BLUE WATERS

SUSTAINED PETASCALE COMPUTING

Application I/O on Blue Waters

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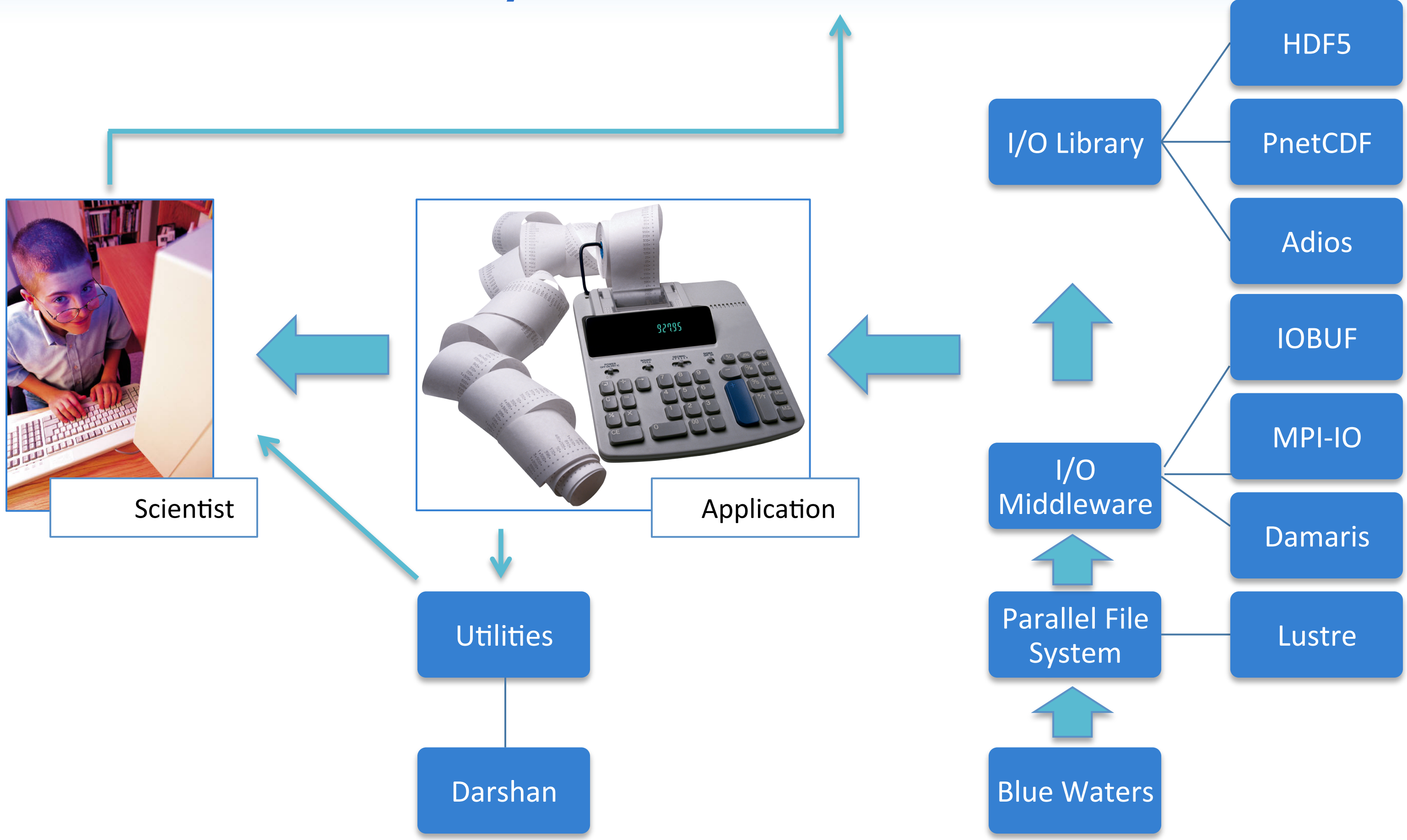
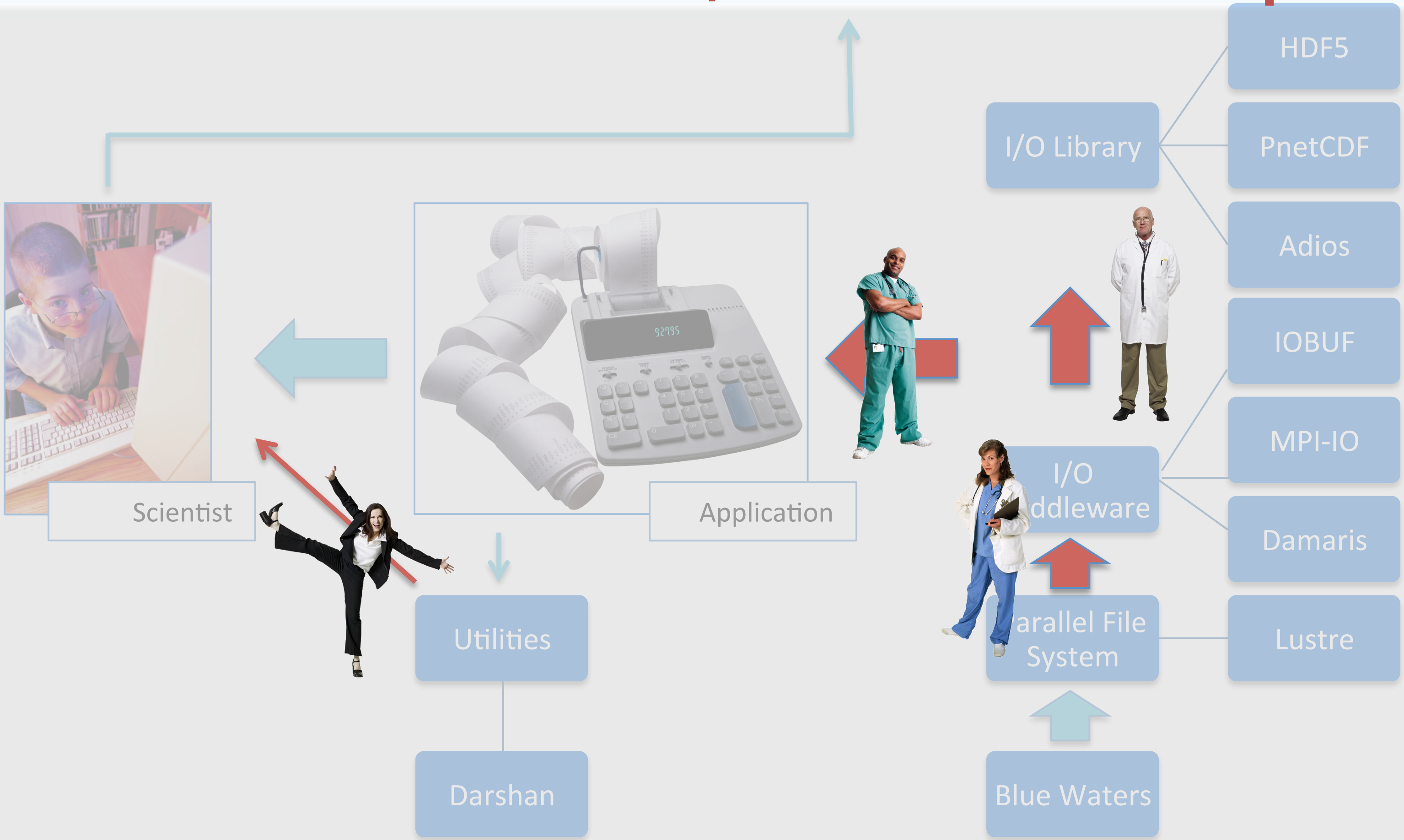
GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION

