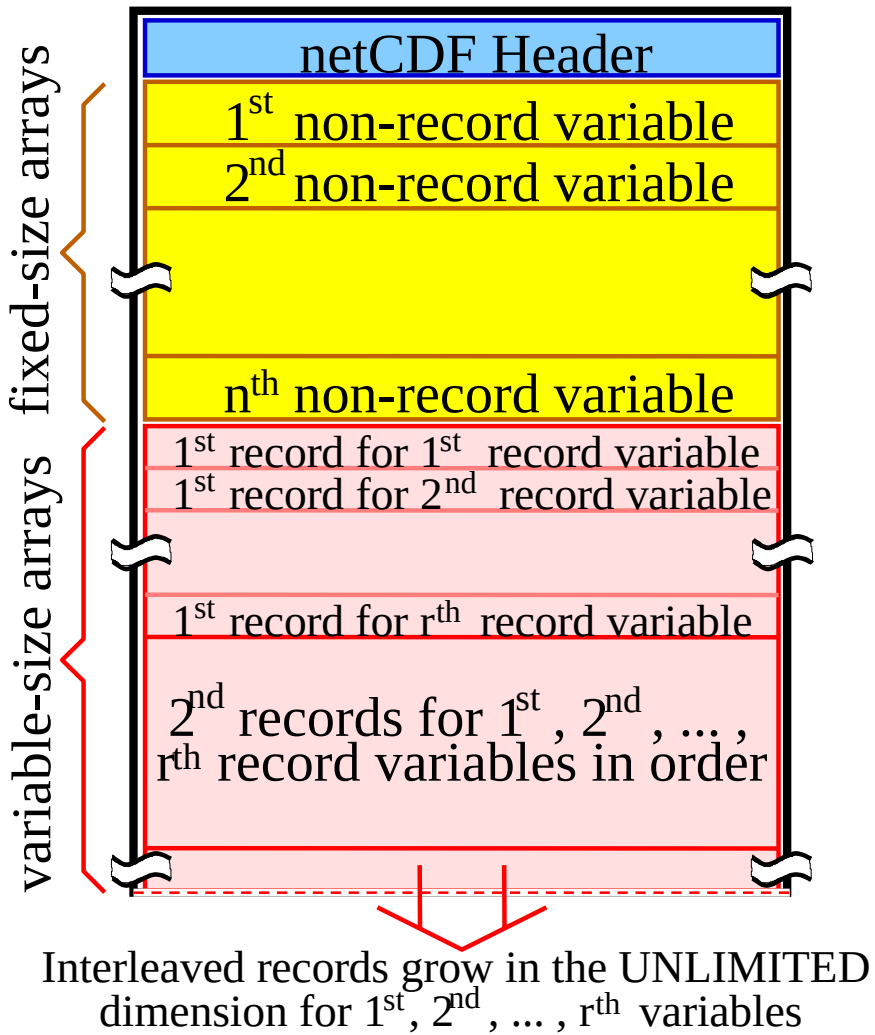
n fixed-size variables:

arrays of fixed dimensions

r record variables:

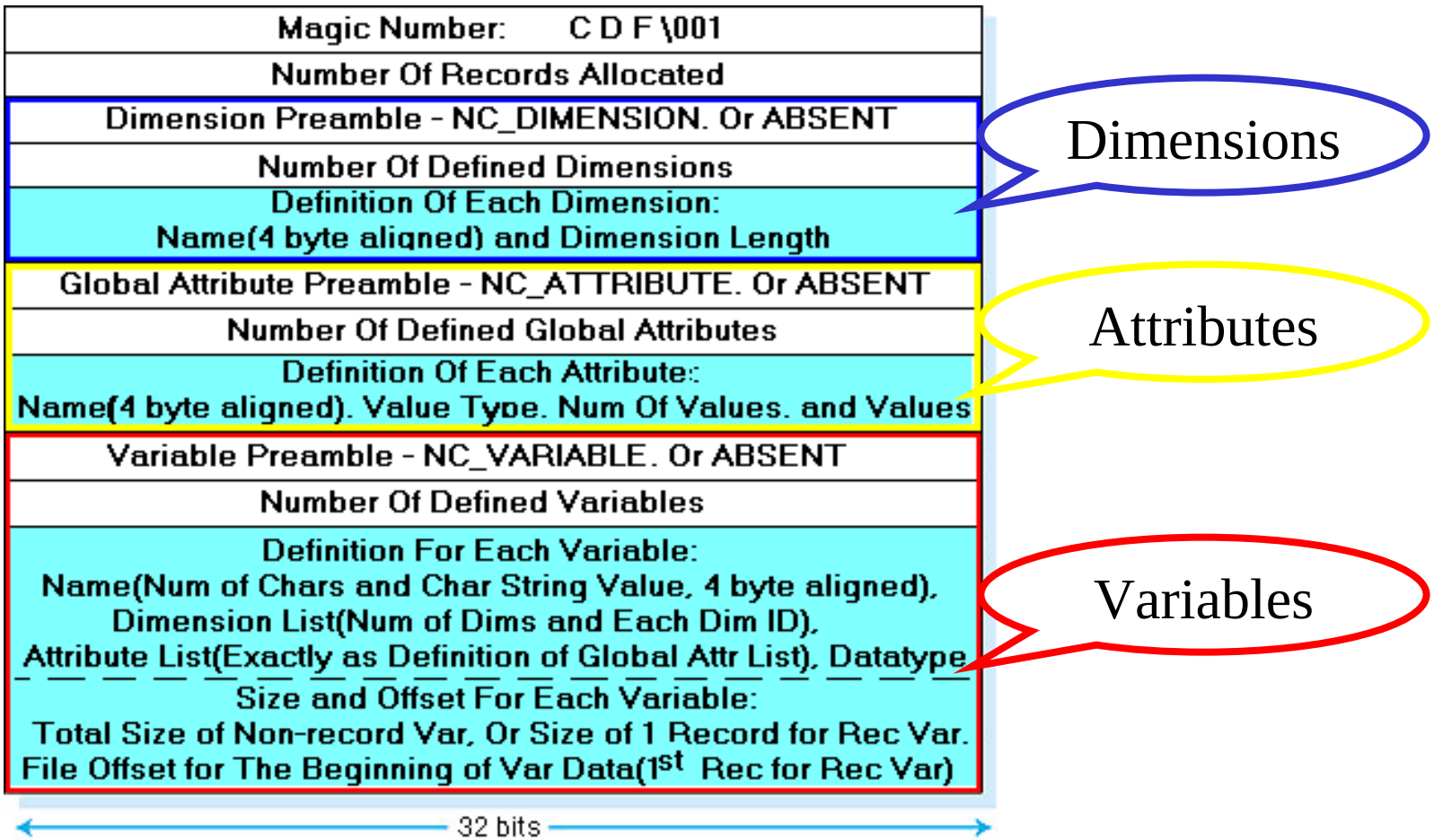
arrays with its most-significant dimension UNLIMITED,

