The MPI-IO Interface

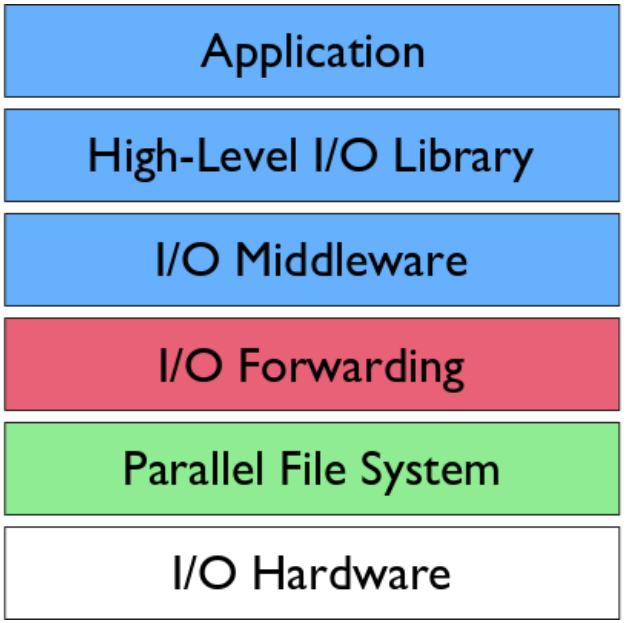
I/O for Computational Science

High-Level I/O Library
maps application abstractions onto storage abstractions and provides data portability.

HDF5, Parallel netCDF, ADIOS

I/O Forwarding
bridges between app. tasks and storage system and provides aggregation for uncoordinated I/O.

IBM ciod, IOFSL, Cray DVS



I/O Middleware
organizes accesses from many processes, especially those using collective I/O.

MPI-IO

Parallel File System
maintains logical space and provides efficient access to data.

PVFS, PanFS, GPFS, Lustre

Additional I/O software provides improved performance and usability over directly accessing the parallel file system. Reduces or (ideally) eliminates need for optimization in application codes.

MPI-IO

- I/O interface specification for use in MPI apps
- Data model is same as POSIX
  - Stream of bytes in a file
- Features:
  - Collective I/O
  - Noncontiguous I/O with MPI datatypes and file views
  - Nonblocking I/O
  - Fortran bindings (and additional languages)
  - System for encoding files in a portable format (external32)
    - Not self-describing - just a well-defined encoding of types
- Implementations available on most platforms (more later)

Simple MPI-IO

- Collective open: all processes in communicator
- File-side data layout with *file views*
- Memory-side data layout with *MPI datatype* passed to write

```
MPI_File_open(COMM, name, mode,
    info, fh);
MPI_File_set_view(fh, disp, etype,
    filetype, datarep, info);
MPI_File_write_all(fh, buf, count,
    datatype, status);
```