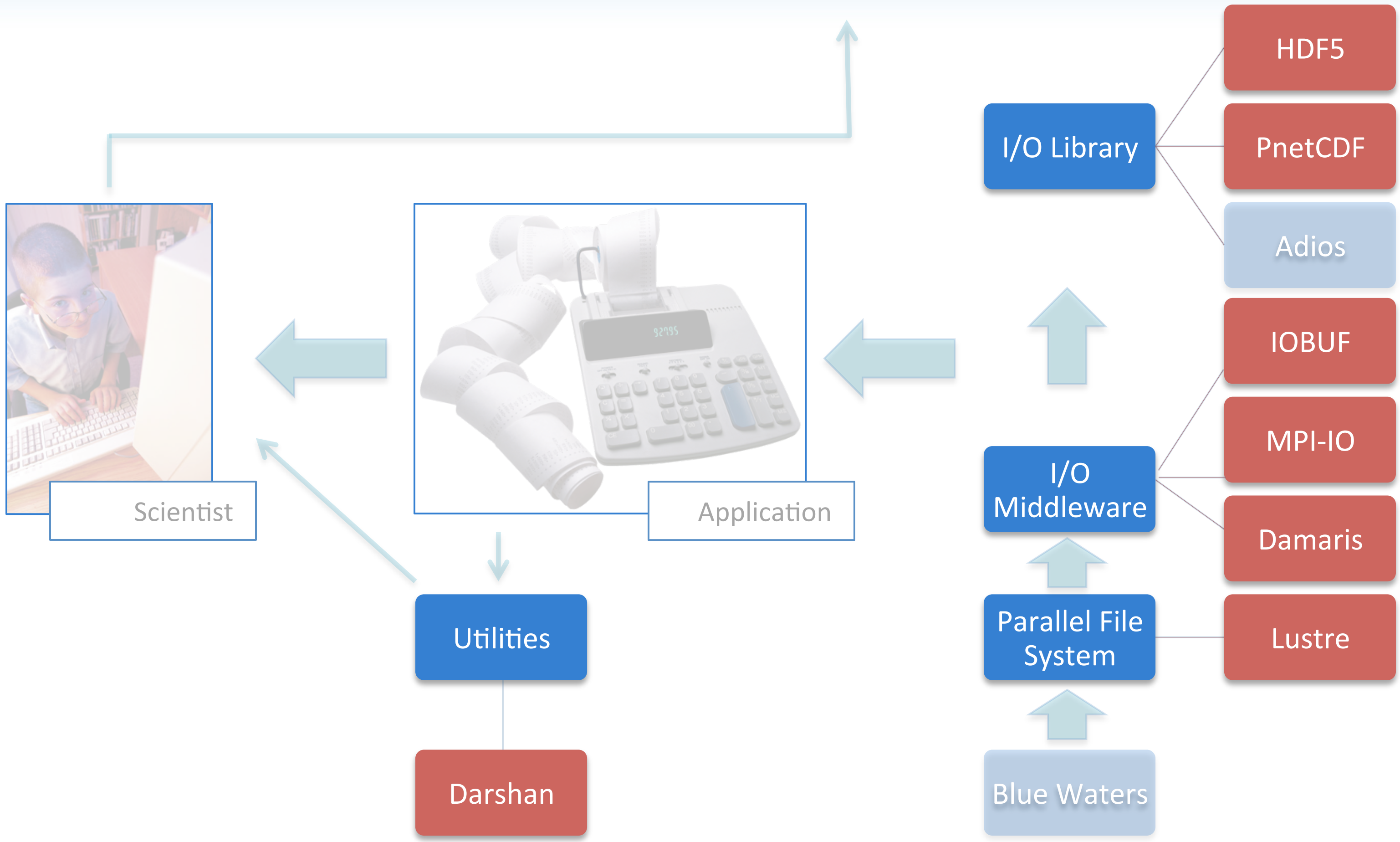
I/O For Science!



Where the BW I/O Team Can Help



This Talk


Scientist
Application
Utilities
Darshan
I/O Library
HDF5
PnetCDF
Adios
I/O Middleware
IOBUF
MPI-IO
Damaris
Parallel File System
Lustre
Blue Waters

PARALLEL I/O

Lustre

Common I/O Usage

- Checkpoint files
  - Write-close
  - Size varies
  - Must be written to disk
- Log / history / state files
  - Simple appends
  - Small writes (~kb - ~MB)
  - Can be buffered
- Write-read not very common

- Optimize for write
- Synchronous write

- Optimize for write
- Asynchronous write
- Explicit buffer management or
- Use a library

Available File Systems

- home
  - 2.2 PB
  - 1TB quota
- project
  - 2.2 PB
  - 3TB quota
- scratch
  - 22 PB
  - 500 TB quota

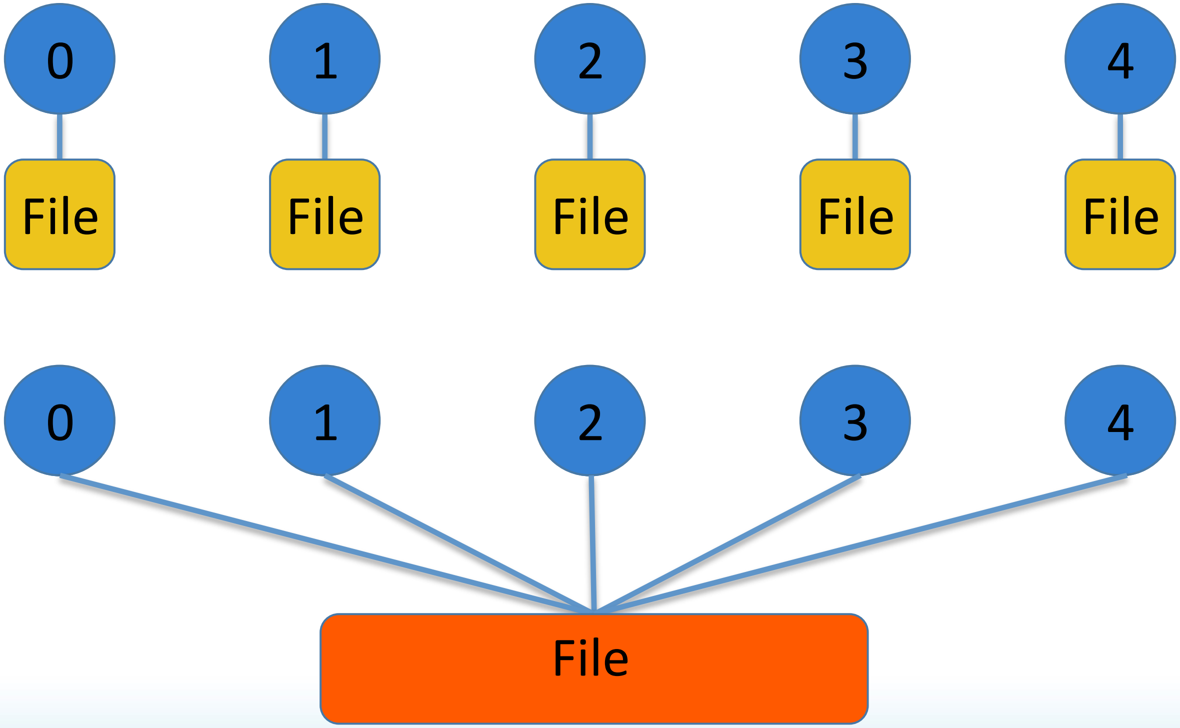
- Three separate file systems
- Three separate metadata servers
- User operations in home won't interfere with application IO
- Project space controlled by the PI