records defined by the rest of the dimensions.



File Header

Defines the 3 components of a netCDF dataset:



An Example NetCDF File

```
netCDF_example { // CDL notation for netCDF dataset
   dimensions: // dimension (names and lengths)
        lat = 5, lon = 10, level = 4, time = unlimited;
   variables: // var (types, names, shapes, attributes)
        float temp(time,level,lat,lon);
                temp:long_name = "temperature";
                temp:units = "celsius";
        float rh(time,lat,lon);
                rh:long_name = "relative humidity";
                rh:valid_range = 0.0, 1.0; // min and max
   // global attributes:
        :source = "Fictional Model Output";
   data: // optional data assignments
        temp =  0, ..., 0;
        rh   =  .5,.2,.4,.2,.3,.2,.4,.5,.6,.7,
                .1,.3,.1,.1,.1,.1,.5,.7,.8,.8,
                .1,.2,.2,.2,.2,.5,.7,.8,.9,.9,
                .1,.2,.3,.3,.3,.3,.7,.8,.9,.9,
                 0,.1,.2,.4,.4,.4,.4,.7,.9,.9;  // 1 record allocated
}
```

Serial NetCDF API

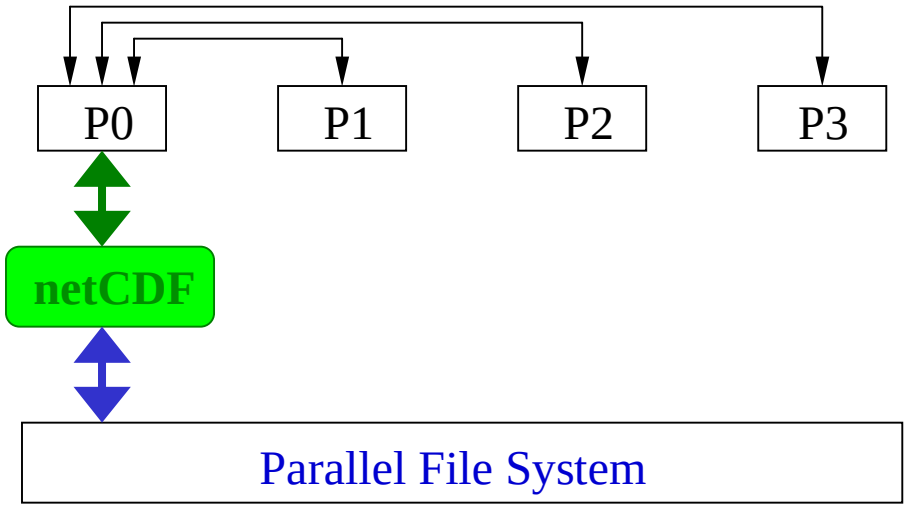
- **Dataset Functions**
  - create/open/close/abort a dataset
  - set the dataset to define/data mode
  - synchronize dataset changes to storage
- **Define Mode Functions**
  - define dataset dimensions and variables
- **Attribute Functions**
  - manage adding, changing, and reading attributes of the dataset
- **Inquiry Functions**
  - return dataset metadata:

    dim(id, name, len), var(id, name, ndims, shape, etype), # of dims/vars/attributes, etc.
- **Data Access Functions**
  - read/write variable data in one of the five access methods (patterns):

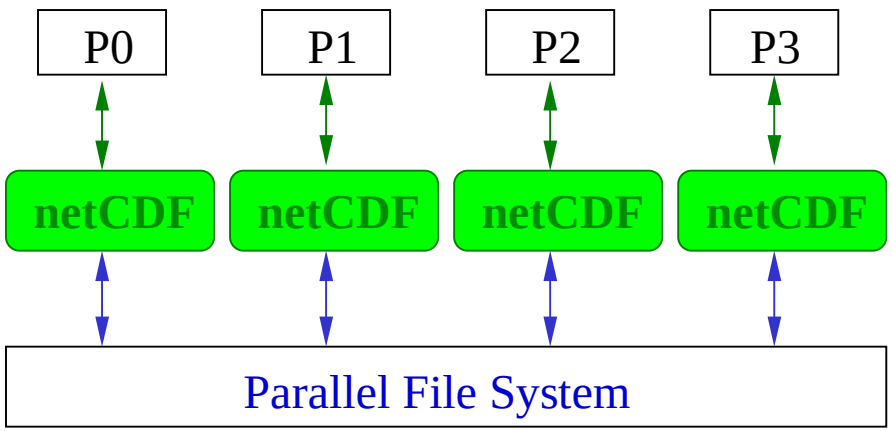
    single element, whole array, subarray, strided subarray, or mapped strided subarray

Built on native I/O and designed for serial access

Parallel Access to NetCDF Files?

