# BLUE WATERS SUSTAINED PETASCALE COMPUTING

# Optimizing Applications on Blue Waters

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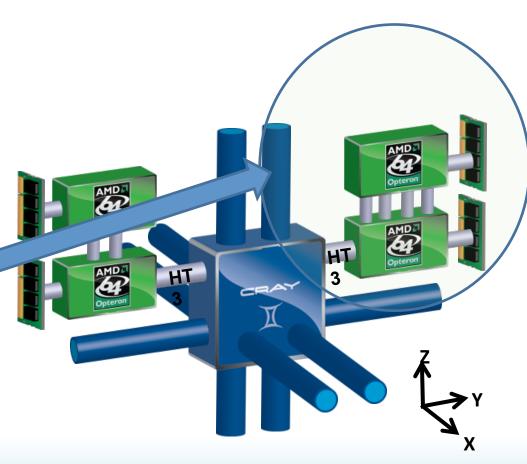


## Cray XE6 Blade and Node



#### **Node Characteristics**

Number of Cores	16 Core modules (2 AMD 6276 Interlagos processors @2.3 GHz)
Peak Performance	313 Gflops/sec
Memory Size	4 GB per core-mod 64 GB per node
Memory Bandwidth (Peak)	102.4 GB/sec







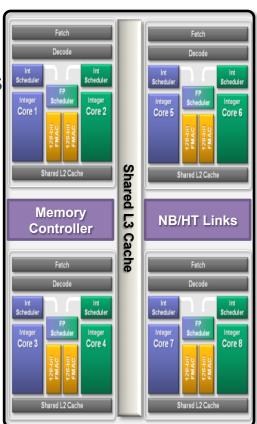


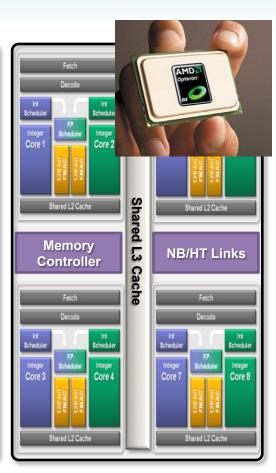




## **AMD 6276 Interlagos Processor**

- Each processor die is composed of 4 core modules
- The 4 core modules share a memory controller and 8 MB L3 data cache on one die
- Two die are packaged on a multi-chip module to form a G34-socket Interlagos processor
- Package contains
  - 8 core modules
  - 16 MB L3 Cache
  - 4 DDR3 1600 memory channels











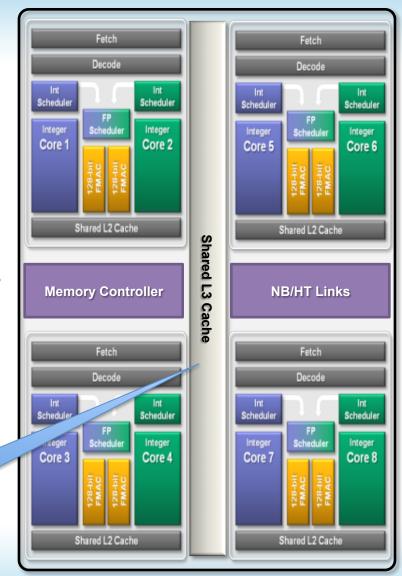




## Interlagos

- Four Core Modules per die
- Two Integer cores and one FP core per Core Module
- OS treats each Interlagos as 16 cores (i.e. 32 per XE6 node)
- Each die shares L3 cache

1 of 2 dies















## **Compiler Options - Topics**

- Available (Supported) Compilers
- Where to Start
- Compiler Choices Relative Strength
- Compiler Options focused on
  - Optimization
  - Debugging













## **Available Compilers**

- Cray Compilers (Cray Compiling Environment (CCE))
  - Provided additional support for Fortran 2003, Co-arrays, UPC, PGAS
- GNU Compiler Collection (GCC)
- Portland Group Inc (PGI) Compilers
- All provide Fortran, C, C++, OpenMP support
- UPC, PGAS, (limited) OpenACC support (Cray, PGI)
- So which compiler do I choose?
  - Experiment with various compilers
  - Work with your BW POC
  - Mixing libraries created by different compilers may cause issues













