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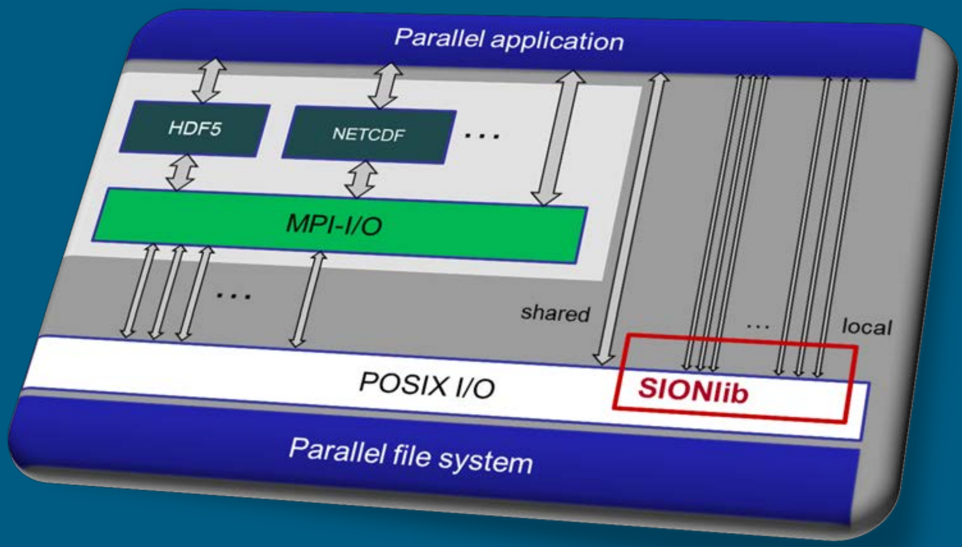
Parallel file I/O bottlenecks and solutions

→ Views to Parallel I/O: Hardware, Software, Application
→ Challenges at Large Scale
→ Introduction SIONlib
→ Pitfalls, Darshan, I/O-Strategies



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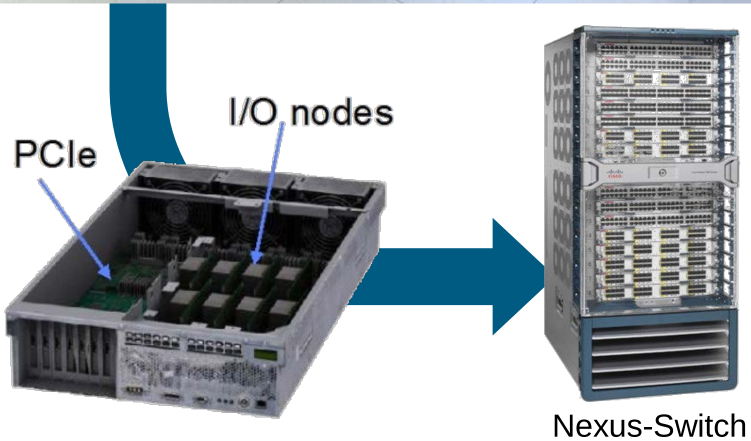
Overview

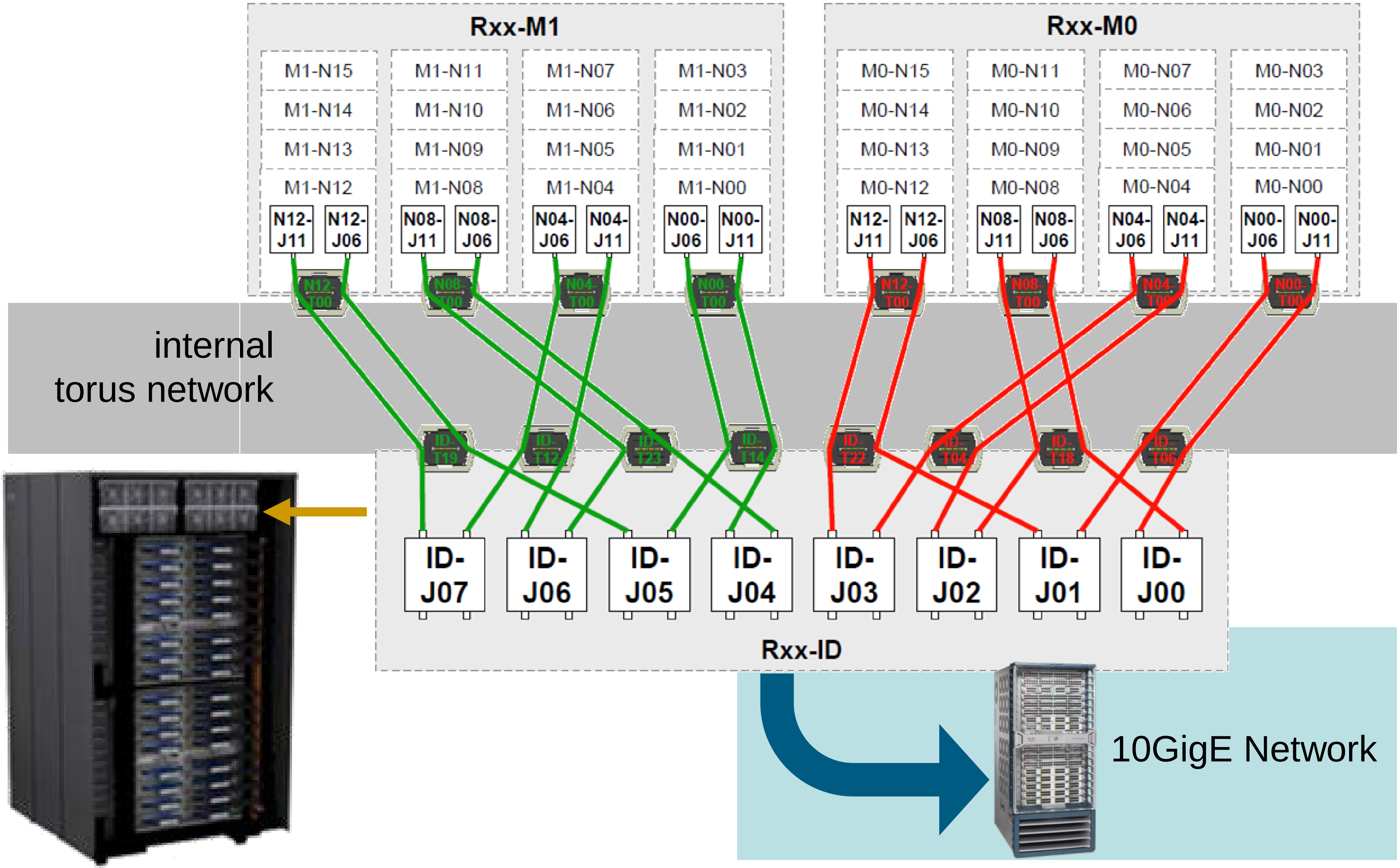
- Parallel I/O from different views
  - Hardware: Example: IBM BG/Q I/O infrastructure
  - System Software: IBM GPFS, I/O-forwarding
  - Application: Parallel I/O libraries
- Pitfalls
  - Small blocks, I/O to individual files, false sharing
  - Tasks per shared File, portability
- *SIONlib* Overview
- I/O characterization with *darshan*
- I/O strategies