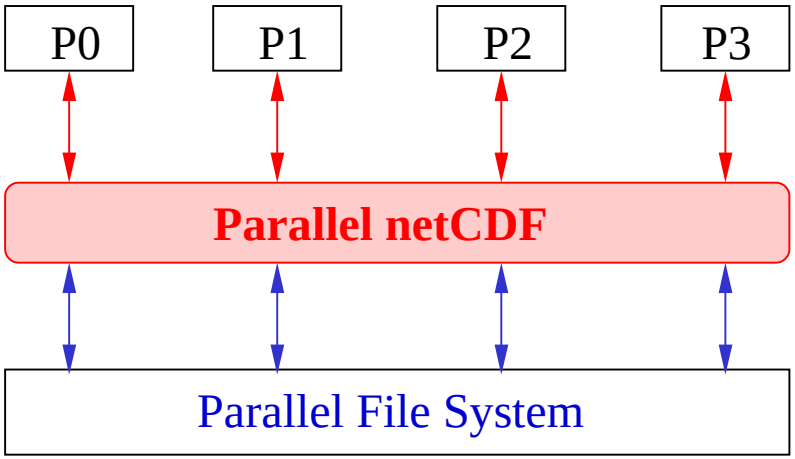


- Slow and cumbersome
- Data shipping
- I/O bottleneck
- Memory requirement



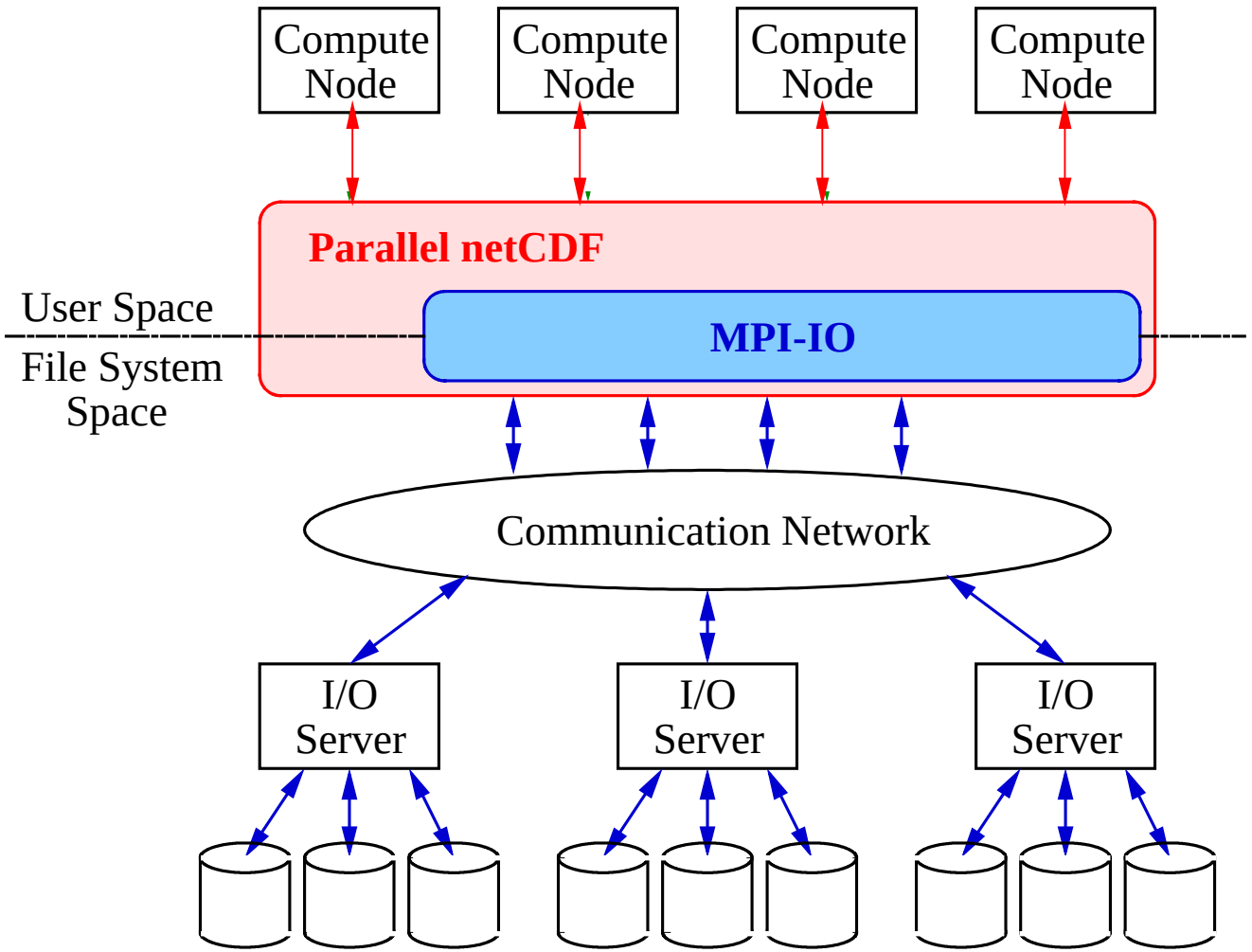
- Multiple file pieces
- Breaks the netCDF dataset
- Independent Access

Access through Parallel NetCDF!



