Parallel I/O on JUQUEEN

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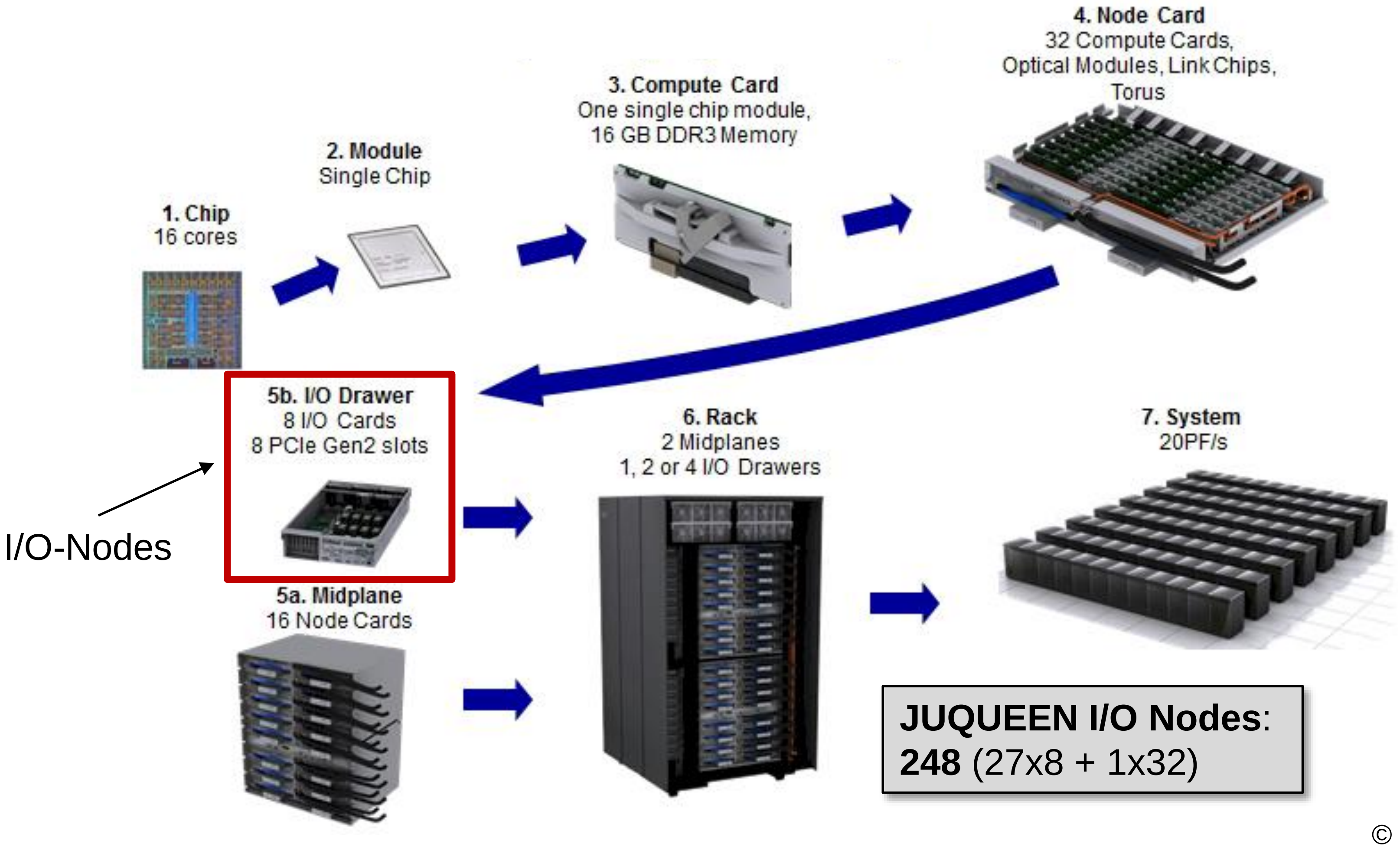
Overview

- Blue Gene/Q I/O Hardware
  - Overview, Cabling, I/O Services
- GPFS architecture and data path
- Pitfalls
- The Parallel I/O Software Stack
- Darshan
  - Overview, Usage, Interpretation
- SIONlib
- Parallel HDF5
- I/O Hints

Blue Gene/Q Packaging Hierarchy



1. Chip
16 cores

2. Module
Single Chip

3. Compute Card
One single chip module,
16 GB DDR3 Memory

4. Node Card
32 Compute Cards,
Optical Modules, Link Chips,
Torus

5b. I/O Drawer
8 I/O Cards
8 PCIe Gen2 slots

I/O-Nodes

5a. Midplane
16 Node Cards

6. Rack
2 Midplanes
1, 2 or 4 I/O Drawers

7. System
20PF/s

JUQUEEN I/O Nodes:
248 (27x8 + 1x32)