Application I/O: Big Picture Considerations

- Maximize both client I/O and communication bandwidth (without breaking things)
- Minimize management of an unnecessarily large number of files
- Minimize costly post-processing
- Exploit parallelism in the file system
- Maintain portability

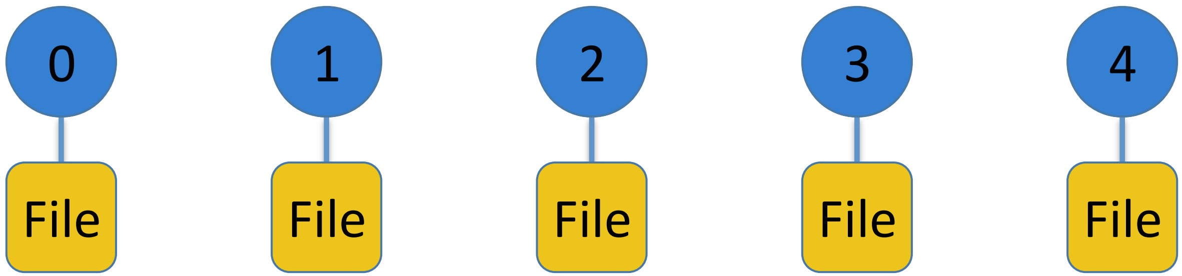
Large Scale I/O in Practice

- Serial I/O is limited by both the I/O bandwidth of a single process as well as that of a single OST
- Two ways to increase bandwidth:



File-Per-Process

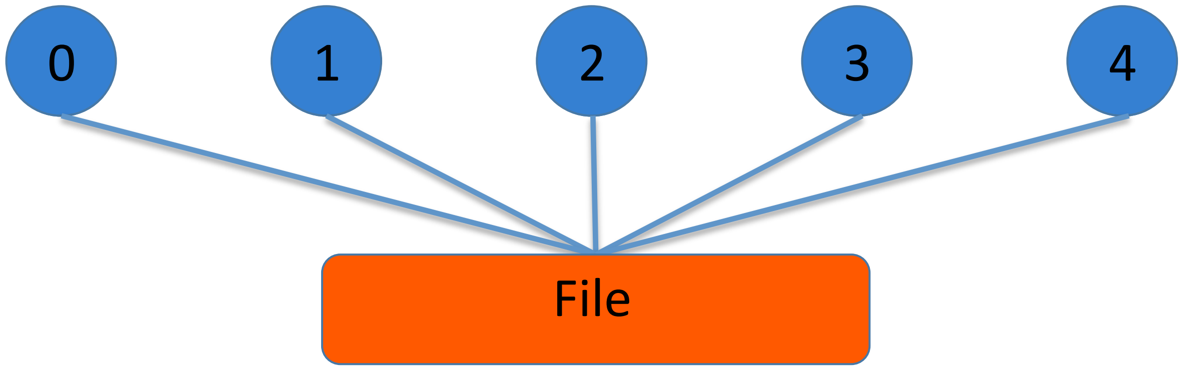
- Each process performs I/O on its own file



- Advantages
  - Straightforward implementation
  - Typically leads to reasonable bandwidth quickly
- Disadvantages
  - Limited by single process
  - Difficulty in managing a large number of files
  - Likely requires post processing to acquire useful data
  - Can be taxing on the file system metadata and ruin everybody’s day

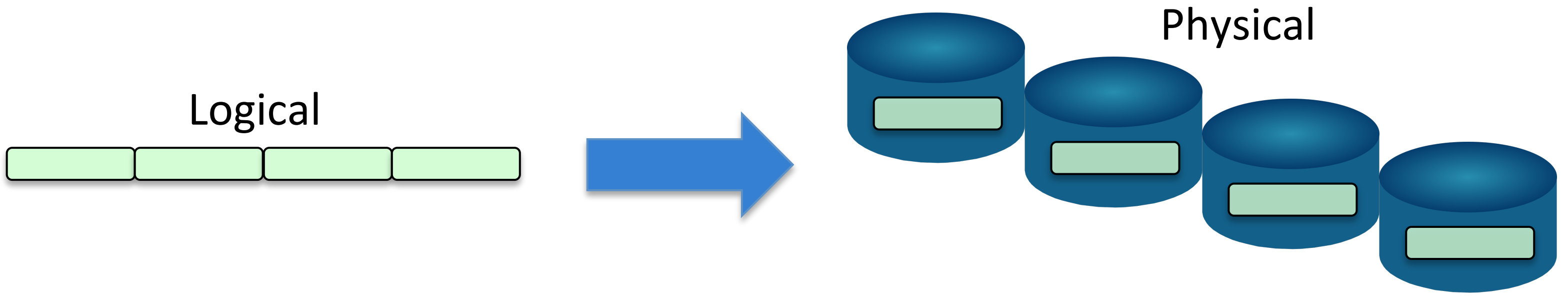
Shared-File

- There is one, large file shared among all processors which access the file concurrently



- Advantages
  - Results in easily managed data that is useful with minimal preprocessing
- Disadvantages
  - Likely slower than file-per-process, if not used properly
  - Additional (one-time!) programing investment

Lustre File System: Striping



- **File striping:** single files are distributed across a series of OSTs
  - File size can grow to the aggregate size of available OSTs (rather than a single disk)
  - Accessing multiple OSTs concurrently increases I/O bandwidth

Performance Impact: Configuring File Striping

- `lfs` is the Lustre utility for viewing/setting file striping info
  - **Stripe count** – the number of OSTs across which the file can be striped
  - **Stripe size** – the size of the blocks that a file will be broken into
  - **Stripe offset** – the ID of an OST for Lustre to start with, when deciding which OSTs a file will be striped across
- Configurations should focus on stripe count/size
- Blue Waters defaults:

```
$> touch test
$> lfs getstripe test
test
lmm_stripe_count:   1
lmm_stripe_size:    1048576
lmm_stripe_offset:  708
   obdidx        objid         objid          group
      708      2161316      0x20faa4              0
```