- New parallel interface
- Perform I/O cooperatively or collectively
- Potential parallel I/O optimizations for better performance
- NetCDF data integration and management

Architecture for Parallel NetCDF



Parallel NetCDF API

- The same netCDF file format
- Maintains the look and feel of the serial netCDF API
  - Same syntax & semantics for:
    - Dataset functions (except create/open)
    - Define mode functions, attribute functions and inquiry functions
    - High-level data access functions
  - Distinguish by prefixing function calls with “ncmpi_”/“nfmpi_”
- Parallel access through MPI-IO
  - Benefit from MPI-IO optimizations (data shipping, two-phase I/O, etc.)
  - MPI communicator added in the argument list for create/open
  - MPI_Info used for parallel I/O management and further optimization
  - Collective I/O (function names end with “_all”) vs noncollective I/O
- New flexible data access functions
  - Accept non-contiguous memory regions described by MPI datatypes

PnetCDF Example Code

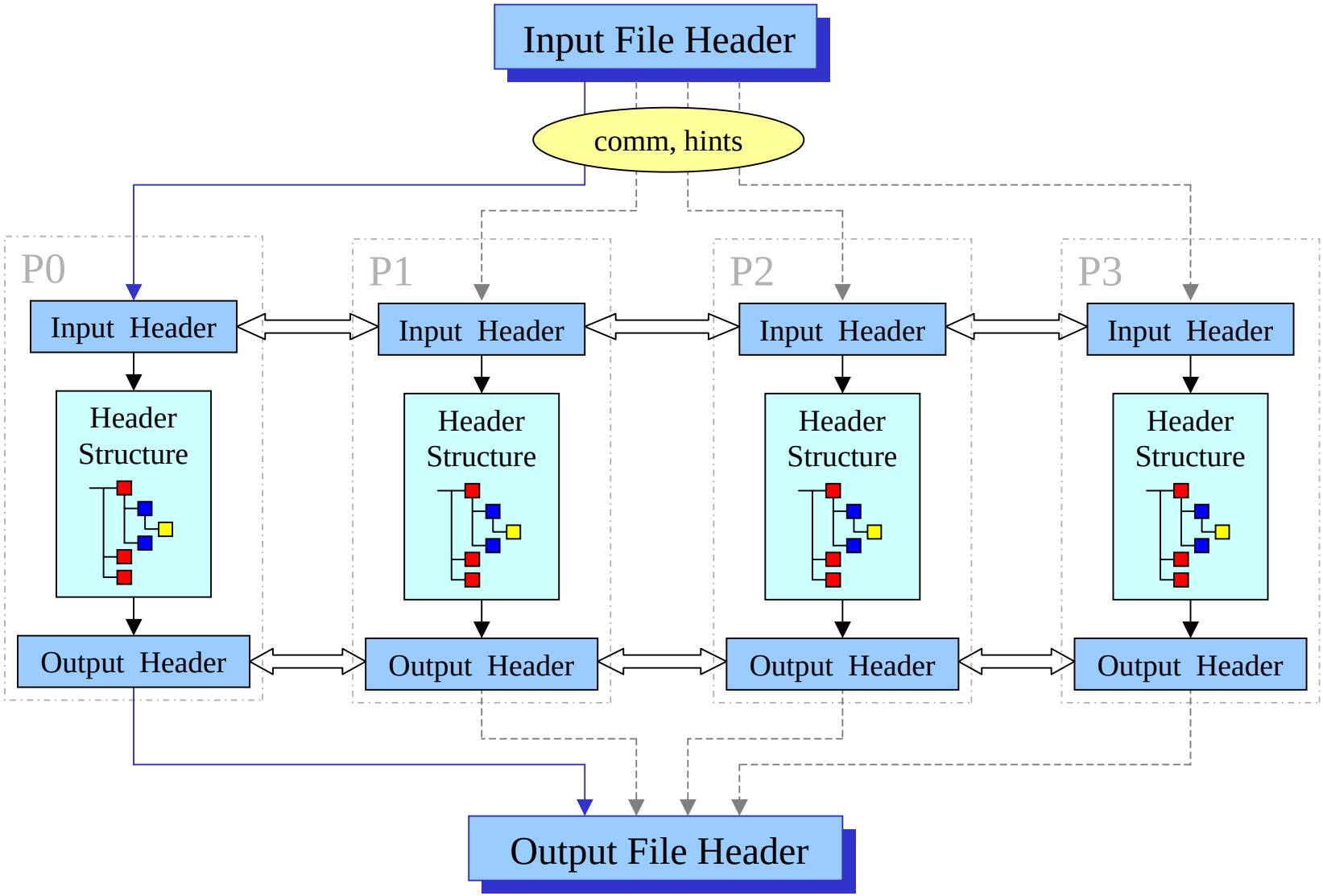
File write

```
1. ncmpi_create(mpi_comm, filename, open_mode, mpi_info, &file_id);
2. ncmpi_def_var(file_id, ...);
   . . .      . . .
   ncmpi_enddef(file_id);
3. ncmpi_put_vara_all(file_id, var_id, start[], count[], buffer, bufcount, mpi_datatype);
4. ncmpi_close(file_id);
```