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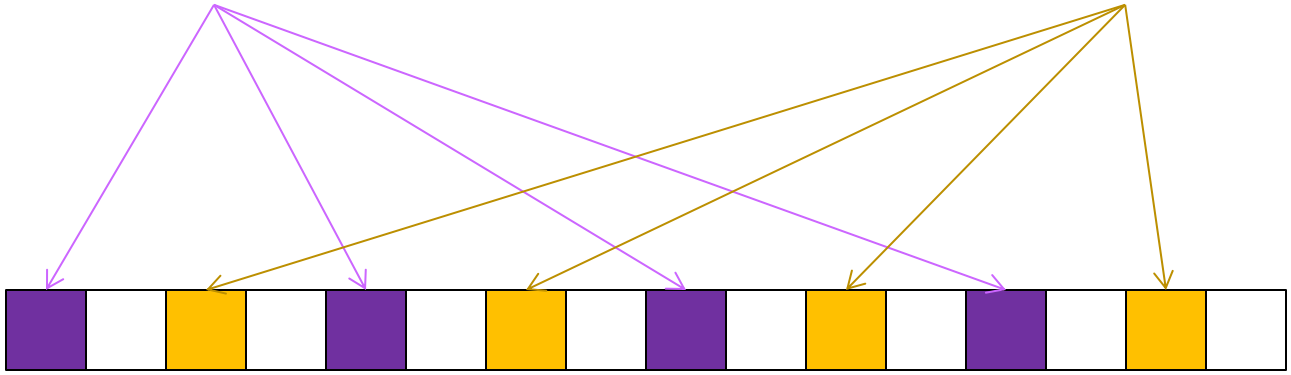
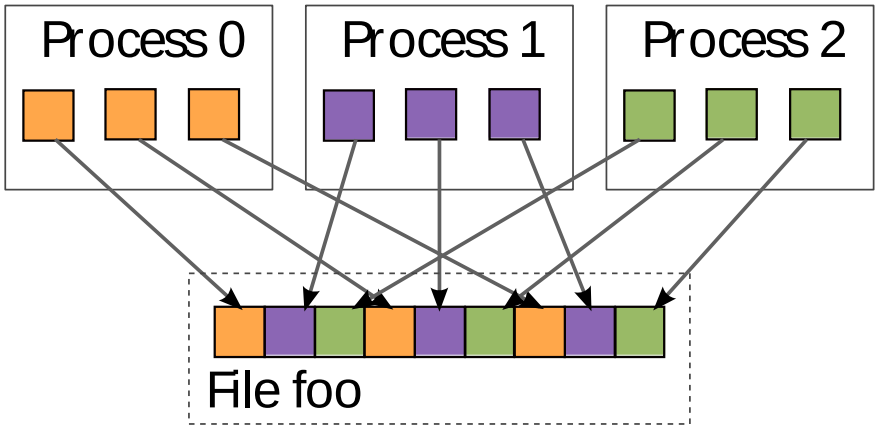


I/O Transformations

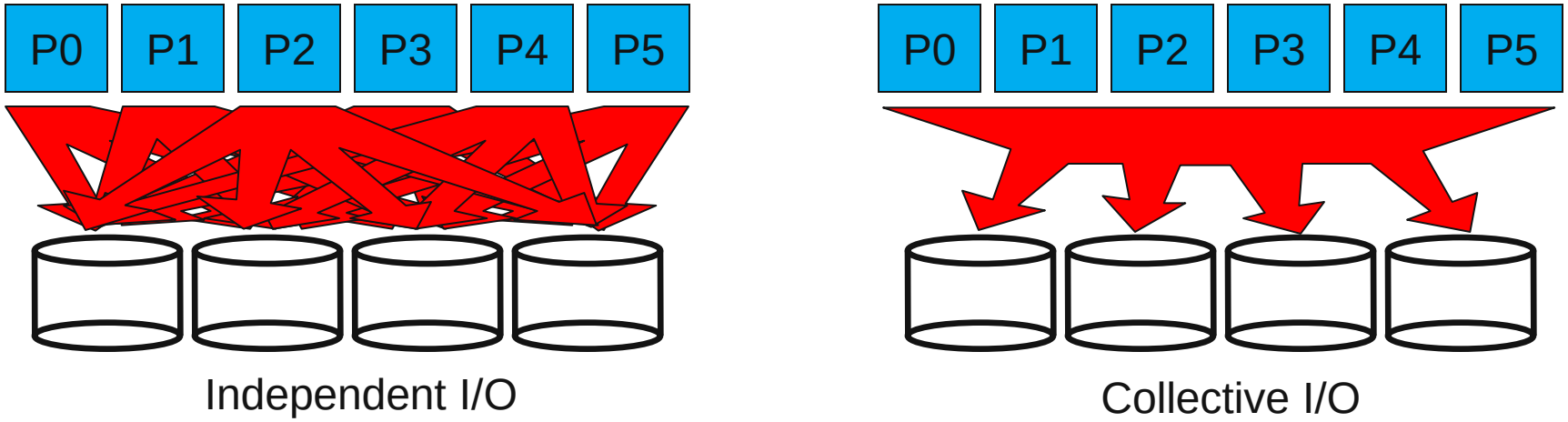
Software between the application and the PFS performs transformations, primarily to improve performance.