IBM Blue Gene/Q (JUQUEEN) & I/O

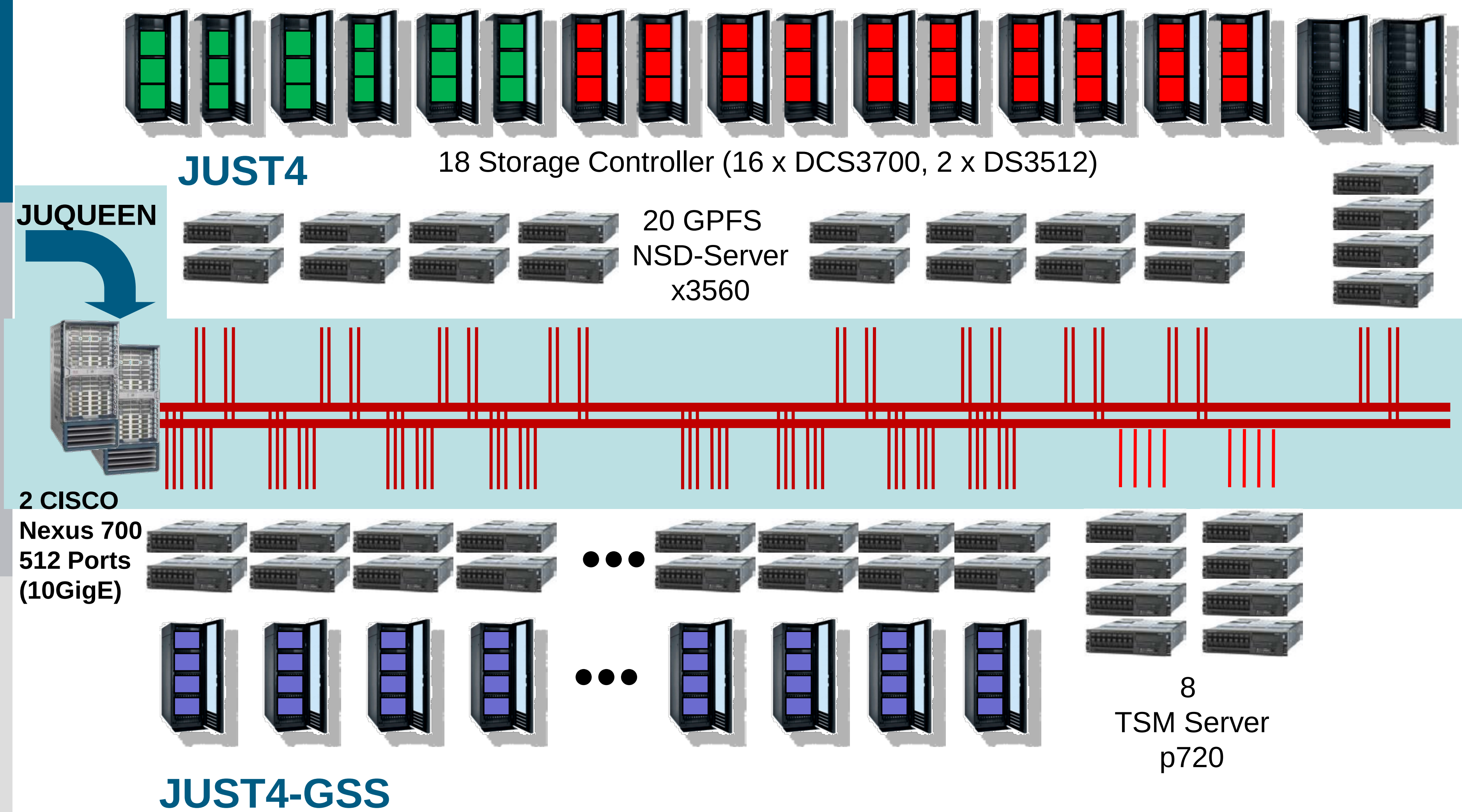
- IBM Blue Gene/Q JUQUEEN
- IBM PowerPC® A2 1.6 GHz,
  16 cores per node
  28 racks (7 rows à 4 racks)
  28,672 nodes (**458,752 cores**)
- 5D torus network
- 5.9 Pflop/s peak
  5.0 Pflop/s Linpack
- Main memory: **448 TB**
- **I/O Nodes**: **248** (27x8 + 1x32)
- **Network**: 2x CISCO Nexus 7018
  Switches (connect I/O-nodes)
  Total ports: **512 10 GigEthernet**



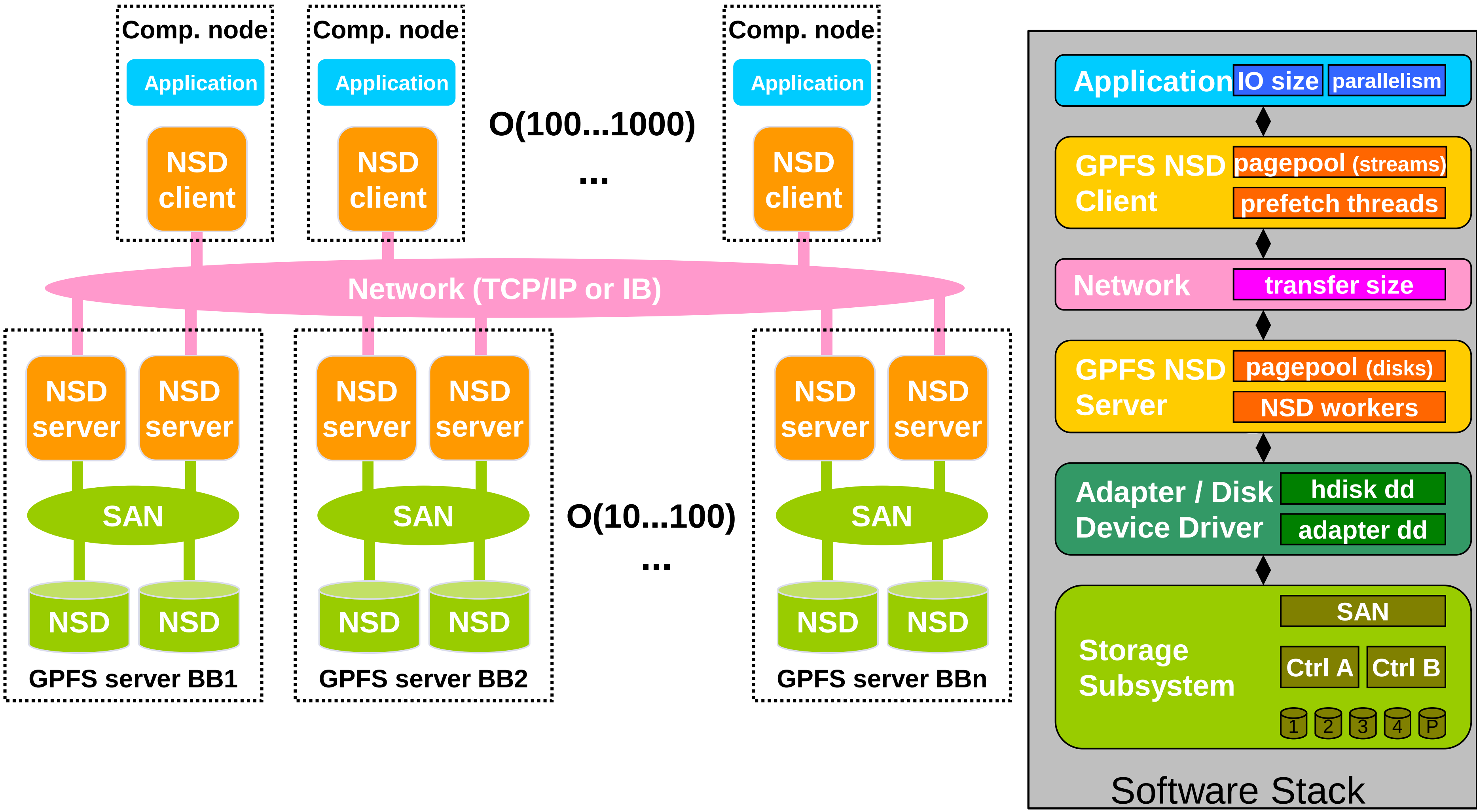
Blue Gene/Q: I/O-node cabling (8 ION/Rack)



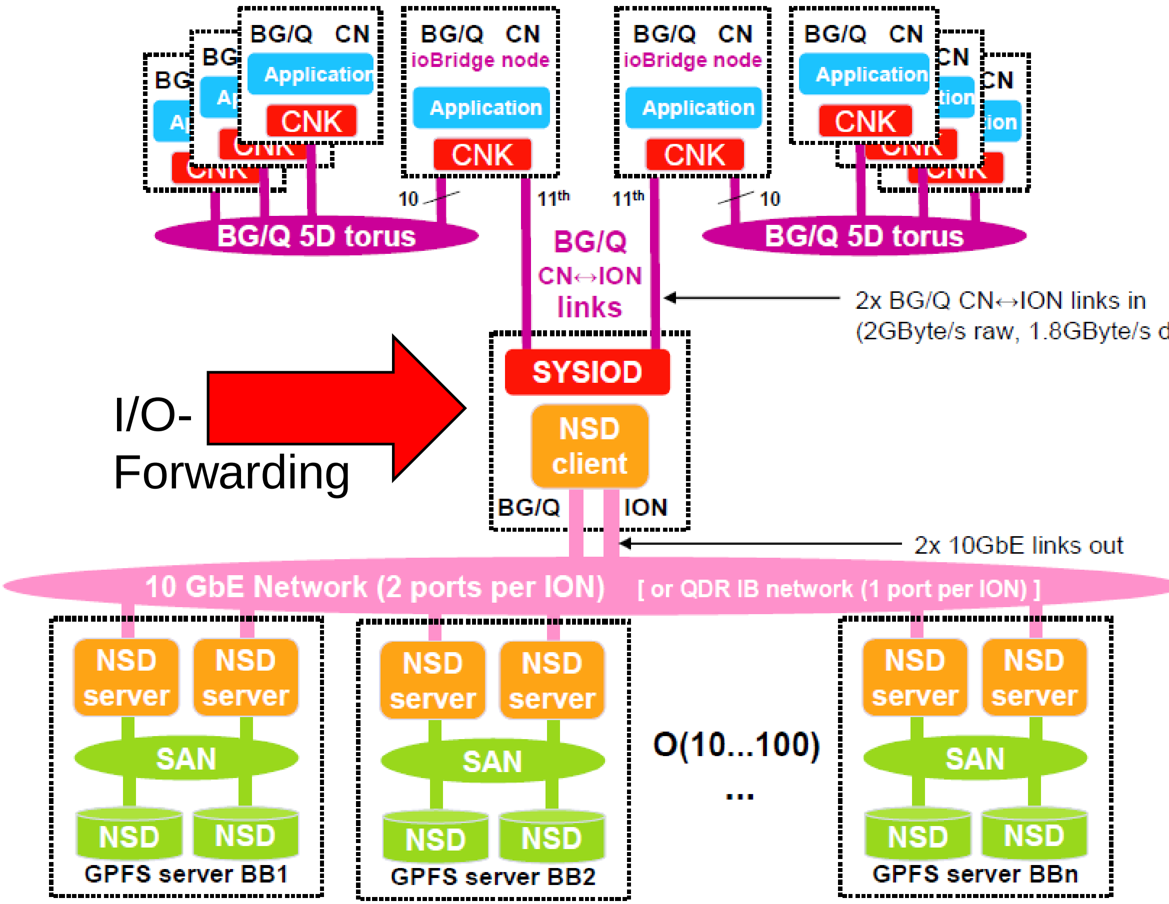
I/O-Network & File Server (JUST)