Setting Striping Patterns

```
$> lfs setstripe -c 5 -s 32m test
$> lfs getstripe test
test
lmm_stripe_count:   5
lmm_stripe_size:    33554432
lmm_stripe_offset:  1259
   obdidx         objid         objid          group
     1259       2162557      0x20ff7d              0
     1403       2165796      0x210c24              0
      955       2163063      0x210177              0
     1139       2161496      0x20fb58              0
      699       2161171      0x20fa13              0
```

- Note: a file's striping pattern is permanent, and set upon creation
  - `lfs setstripe` creates a new, 0 byte file
  - The striping pattern *can* be changed for a directory; every *new* file or directory created within will inherit its striping pattern
  - Simple API available for configuring striping – portable to other Lustre systems

Striping Case Study

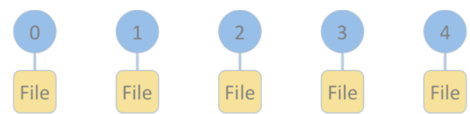
- Reading 1 TB input file using 2048 cores

Function	Stripe Count = 1	Stripe Count = 64	Improvement
Total	4551.620s	268.209s	94.1%
loadKernel	4296.118s	85.331s	98.0%
loadDamp	33.767s	6.144s	81.8%
loadDamp_bycol	30.085s	5.712s	81.0%

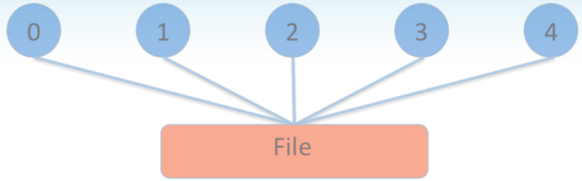
- Code is now CPU bound instead of I/O bound
- Optimization "effort": `lfs setstripe -c 64`

Striping, and You

- When to use the default stripe count of 1
  - Serial I/O or small files
    - Inefficient use of bandwidth + overhead of using multiple OSTs will degrade performance
  - File-per-process I/O Pattern



    - Each core interacting with a single OST reduces network costs of hitting OSTs (which can eat your lunch at large scales)
- Stripe size is unlikely to vary performance unless unreasonably small/large
  - Err on the side of small
    - This helps keep stripes **aligned**, or within single OSTs
    - Can lessen OST traffic
  - Default stripe size should be adequate



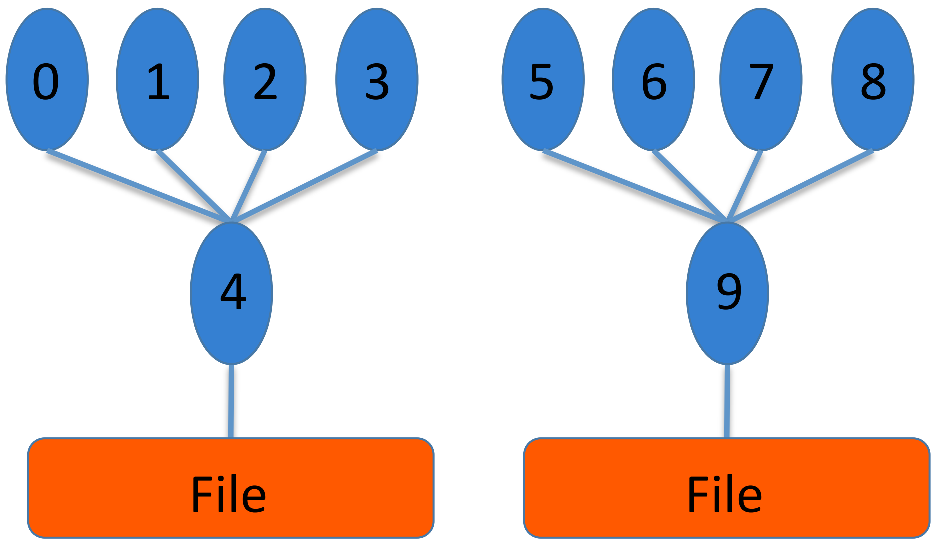
- Large shared files:
  - Processes ideally access exclusive file regions
  - Stripe size
    - Application dependent
    - Should maximize stripe alignment (localize a process to an OST to reduce contention and connection overhead)
  - Stripe count
    - Should equal the number of processes performing I/O to maximize I/O bandwidth
    - Blue Waters contains 1440 OSTs, the maximum possible for file stripe count is currently 160 (likely to increase soon pending a software update)

```
 $> lfs osts
 OBDS
 0: snx11001-OST0000_UUID ACTIVE
 1: snx11001-OST0001_UUID ACTIVE
  ……
1438: snx11003-OST059e_UUID ACTIVE
1439: snx11003-OST059f_UUID ACTIVE
```

And the Winner is… Neither?

- Both patterns increase bandwidth through the addition of I/O processes
  - There are a limited number of OSTs to stripe a file across
  - The likelihood of OST contention grows with the ratio of I/O processes to OSTs
  - Eventually, the benefit of another I/O process is offset by added OST traffic
- Both routinely use all processes to perform I/O
  - A small subset of a node’s cores can consume a node’s I/O bandwidth
  - This is an inefficient use of resources
- The answer? It depends… but,
  - Think aggregation, a la *file-per-node*

I/O Delegates



- Advantages
  - More control - customize per job size
    - Ex: One file per node, one file per OST
- Disadvantages
  - Additional (one-time!) programing investment

I/O MIDDLEWARE

Damaris, MPI-IO & IOBUF

Why use I/O Middleware?

- Derived data types
- Easy to work with shared files
- Derived types + shared files
  - Data is now a series of objects, rather than a number of files
  - On restart from checkpoint, the number of processors need not match the number of files
- Easy read-write of non-contiguous data
- Optimizations possible with little effort