- Goals of transformations:
  - Reduce number of operations to PFS (avoiding latency)
  - Avoid lock contention (increasing level of concurrency)
  - Hide number of clients (more on this later)
- With “transparent” transformations, data ends up in the same locations in the file
  - i.e., the file system is still aware of the actual data organization



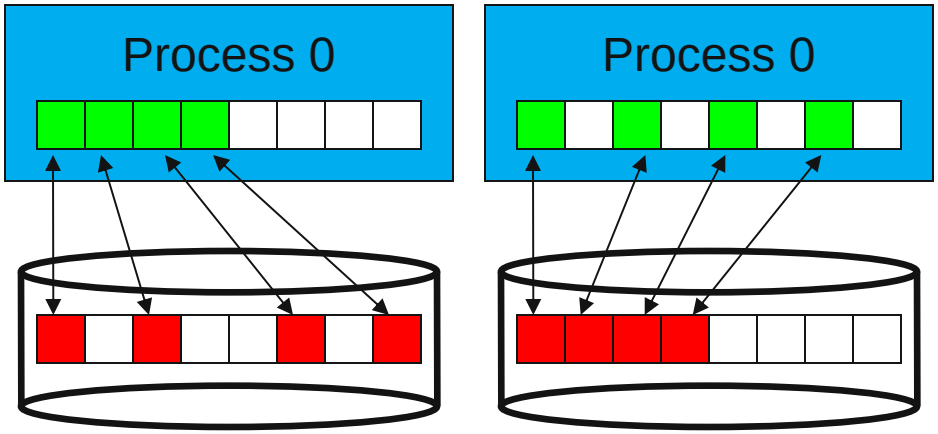
When we think about I/O transformations, we consider the mapping of data between application processes and locations in file.

Independent and Collective I/O



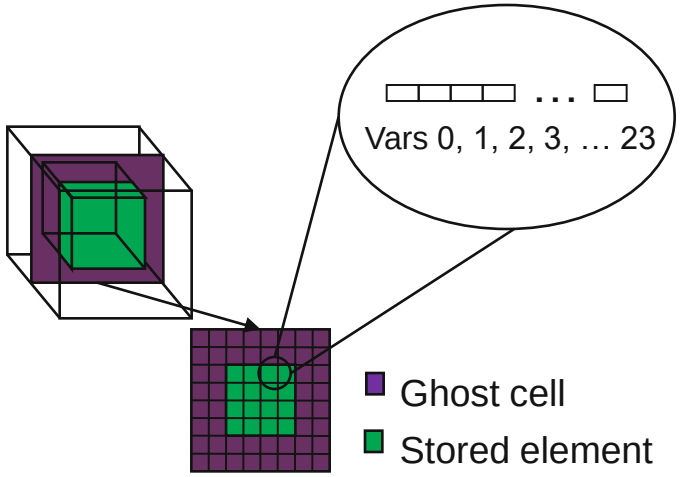
- Independent I/O operations specify only what a single process will do
  - Independent I/O calls do not pass on relationships between I/O on other processes
- Many applications have phases of computation and I/O
  - During I/O phases, all processes read/write data
  - We can say they are collectively 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

