Parallel I/O: Not Your Job

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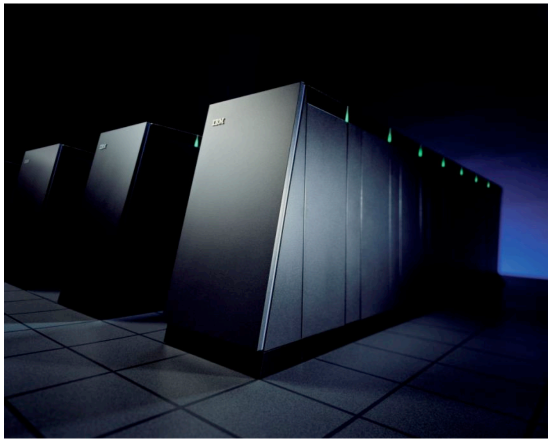
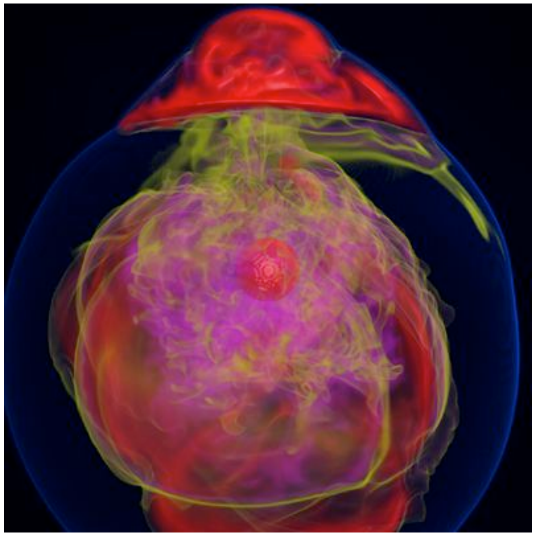
Computational Science

- Use of computer simulation as a tool for greater understanding of the real world
- Complements experimentation and theory
- As our simulations become ever more complicated
  - Large parallel machines needed to perform calculations
  - Leveraging parallelism becomes more important
- Managing code complexity bigger issue as well
  - Use of libraries increases (e.g. MPI, BLAS)
- Data access is a huge challenge
  - Using parallelism to obtain performance
  - Providing usable and efficient interfaces



IBM BG/L system.



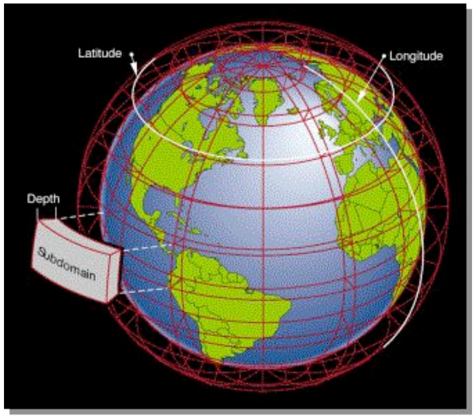
Visualization of entropy in Terascale Supernova Initiative application. Image from Kwan-Liu Ma's visualization team at UC Davis.

Outline

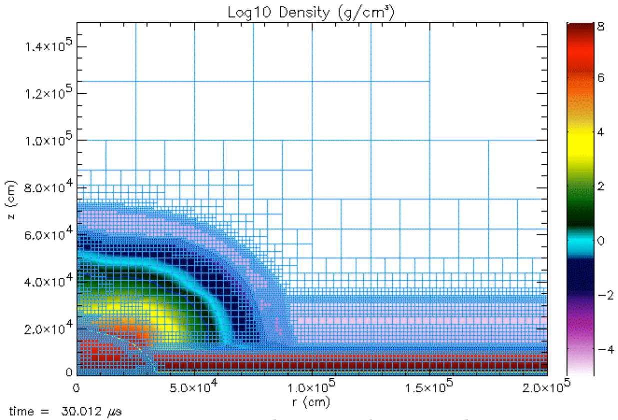
- Introduction
- I/O software stacks
- Interfaces
  - MPI-IO
  - Parallel netCDF
  - HDF5
- Best practice
- Wrapping up

Application I/O

- Applications have data models appropriate to domain
  - Multidimensional typed arrays, images composed of scan lines, variable length records
  - Headers, attributes on data
- I/O systems have very simple data models
  - Tree-based hierarchy of containers
  - Some containers have streams of bytes (files)
  - Others hold collections of other containers (directories or folders)
- Someone has to map from one to the other!



Graphic from J. Tannahill, LLNL



Graphic from A. Siegel, ANL

Common Approaches to Application I/O

- Root performs I/O
  - *Pro: trivially simple for "small" I/O*
  - *Con: bandwidth limited by rate one client can sustain*
  - *Con: may not have enough memory on root to hold all data*
- All processes access their own file
  - *Pro: no communication or coordination necessary between processes*
  - *Pro: avoids some file system quirks (e.g. false sharing)*
  - *Con: for large process counts, lots of files created*
  - *Con: data often must be post-processed to recreate canonical dataset*
  - *Con: uncoordinated I/O from all processes may swamp I/O system*
- All processes access one file
  - *Pro: only one file (per timestep etc.) to manage: fewer files overall*
  - *Pro: data can be stored in canonical representation, avoiding post-processing*
  - *Con: can uncover inefficiencies in file systems (e.g. false sharing)*
  - *Con: uncoordinated I/O from all processes may swamp I/O system*

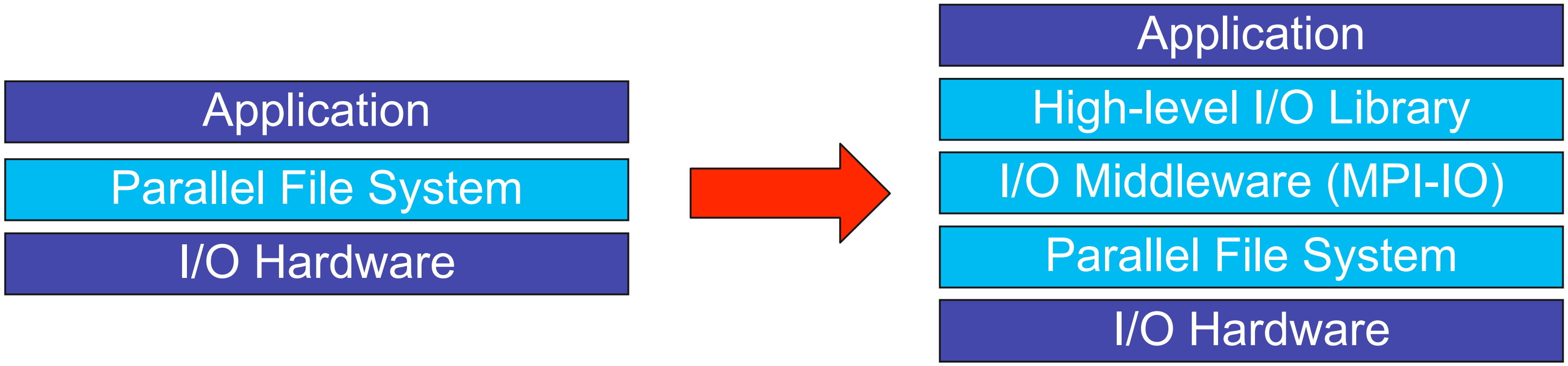
Challenges in Application I/O

- Leveraging aggregate communication and I/O bandwidth of clients
- …But not overwhelming a resource limited I/O system with uncoordinated accesses!
- Limiting number of files that must be managed (also a performance issue)
- Avoiding unnecessary post-processing
- Avoiding file system quirks

- Often application teams spend so much time on this that they never get any further:
  - Interacting with storage through convenient abstractions
  - Storing in portable formats

- Computer science teams that are experienced in parallel I/O have developed software to tackle all of these problems
  - **Not your job.**

I/O for Computational Science



Application

Parallel File System

I/O Hardware

Application

High-level I/O Library

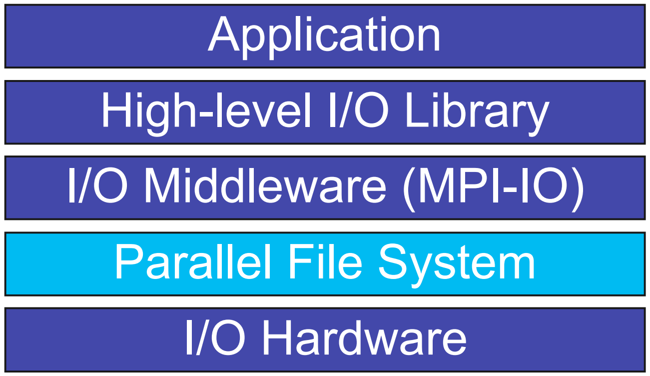
I/O Middleware (MPI-IO)