I/O Middleware: Damaris

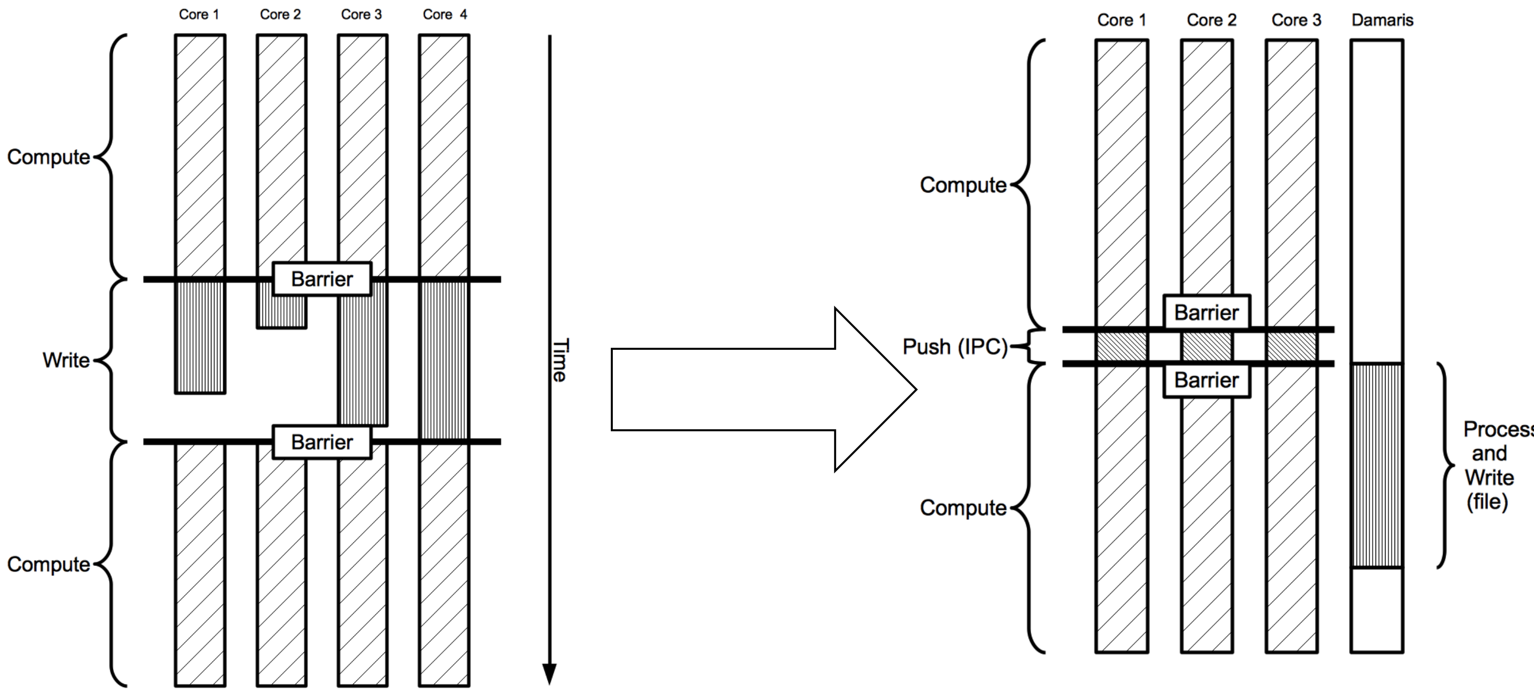
Damaris -- **D**edicated **A**daptable **M**iddleware for **A**pplication **R**esources **I**nline **S**teering

- Started in 2010 by Matthieu Dorier during an internship at NCSA
- The purpose: decouple I/O and computation to enable scalable asynchronous I/O
- The approach: dedicated I/O core(s) on each node
  - Limits OST contention to the node level
  - Leverages shared memory for efficient interaction
  - When simulation “writes” data, Damaris utilizes shared memory to effectively aggregate writes to the “right” size

Application: Reducing I/O Jitter in CM1

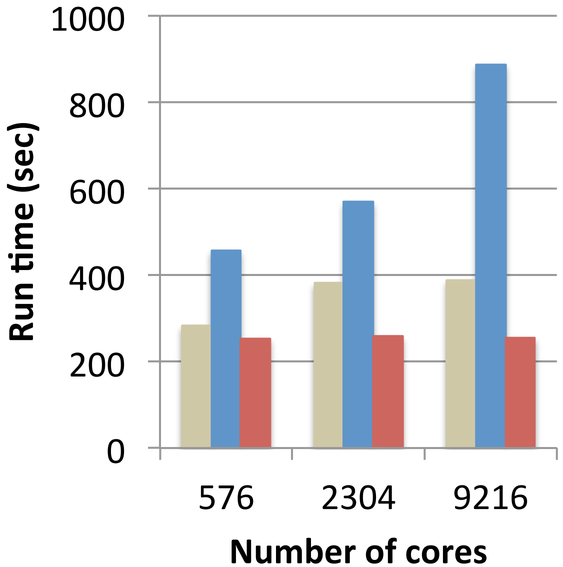
- I/O **Jitter** is the variability in I/O operations that arise from any number of common interferences
- CM1
  - Atmospheric simulation
  - Current Blue Waters allocation
  - Uses serial and parallel HDF5

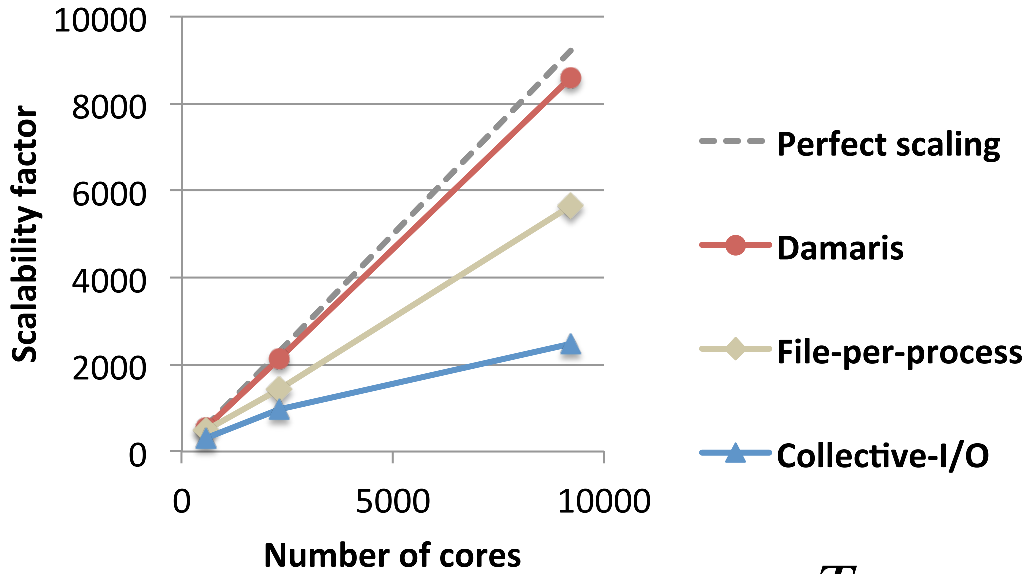
How Damaris Helps with I/O Jitter



- Jitter is “moved” to the dedicated core
- Even with the reduction in number of cores performing computation, performance is not adversely affected, in fact….