Contiguous and Noncontiguous I/O



Noncontiguous in File

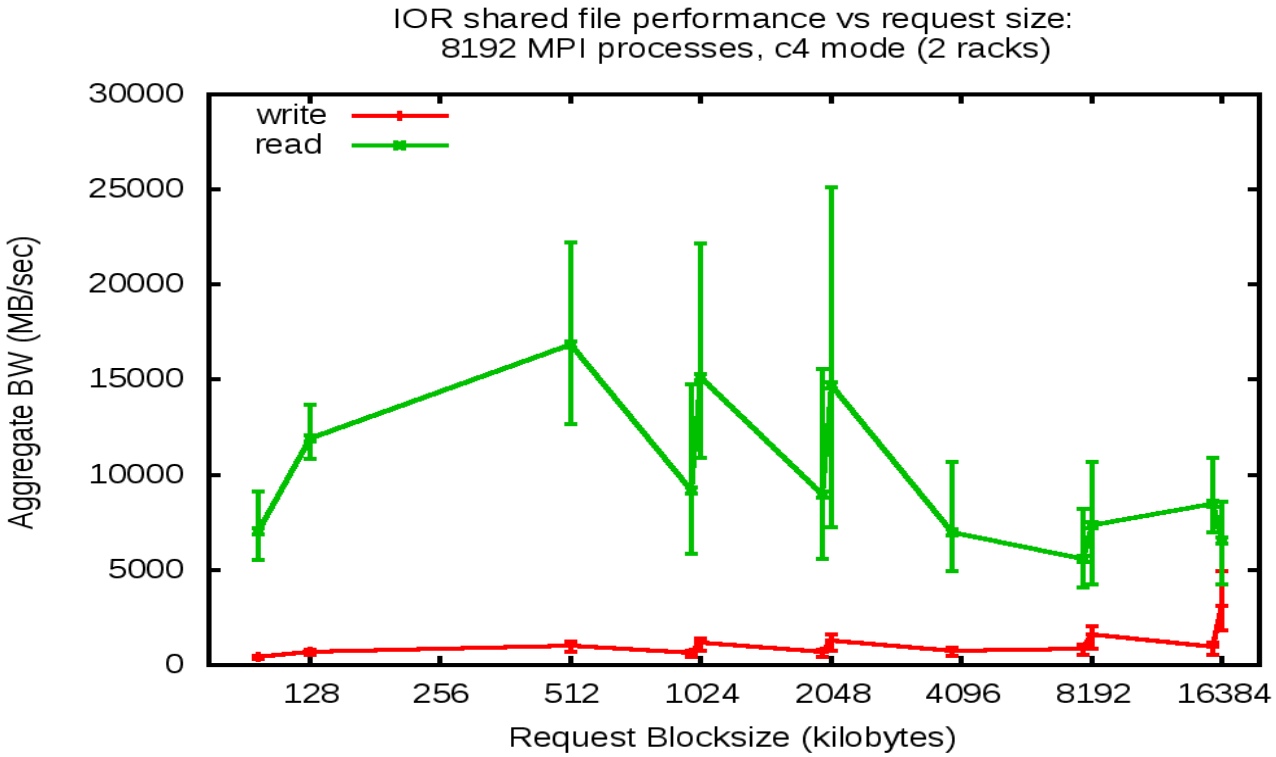
Noncontiguous in Memory



Extracting variables from a block and skipping ghost cells will result in 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

Request Size and I/O Rate



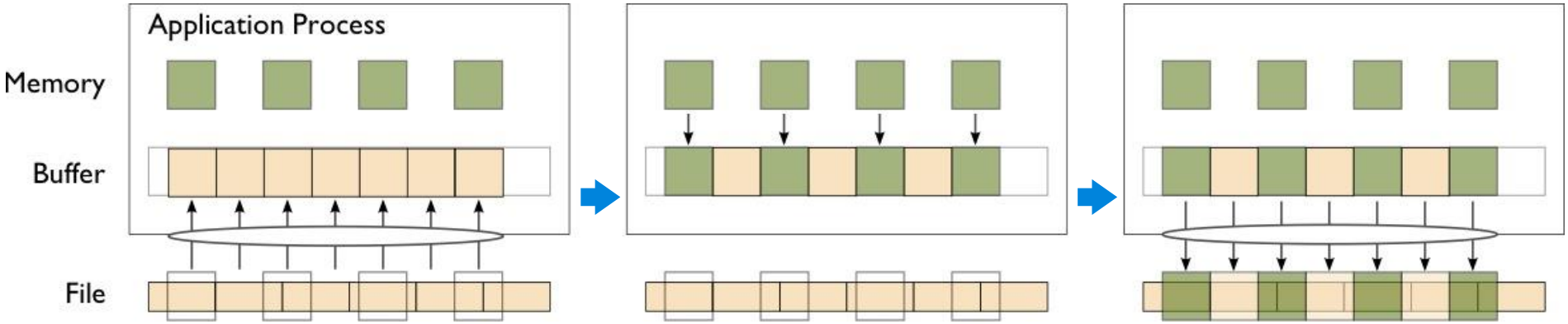
Interconnect latency has a significant impact on effective rate of I/O. Typically I/O should be in the O(Mbytes) range (at least 16 MiB on this GPFS config).