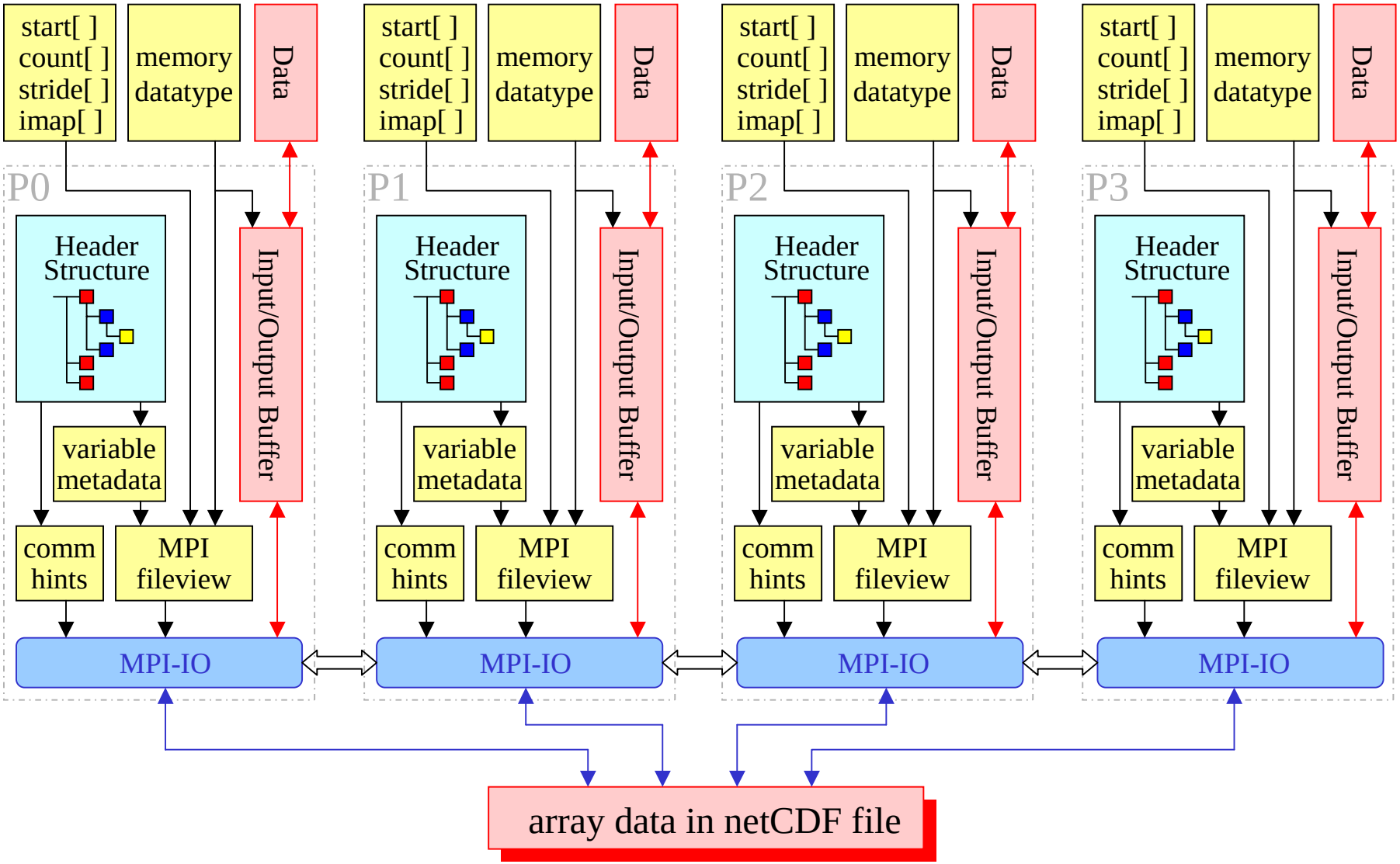
File read

```
1. ncmpi_open(mpi_comm, filename, open_mode, mpi_info, &file_id);
2. ncmpi_inq(file_id, ... );
   . . .      . . .
3. ncmpi_get_vars(file_id, var_id, start[], count[], stride[], buffer, bufcount, mpi_datatype);
4. ncmpi_close(file_id);
```

Access to File Header

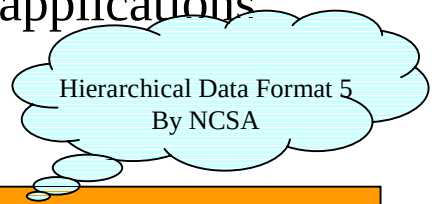


Parallel I/O for Array Data



Compare with Parallel HDF5

- Both define portable, self-describing file formats
- Both serve as data access standards for parallel scientific applications
- Both have parallel I/O built on top of MPI-IO