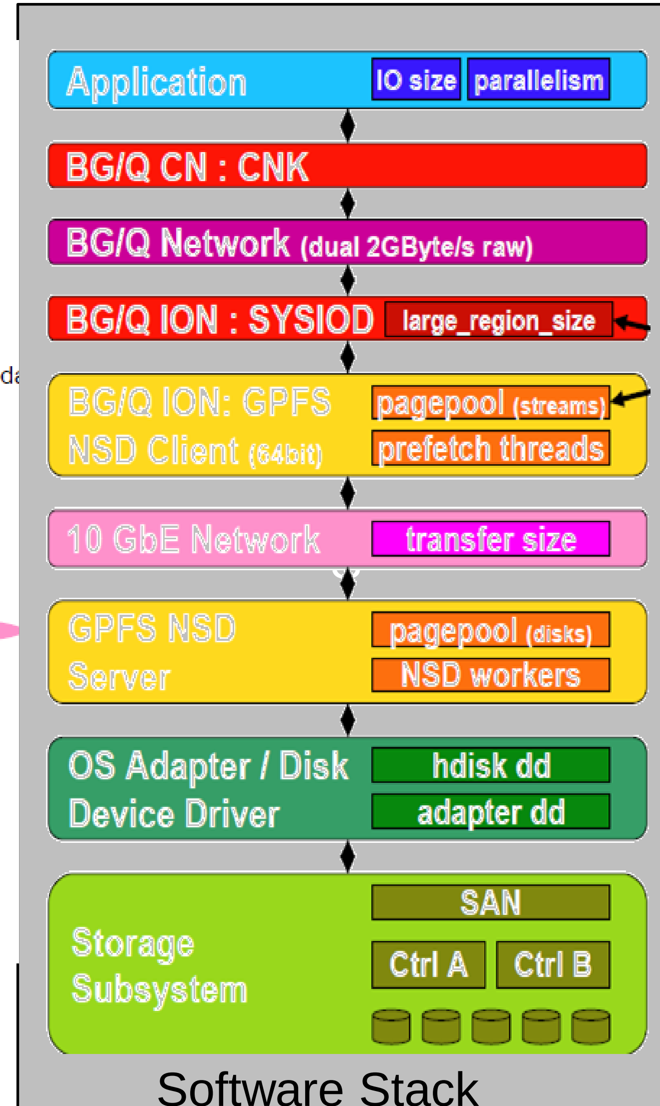


Software View to Parallel I/O:
… GPFS Architecture and I/O Data Path

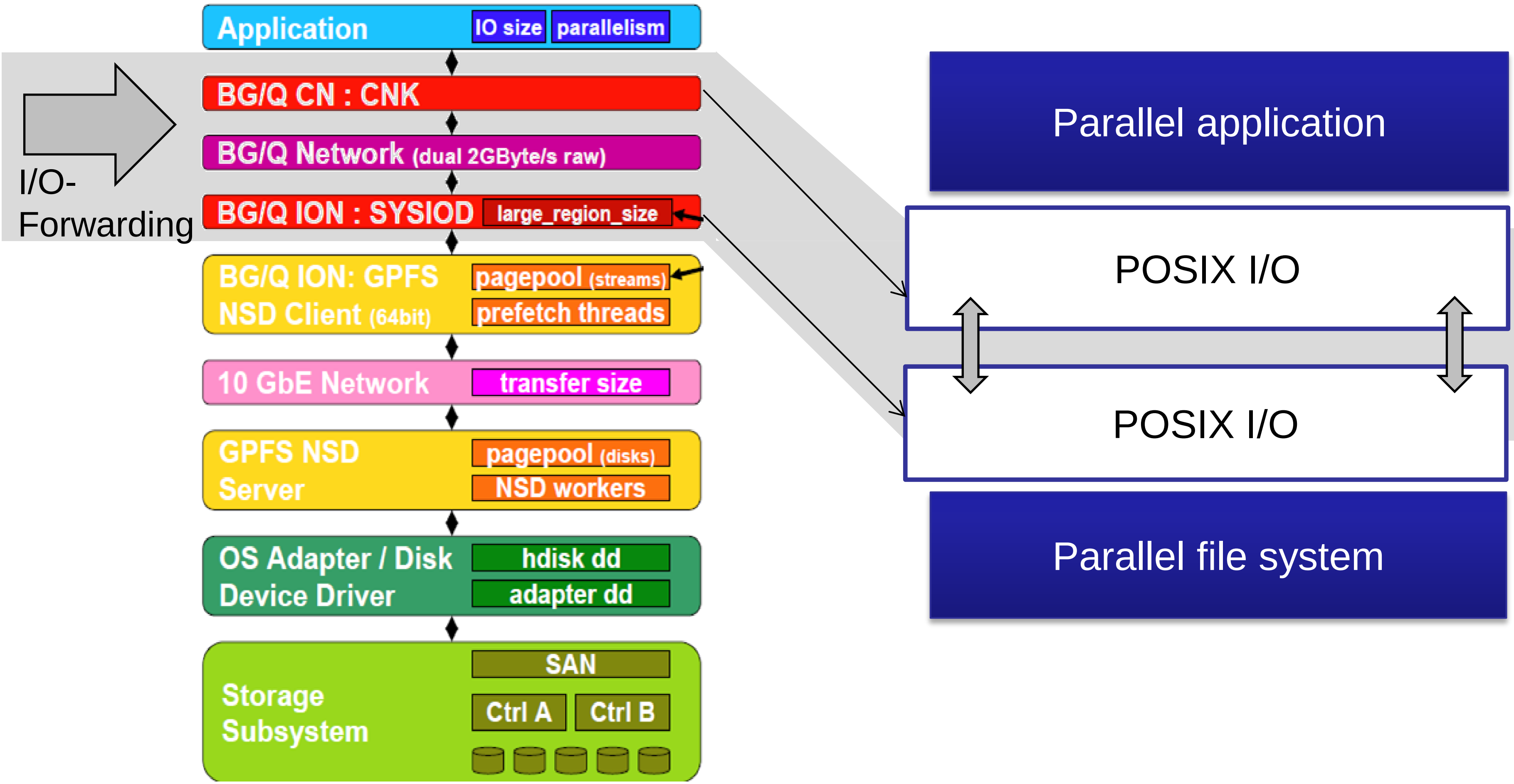


Software View to Parallel I/O: … GPFS on IBM Blue Gene/Q (I)