Tests run on 8K processes of IBM Blue Gene/Q at ANL.

Reducing Number of Operations

Since most operations go over the network, I/O to a PFS incurs more latency than with a local FS. *Data sieving* is a technique to address I/O latency by combining operations:

- When reading, application process reads a large region holding all needed data and pulls out what is needed
- When writing, three steps required (below)



Step 1: Data in region to be modified are read into intermediate buffer (1 read).

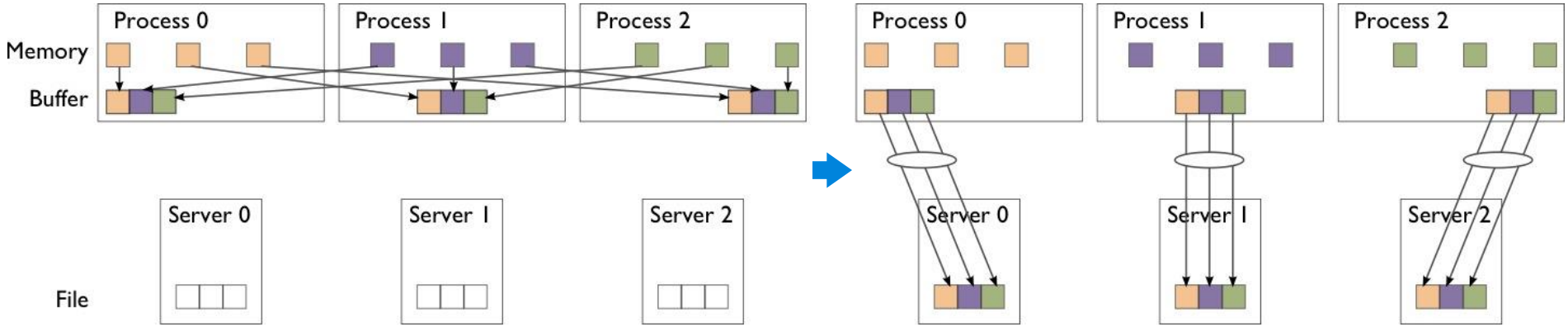
Step 2: Elements to be written to file are replaced in intermediate buffer.

Step 3: Entire region is written back to storage with a single write operation.

Avoiding Lock Contention

To avoid lock contention when writing to a shared file, we can reorganize data between processes. *Two-phase I/O* splits I/O into a data reorganization phase and an interaction with the storage system (two-phase write depicted):

- Data exchanged between processes to match file layout

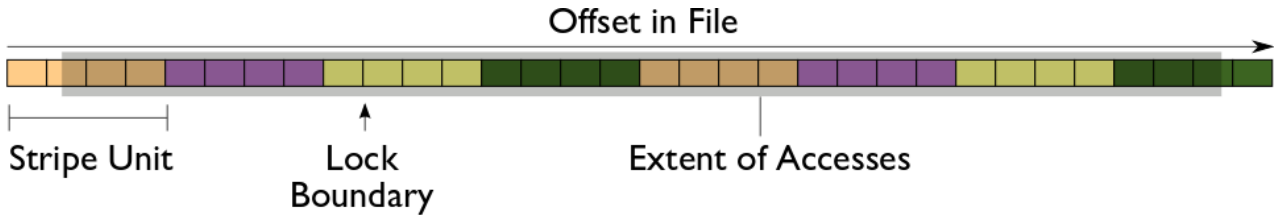


Phase 1: Data are exchanged between processes based on organization of data in file.