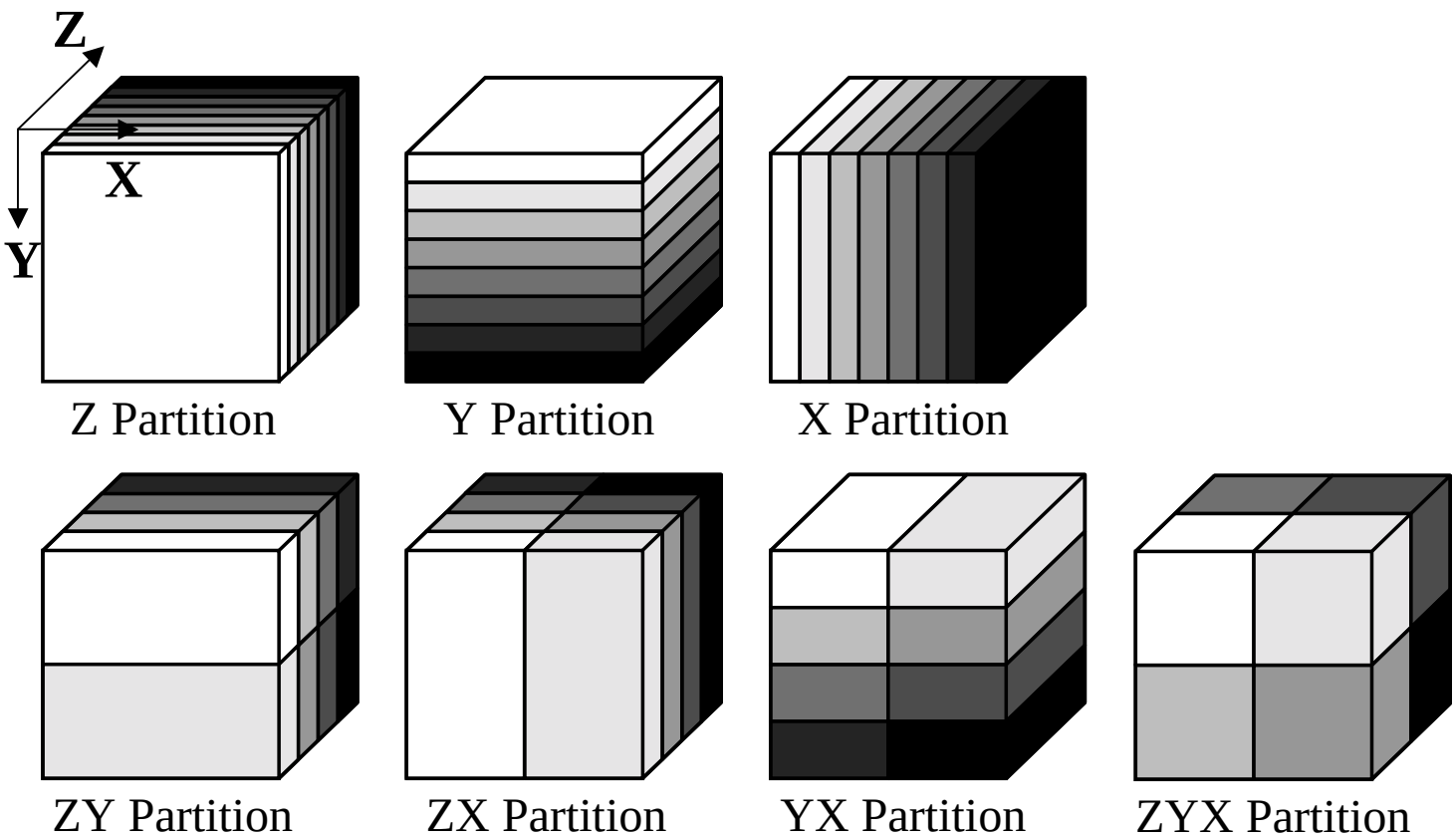


Parallel netCDF	Parallel HDF5
• Contiguous or interleaved data layout; • Sits on top of MPI-IO, transferring user access patterns directly to MPI fileview, little overhead.	• Tree-like file structure; • Use dataspace and hyperslabs to define data organization, map and transfer data between memory and filespace, pack or unpack.
• One time header I/O gets all necessary info for direct access of each data array; • By maintaining a local copy of header, each process can access any array identified by its permanent ID at any time, without any collective open/close operation of the object. Saves a lot of inter-process communication.	• Iterate through entire namespace to get the header info to access each object; • Need collective open/close operation when accessing each single object, and for file write, the metadata need to be updated in a synchronous way. So lots of communication overhead.

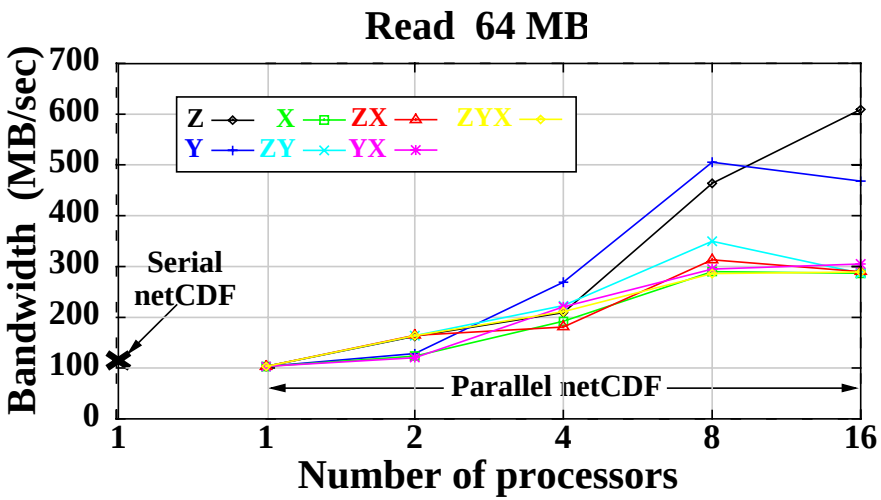
Performance Evaluation

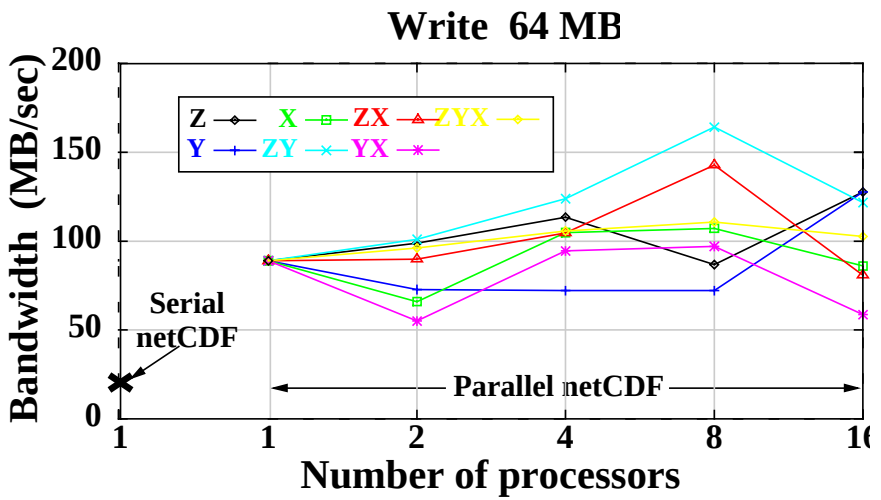
- A micro-benchmark accessing a 3-D array
  - Platform: Bluehorizon (IBM SP-2) @ SDSC
    - IBM's MPI, GPFS file system
  - Performance scalability of our PnetCDF
  - Compare Parallel netCDF with Serial netCDF
- FLASH I/O benchmark writing a number of multi-dimensional arrays
  - Platform: ASCI White (Frost) @ LLNL
    - IBM's MPI, GPFS file system
  - Compare PnetCDF with PHDF5