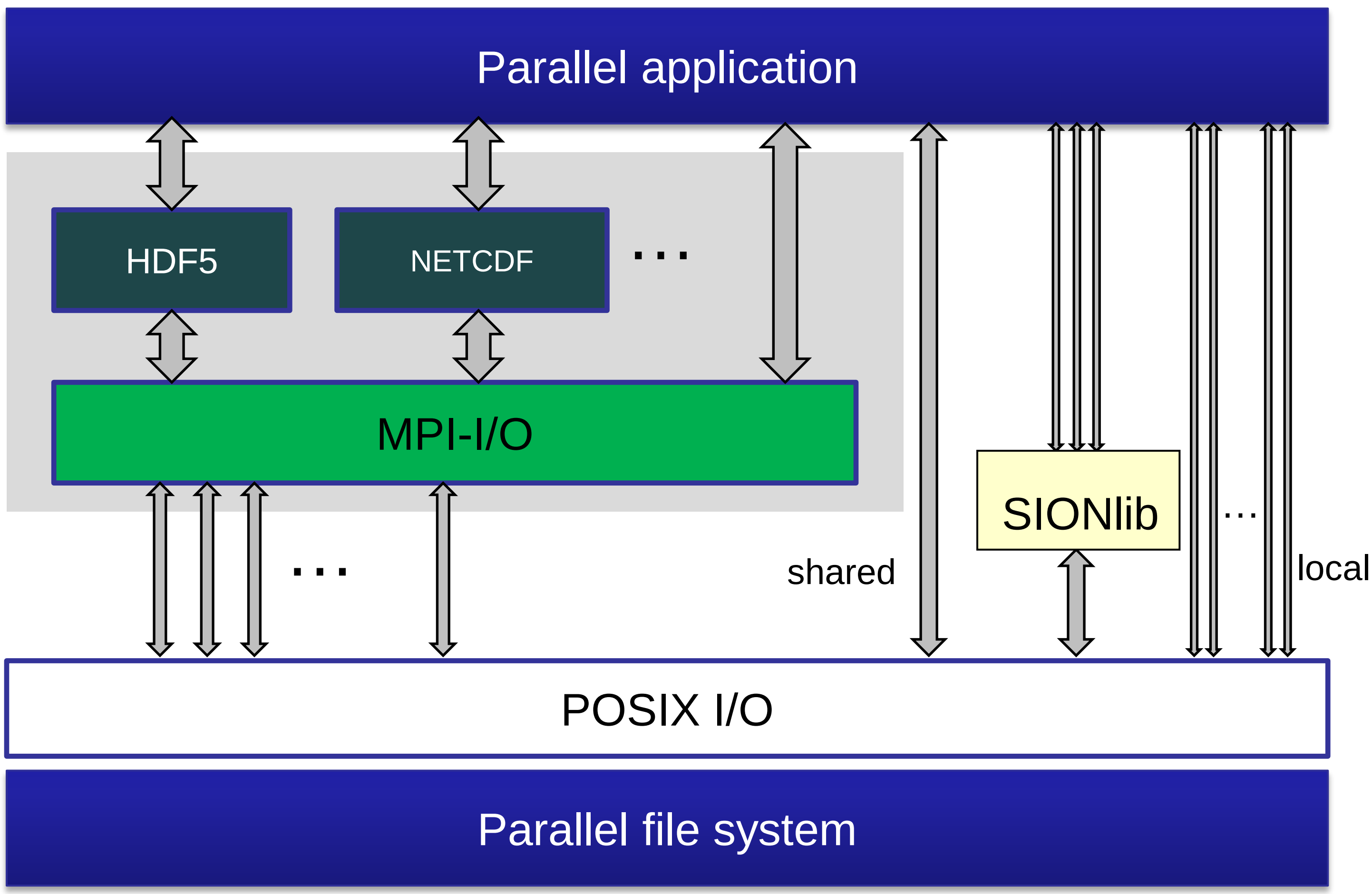




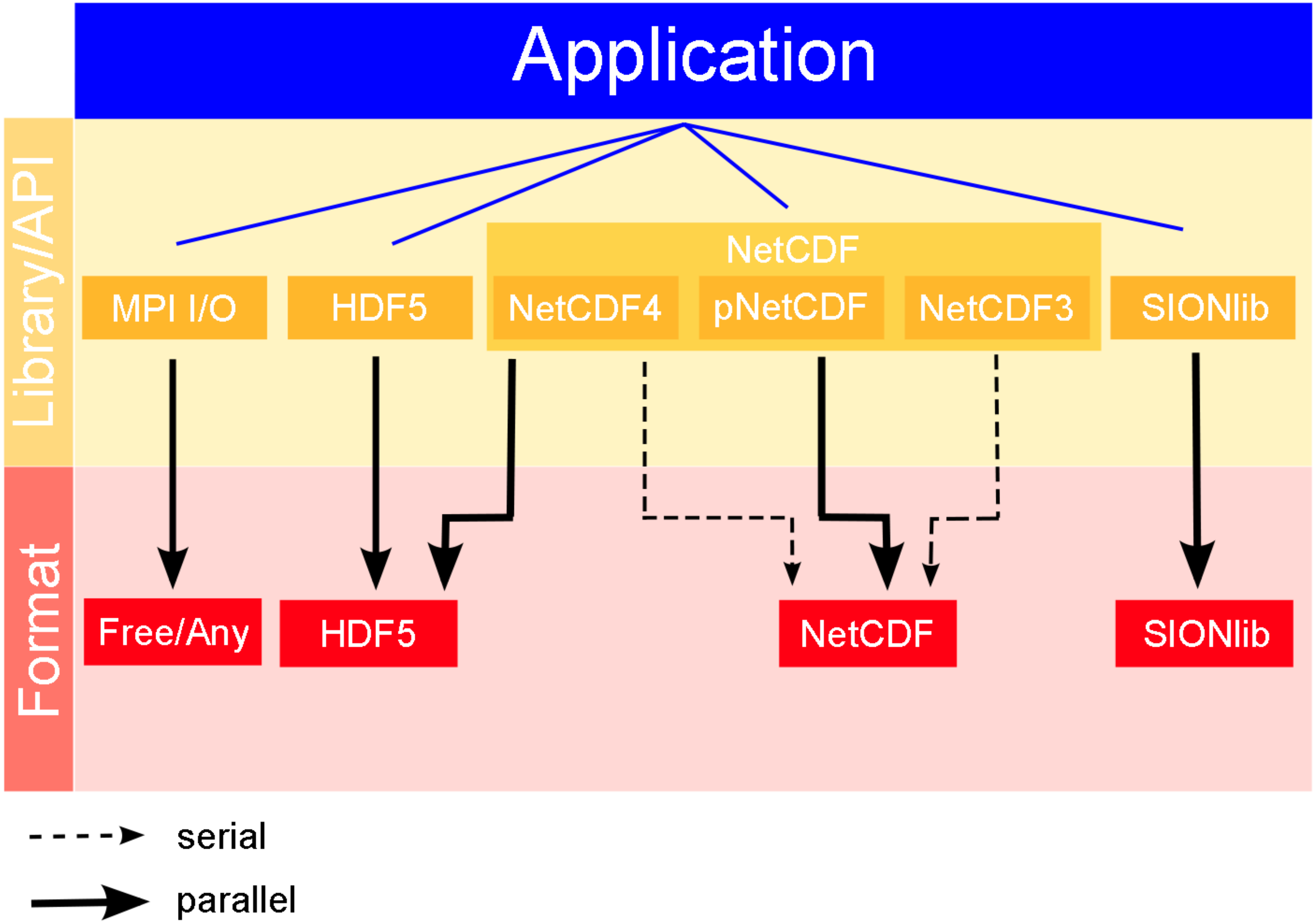
Software View to Parallel I/O: … GPFS on IBM Blue Gene/Q (II)