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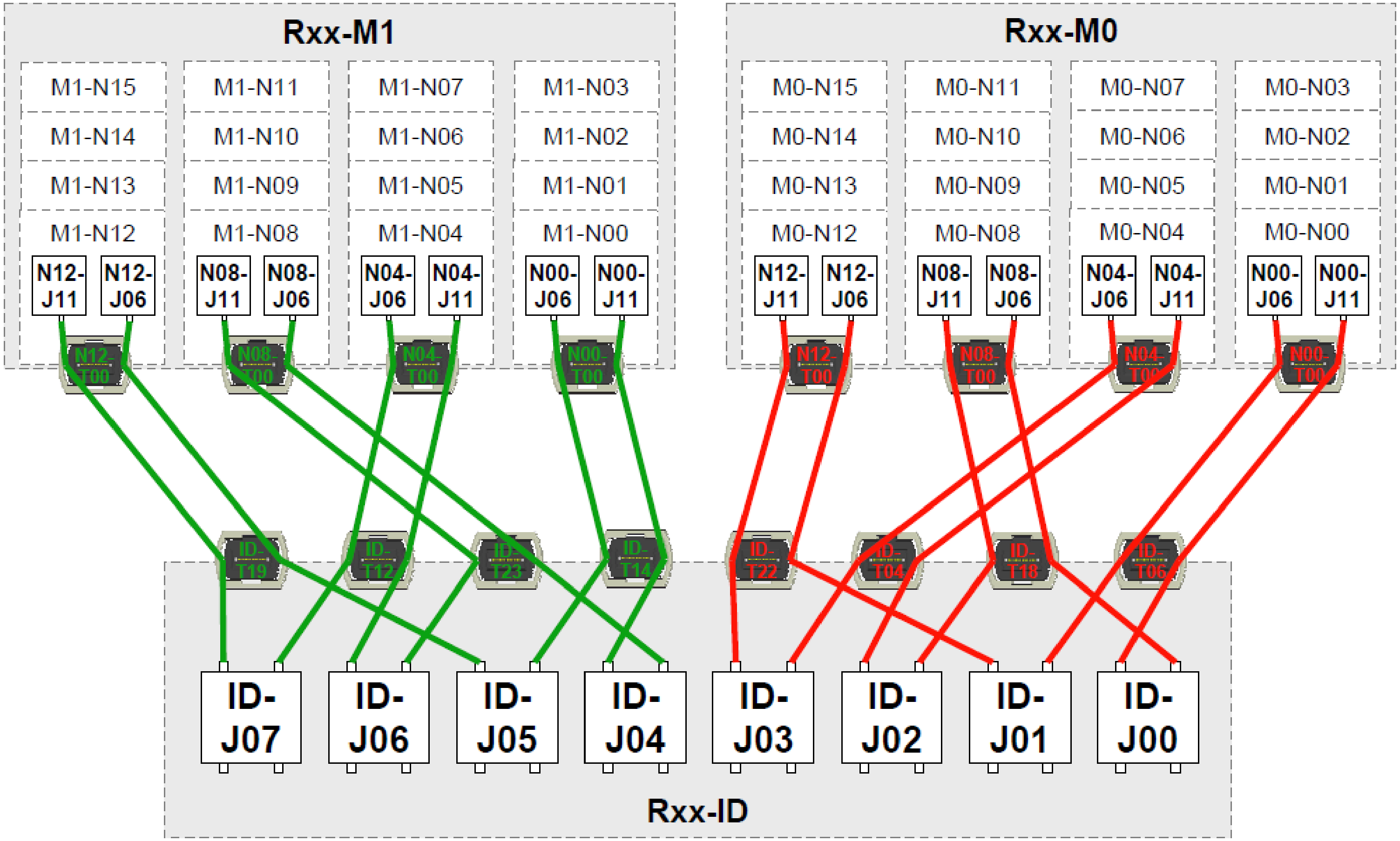
Blue Gene/Q: I/O-node cabling (8 ION/Rack)