#### Where to Start

- Unless you have a very good reason, always use compiler wrappers
  - "module load PrgEnv-[cray,gnu,pgi]"
  - Compiler wrappers: ftn, cc, CC
  - Additional libraries are automatically linked in
  - Optimization targets automatically set
- For most applications, using default settings work very well
- The OpenMP threaded BLAS/LAPACK libraries are used
  - The serial version is used if "OMP\_NUM\_THREADS" is not set or set to 1













## **Use the Best Compiler**

- The best compiler may not be the same for every application.
- Work with BW staff to compare compilers













## Compiler Choices – Relative Strength

- CCE Outstanding Fortran, Very good C and okay C++
  - Very good vectorization
  - Very good Fortran language support; only real choice for coarrays
  - C support is very good, with UPC support
  - Very good scalar optimization and automatic parallelization
  - Clean implementation of OpenMP 3.0 with tasks
  - Cleanest integration with other Cray tools (Performance tools, debuggers, upcoming productivity tools)
  - No inline assembly support
  - Excellent support from Cray (bugs, issues, performance etc)











## Compiler Choices – Relative Strength

- PGI Very good Fortran, okay C and C++
  - Good vectorization
  - Good functional correctness with optimization enabled
  - Good manual and automatic prefetch capabilities
  - Company focused on HPC market
  - Excellent working relationship with Cray, good bug responsiveness













## Compiler Choices – Relative Strength

- GNU so-so Fortran, outstanding C and C++ (If you ignore vectorization)
  - Obviously, the best gcc compatibility
  - Scalable optimizer was recently rewritten and is very good
  - Vectiorization capabilities focus mostly on inline assembly
  - Few releases have been incompatible with each other and require recompilation of modules (4.3, 4.4, 4.5)











## **Recommended CCE Compilation Options**

- Use default optimization levels
  - It's the equivalent of most other compilers –O3 or –fast
- Use –O3, fp3 (or –O3 –hfp3 or some variation)
  - -O3 gives slightly more than –O2
  - -hfp3 gives a lot more floating point optimizations, esp 32 bit
- If an application is intolerant of floating point reassociation, try lower hfp number, try hfp1 first, only hfp0 if absolutely necessary
  - Might be needed for tests that require strict IEEE conformance
  - Or applications that have validated results from diffferent compiler
- Do not suggest using -Oipa5, -Oaggress and so on; higher numbers are not always correlated with better performance
- Compiler feedback : -rm (fortran), -hlist=m ( C )
- If don't want OpenMP: -xomp or -Othread0 or -hnoomp
- Manpages: crayftn, craycc, crayCC













## Loopmark: Compiler Feedback (CCE)

- Compiler can generate an filename.lst file
- Contains annotated listing of your source code with letter indicating important optimizations
- Loopmark legend

Primary Loop Type	Modifiers
A - Pattern matched	a - atomic memory operation b – blocked
C – Collapsed D – Deleted	c - conditional and/or computed
E – Cloned	f – fused
G – Accelerated	g – partitioned
I - Inlined	i – interchanged
M - Multithreaded	m – partitioned
V – Vectorized	n - non-blocking remote transfer p – partial
	r – unrolled
	s – shortloop
	w - unwound











## Starting Point for PGI Compilers

- Suggested Option : -fast
- Interprocedural analysis allows the compiler to perform whole program optimizations: –Mipa=fast(,safe)
- If you can be flexible with precision, also try –Mfprelaxed
- Option –Msmartalloc, calls the subroutine mallopt in the main routine, can have a dramatic impact on the performance of program that uses dynamic allocation of memory
- Compiler feedback : -Minfo=all, -Mneginfo
- Manpages : pgf90, pgcc, pgCC











# **PGI Compiler Flags**

- -default64: Fortran driver option for –i8 and –r8
- -i8, -r8: Treats INTEGER and REAL variables in Fortran as 8 bytes (use ftn –default64 option to link the right libraries
- -byteswapio : Reads big endian files in fortran
- -Mnomain: Uses ftn driver to link programs with the main program (written in C or C++) and one or more subroutines (written in fortran)













## **PGI Compiler Flags**

- It is possible to disable optimizations included with –fast, for example –fast –Mnolre enables –fast and then disables loop redundant optimizations
- -Mconcur, -mprof=mpi, -Mmpi and -Mscalapack are no more supported
- Fortran interfaces can be called from C program by inserting an underscore to the respective name
- Pass argument by reference rather than by value
- For example to call dgetrf()
- Dgetrf\_(&uplo, &M, &n, .....);
- To debug an optimized code, the –opt flag will insert debugging information without disabling optimizations