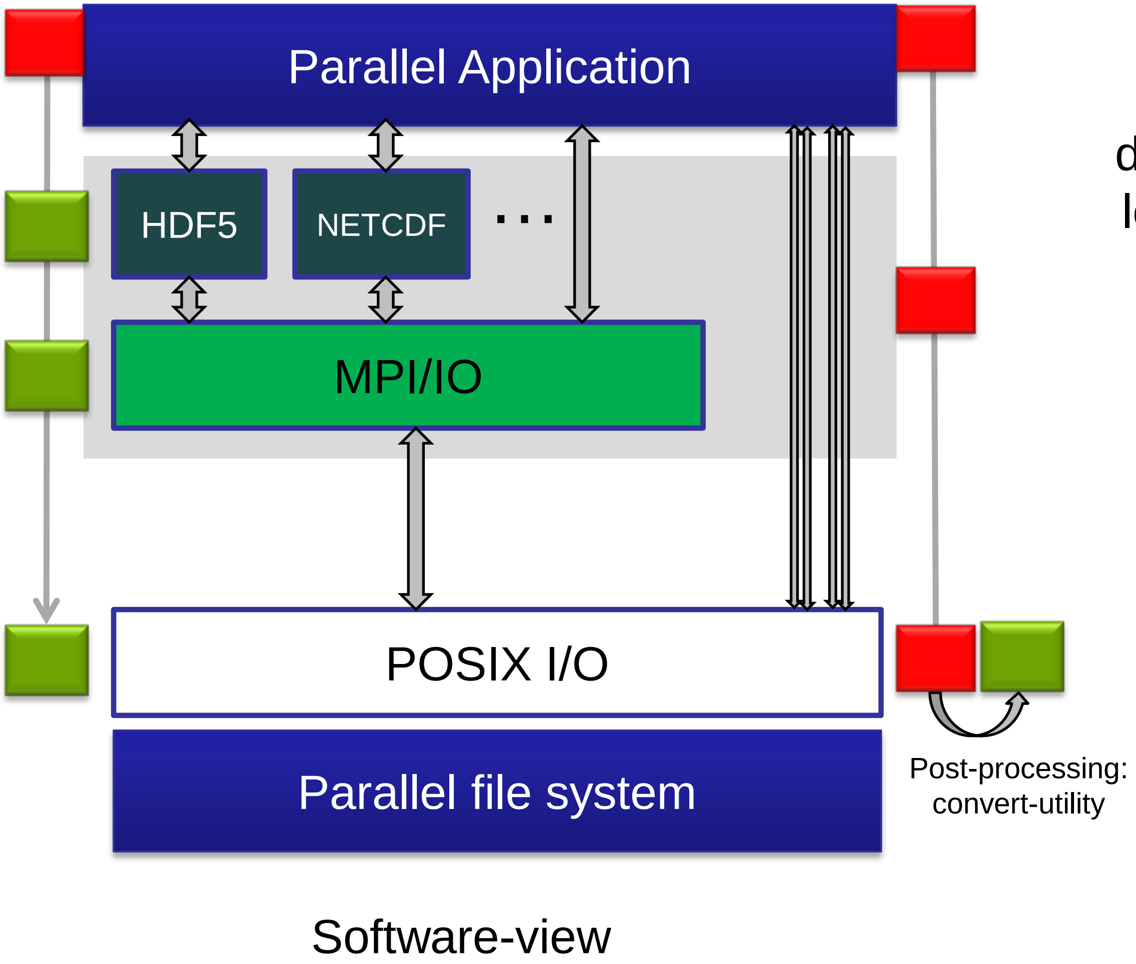
Application View to Parallel I/O

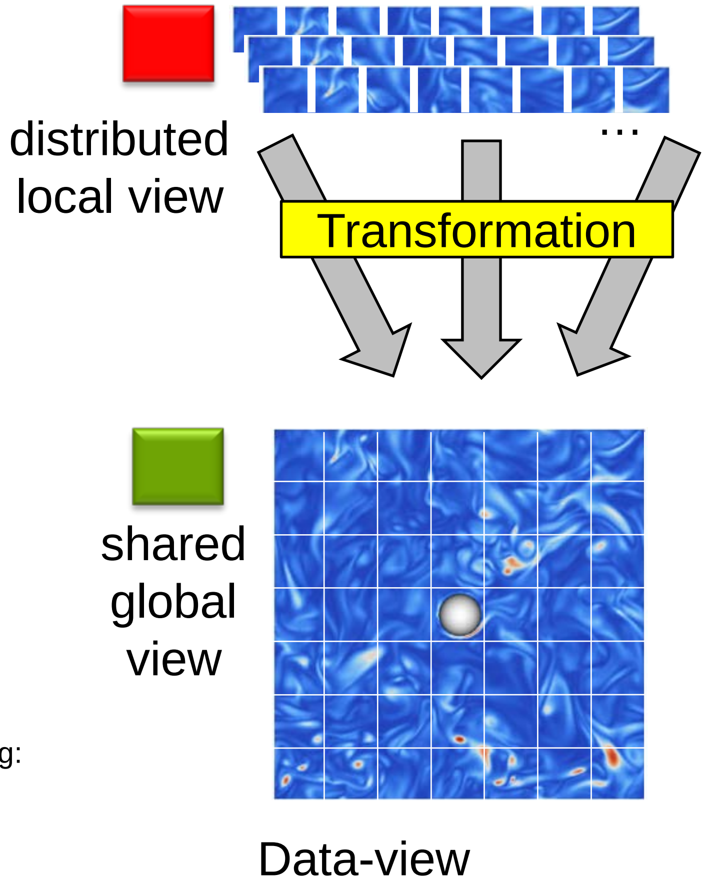


Application View: Data Formats



Application View: Data Distribution





Parallel Task-local I/O at Large Scale

Usage Fields:

- Check-point files, restart files
- Result files, post-processing
- Parallel Performance-Tools

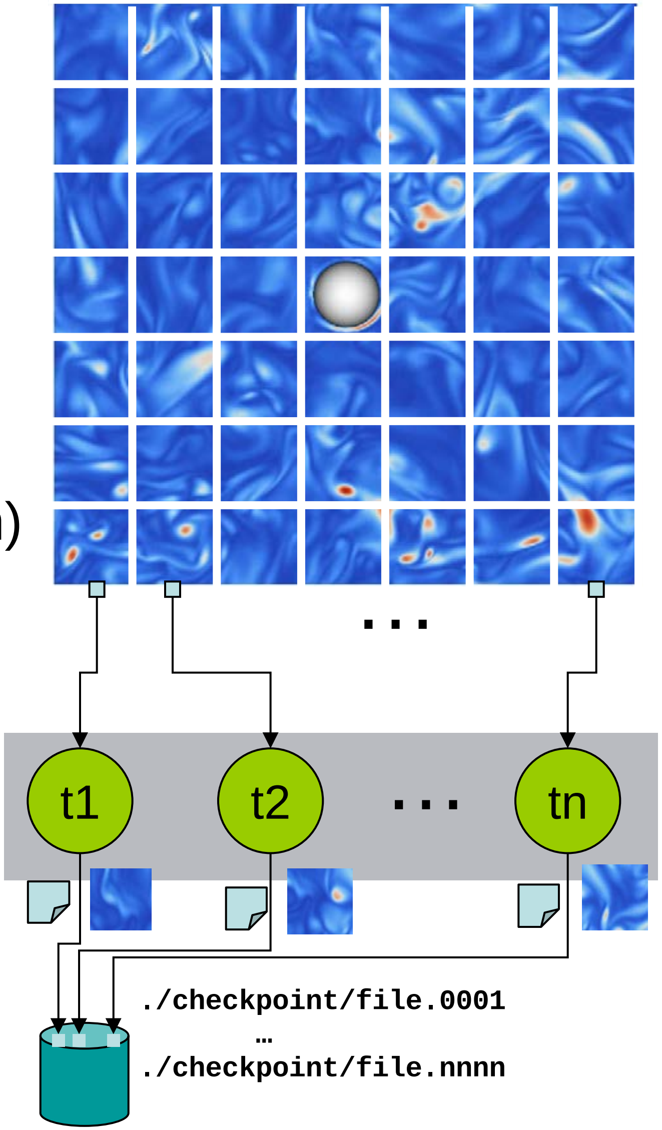
Data types:

- Simulation data (domain-decomposition)
- Trace data (parallel performance tools)

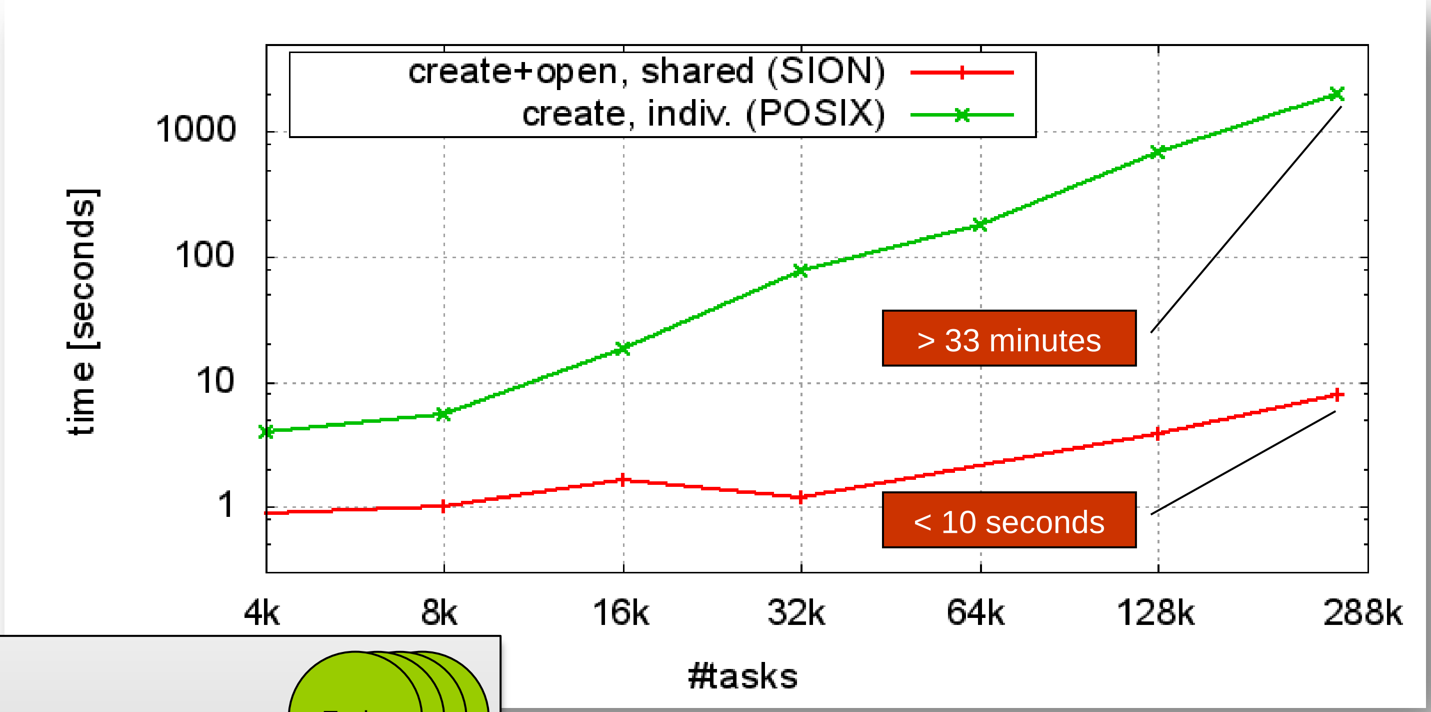
Bottlenecks:

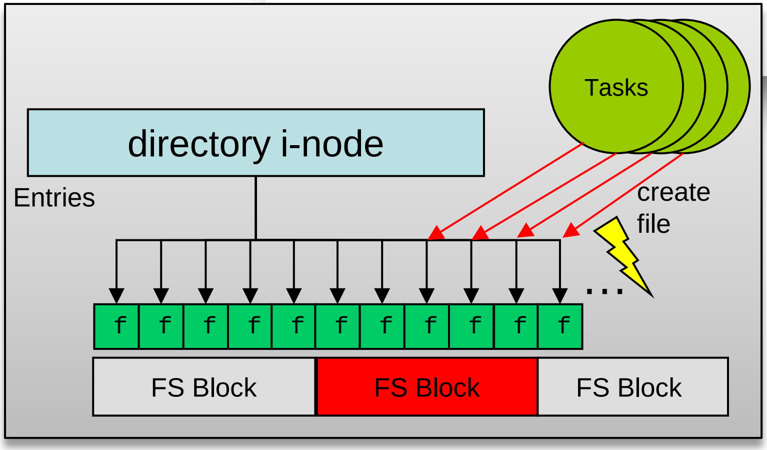
- File creation
- File management

→ #files: $O(10^5)$



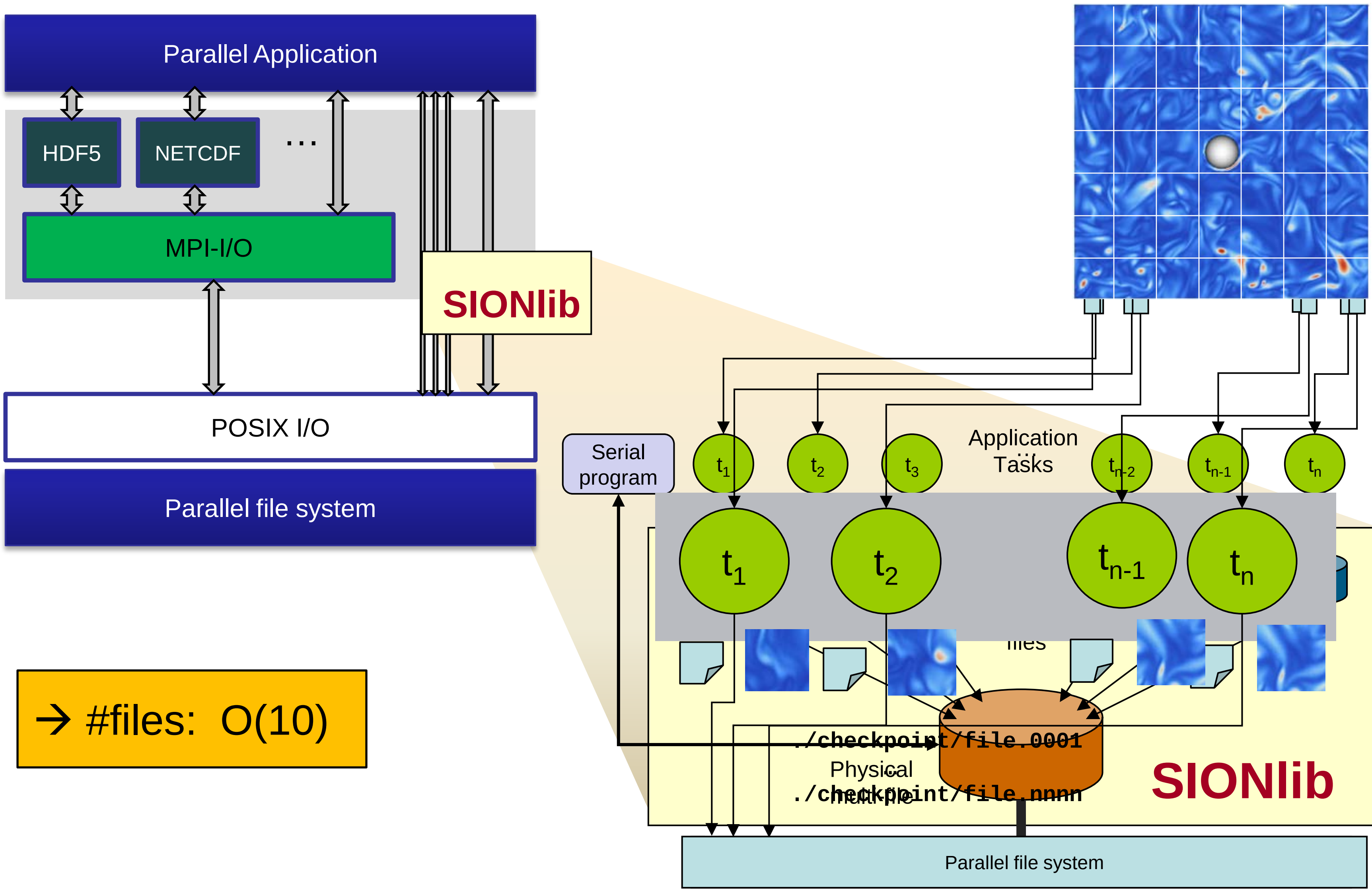
The Showstopper for Task-local I/O: … Parallel Creation of Individual Files





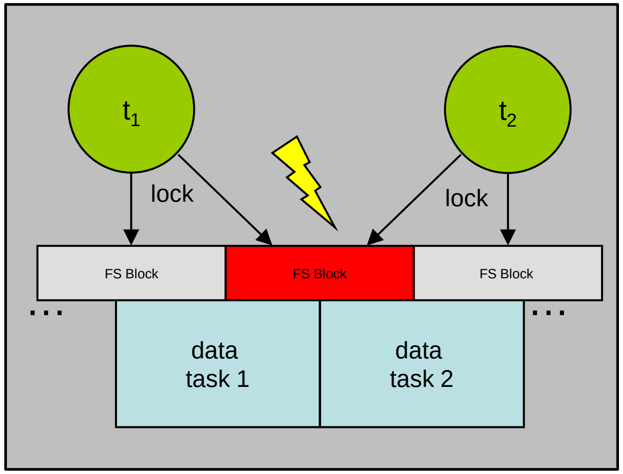
Jugene + GPFS: file create+open, one file per task versus one file per I/O-node

SIONlib: Shared Files for Task-local Data



→ #files: O(10)

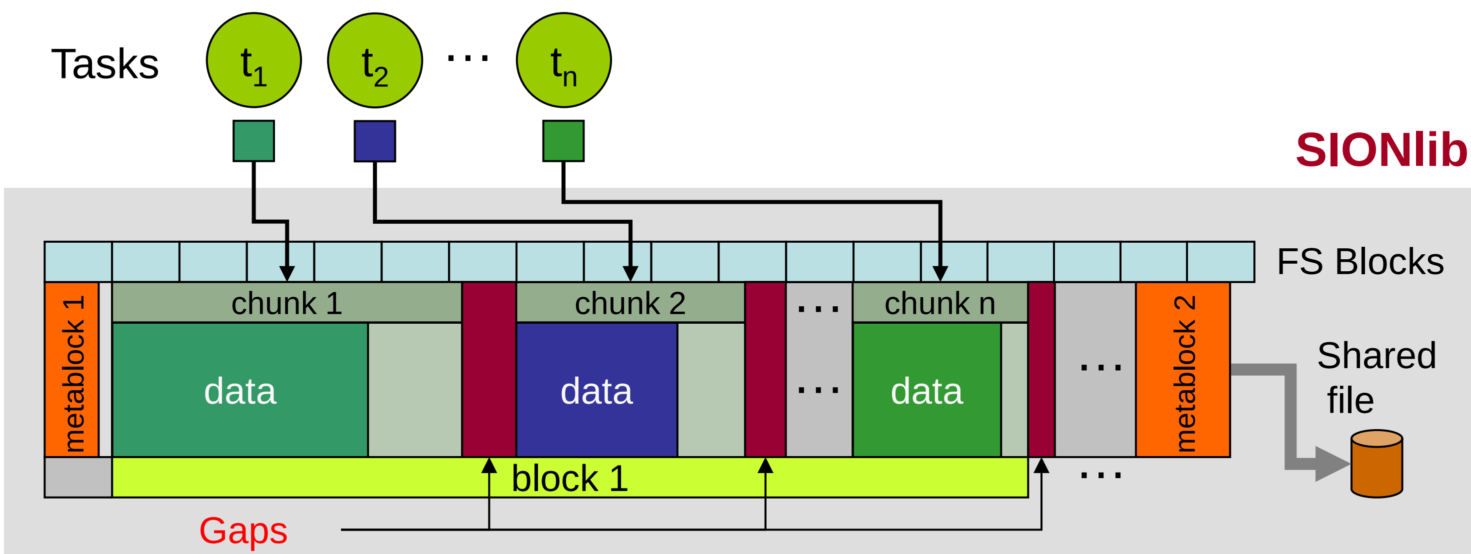
The Showstopper for Shared File I/O: … Concurrent Access & Contention