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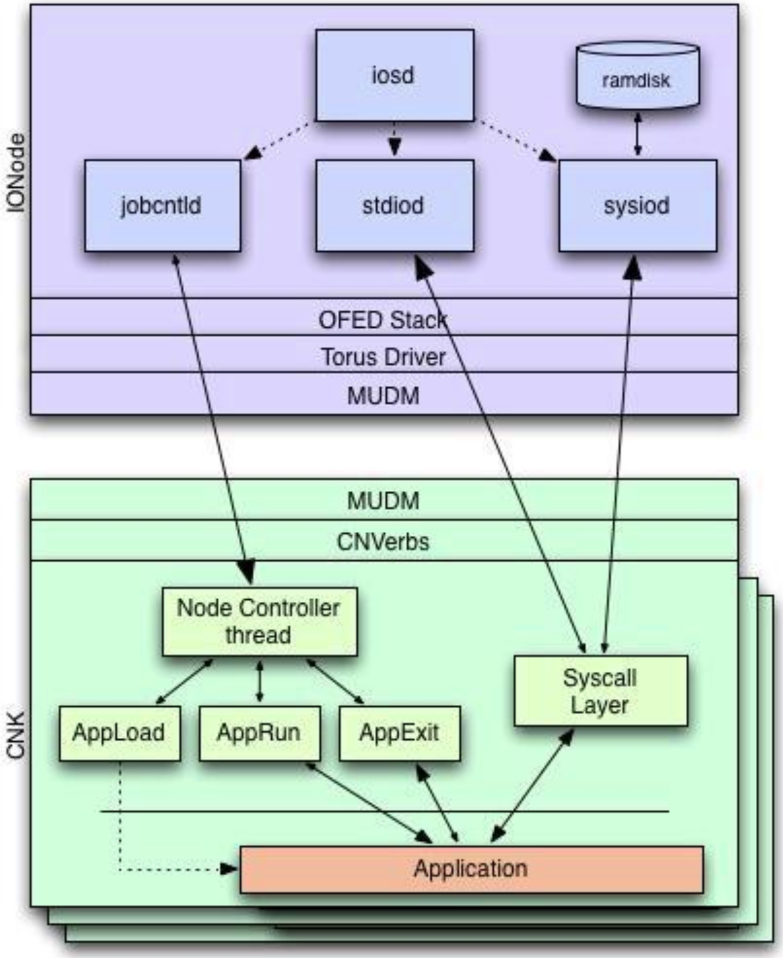
Blue Gene/Q: I/O Services

- Function shipping system calls to I/O-node
- Support NFS, GPFS, Lustre and PVFS2 filesystems
- Supports ratio of **8192:1** compute task to I/O-node
  - Only 1 I/O-Proxy per compute node
- Standard communications protocol
  - OFED verbs
  - Using Torus DMA hardware for performance



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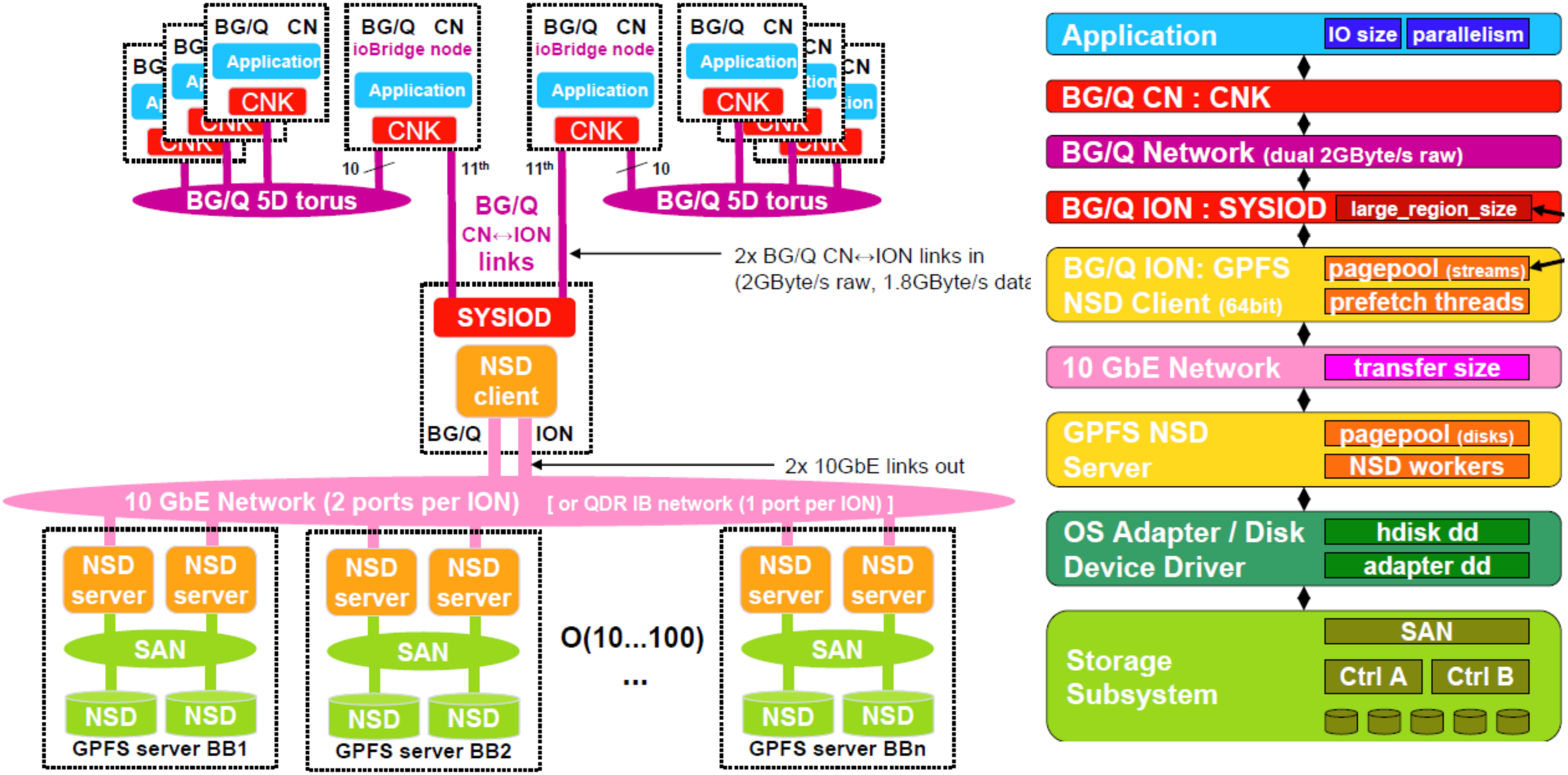
IBM General Parallel File System : Architecture and I/O Data Path on BG/Q