Parallel File System

I/O Hardware

- Applications require more software than just a parallel file system
- Break up support into multiple layers with distinct roles:
  - Parallel file system maintains logical space, provides efficient access to data (e.g. PVFS, GPFS, Lustre)
  - Middleware layer deals with organizing access by many processes (e.g. MPI-IO, UPC-IO)
  - High level I/O library maps app. abstractions to a structured, portable file format (e.g. HDF5, Parallel netCDF)

Parallel File System


Application

High-level I/O Library

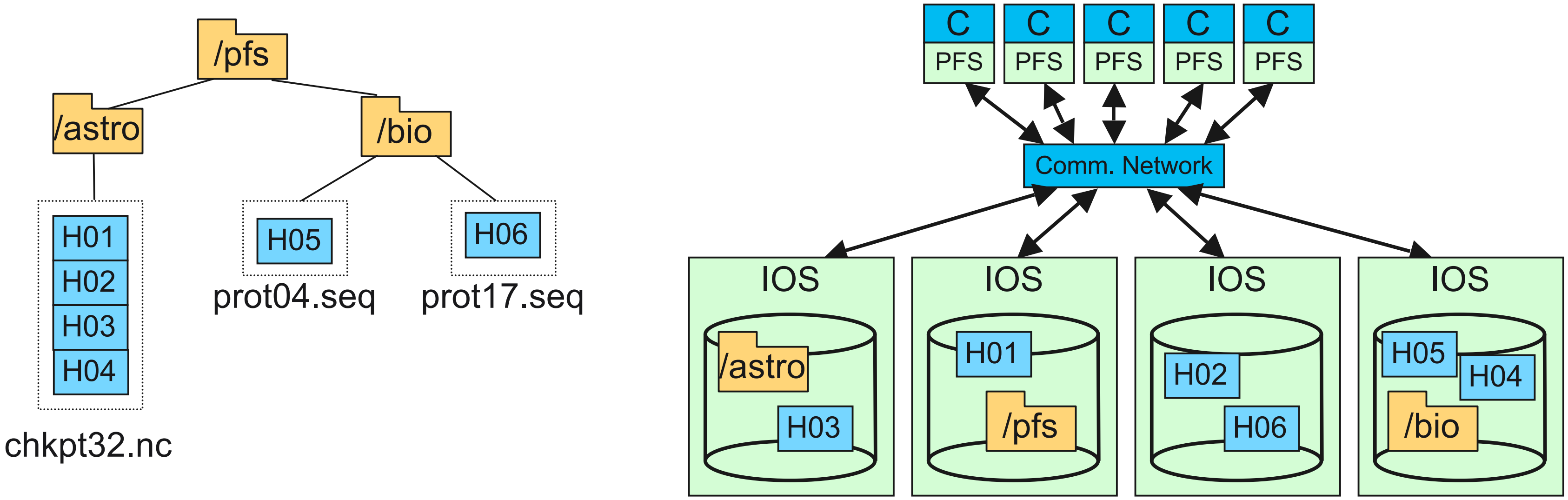
I/O Middleware (MPI-IO)

Parallel File System

I/O Hardware

- Manage storage hardware
  - Present single view
  - Stripe files for performance
- In the context of the I/O software stack
  - Focus on concurrent, independent access
  - Publish an interface that middleware can use effectively
    - *Rich I/O language*
    - *Relaxed but sufficient semantics*
  - Knowledge of collective I/O usually very limited

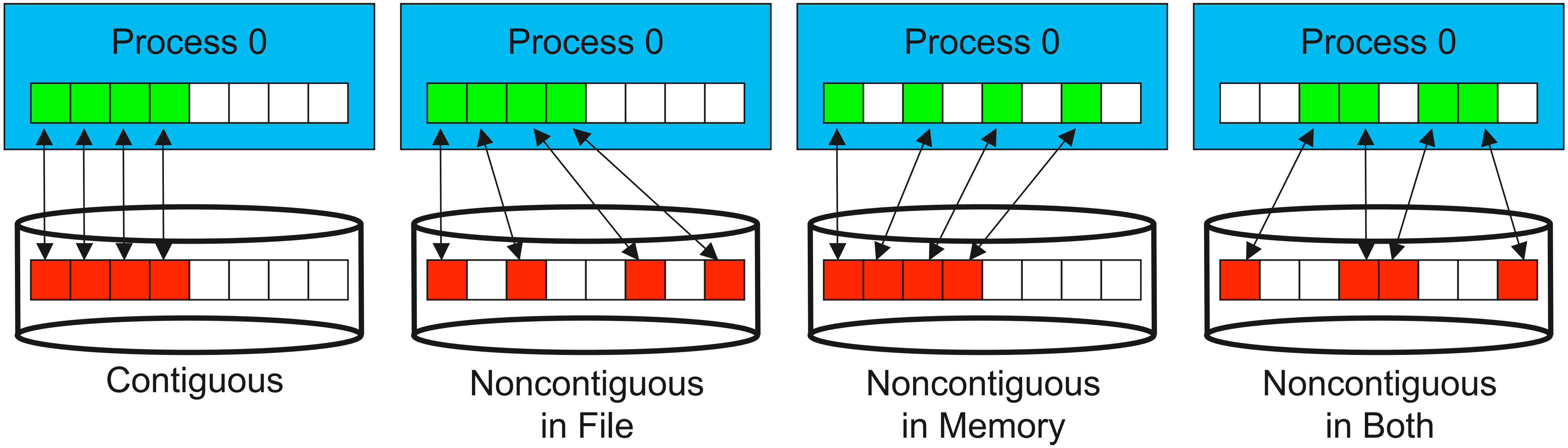
Parallel File Systems



An example parallel file system, with large astrophysics checkpoints distributed across multiple I/O servers (IOS) while small bioinformatics files are each stored on a single IOS.

- Block-based or region-oriented accesses
- Stripe data across multiple resources
  - Simultaneous use of multiple servers, disks, and network links
- Tradeoffs between performance and consistency
  - POSIX: strict consistency hurts performance
  - NFS: consistency too weak: much time spent flushing buffers
  - More on this later

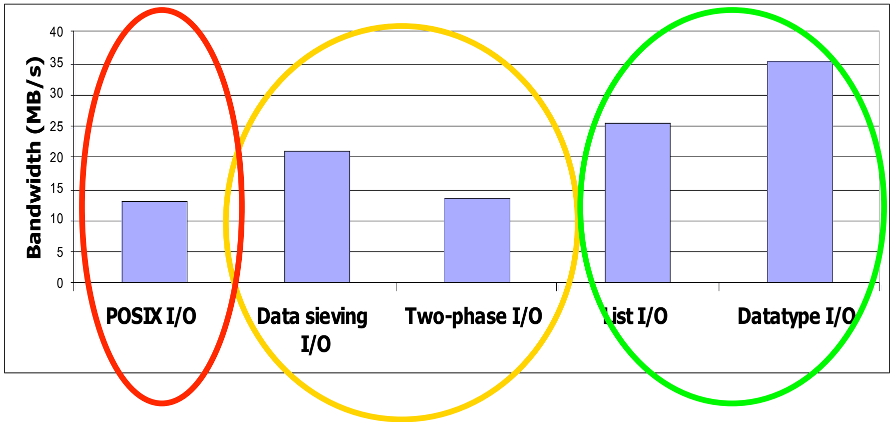
Contiguous and Noncontiguous I/O



- Contiguous I/O moves data from a single memory block into a single file region
- Noncontiguous I/O has three forms:
  - Noncontiguous in memory, noncontiguous in file, or noncontiguous in both
- Structured data leads naturally to noncontiguous I/O (e.g. block decomposition)
- Describing noncontiguous accesses with a single operation passes more knowledge to I/O system

Supporting Noncontiguous I/O

- Three approaches for noncontiguous I/O
  - Use POSIX and suffer
  - Perform optimizations at the MPI-IO layer as work-around
  - Augment the parallel file system
- Augmenting the parallel file system API is most effective