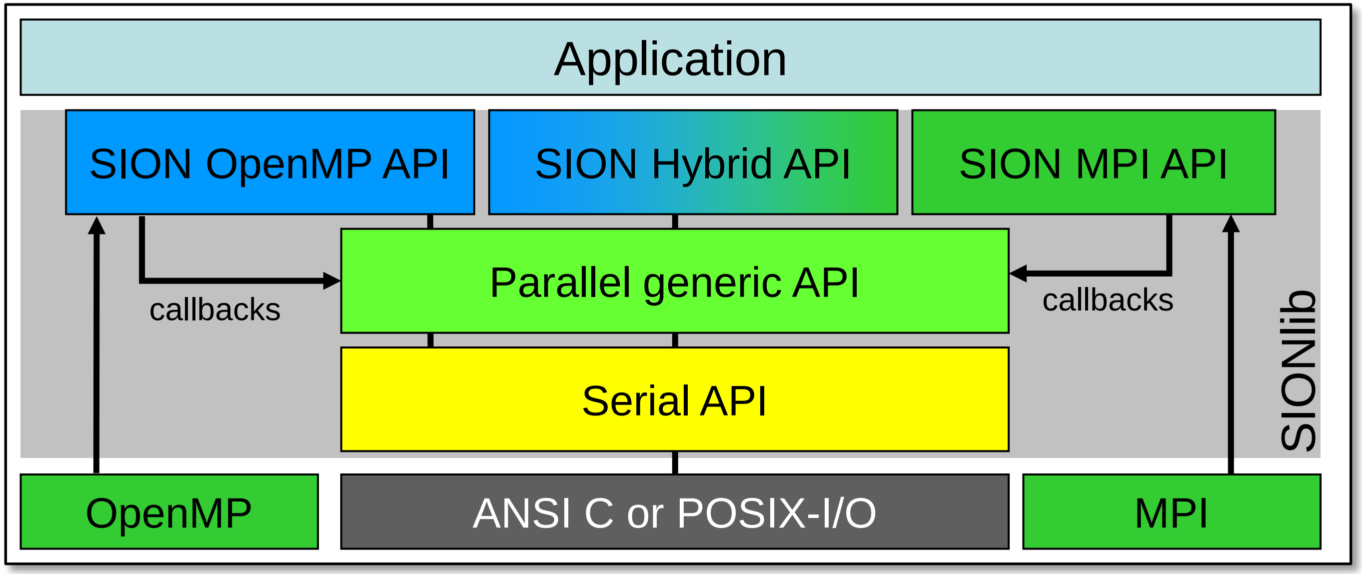
File System Block Locking → Serialization

SIONlib: Logical partitioning of Shared File:

- Dedicated data chunks per task
- Alignment to boundaries of file system blocks → no contention



SIONlib: Architecture & Example



- Extension of I/O-API (ANSI C or POSIX)
- C and Fortran bindings, implementation language C
- Current versions: 1.4p3
- Open source license: 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)
```

SIONlib in a NutShell:
... Task local I/O

```
/* Open */
sprintf(tmpfn, "%s.%06d",filename,my_nr);
fileptr=fopen(tmpfn, "bw", ...);

...
/* Write */
fwrite(bindata,1,nbytes,fileptr);
...

/* Close */
fclose(fileptr);
```

- Original ANSI C version
- no collective operation, no shared files
- data: stream of bytes

SIONlib in a NutShell:
… Add SIONlib calls

```
/* Collective Open */
nfiles=1;chunksize=nbytes;
sid=sion_paropen_mpi( filename, "bw", &nfiles ,
                      &chunksize , MPI_COMM_WORLD,
                      &lcomm , &fileptr , ...);
...
/* Write */
fwrite(bindata,1,nbytes,fileptr);
...
/* Collective Close */
sion_parclose_mpi(sid);
```

- Collective (SIONlib) open and close
- Ready to run ...
- Parallel I/O to one shared file

SIONlib in a NutShell:
… Variable Data Size

```
/* Collective Open */
nfiles=1;chunksize=nbytes;
sid=sion_paropen_mpi( filename, "bw", &nfiles ,
                      &chunksize , MPI_COMM_WORLD,
                      &lcomm , &fileptr , ...);
...
/* Write */
if(sion_ensure_free_space(sid, nbytes)) {
   fwrite(bindata,1,nbytes,fileptr);
}
...
/* Collective Close */
sion_parclose_mpi(sid);
```

- Writing more data as defined at open call
- SIONlib moves forward to next chunk, if data to large for current block

SIONlib in a NutShell:
… Wrapper function

```
/* Collective Open */
nfiles=1;chunksize=nbytes;
sid=sion_paropen_mpi( filename, "bw", &nfiles ,
                      &chunksize , MPI_COMM_WORLD,
                      &lcomm , &fileptr , ...);
...

/* Write */
sion_fwrite(bindata,1,nbytes,sid);