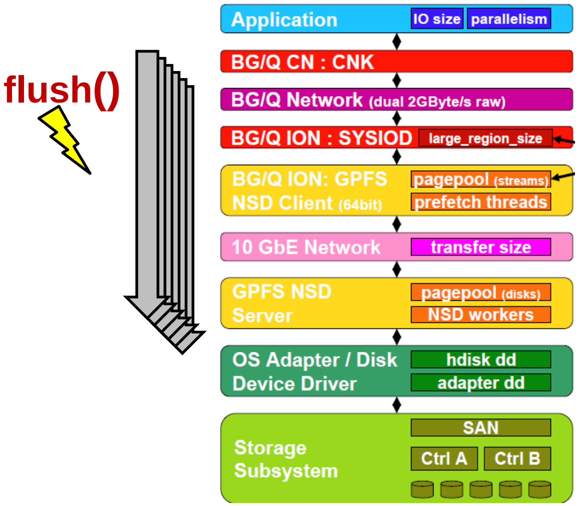


2x BG/Q CN↔ION links in (2GByte/s raw, 1.8GByte/s data

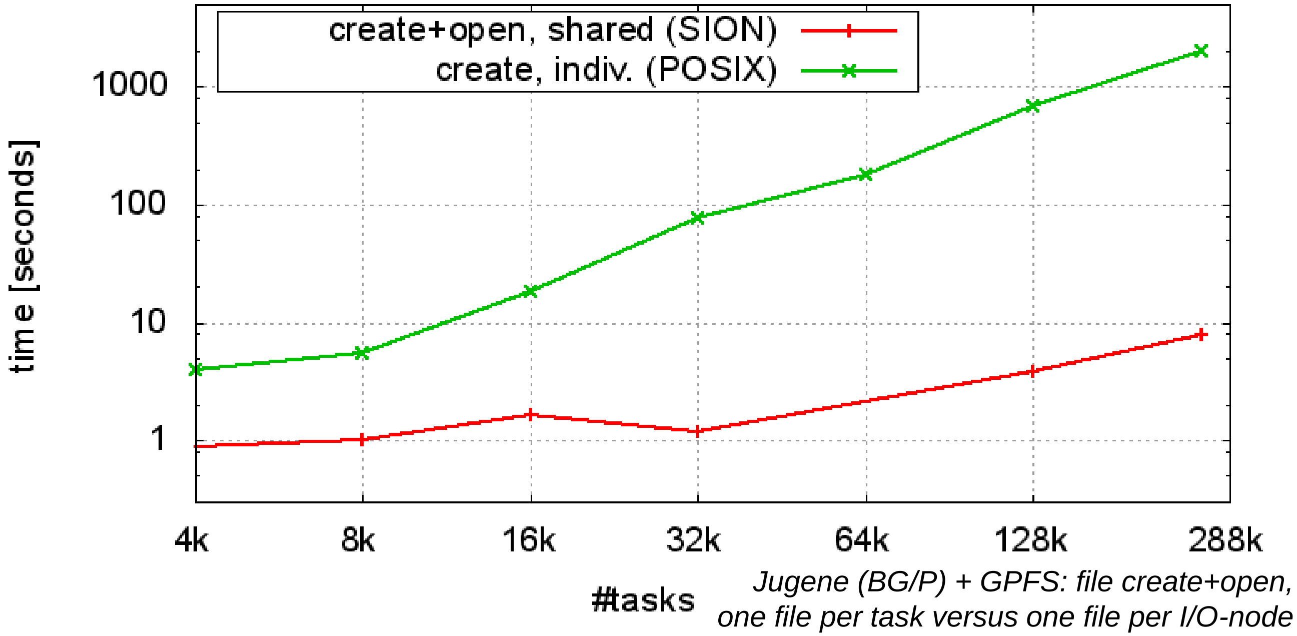
2x 10GbE links out

Pitfall 1: Frequent flushing on small blocks

- Modern file systems in HPC have large file system blocks
- A flush on a file handle forces the file system to perform all pending write operations
- If application writes in small data blocks the same file system block it has to be read and written multiple times
- Performance degradation due to the inability to combine several write calls