## **PGI Compiler Flags**

- Some compiler options mat affect both performance and accuracy
- Lower accuracy is often higher performance, but it also able to enforce accuracy
  - -Kieee: all floating point (FP) math strictly conforms to IEEE, off by default
  - -Ktrap: Turns processor trapping of FP exceptions
  - -Mdaz : Treat all denormalized numbers as zeros
  - Mflushz: Set SSE to flush-to-zero (on with –fast)
  - -Mfprelaxed: allow to use relaxed (reduced) precision to speed up some floating point optimizations
    - Some compilers turn this on by default, PGI chooses to favor accuracy to speed, by default













## **Starting Point for GNU Compilers**

- -O3 –ffast-math –funroll-loops
- Compiler feedback : -ftree-vectorizer-verbose=2
- Manpages: gfortran, gcc, g++













#### **Numerical Libraries Overview**

- Many commonly-used packages are available on Blue Waters
- Typically can link with most or all combinations of compiler, language, and parallel programming model
- Use the "module" command to select a particular version
- Will try to accommodate special installation requests (can't install "Everything under the Sun" due to scalibility and other considerations)













## Cray Scientific Library (libsci)

- Contains optimized versions of several popular scientific software routines
- Available by default; can change versions with "module avail" and "module load xt-libsci[/version]"
  - BLAS, BLACS
  - LAPACK, ScaLAPACK
  - FFT, FFTW
- Unique to Cray (affects portability)
  - CRAFFT, CASE, IRT













## PETSc (Argonne National Laboratory)

- Programmable, <u>Extensible Toolkit for Scientific Computing</u>
- Widely-used collection of many different types of linear and non-linear solvers
- Actively under development; very responsive team
- Can also interface with numerous optional external packages (e.g., SLEPC, HYPRE, ParMETIS, ...)
- Optimized version installed by Cray, along with many external packages
- Use "module load petsc[/version]"













#### Other Numerical Libraries

- ACML (AMD Core Math Library)
  - BLAS, LAPACK, FFT, Random Number Generators
- Trilinos (from Sandia National Laboratories)
  - Somewhat similar to PETSc, interfaces to a large collection of preconditioners, solvers, and other computational tools
- GSL (GNU Scientific Library)
  - Collection of numerous computational solvers and tools for C and C++ programs
- All available using "module load"











## **Optimization options**

- Hybrid programming model (MPI+OpenMP, et al) is usually better
- Try 1, 2, 4, 16, 32 tasks per node

For 1024 nodes:

```
32 tasks+threads/node:
```

```
aprun -n 4096 -N 4 -d 8 ./myprog
16 tasks+threads/node:
aprun -n 4096 -N 4 -d 4 \
   -cc 0,2,4,6:8,10,12,14:16,18,20,22:24,26,28,30 \
   ./myprog
```

Try using –r 1 to reserve a core for the OS

```
aprun -n 4096 -N 4 -d 7 -r 1 \
-cc 0-6:8-14:16-22:24-30 ./myprog
```