MPI-IO Optimizations

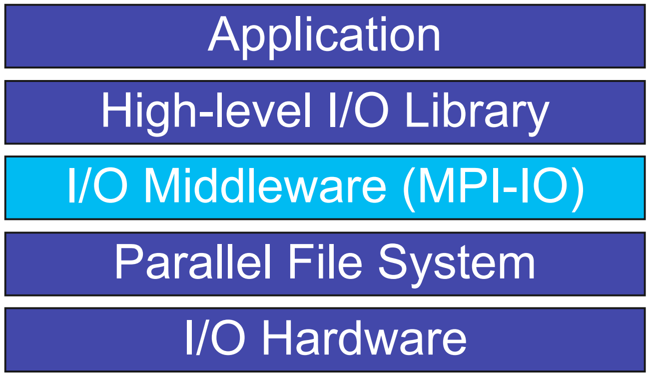
PFS Enhancements

POSIX I/O

Results from "Datatype I/O" prototype in PVFS1 with tile example

I/O Middleware

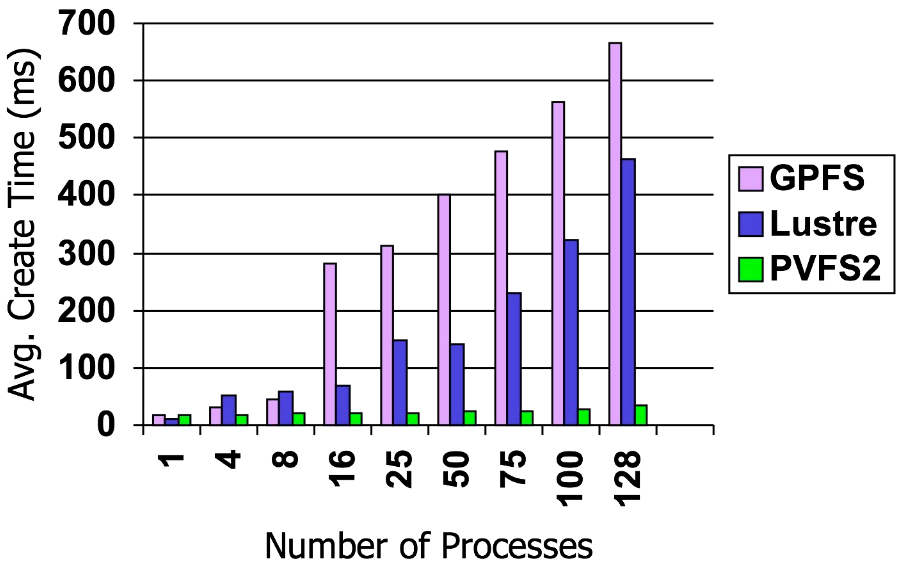
- Match the programming model (e.g. MPI)
- Facilitate concurrent access by groups of processes
  - Collective I/O
  - Atomicity rules
- Expose a generic interface
  - Good building block for high-level libraries
- Efficiently map middleware operations into PFS ones
  - Leverage any rich PFS access constructs, such as:
    - *Scalable file name resolution*
    - *Rich I/O descriptions*

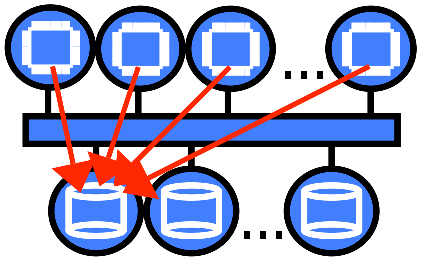

Application
High-level I/O Library
I/O Middleware (MPI-IO)
Parallel File System
I/O Hardware

Creating Files Efficiently

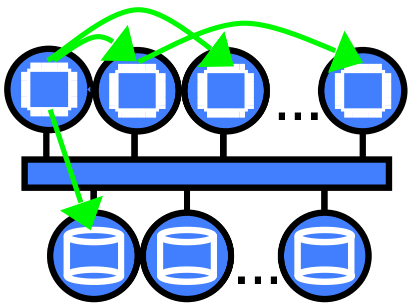
- File create rates can actually have a significant performance impact
- Improving the file system interface improves performance for computational science
  - Leverage communication in MPI-IO layer

Time to Create Files Through MPI-IO



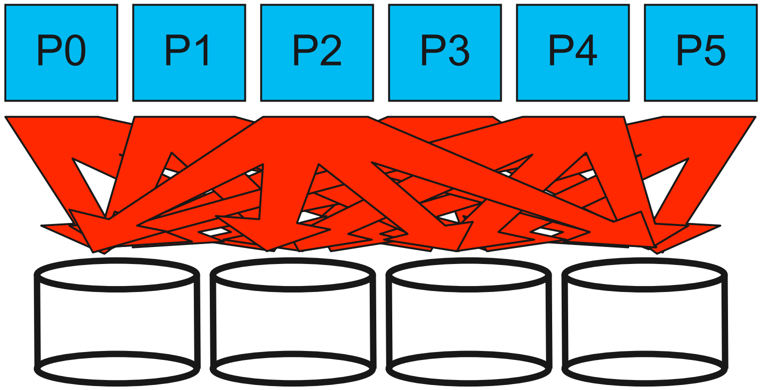


File system interfaces force all processes to open a file, causing a storm of system calls.

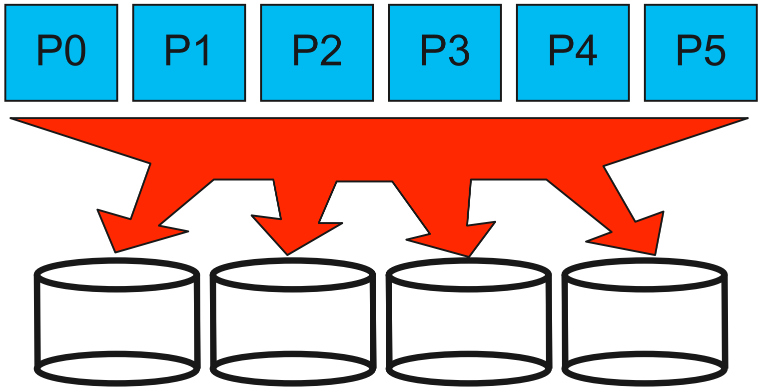


MPI-IO can leverage other interfaces, avoiding this behavior.

Independent and Collective I/O



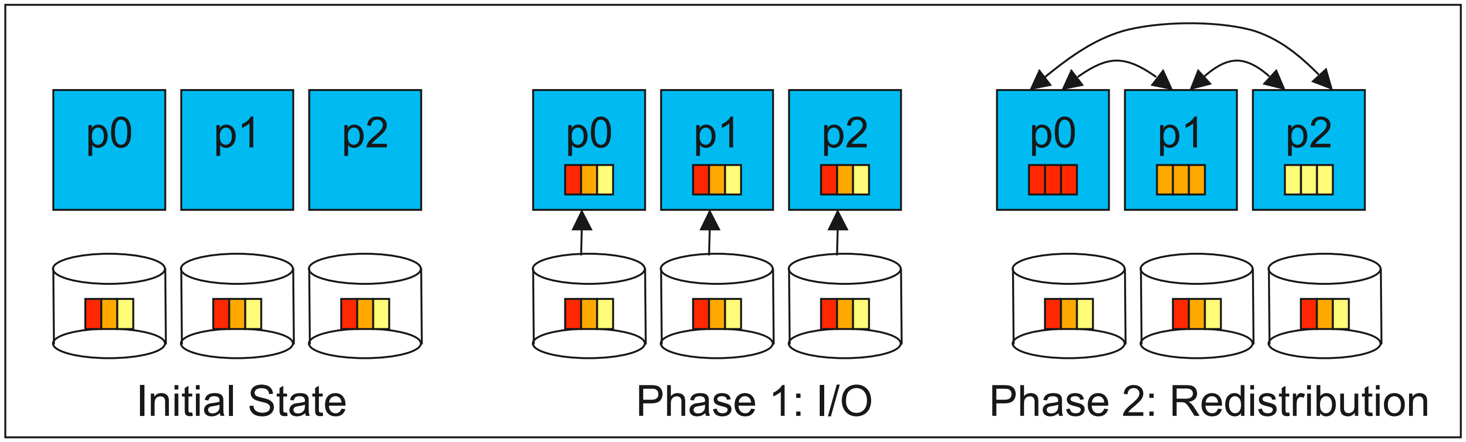
Independent I/O



Collective I/O

- Independent I/O operations specify only what a single process will do
  - Independent I/O calls do not pass on relationships between I/O on other processes
- Many applications have phases of computation and I/O
  - During I/O phases, all processes read/write data
  - We can say they are collectively accessing storage
- Collective I/O is coordinated access to storage by a group of processes
  - Collective I/O functions are called by all processes participating in I/O
  - Allows I/O layers to know more about access as a whole, more opportunities for optimization in lower software layers, better performance