Pitfall 2: Parallel Creation of Individual Files



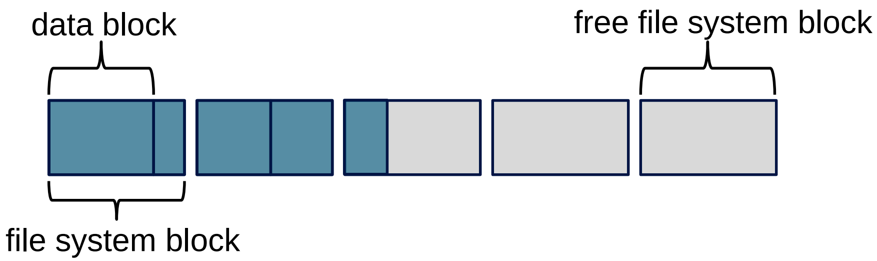
Jugene (BG/P) + GPFS: file create+open, one file per task versus one file per I/O-node

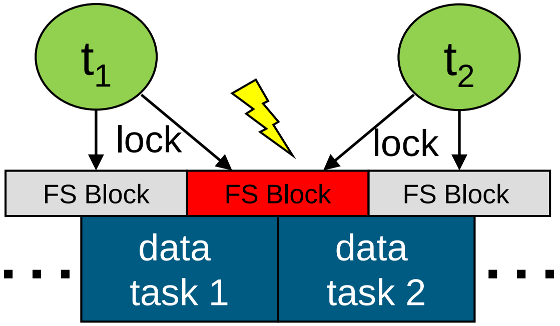
- Contention at node doing directory updates (directory meta-node)
- Pre-created files or own directory per task may help performance, but does not simplify file handling
- Complicates file management (e.g. archive)

→ **shared files are mandatory**

Pitfall 3: False sharing of file system blocks

- Parallel I/O to shared files (POSIX)

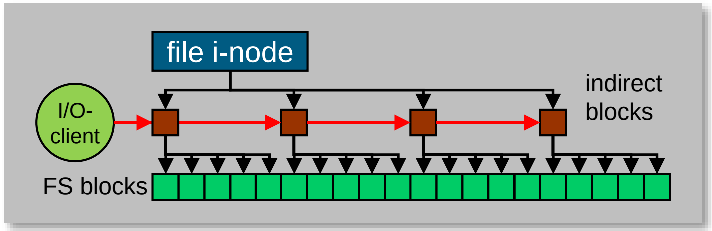




- Data blocks of individual processes do not fill up a complete file system block
- Several processes share a file system block
- Exclusive access (e.g. write) must be serialized
- The more processes have to synchronize the more waiting time will propagate

Pitfall 4: Number of Tasks per Shared File

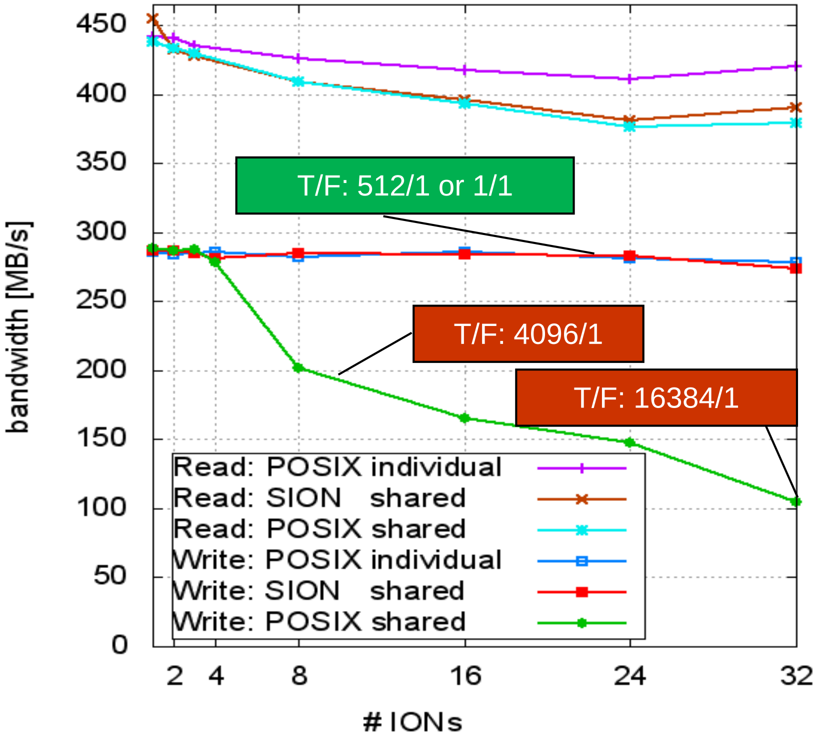
- Meta-data wall on file level
  - File meta-data management
  - Locking