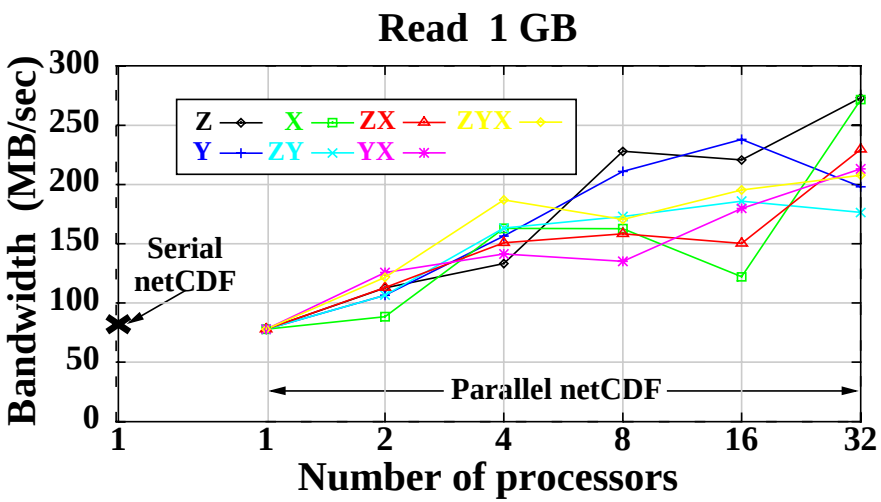
Data Partition of Micro-benchmark

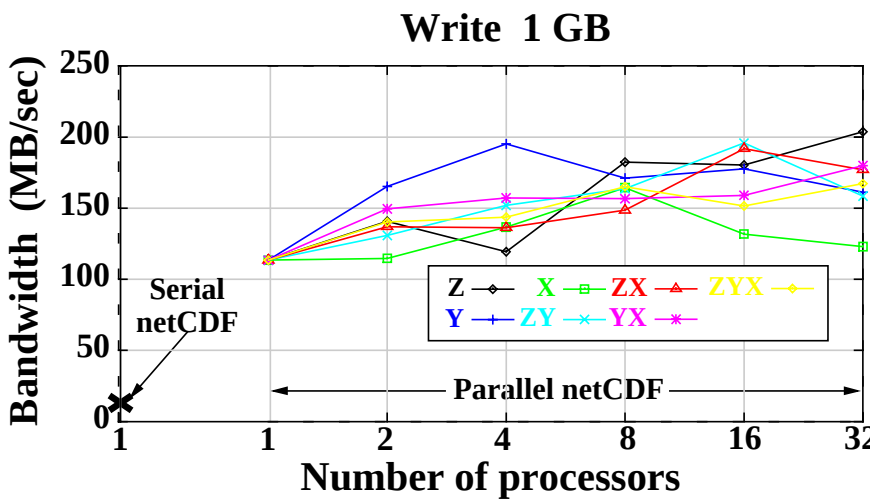


Performance Scalability





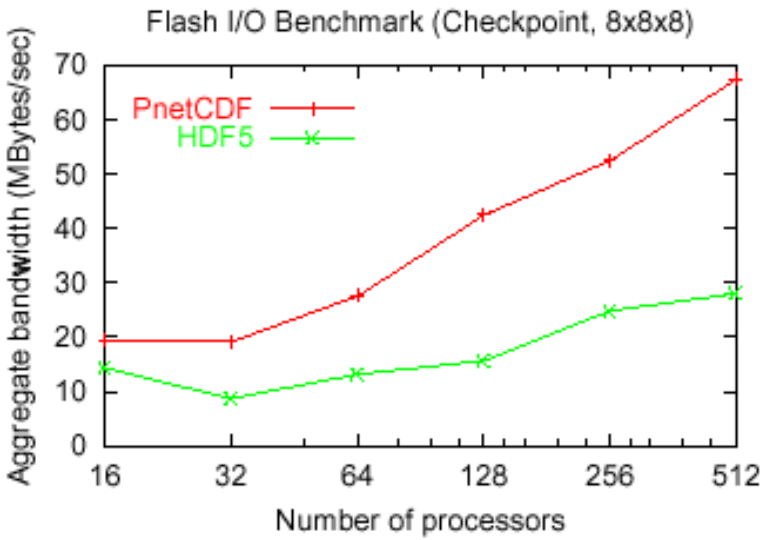


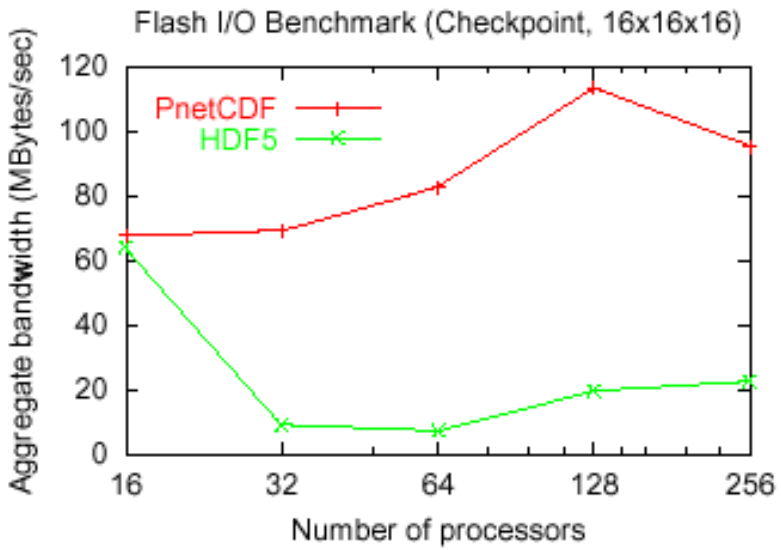


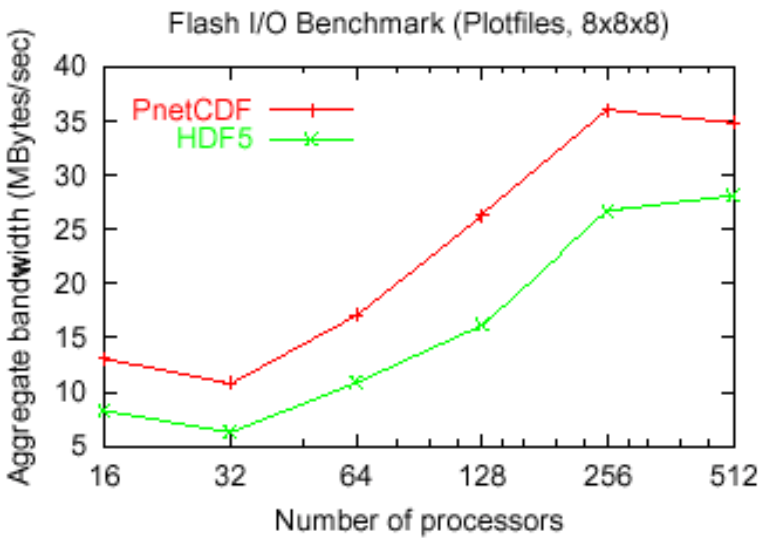
FLASH I/O Benchmark

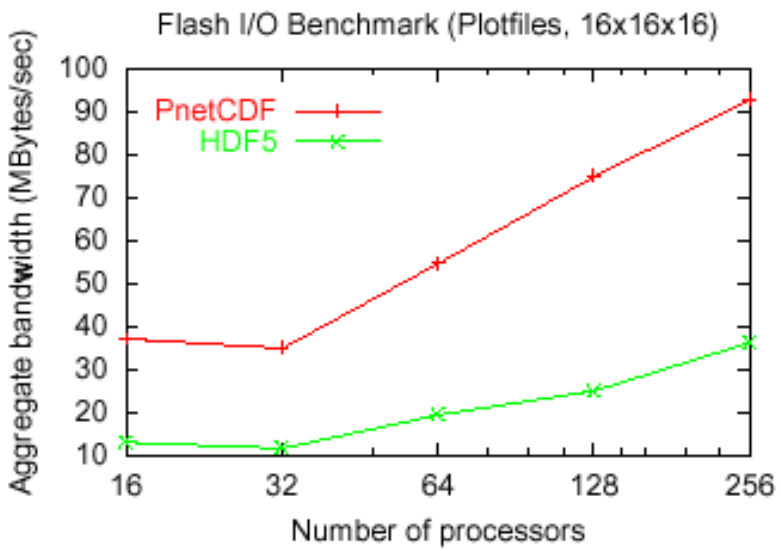
- FLASH – parallel hydrodynamics code
  - Simulate astrophysical thermonuclear flashes in 2/3D
  - Use structured adaptive mesh refinement method to solve some physics equations
  - Produce checkpoint files and visualization plotfiles
- FLASH I/O benchmark
  - Simulate the I/O pattern of FLASH
  - 3D AMR subblocks with a perimeter of four guard cells (In the simulation, 80 blocks by each process, 8*8*8 or 16*16*16)
  - Generate a checkpoint file, a plotfile with centered data, and a plotfile with corner data
  - A series of multi-dimensional arrays, each partitioned in the most significant dimension