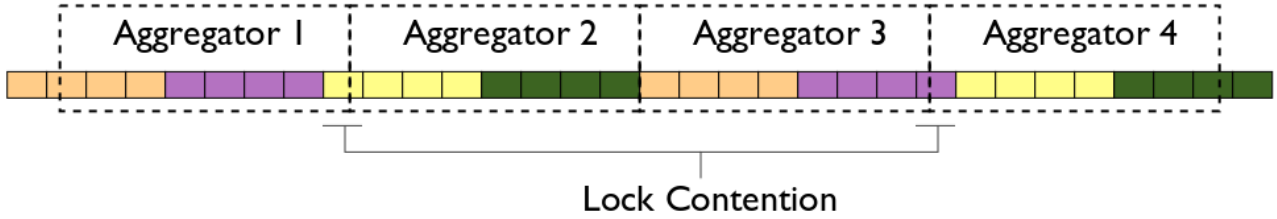
Phase 2: Data are written to file (storage servers) with large writes, no contention.

Two-Phase I/O Algorithms

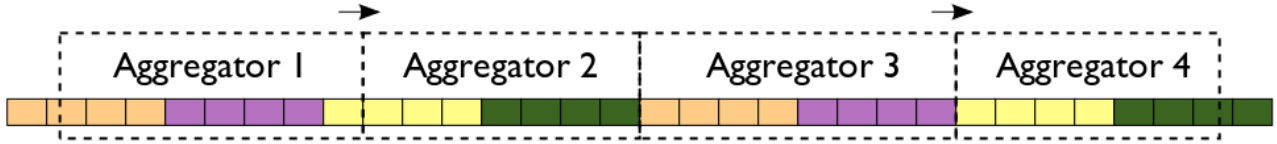
Imagine a collective I/O access using four aggregators to a file striped over four file servers (indicated by colors):



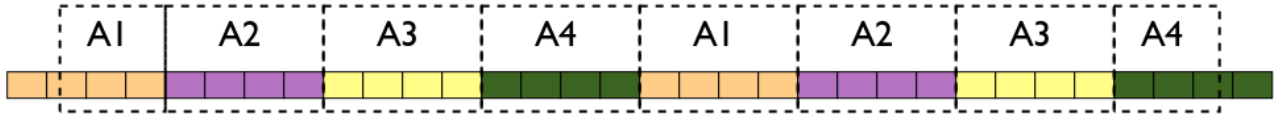
One approach is to evenly divide the region accessed across aggregators.



Aligning regions with lock boundaries eliminates lock contention.



Mapping aggregators to servers reduces the number of concurrent operations on a single server and can be helpful when locks are handed out on a per-server basis (e.g., Lustre).



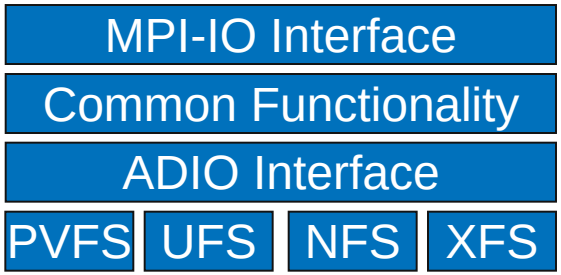
For more information, see W.K. Liao and A. Choudhary, “Dynamically Adapting File Domain Partitioning Methods for Collective I/O Based on Underlying Parallel File System Locking Protocols,” SC2008, November, 2008.