- Example Blue Gene/P
  - Jugene (72 racks)
  - I/O forwarding nodes (ION)
  - GPFS client on ION
  - Solution:

    → tasks : files ratio ~ const

    → SIONlib:
    one file per ION
    implicit task-to-file mapp



Pitfall 5: Portability

- Endianess (byte order) of binary data
- Example (32 bit):

2.712.847.316

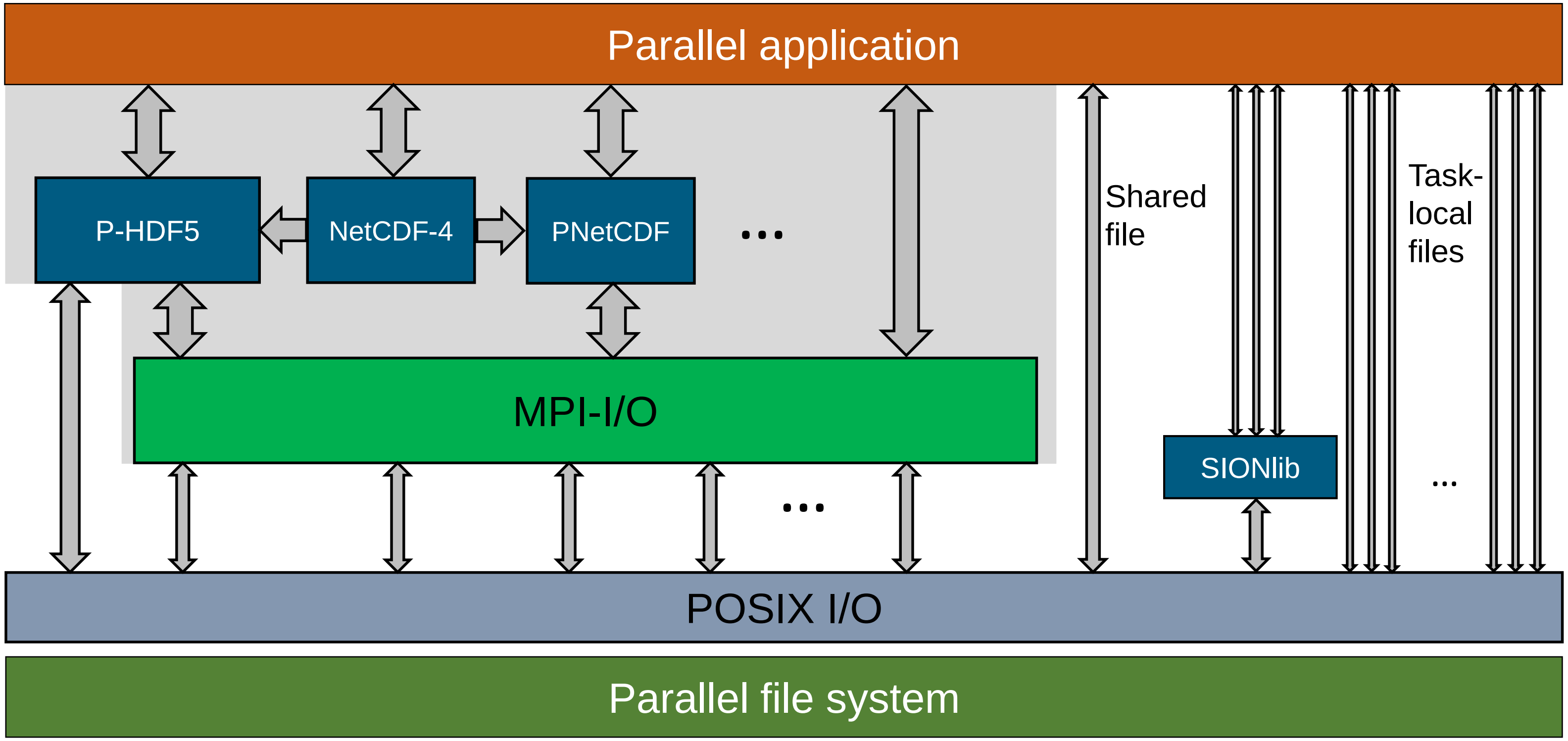
=

10100001 10110010 11000011 11010100

Address	Little Endian	Big Endian
1000	**11010100**	**10100001**
1001	**11000011**	**10110010**
1002	**10110010**	**11000011**
1003	**10100001**	**11010100**

- Conversion of files might be necessary and expensive
- Solution: Choosing a portable data format (HDF5, NetCDF)

The Parallel I/O Software Stack



How to choose an I/O strategy?