- Test different compilers, flags
- Use accelerators



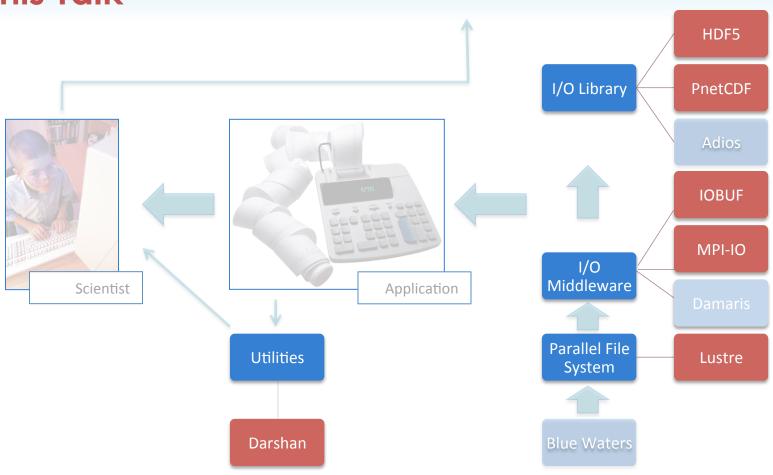








#### This Talk















## 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







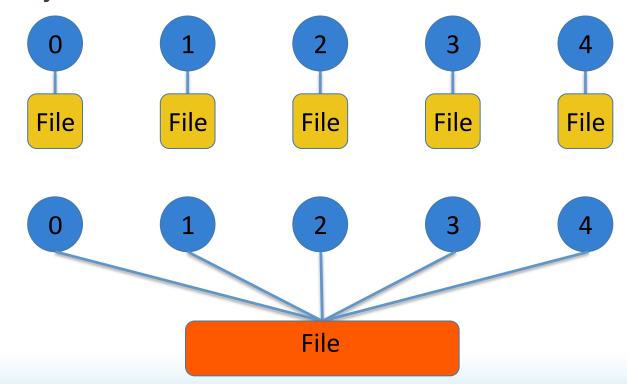






## Large Scale I/O in Practice

- 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:







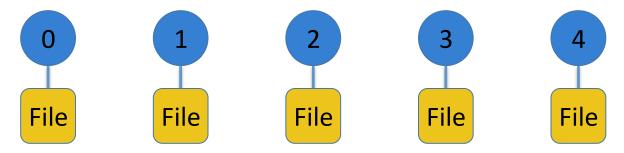






#### File-Per-Process

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





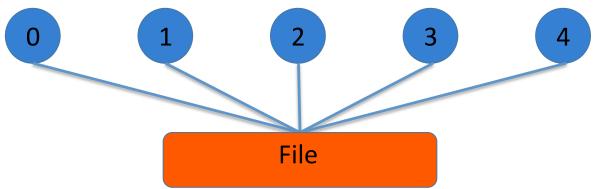






#### **Shared-File**

 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





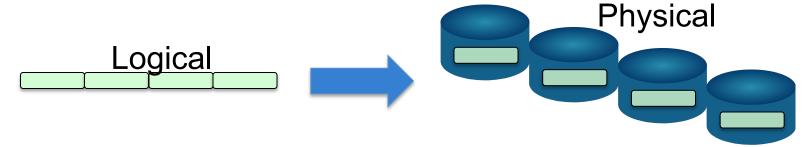








## Lustre File System: Striping



- 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

group	objid	objid	obdidx
0	0x20ff7d	2162557	1259
0	0x210c24	2165796	1403
0	0x210177	2163063	955
0	0x20fb58	2161496	1139
0	0x20fa13	2161171	699

- Note: a file's striping pattern is permanent, and set upon creation
  - Ifs 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**