Impact of Optimizations on S3D I/O

- Testing with PnetCDF output to single file, three configurations, 16 processes
  - All MPI-IO optimizations (collective buffering and data sieving) disabled
  - Independent I/O optimization (data sieving) enabled
  - Collective I/O optimization (collective buffering, a.k.a. two-phase I/O) enabled

	Coll. Buffering and Data Sieving Disabled	Data Sieving Enabled	Coll. Buffering Enabled (incl. Aggregation)
POSIX writes	102,401	81	**5**
POSIX reads	0	80	0
MPI-IO writes	64	64	64
Unaligned in file	102,399	80	4
Total written (MB)	6.25	**87.11**	6.25
Runtime (sec)	1443	11	6.0
Avg. MPI-IO time per proc (sec)	**1426.47**	4.82	0.60

MPI-IO Implementations

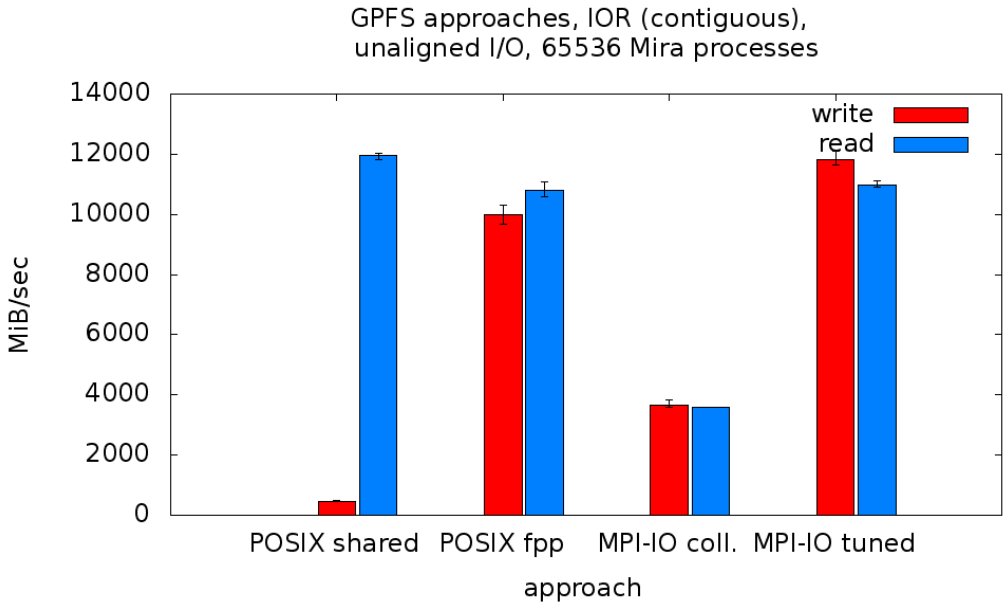


ROMIO's layered architecture.

- Different MPI-IO implementations exist
- Four better-known ones are:
  - ROMIO from Argonne National Laboratory
    - Leverages MPI-1 communication
    - Supports local file systems, network file systems, parallel file systems
      - UFS module works GPFS, Lustre, and others
    - Includes data sieving and two-phase optimizations
  - MPI-IO/GPFS from IBM (for AIX only)
    - Includes two special optimizations
      - Data shipping -- mechanism for coordinating access to a file to alleviate lock contention (type of aggregation)
      - Controlled prefetching -- using MPI file views and access patterns to predict regions to be accessed in future
  - MPI from NEC
    - For NEC SX platform and PC clusters with Myrinet, Quadrics, IB, or TCP/IP
    - Includes listless I/O optimization -- fast handling of noncontiguous I/O accesses in MPI layer
  - OMPIO from OpenMPI
    - Emphasis on modularity and tighter integration into MPI implementation

GPFS Access three ways

- POSIX shared vs MPI-IO collective
  - Locking overhead for unaligned writes hits POSIX hard
- Default MPI-IO parameters not ideal
  - Reported to IBM; simple tuning brings MPI-IO back to parity
  - “Vendor Defaults” might give you bad first impression
- File per process (fpp) extremely seductive, but entirely untenable on current generation.



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
- Ideal location in software stack for file system specific quirks or optimizations
- Also forms solid basis for high-level I/O libraries
  - But they must take advantage of these features!