- Performance considerations
  - Amount of data
  - Frequency of reading/writing
  - Scalability
- Portability
  - Different HPC architectures
  - Data exchange with others
  - Long-term storage
- E.g. use two formats and converters:
  - Internal: Write/read data “as-is”
    → Restart/checkpoint files
  - External: Write/read data in non-decomposed format
    (portable, system-independent, self-describing)
    → Workflows, Pre-, Postprocessing, Data exchange, …

Darshan: Overview

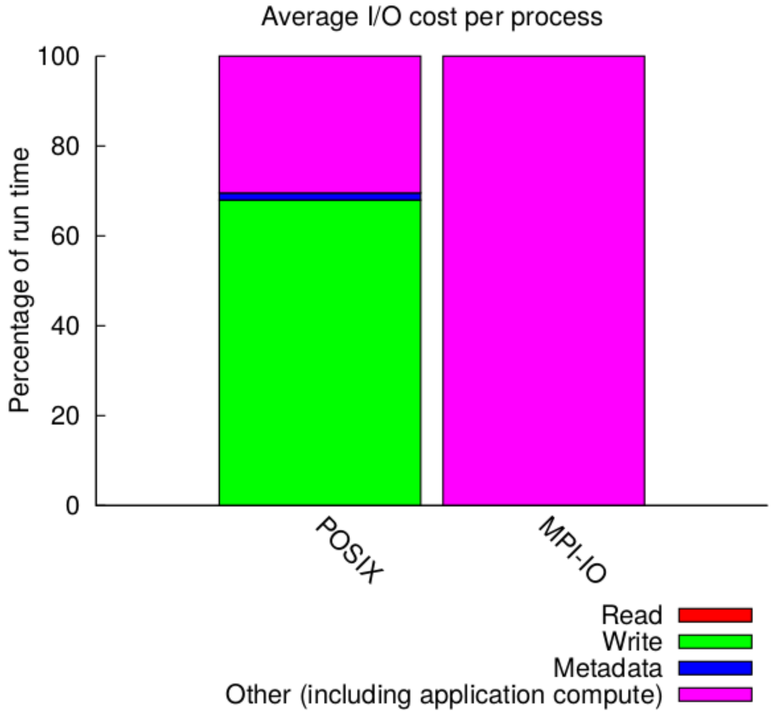
- Developed at ANL: http://www.mcs.anl.gov/darshan
- “HPC I/O Characterization Tool“ instruments I/O
    - Uses modified versions of I/O libraries during linking
        - No code changes needed only recompilation with wrapped compiler
    - Helps analysing I/O patterns and identifying bottlenecks
    - Analyses parallel I/O with MPI-IO and standard POSIX I/O
- Ready to use version available on JUQUEEN

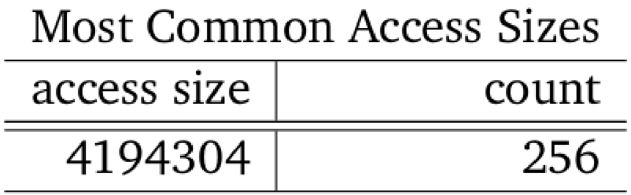
Darshan: Usage example on JUQUEEN

- Load module
  - module load darshan
- Recompile
  - make MPICC=mpicc.darshan
- Tell runjob where to save the output (in submit script)
  - runjob ... --envs \
    DARSHAN_LOG_PATH=$HOME/darshanlogs …
- Analyse output
  - darshan-job-summary.pl mylog.darshan.gz
  - evince mylog.pdf

Darshan: Interpret the summary

- Average and statistical information on I/O patterns
  - Relative time for I/O
  - Most common access sizes
- Additional metrics
  - File count
  - I/O size histogram
  - Timeline for read / write per task
  - …