The Two-Phase I/O Optimization

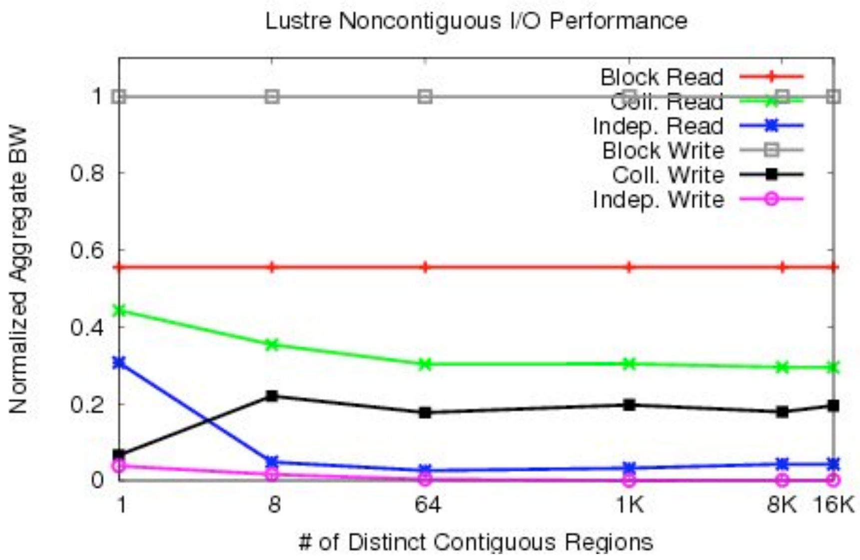


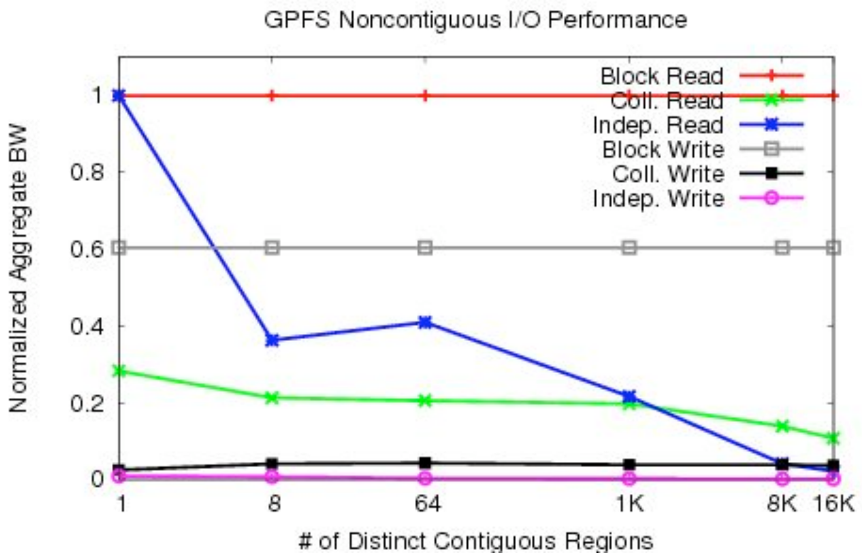
Two-Phase Read Algorithm

- Problems with independent, noncontiguous access
  - Lots of small accesses
  - Independent data sieving reads lots of extra data, can exhibit false sharing
- Idea: Reorganize access to match layout on disks
  - Single processes use data sieving to get data for many
  - Often reduces total I/O through sharing of common blocks
- Second “phase” redistributes data to final destinations
- Two-phase writes operate in reverse (redistribute then I/O)
  - Typically read/modify/write (like data sieving)
  - Overhead is lower than independent access because there is little or no false sharing
- Aggregating to fewer nodes as part of this process is trivial (and implemented!)

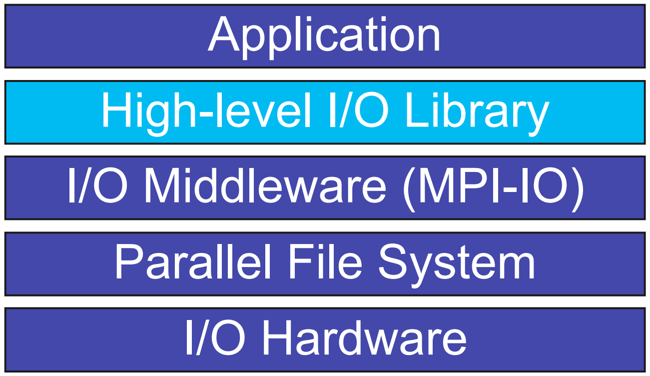
noncontig Collective I/O Results

- Benchmark that tests file system performance with increasingly small contiguous regions (keeping total size same)
- All file systems benefit from collective I/O optimizations for all but the most contiguous patterns
  - Collective I/O optimizations can be absolutely critical to performance


Lustre Noncontiguous I/O Performance


GPFS Noncontiguous I/O Performance

High Level Libraries


Application

High-level I/O Library

I/O Middleware (MPI-IO)

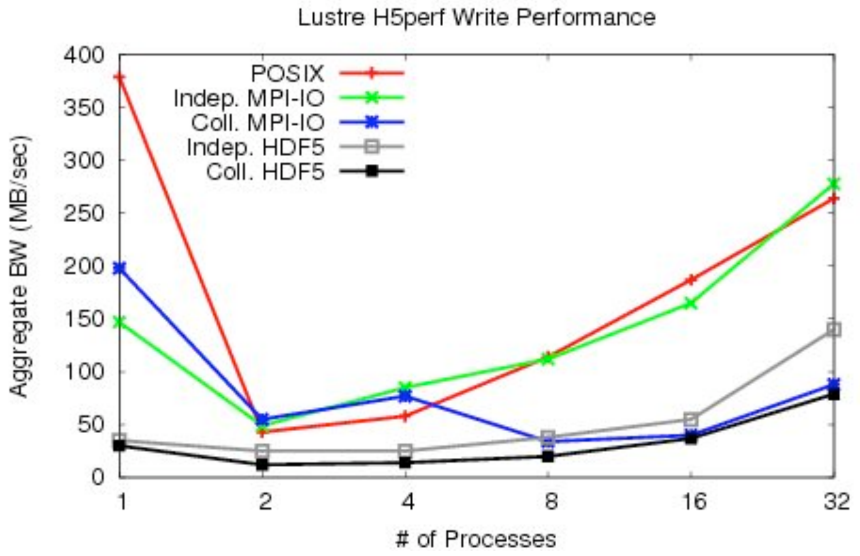
Parallel File System

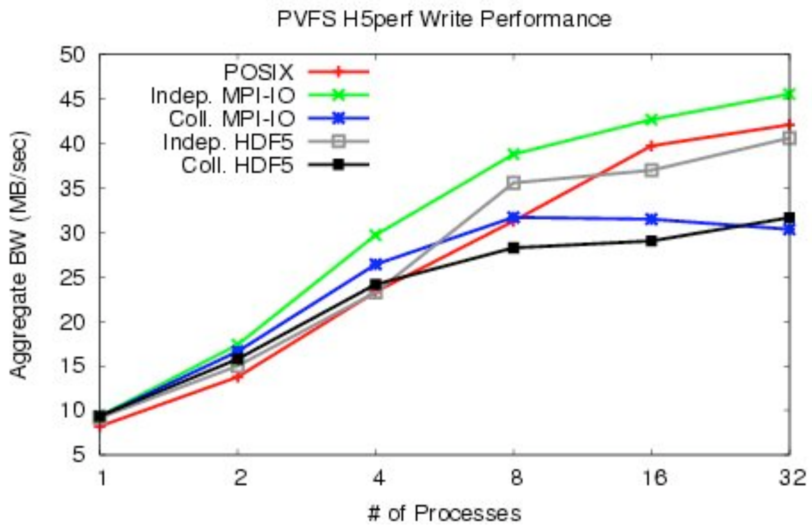
I/O Hardware

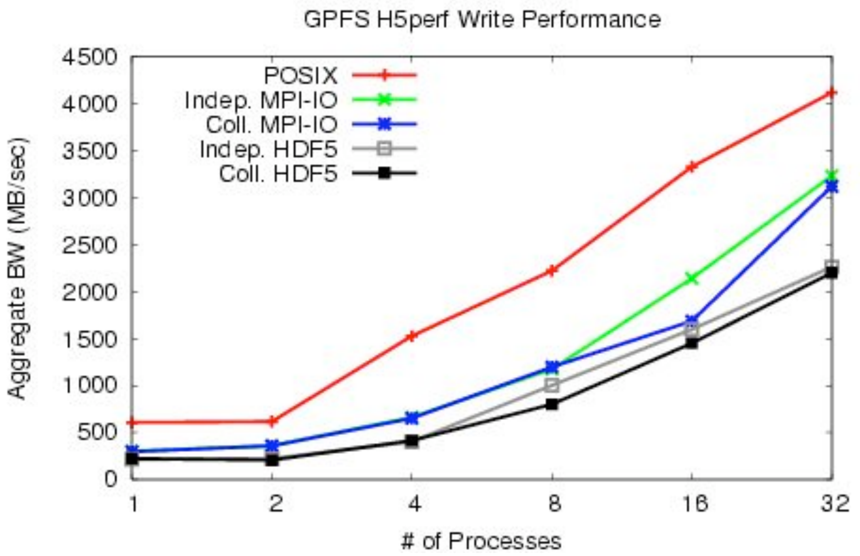
- Match storage abstraction to domain
  - Multidimensional datasets
  - Typed variables
  - Attributes
- Provide self-describing, structured files
- Map to middleware interface
  - Encourage collective I/O
- Implement optimizations that middleware cannot, such as
  - Caching attributes of variables
  - Chunking of datasets