•	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





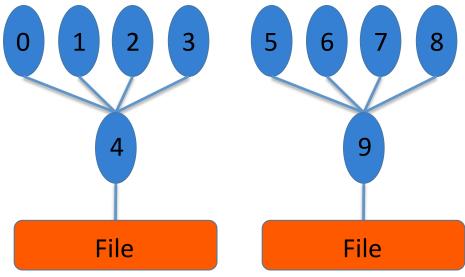








I/O Delegates



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













MPI-IO & IOBUF

# I/O MIDDLEWARE













## 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: 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





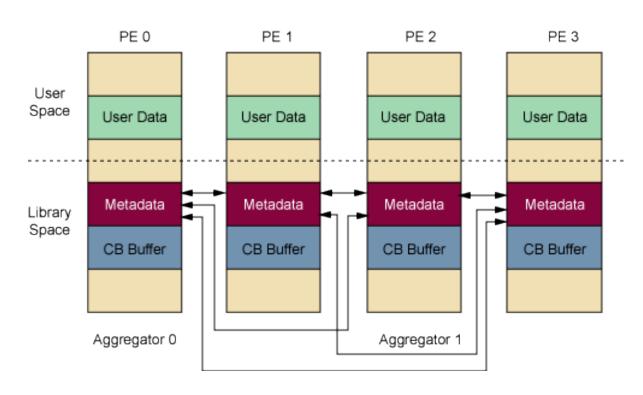






#### Collective Buffering (1)

Exchange metadata









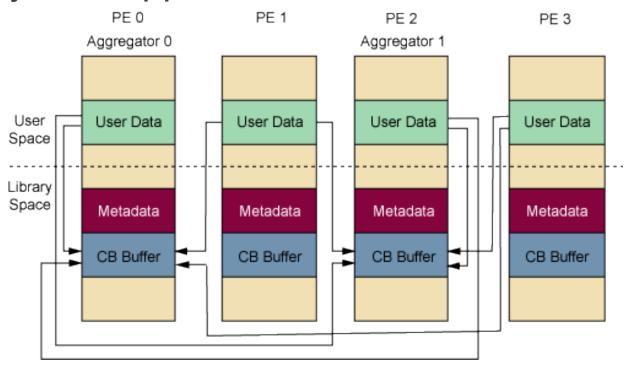






## Collective Buffering (2)

Copy user/application data







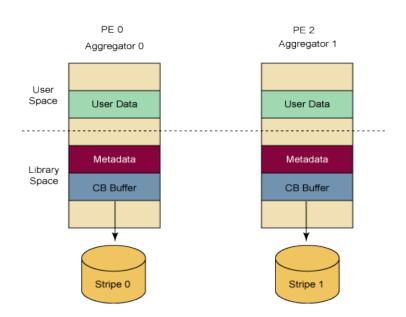






## Collective Buffering (3)

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	<ul><li>if true, MPI-IO knows all I/O is collective</li><li>Only aggregators will open files</li></ul>	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

Application **IOBUF** Linux IO infrastructure File Systems / Lustre

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 Avg Size Megabytes Megabytes/sec 0.000756 0pen 1 Close 1 0.000318 Buffers used 1 (1 MB) PE 0: File "outc-iob.1" Calls Seconds Megabytes Megabytes/sec Avg Size 0.065536 65536 Read 0.000663 98.841390 0pen 0.000710 Close 0.000361 1 Buffer Read 147.308632 0.000445 0.065536 65536 I/O Wait 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 0.000694 0.065536 94.427313 65536 0pen 1 0.000844 Close 1 0.000189 Buffer Read 1 0.000433 0.065536 151.364486 65536 I/O Wait 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













HDF5 & PnetCDF

# I/O LIBRARIES













## 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 selfdescribing 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:

Dataset.c is a test code from the HDF Group:

http://www.hdfgroup.org/ftp/HDF5/examples/parallel/Dataset.c













#### Darshan

# I/O UTILITIES













#### **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



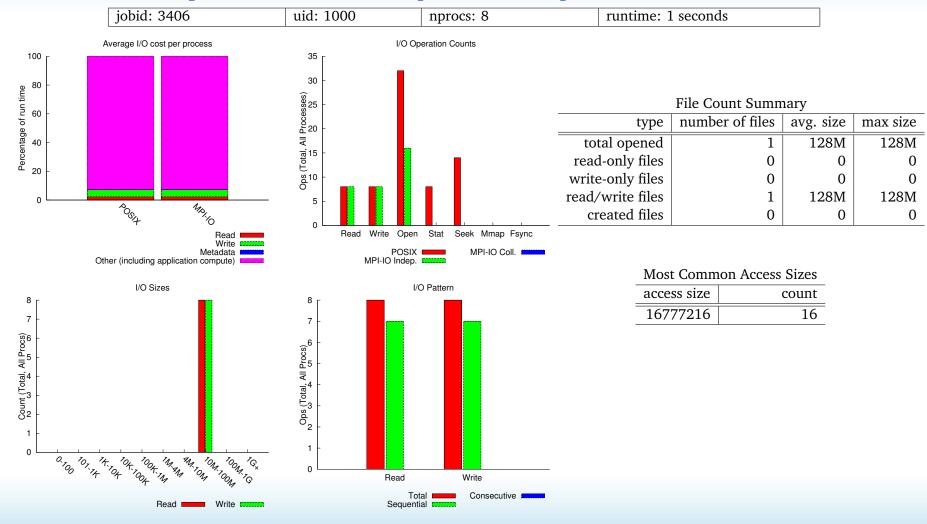








## **Summary Tool Example Output**





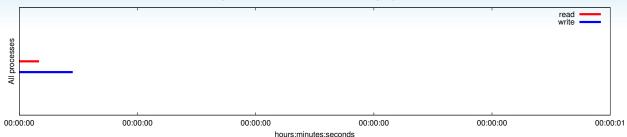




GREAT LAKES CONSORTIUM



#### Timespan from first to last access on files shared by all processes



#### Average I/O per process

	Cumulative time spent in	Amount of I/O (MB)
	I/O functions (seconds)	
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	Writ	:e	Read			
	MiB	Ratio	MiB	Ratio		
/	128.00000	1.00000	128.00000	1.00000		

#### Variance in Shared Files

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













Two slides left.

# THE SUMMARY











# 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 -1 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













#### The End

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