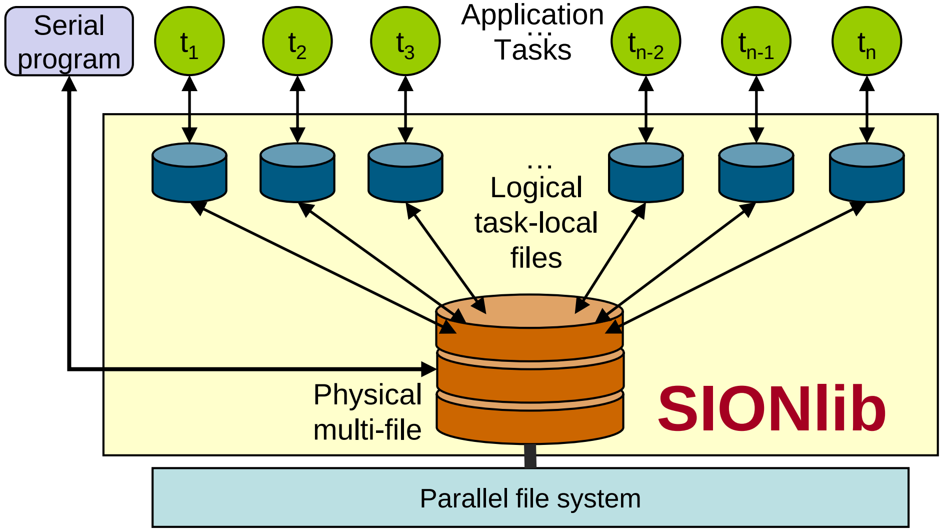


Most Common Access Sizes

access size	count
4194304	256

SIONlib: Overview

- Shared file I/O with automatic file system block alignment
  - One single or few large files (e.g. one per ION)
    - Only open and close calls are collective
  - Support for file coalescing
    - For data sizes << file system block size
- http://www.fz-juelich.de/jsc/sionlib



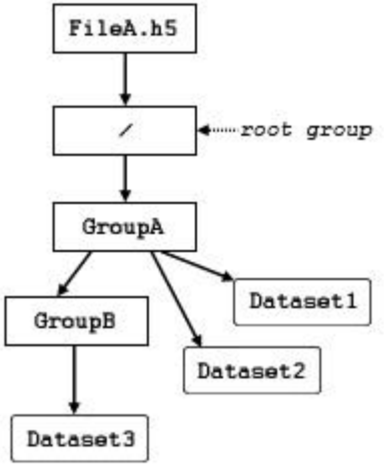
```
/* fopen() → */
sid=sion_paropen_mpi( filename , “bw“,
                     &numfiles, &chunksize,
                     gcom, &lcom, &fileptr, ...);

/* fwrite(bindata,1,nbytes, fileptr) → */
sion_fwrite(bindata,1,nbytes, sid);

/* fclose() → */
sion_parclose_mpi(sid)
```

Parallel HDF5: Overview

- Self-describing file format
  - Hierarchical, filesystem-like data format
  - Support of additional metadata for datasets
- Portable
  - Builds on top of standard MPI-I/O or POSIX-I/O
  - Move between system architectures
    - Automatic conversion of data representation
  - Move between parallel/serial applications
    - e.g. 4096 MPI processes → 65.536 MPI processes
    - e.g. simulation → post-processing
  - Complex data selections possible for read or write
    - e.g. read only sub-array of dataset with stride



slide provided by Jens Henrik Göbbert

Parallel HDF5: I/O Hints

- Align datasets to file system block size

```
H5Pset_alignment(...);
```

- Use hyperslabs

```
H5Sselect_hyperslab(...);
```

- Chunk datasets

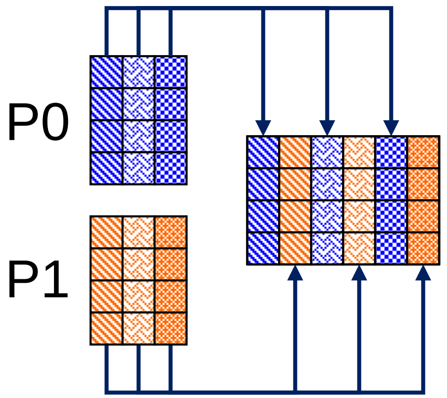
```
H5Pset_cache(...);
H5Pset_chunk_cache(...);
```

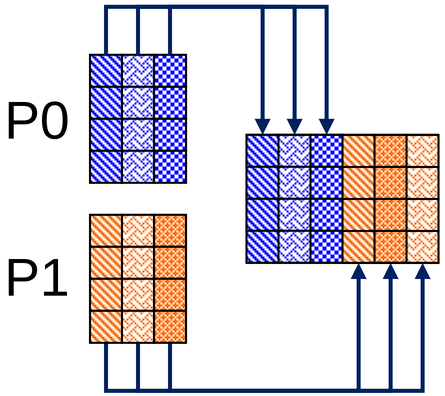
- Increase transfer buffer

```
H5Pset_buffer(...);
```

- Improve metadata handling

```
H5Pset_istore_k(...);
H5Pset_meta_block_size(…);
```





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I/O Hints

- Reduce locking for MPI-IO
  - export BGLOCKLESSMPIO_F_TYPE="0x47504653“
- ROMIO hints
  - echo " IBM_largeblock_io true" > romio.hints
  - echo " cb_buffer_size 33554432" >> romio.hints
  - export ROMIO_HINTS=romio.hints
- Note: don’t forget to add exports to runjob, via “--exp-env X”
- MPIX_Calls: splitting communicators per I/O-bridge

```
FORTRAN: MPIX_PSET_SAME_COMM_CREATE(INTEGER pset_comm_same,
                                    INTEGER ierr)
C: #include <mpix.h>
   int MPIX_Pset_same_comm_create( MPI_Comm *pset_comm_same )
```

```
sid=sion_paropen_mpi( filename , “bw“, &numfiles, &chunksize, gcom, &lcom, ...);
```