H5perf Write Results

- Performance of high-level I/O libraries can approach that of well-formed POSIX and MPI-IO, but doesn't always
  - Complexities of HLL storage formats can cause some performance degradation
  - Obviously developers are sensitive to this potential


Lustre H5perf Write Performance


PVFS H5perf Write Performance


GPFS H5perf Write Performance

What we’ve said so far…

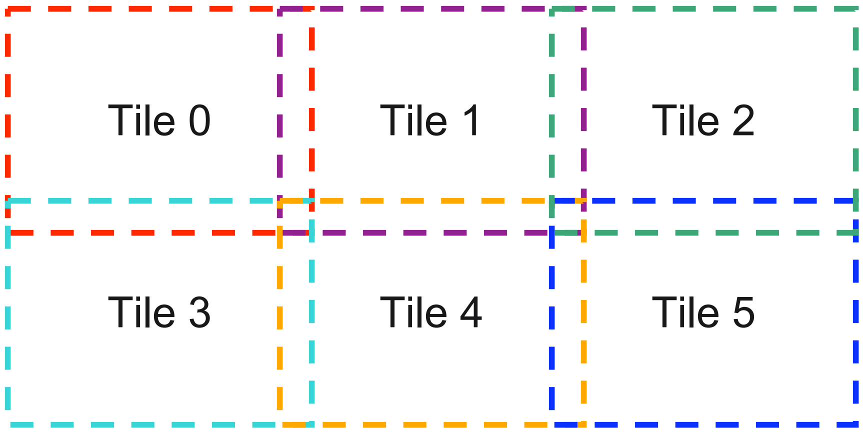
- Application scientists have basic goals for interacting with storage
  - Keep productivity high (meaningful interfaces)
  - Keep efficiency high (performant systems)
- Many solutions have been pursued by application teams, with limited success
  - This is largely due to reliance on file system APIs, which are poorly designed for computational science
- Parallel I/O teams have developed software to address these goals
  - Provide meaningful interfaces with common abstractions
  - Interact with the file system in the most efficient way possible

MPI-IO Interface

MPI-IO

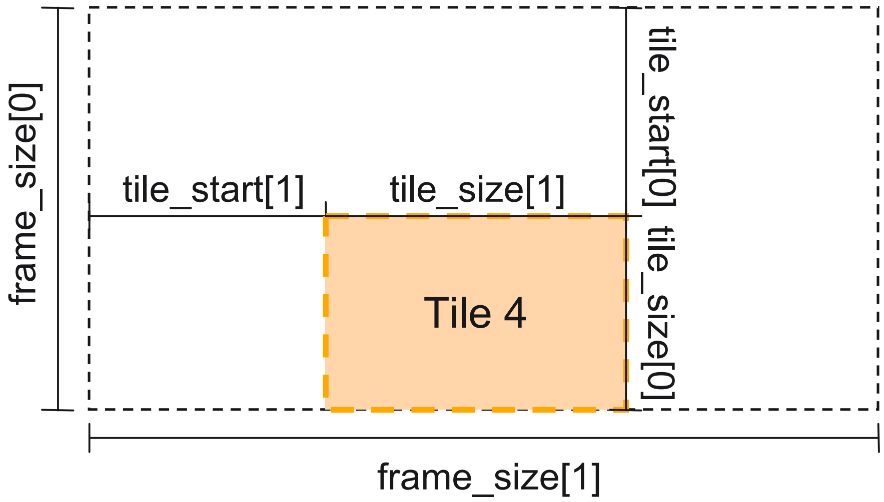
- I/O interface **specification** for use in MPI apps
- Data Model:
  - Stream of bytes in a file
  - Portable data format (external32)
    - *Not self-describing - just a well-defined encoding of types*
- Features:
  - Collective I/O
  - Noncontiguous I/O with MPI datatypes and file views
  - Nonblocking I/O
  - Fortran bindings (and additional languages)
- Implementations available on most platforms

Example: Visualization Staging



- Often large frames must be preprocessed before display on a tiled display
- First step in process is extracting “tiles” that will go to each projector
  - Perform scaling, etc.
- Parallel I/O can be used to speed up reading of tiles
  - One process reads each tile
- We’re assuming a raw RGB format with a fixed-length header

MPI Subarray Datatype



- MPI_Type_create_subarray can describe any N-dimensional subarray of an N-dimensional array
- In this case we use it to pull out a 2-D tile
- Tiles can overlap if we need them to
- Separate MPI_File_set_view call uses this type to select the file region

Opening the File, Defining RGB Type

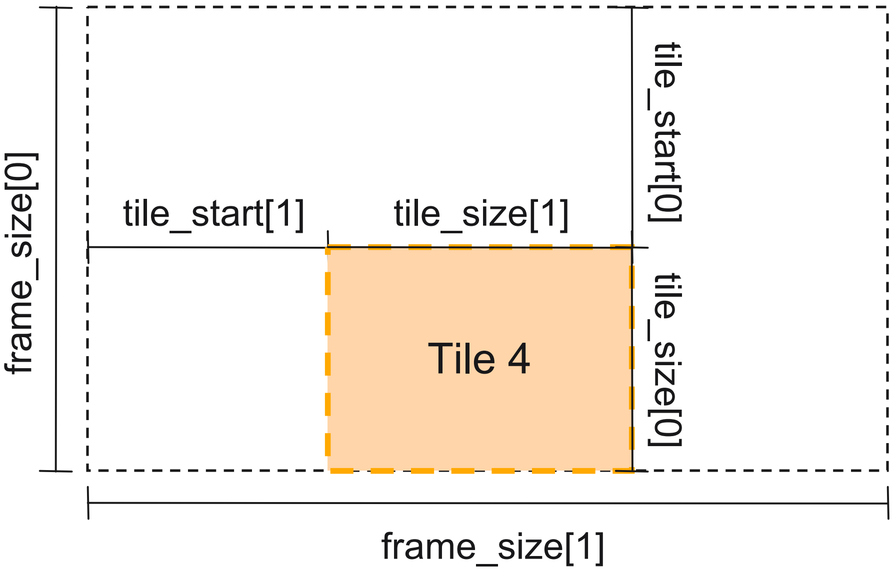
```
MPI_Datatype rgb, filetype;
MPI_File filehandle;
ret = MPI_Comm_rank(MPI_COMM_WORLD, &myrank);

/* collectively open frame file */
ret = MPI_File_open(MPI_COMM_WORLD, filename,
  MPI_MODE_RDONLY, MPI_INFO_NULL, &filehandle);

/* first define a simple, three-byte RGB type */
ret = MPI_Type_contiguous(3, MPI_BYTE, &rgb);
ret = MPI_Type_commit(&rgb);
/* continued on next slide */
```

Defining Tile Type Using Subarray

```
/* in C order, last array
 * value (X) changes most
 * quickly
 */
frame_size[1] = 3*1024;
frame_size[0] = 2*768;
tile_size[1] = 1024;
tile_size[0] = 768;
tile_start[1] = 1024 * (myrank % 3);
tile_start[0] = (myrank < 3) ? 0 : 768;
ret = MPI_Type_create_subarray(2, frame_size,
   tile_size, tile_start, MPI_ORDER_C, rgb, &filetype);
ret = MPI_Type_commit(&filetype);
```



Reading Noncontiguous Data

```
/* set file view, skipping header */
ret = MPI_File_set_view(filehandle, file_header_size,
    rgb, filetype, "native", MPI_INFO_NULL);
/* collectively read data */
ret = MPI_File_read_all(filehandle, buffer,
    tile_size[0] * tile_size[1], rgb, &status);
ret = MPI_File_close(&filehandle);
```

- MPI_File_set_view is the MPI-IO mechanism for describing noncontiguous regions in a file
  - In this case we use it to skip a header and read a subarray
- Using file views, rather than reading each individual piece, gives the implementation more information to work with (more later)
- Likewise, using a collective I/O call (MPI_File_read_all) provides additional information for optimization purposes (more later)

MPI-IO Wrap-Up

- MPI-IO provides a rich interface allowing us to describe
  - Noncontiguous accesses in memory, file, or both
  - Collective I/O
- This allows implementations to perform many transformations that result in better I/O performance
- Also forms solid basis for high-level I/O libraries
  - But they must take advantage of these features!