How Damaris Helps CM1





Weak scalability factor: $S = N \frac{T_{base}}{T}$

N: number of cores
T_{base}: time of an iteration on one core w/ write
T: time of an iteration + a write

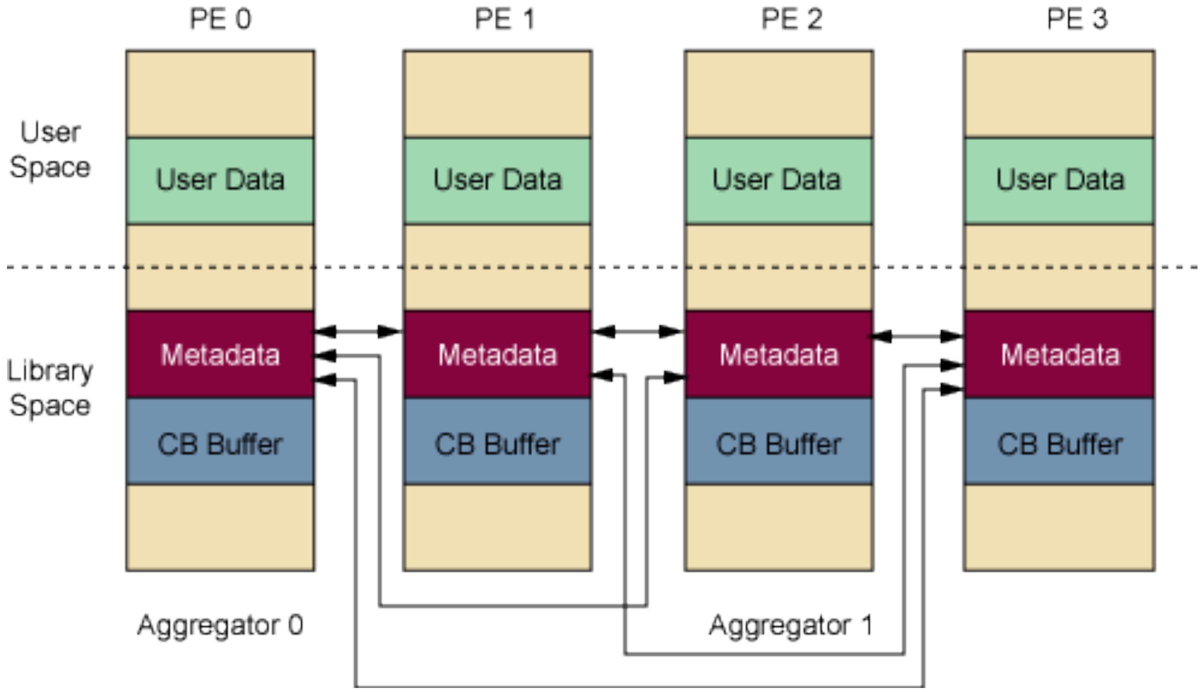
- In these runs, Damaris spent at least 75% its time waiting!
- A plugin system was implemented such that this time may be used for other tasks – We are collaborating with the developer to identify alternate uses.

I/O Middleware: MPI-IO

- MPI standard's implementation of **collective** I/O (shared-file)
  - A file is opened by a group of processes, partitioned among them, and I/O calls are collective among all processes in the group
  - Files are composed of native MPI data types
  - Non-collective I/O is also possible
- Uses **collective buffering** to consolidate I/O requests
  - All data is transferred to a subset of processes and aggregated
  - Use MPICH_MPIIO_CB_ALIGN=2 to enable Cray's collective buffering algorithm
    - *automatic* Lustre stripes alignment & minimize lock contention
    - May not be beneficial when writing small data segments
    - Verified to deliver 25% improvement on BlueWaters for a 1000 rank job
- Use MPICH_MPIIO_XSTATS [0, 1, 2] to obtain MPI-IO statistics
- I/O optimizations in high level libraries are often implemented here – be sure any monkeying is careful monkeying

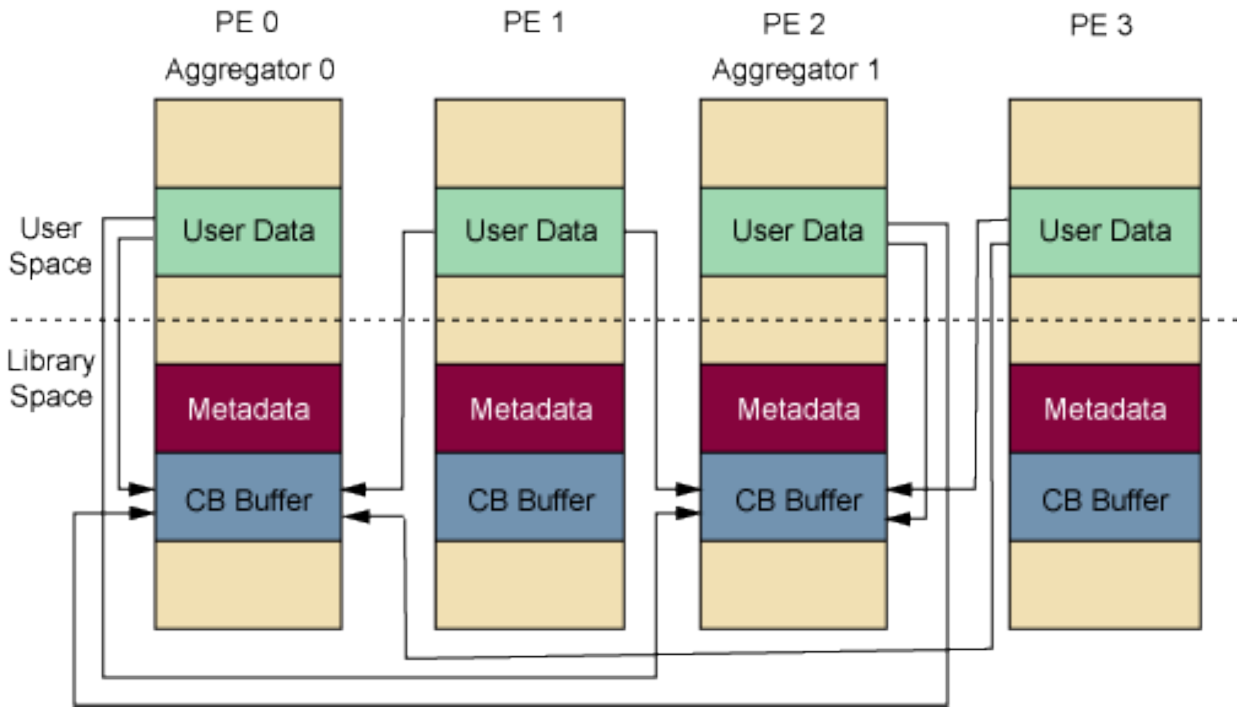
Collective Buffering (1)

- Exchange metadata



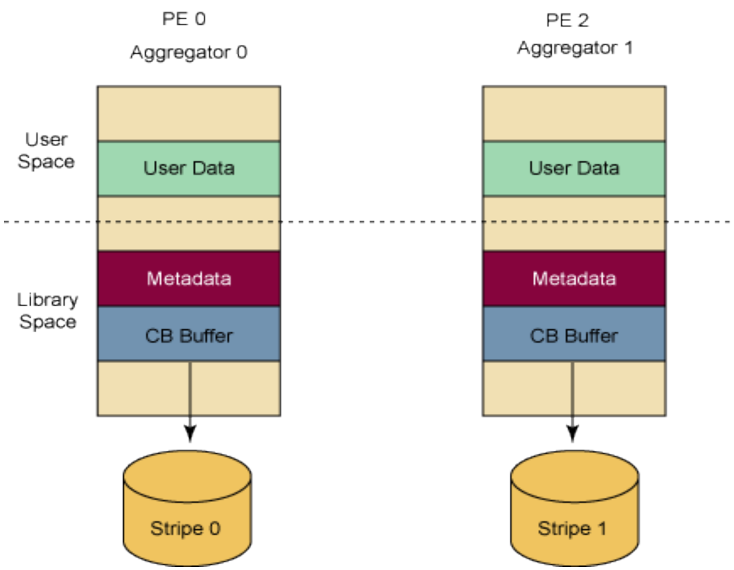
Collective Buffering (2)