FLASH I/O Performance

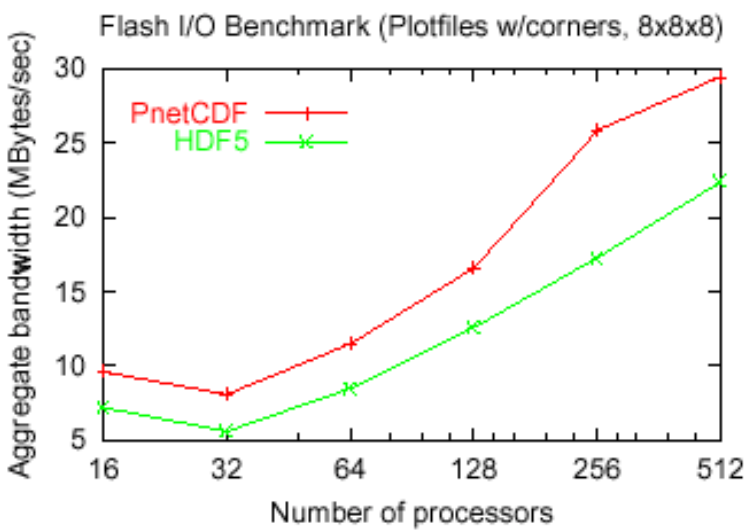


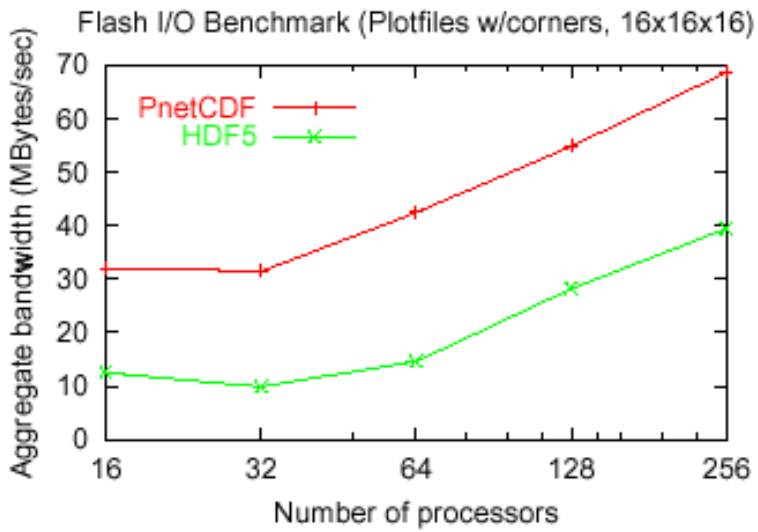






FLASH I/O Performance (cont.)





Summary and Future Work

- PnetCDF - A new high-level I/O library
  - Uses same data format as netCDF
  - Maintains the flavor of the netCDF API
  - Provides parallel access semantics
- Current status
  - Distributions of code available, w/ basic test suite
  - Mailing list for users, support
  - External groups are already adopting this software
  - Performance is already competitive w/out any tuning
- Future work
  - Perfect the library, improving our test suite, support
  - Performance tuning for key platforms (IBM SP, Linux)

More Information

- Learn more about netCDF

  http://www.unidata.ucar.edu/packages/netcdf/
- Download the PnetCDF software & docs

  http://www.mcs.anl.gov/parallel-netcdf/

Thank you!

>> Questions???