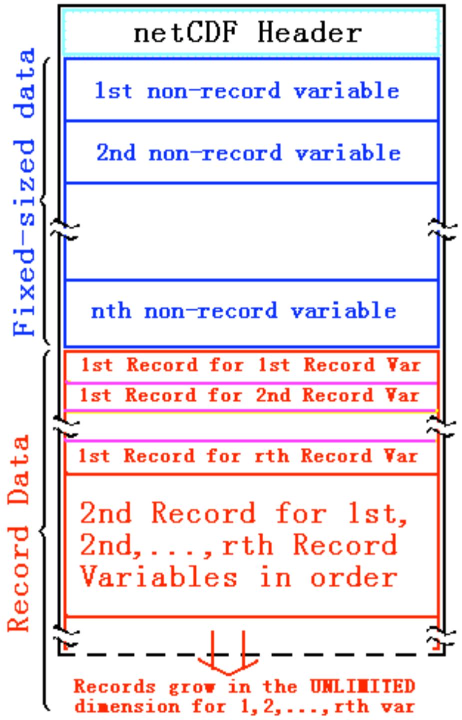
PnetCDF Interface and File Format

Parallel netCDF (PnetCDF)

- Based on original “Network Common Data Format” (netCDF) work from Unidata
  - Derived from their source code
- Data Model:
  - Collection of variables in single file
  - Typed, multidimensional array variables
  - Attributes on file and variables
- Features:
  - C and Fortran interfaces
  - Portable data format (identical to netCDF)
  - Noncontiguous I/O in memory using MPI datatypes
  - Noncontiguous I/O in file using sub-arrays
  - Collective I/O
- Unrelated to netCDF-4 work

netCDF/PnetCDF Files

- PnetCDF files consist of three regions
  - Header
  - Non-record variables (all dimensions specified)
  - Record variables (ones with an unlimited dimension)
- Record variables are interleaved, so using more than one in a file is likely to result in poor performance due to noncontiguous accesses
- Data is always written in a big-endian format

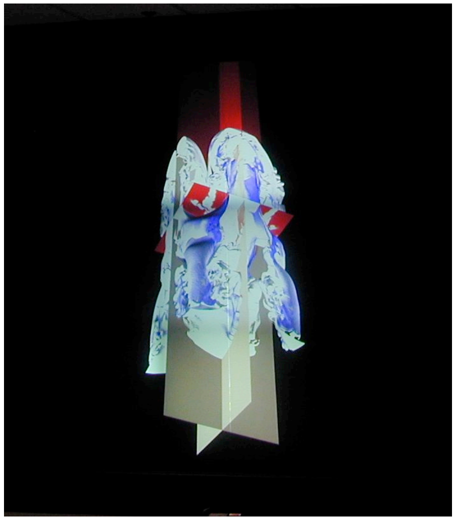


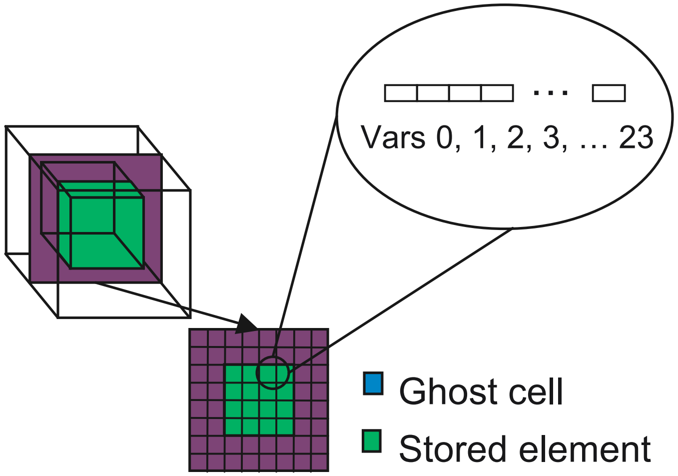
Storing Data in PnetCDF

- Create a dataset (file)
  - Puts dataset in define mode
  - Allows us to describe the contents
    - *Define dimensions for variables*
    - *Define variables using dimensions*
    - *Store attributes if desired (for variable or dataset)*
- Switch from define mode to data mode to write variables
- Store variable data
- Close the dataset

Example: FLASH Astrophysics

- FLASH is an astrophysics code for studying events such as supernovae
  - Adaptive-mesh hydrodynamics
  - Scales to 1000s of processors
  - MPI for communication
- Frequently checkpoints:
  - Large blocks of typed variables from all processes
  - Portable format
  - Canonical ordering (different than in memory)
  - Skipping ghost cells





Example: FLASH with PnetCDF

- FLASH AMR structures do not map directly to netCDF multidimensional arrays
- Must create mapping of the in-memory FLASH data structures into a representation in netCDF multidimensional arrays
- Chose to
  - Place all checkpoint data in a single file
  - Impose a linear ordering on the AMR blocks
    - *Use 4D variables*
  - Store each FLASH variable in its own netCDF variable
    - *Skip ghost cells*
  - Record attributes describing run time, total blocks, etc.

Defining Dimensions

```
int status, ncid, dim_tot_blks, dim_nxb,
   dim_nyb, dim_nzb;
MPI_Info hints;
/* create dataset (file) */
status = ncmpi_create(MPI_COMM_WORLD, filename,
   NC_CLOBBER, hints, &file_id);
/* define dimensions */
status = ncmpi_def_dim(ncid, "dim_tot_blks",
   tot_blks, &dim_tot_blks);
status = ncmpi_def_dim(ncid, "dim_nxb",
   nzones_block[0], &dim_nxb);
status = ncmpi_def_dim(ncid, "dim_nyb",
   nzones_block[1], &dim_nyb);
status = ncmpi_def_dim(ncid, "dim_nzb",
   nzones_block[2], &dim_nzb);
```

Each dimension gets
a unique reference

Creating Variables

```
int dims = 4, dimids[4];
int varids[NVARS];
/* define variables (X changes most quickly) */
dimids[0] = dim_tot_blks;
dimids[1] = dim_nzb;
dimids[2] = dim_nyb;
dimids[3] = dim_nxb;
for (i=0; i < NVARS; i++) {
    status = ncmpi_def_var(ncid, unk_label[i],
      NC_DOUBLE, dims, dimids, &varids[i]);
}
```

Same dimensions used for all variables

Storing Attributes

```
/* store attributes of checkpoint */
status = ncmpi_put_att_text(ncid, NC_GLOBAL,
  "file_creation_time", string_size, file_creation_time);
status = ncmpi_put_att_int(ncid, NC_GLOBAL,
  "total_blocks", NC_INT, 1, tot_blks);
status = ncmpi_enddef(file_id);

/* now in data mode … */
```

Writing Variables

```
double *unknowns; /* unknowns[blk][nzb][nyb][nxb] */
size_t start_4d[4], count_4d[4];
start_4d[0] = global_offset; /* different for each process */
start_4d[1] = start_4d[2] = start_4d[3] = 0;
count_4d[0] = local_blocks;
count_4d[1] = nzb;  count_4d[2] = nyb;  count_4d[3] = nxb;
for (i=0; i < NVARS; i++) {
    /* ... build datatype “mpi_type” describing values of a
      single variable ... */
    /* collectively write out all values of a single variable
      */
    ncmpi_put_vara_all(ncid, varids[i], start_4d, count_4d,
      unknowns, 1, mpi_type);
}
status = ncmpi_close(file_id);
```

Typical MPI buffer-count-type tuple

Inside PnetCDF Define Mode

- In define mode (collective)
  - Use `MPI_File_open` to create file at create time
  - Set hints as appropriate (more later)
  - Locally cache header information in memory
    - *All changes are made to local copies at each process*
- At `ncmpi_enddef`
  - Process 0 writes header with `MPI_File_write_at`
  - `MPI_Bcast` result to others
  - Everyone has header data in memory, understands placement of all variables
    - *No need for any additional header I/O during data mode!*

Inside PnetCDF Data Mode

- Inside `ncmpi_put_vara_all` (once per variable)
  - Each process performs data conversion into internal buffer
  - Uses `MPI_File_set_view` to define file region
    - *Contiguous region for each process in FLASH case*
  - `MPI_File_write_all` collectively writes data
- At `ncmpi_close`
  - `MPI_File_close` ensures data is written to storage

- MPI-IO performs optimizations
  - Two-phase possibly applied when writing variables
- MPI-IO makes PFS calls
  - PFS client code communicates with servers and stores data