- Copy user/application data



Collective Buffering (3)

- Aggregators write to disk



Tuning MPI-IO: CB Hints

- Hints are specified in application code [`MPI_Info_set()`] or as environment variables (`MPICH_MPIIO_HINTS`)
- Collective buffering hints

Hint	Description	Default
`cb_buffer_size`	set the maximum size of a single I/O operation	4MB
`cb_nodes`	set maximum number of aggregators	stripe count of file
romio_cb_read romio_cb_write	enable or disable collective buffering	automatic
romio_no_indep_rw	• if `true`, MPI-IO knows all I/O is collective • Only aggregators will open files	`false`
cb_config_list	a list of independent configurations for nodes	N/A
striping_factor	Specifies the number of Lustre stripes	File system
striping_unit	Specifies the size of the Lustre stripe	File system

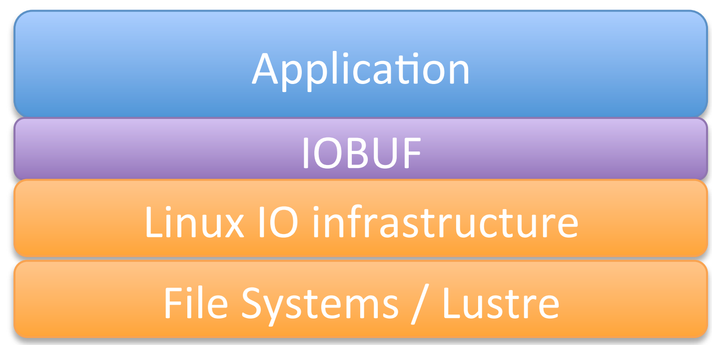
Other Useful Hints

Hint	Description	Default
`romio_lustre_co_ratio`	tell MPI-IO the maximum number of processes (clients, here) that will access an OST	1
`romio_lustre_coll_threshold`	Turns off collective buffering when transfer sizes are above a certain threshold	0 (never)
mpich_mpiio_hints_display	when true a summary of all hints to stderr each time a file is opened	`false`

IOBUF – I/O Buffering Library

- Optimize I/O performance with minimal effort
  - Asynchronous prefetch
  - Write back caching
  - stdin, stdout, stderr disabled by default

- No code changes needed
  - Load module
  - Recompile & relink the code
- Ideal for sequential read or write operations



IOBUF – I/O Buffering Library

- Globally (dis)enable by (un)setting IOBUF_PARAMS
- Fine grained control
  - Control buffer size, count, synchronicity, prefetch
  - Disable iobuf per file
- Some calls in C, C++ can be enabled using iobuf.h, use the compiler macro, USE_IOBUF_MACROS

```
export IOBUF_PARAMS='*.in:count=4:size=32M,*.out:count=8:size=64M:preflush=1'
```

IOBUF – MPI-IO Sample Output

```
IOBUF parameters: file="outc-iob.4":size=1048576:count=4:vbuffer_count=4096:prefetch=1:verbose
PE 0: File "outc-iob.2"
                Calls        Seconds      Megabytes   Megabytes/sec   Avg Size
Open                1       0.000756
Close               1       0.000318
Buffers used             1 (1 MB)
PE 0: File "outc-iob.1"
                Calls        Seconds      Megabytes   Megabytes/sec   Avg Size
Read                1       0.000663       0.065536       98.841390      65536
Open                1       0.000710
Close               1       0.000361
Buffer Read         1       0.000445       0.065536      147.308632      65536
I/O Wait            1       0.000474       0.065536      138.268565
Buffers used             1 (1 MB)
PE 0: File "outc-iob.3"
                Calls        Seconds      Megabytes   Megabytes/sec   Avg Size
Read                1       0.000694       0.065536       94.427313      65536
Open                1       0.000844
Close               1       0.000189
Buffer Read         1       0.000433       0.065536      151.364486      65536
I/O Wait            1       0.000460       0.065536      142.497619
Buffers used             1 (1 MB)
IOBUF parameters: file="outc-iob.2":size=1048576:count=4:vbuffer_count=4096:prefetch=1:verbose
```

I/O LIBRARIES

HDF5 & PnetCDF

Benefits of I/O Libraries

- There are many benefits to using higher level I/O libraries
  - They provide a well-defined, base structure for files that is self-describing and organizes data intuitively
  - Has an API that represents data in a way similar to a simulation
  - Often built on MPI-IO and handle (some) optimization
  - Easy serialization/deserialization of user data structures
  - Portable

- Currently supported: (Parallel) HDF5, (Parallel) netCDF, Adios

I/O Libraries – Some Details

- Parallel netCDF
  - Derived from and compatible with the original "Network Common Data Format"
  - Offers collective I/O on single files
  - Variables are typed, multidimensional, and (with files) may have associated attributes
  - Record variables – "unlimited" dimensions allowed if dimension size is unknown
- Parallel HDF5
  - "Hierarchical Data Format" with data model similar to PnetCDF, and also uses collective I/O calls
  - Can use compression (only in serial I/O mode)
  - Can perform data reordering
  - Very flexible
  - Allows some fine tuning, e.g. enabling buffering

Example Use on Blue Waters

- Under PrgEnv-cray:

```
$> module avail hdf5
------------------------ /opt/cray/modulefiles ------------------------
hdf5/1.8.7   hdf5/1.8.8(default)   hdf5-parallel/1.8.7   hdf5-parallel/1.8.8
(default)

$> module load hd5-parallel

$> cc Dataset.c

$> qsub -I -lnodes=1:ppn=16 -lwalltime=00:30:00
$> aprun -n 2 ./a.out
Application 1293960 resources: utime ~0s, stime ~0s

$> ls *.h5
SDS.h5
```

- Dataset.c is a test code from the HDF Group:
  http://www.hdfgroup.org/ftp/HDF5/examples/parallel/Dataset.c

I/O UTILITIES

Darshan

Example I/O Utility: Darshan

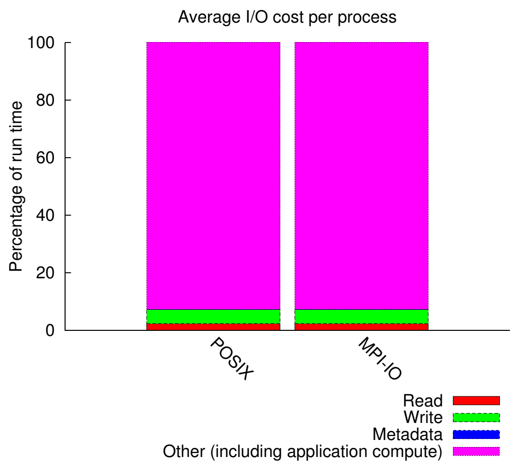
- We will support tools for I/O Characterization
  - Sheds light on the intricacies of an application's I/O
  - Useful for application I/O debugging
  - Pinpointing causes of extremes
  - Analyzing/tuning hardware for optimizations
- Darshan was developed at Argonne, and
- is "a scalable HPC I/O characterization tool… designed to capture an accurate picture of application I/O behavior… with minimum overhead"
- http://www.mcs.anl.gov/research/projects/darshan/