PnetCDF Wrap-Up

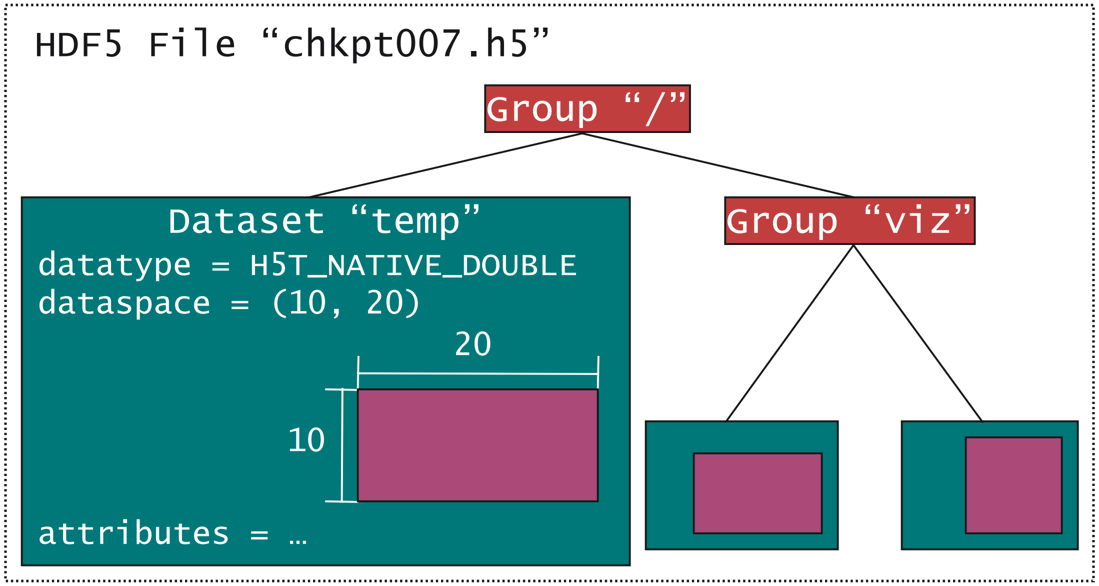
- PnetCDF gives us
  - Simple, portable, self-describing container for data
  - Collective I/O
  - Data structures closely mapping to the variables described
- If PnetCDF meets application needs, it is likely to give good performance
  - Type conversion to portable format does add overhead

HDF5 Interface and File Format

HDF5

- Hierarchical Data Format, from the HDF Group (formerly of NCSA)
- Data Model:
  - Hierarchical data organization in single file
  - Typed, multidimensional array storage
  - Attributes on dataset, data
- Features:
  - C, C++, and Fortran interfaces
  - Portable data format
  - Optional compression (not in parallel I/O mode)
  - Data reordering (chunking)
  - Noncontiguous I/O (memory and file) with hyperslabs

HDF5 Files

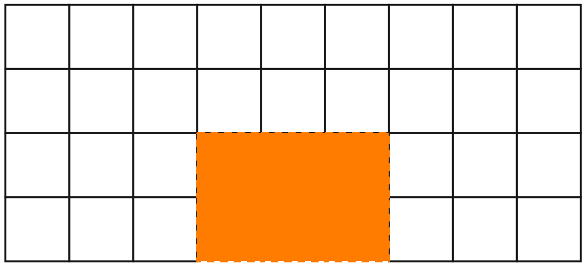


- HDF5 files consist of groups, datasets, and attributes
  - Groups are like directories, holding other groups and datasets
  - Datasets hold an array of typed data
    - *A datatype describes the type (not an MPI datatype)*
    - *A dataspace gives the dimensions of the array*
  - Attributes are small datasets associated with the file, a group, or another dataset
    - *Also have a datatype and dataspace*
    - *May only be accessed as a unit*

HDF5 Data Chunking

- Apps often read subsets of arrays (subarrays)
- Performance of subarray access depends in part on how data is laid out in the file
  - e.g. column vs. row major
- Apps also sometimes store sparse data sets
- Chunking describes a reordering of array data
  - Subarray placement in file determined lazily
  - Can reduce worst-case performance for subarray access
  - Can lead to efficient storage of sparse data
- Dynamic placement of chunks in file requires coordination
  - Coordination imposes overhead and can impact performance

Simplified Hyperslab Example



```
/* define dataspace of entire region */
dims[0] = 9; dims[1] = 4;
filespace = H5Screate_simple(NR_DIMS,
   dims, NULL);

/* create dataset from dspace */
fileset = H5Dcreate(file_id, “subtile”, H5T_NATIVE_INT,
   filespace, H5P_DEFAULT);

/* define region of interest */
count[0] = 2; count[1] = 3;
offset[0] = 2; offset[1] = 3;

/* define hyperslab: modified fileset passed to H5Dwrite */
H5Sselect_hyperslab(fileset, H5S_SELECT_SET,
   offset, NULL, count, NULL);
```

logically contiguous:
no stride

Example: FLASH with HDF5

- FLASH AMR structures do not map directly to HDF5 datasets
- Must create mapping of the in-memory FLASH data structures into a representation in HDF5 datasets
- Chose to
  - Place all checkpoint data in a single file
  - Impose a linear ordering on the AMR blocks
    - *Use 1D arrays of 3D blocks (so 4D overall)*
  - Store each FLASH variable in its own HDF5 dataset
    - *Skip ghost cells*
  - Record attributes describing run time, total blocks, etc.

Note: We will just show code storing an attribute and collectively writing a variable.

Noncontiguous I/O with Hyperslabs (1 of 2)

```
hsize_t dimens_4d[4];

/* Step 1: set up dataspace */
dimens_4d[0] = dim_tot_blks;
dimens_4d[1] = nzb;  dimens_4d[2] = nyb;  dimens_4d[3] =
   nxb;

dspace = H5Screate_simple(4, dimens_4d, NULL);
dset = H5Dcreate(file_id, variable_name,
   H5T_NATIVE_DOUBLE, dspace, H5P_DEFAULT);
```

Remember:
“S” is for dataspace,
“T” is for datatype,
“D” is for dataset!

Noncontiguous I/O with Hyperslabs (2 of 2)

```
hsize_t count_4d[4];
hsize_t start_4d[4] = {0, 0, 0, 0},
       stride_4d[4] = {1, 1, 1, 1};

/* Step 2: setup hyperslab for dataset in file */
start_4d[0]  = global_offset; /* different for each
process */
count_4d[0]  = local_blocks;
count_4d[1]  = nzb; count_4d[2] = nyb; count_4d[3] = nxb;

status = H5Sselect_hyperslab(dspace,
                             H5S_SELECT_SET,
                             start_4d,
                             stride_4d,
                             count_4d,
                             NULL);
```

dataspace from last slide

Collectively Writing a Variable

```
/* Step 1: specify collective I/O */
dxfer_template = H5Pcreate(H5P_DATASET_XFER);
ierr = H5Pset_dxpl_mpio(dxfer_template,
   H5FD_MPIO_COLLECTIVE);

/* Step 2: perform collective write */
status = H5Dwrite(dataset,
                 H5T_NATIVE_DOUBLE,
                 memspace,
                 dspace,
                 dxfer_template,
                 unknowns);
```

"P" is for property list; tuning parameters

dataspace describing memory, could also use a hyperslab

dataspace describing region in file, with hyperslab

Remember:
"S" is for dataspace,
"T" is for datatype,
"D" is for dataset!

Inside HDF5

- `MPI_File_open` used to open file
- Because there is no “define” mode, file layout is determined at write time
- In `H5Dwrite`:
  - Processes communicate to determine file layout
    - *Process 0 performs metadata updates*
  - Call `MPI_File_set_view`
  - Call `MPI_File_write_all` to collectively write
    - *Only if this was turned on (more later)*
- Memory hyperslab could have been used to define noncontiguous region in memory
- In FLASH application, data is kept in native format and converted at read time (defers overhead)
  - Could store in some other format if desired
- At the MPI-IO layer:
  - Metadata updates at every write are a bit of a bottleneck
    - *MPI-IO from process 0 introduces some skew*

I/O Best Practices

How do I choose an API?

- Your programming model will limit choices
  - Domain might too
  - e.g. Climate community has substantial existing netCDF data and tools to manipulate that data
- Find something that matches your data model
- Avoid APIs with lots of features you won't use
  - Potential for overhead costing performance is high
- Maybe the right API isn't available?
  - Get I/O people interested, consider designing a new library

Summary of API Capabilities

	POSIX	MPI-IO	PnetCDF	HDF5
Noncontig. Memory	Yes	Yes	Yes	Yes
Noncontig. File	Sort-of	Yes	Yes	Yes
Coll. I/O		Yes	Yes	Yes
Portable Format		Yes	Yes	Yes
Self-Describing			Yes	Yes
Attributes			Yes	Yes
Chunking				Yes
Hierarchical File				Yes

Tuning Application I/O (1 of 2)

- Have realistic goals:
  - What is peak I/O rate?
  - What other testing has been done?
- Describe as much as possible to the I/O system:
  - Open with appropriate mode
  - Use collective calls when available
  - Describe data movement with fewest possible operations
- Match file organization to process partitioning if possible
  - Order dimensions so relatively large blocks are contiguous with respect to data decomposition

Tuning Application I/O (2 of 2)

- Know what you can control:
  - What I/O components are in use?
  - What hints are accepted?
- Consider system architecture as a whole:
  - Is storage network faster than communication network?
  - Do some nodes have better storage access than others?

Do’s and Don’ts

- PFSs are not optimized for metadata, instead for moving data
  - Don’t use ‘ls –l’ or ‘du’ on millions of files
    - ***Certainly not to check application progress!***
  - Use your own subdirectory to avoid contention with others
- Keep file creates, opens, and closes to a minimum
  - Open once, close once
  - Use shared files or at least a subset of tasks
- Aggregate writes – PFSs are not databases, they need large transfers (at least 64K)
  - Contiguous data patterns utilize prefetching and write-behind far better than noncontiguous patterns
  - Collective I/O can aggregate for you, transform accesses into contiguous ones
- Avoid overlapped write regions if file systems rely on locks
  - Attempt to use block-aligned data
- Check error codes!

Controlling I/O Stack Behavior: Hints

- Most systems accept hints through one mechanism or another
  - Parameters to file “open” calls
  - Proprietary POSIX `ioctl` calls
  - MPI_Info
  - HDF5 transfer templates
- Allow the programmer to:
  - Explain more about the I/O pattern
  - Specify particular optimizations
  - Impose resource limitations
- Generally pass information that is used only during a particular set of accesses (between open and close, for example)

MPI-IO Hints

- MPI-IO hints may be passed via:
  - `MPI_File_open`
  - `MPI_File_set_info`
  - `MPI_File_set_view`
- Hints are optional - implementations are guaranteed to ignore ones they do not understand
  - Different implementations, even different underlying file systems, support different hints
- `MPI_File_get_info` used to get list of hints

MPI-IO Hints: Collective I/O

- `cb_buffer_size` - Controls the size (in bytes) of the intermediate buffer used in two-phase collective I/O
- `cb_nodes` - Controls the maximum number of aggregators to be used
- `romio_cb_read` - Controls when collective buffering is applied to collective read operations
- `romio_cb_write` - Controls when collective buffering is applied to collective write operations
- `cb_config_list` - Provides explicit control over aggregators (see ROMIO User's Guide)

MPI-IO Hints: FS-Specific

- `striping_factor` - Controls the number of I/O devices to stripe across
- `striping_unit` - Controls the amount of data placed on one device before moving to next device (in bytes)
- `start_iodevice` - Determines what I/O device data will first be written to
- `direct_read` - Controls direct I/O for reads
- `direct_write` - Controls direct I/O for writes

Using MPI_Info

- Example: setting data sieving buffer to be a whole “frame”

```
char info_value[16];
MPI_Info info;
MPI_File fh;
MPI_Info_create(&info);
snprintf(info_value, 15, "%d", 3*1024 * 2*768 * 3);
MPI_Info_set(info, "ind_rd_buffer_size",
  info_value);
MPI_File_open(comm, filename, MPI_MODE_RDONLY, info,
  &fh);
MPI_Info_free(&info);
```

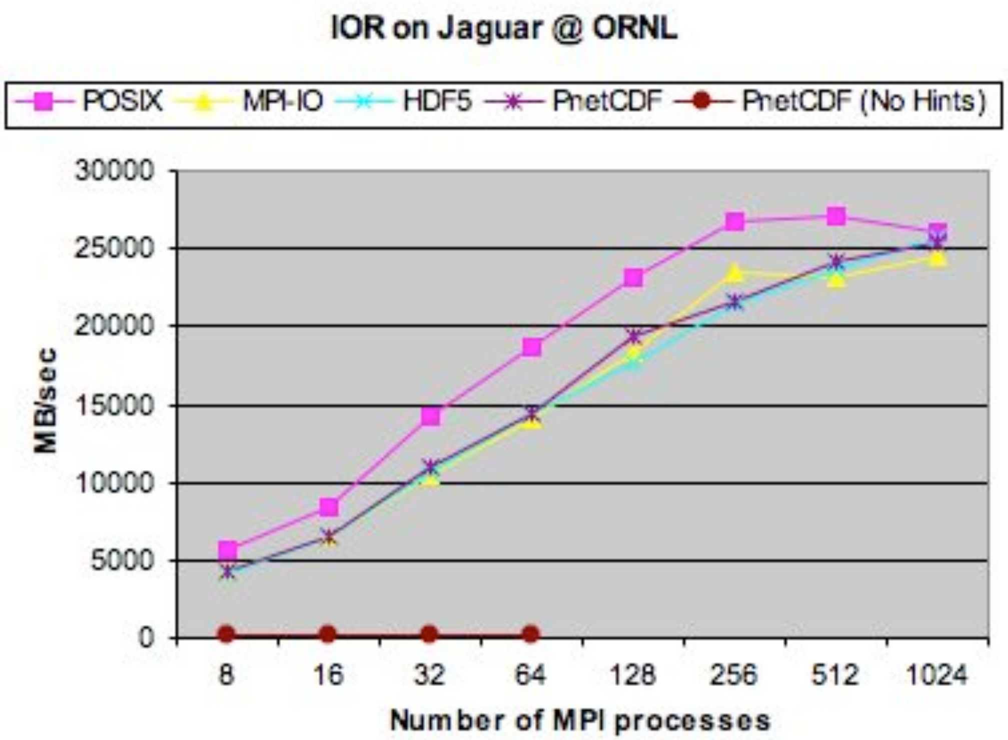
Hints and PnetCDF

- Uses MPI_Info, so almost identical
- For example, reducing I/O to a smaller number of processors (aggregators):

```
MPI_Info info;
MPI_File fh;
MPI_Info_create(&info);
MPI_Info_set(info, ”cb_nodes”, “16”);
ncmpi_open(comm, filename, NC_NOWRITE, info,
  &ncfile);
MPI_Info_free(&info);
```

Surprising Results and Fixing Them

- Recent testing on Jaguar (XT3) showed terrible performance with PnetCDF (bottom of graph)!
- Turned out to be an interaction between a bug in the MPI-IO implementation and a quirk of the file system
- Using a hint allowed programmer to work around the MPI-IO bug, avoiding the FS quirk and getting performance back
- Didn't have to **implement** anything new



Results compliments of W.-K. Liao, NWU

Helping I/O Experts Help You

- Scenarios
  - Explaining logically what you are doing
  - Separate the conceptual structures from their representation on storage
  - Common vs. infrequent patterns
  - Possible consistency management simplifications
- Application I/O kernels
  - Simple codes exhibiting similar I/O behavior
  - Easier for I/O group to work with
  - Useful for acceptance testing!
  - Needs to be pretty close to the real thing...

Concluding Remarks

Wrapping Up

- Computer scientists have developed solutions to many common computational science I/O problems
  - In most cases, these solutions will lead to high efficiency with minimal effort
  - Knowing how these components work will lead you to better performance
- Building this software is not your job, but using it appropriately is!
  - Choosing appropriate APIs
  - Using those APIs well
  - Understanding what you’re asking the system to do
- I/O systems will continue to get more complicated, but hopefully easier to use at the same time!
  - Remote access to data
  - More layers to I/O stack
  - Domain-specific application interfaces

Printed References

- John May, Parallel I/O for High Performance Computing, Morgan Kaufmann, October 9, 2000.
  - Good coverage of basic concepts, some MPI-IO, HDF5, and serial netCDF
- William Gropp, Ewing Lusk, and Rajeev Thakur, Using MPI-2: Advanced Features of the Message Passing Interface, MIT Press, November 26, 1999.
  - In-depth coverage of MPI-IO API, including a very detailed description of the MPI-IO consistency semantics

On-Line References (1 of 3)

- netCDF

  http://www.unidata.ucar.edu/packages/netcdf/
- PnetCDF

  http://www.mcs.anl.gov/parallel-netcdf/
- ROMIO MPI-IO

  http://www.mcs.anl.gov/romio/
- HDF5 and HDF5 Tutorial

  http://www.hdfgroup.org/

  http://hdf.ncsa.uiuc.edu/HDF5/

  http://hdf.ncsa.uiuc.edu/HDF5/doc/Tutor/index.html

On-Line References (2 of 3)

- PVFS

  http://www.pvfs.org/
- Lustre

  http://www.lustre.org/
- GPFS

  http://www.almaden.ibm.com/storagesystems/file_systems/GPFS/

On-Line References (3 of 3)

- LLNL I/O tests (IOR, fdtree, mdtest)
  - http://www.llnl.gov/icc/lc/siop/downloads/download.html
- Parallel I/O Benchmarking Consortium (noncontig, mpi-tile-io, mpi-md-test)
  - http://www.mcs.anl.gov/pio-benchmark/
- FLASH I/O benchmark
  - http://www.mcs.anl.gov/pio-benchmark/
  - http://flash.uchicago.edu/~jbgallag/io_bench/ (original version)
- b_eff_io test
  - http://www.hlrs.de/organization/par/services/models/mpi/b_eff_io/
- mpiBLAST
  - http://www.mpiblast.org

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