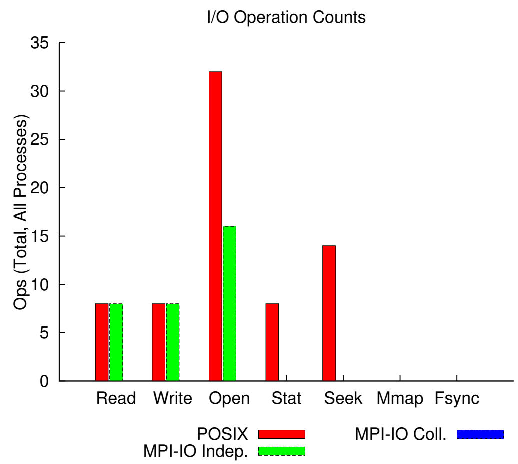
Darshan Specifics

- Darshan collects per-process statistics (organized by file)
  - Counts I/O operations, e.g. unaligned and sequential accesses
  - Times for file operations, e.g. opens and writes
  - Accumulates read/write bandwidth info
  - Creates data for simple visual representation
- More
  - Requires no code modification (only re-linking)
  - Small memory footprint
  - Includes a job summary tool

Summary Tool Example Output

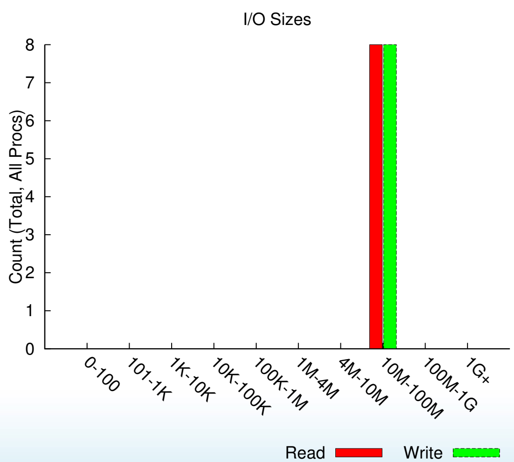
jobid: 3406	uid: 1000	nprocs: 8	runtime: 1 seconds

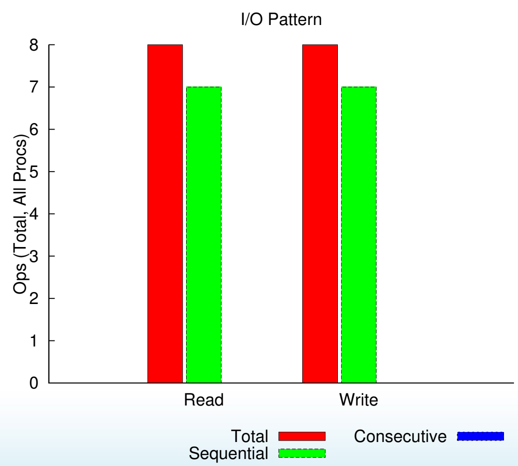




File Count Summary

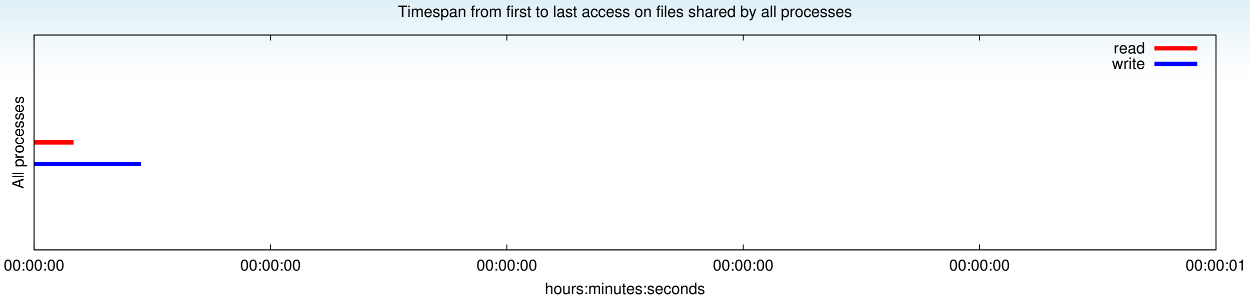
type	number of files	avg. size	max size
total opened	1	128M	128M
read-only files	0	0	0
write-only files	0	0	0
read/write files	1	128M	128M
created files	0	0	0





Most Common Access Sizes

access size	count
16777216	16



Average I/O per process

	Cumulative time spent in I/O functions (seconds)	Amount of I/O (MB)
Independent reads	0.000000	0.000000
Independent writes	0.000000	0.000000
Independent metadata	0.000000	N/A
Shared reads	0.023298	16.000000
Shared writes	0.049300	16.000000
Shared metadata	0.000019	N/A

Data Transfer Per Filesystem

File System	Write		Read	
	MiB	Ratio	MiB	Ratio
/	128.00000	1.00000	128.00000	1.00000

Variance in Shared Files

File Suffix	Processes	Fastest			Slowest			σ	
		Rank	Time	Bytes	Rank	Time	Bytes	Time	Bytes
...test.out	8	0	0.041998	32M	2	0.111384	32M	0.0246	0

THE SUMMARY

Two slides left.

Good Practices, Generally

- Opening a file for writing/appending is expensive, so:
  - If possible, open files as *read-only*
  - Avoid large numbers of small writes

```
while(forever){    open("myfile");
    write(a_byte); close("myfile"); }
```

- Be gentle with metadata (or suffer its wrath)
  - limit the number of files in a single directory
    - Instead opt for hierarchical directory structure
  - `ls` contacts the metadata server, `ls -l` communicates with every OST assigned to a file (for all files)
  - Avoid wildcards: `rm -rf *`, expanding them is expensive over many files
  - It may even be more efficient to pass medata through MPI than have all processes hit the MDS (calling `stat`)
  - Avoid updating last access time for *read-only* operations (NO_ATIME)

Lessons Learned

- **Avoid unaligned I/O and OST contention!**
- Use large data transfers
  - Don't expect performance with non-contiguous, small data transfers. Use buffering when possible
- Consider using MPI-IO and other I/O libraries
  - Portable data formats vs. unformatted files
- Use system specific hints and optimizations
- Exploit parallelism using striping
  - Focus on stripe alignment, avoiding lock contention
- Move away from one-file-per-process model
  - Use aggregation and reduce number of output files
- Talk to your POC about profiling and optimizing I/O