...
/* Collective Close */
sion_parclose_mpi(sid);
```

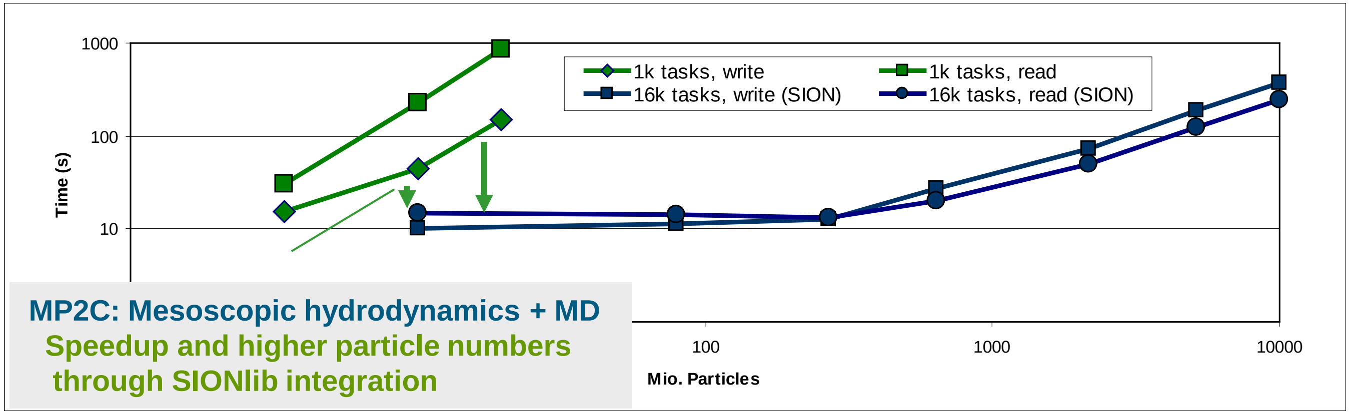
- Includes check for space in current chunk
- Parameter of fwrite: fileptr → sid

SIONlib: Applications

- ## Applications

DUNE-ISTL **(**Multigrid solver, Univ. Heidelberg) **ITM** (Fusion-community),
LBM (Fluid flow/mass transport, Univ. Marburg), **PSC** (particle-in-cell code),
OSIRIS (Fully-explicit particle-in-cell code), **PEPC** (Pretty Efficient Parallel C. Solver)
Profasi: (Protein folding and aggr. simulator) **NEST** (Human Brain Simulation)

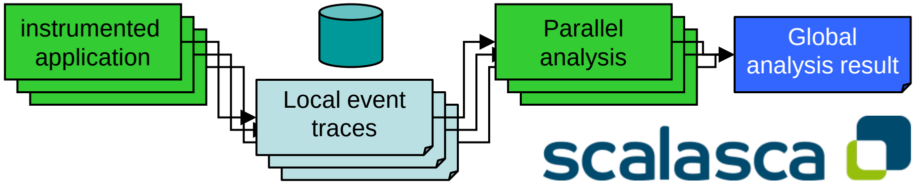
MP2C:



MP2C: Mesoscopic hydrodynamics + MD
Speedup and higher particle numbers through SIONlib integration

- ## Tools/Projects

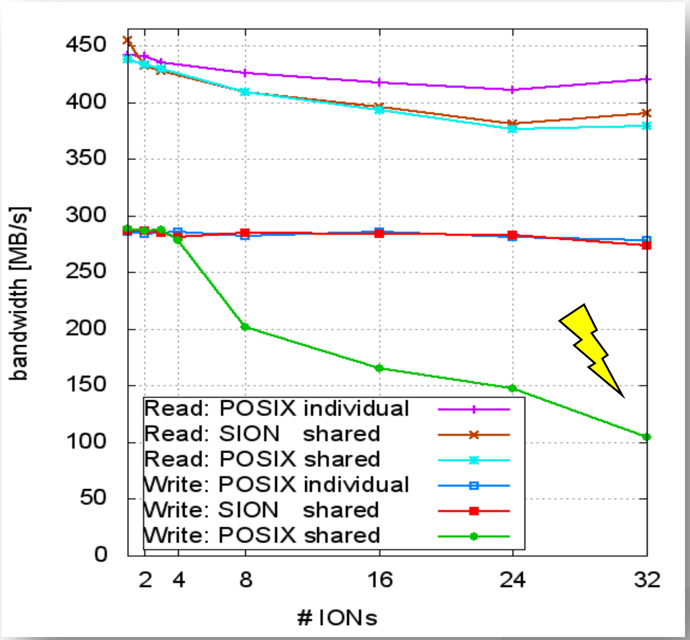
Scalasca: Performance Analysis



Score-P: Scalable Performance Measurement Infrastructure for Parallel Codes

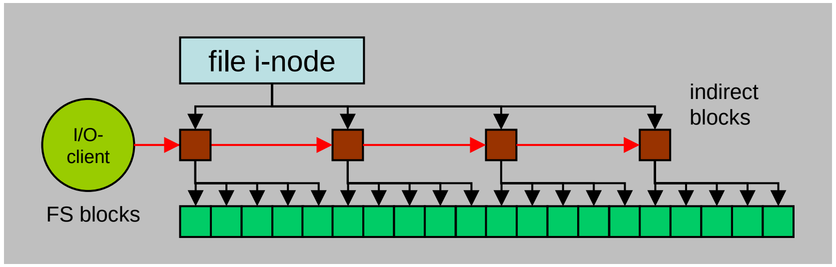
DEEP-ER: Adaption to new platform and parallelization paradigm

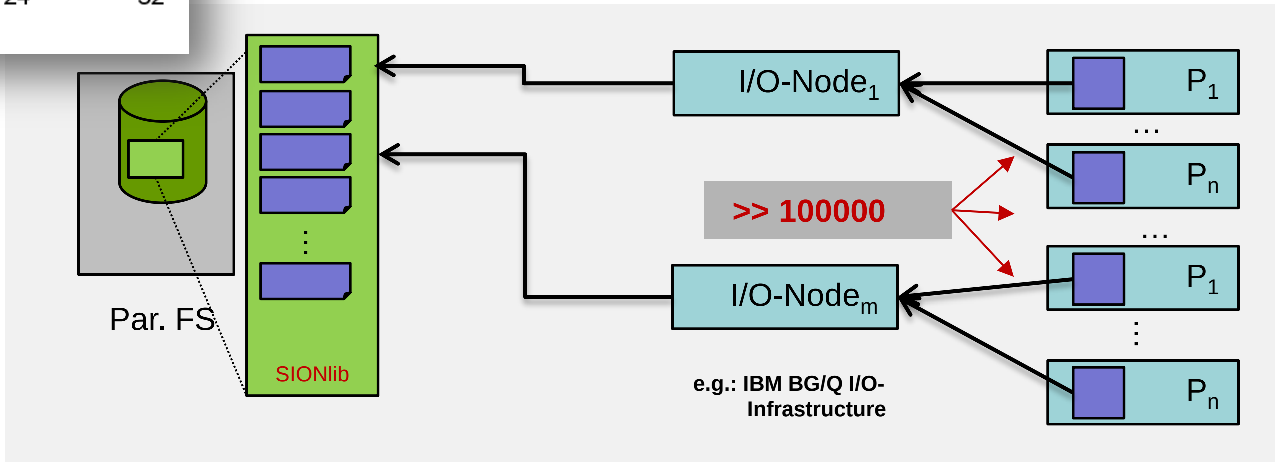
Are there more Bottlenecks?
… Increasing #tasks further …



JUGENE: Bandwidth per ION, comparison individual files (POSIX), one file per ION (SION) and one shared file (POSIX)

- Bottleneck: file meta data management
- by first GPFS client which opened the file



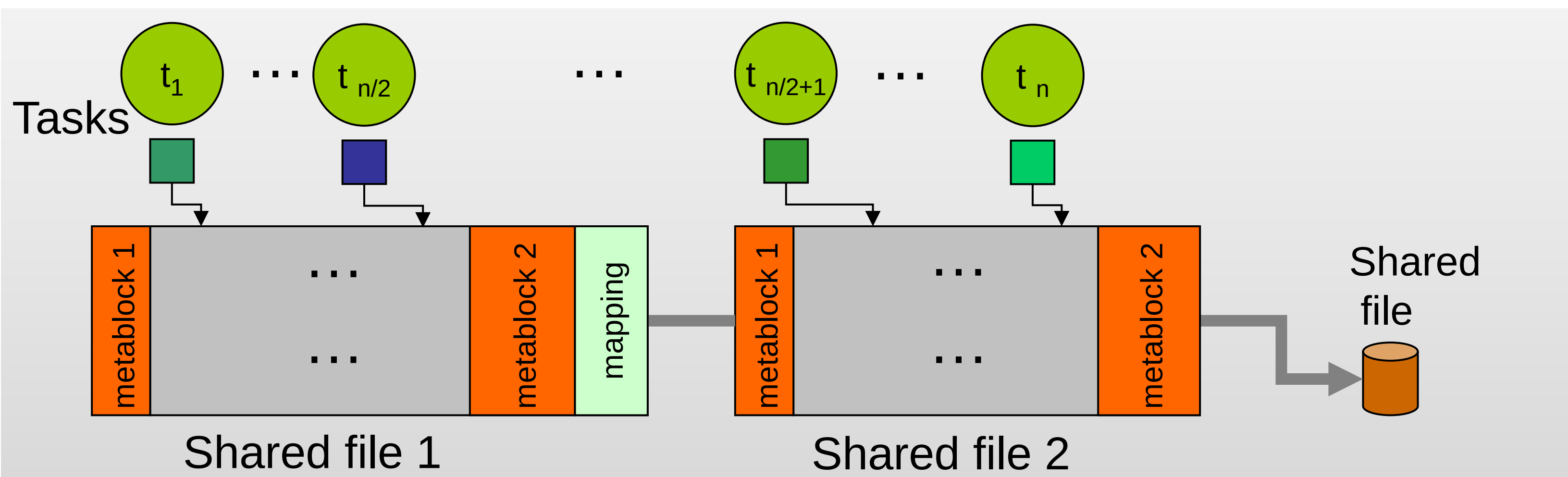


SIONlib: Multiple Underlying Physical Files

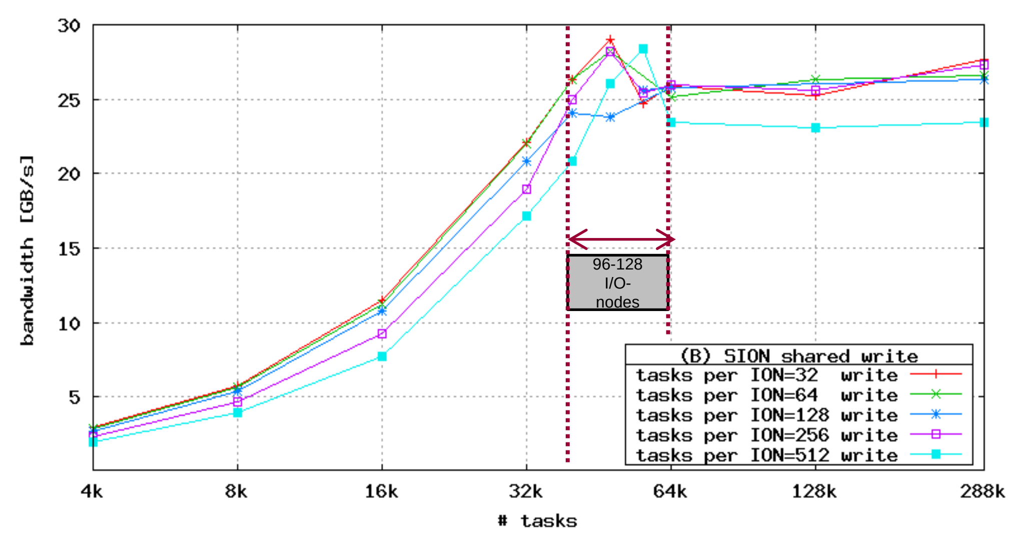
- Parallelization of file meta data handling using multiple physical files
- Mapping: Files : Tasks

1 : n ← **p : n** → n : n

→ IBM Blue Gene: One file per I/O-node (locality)



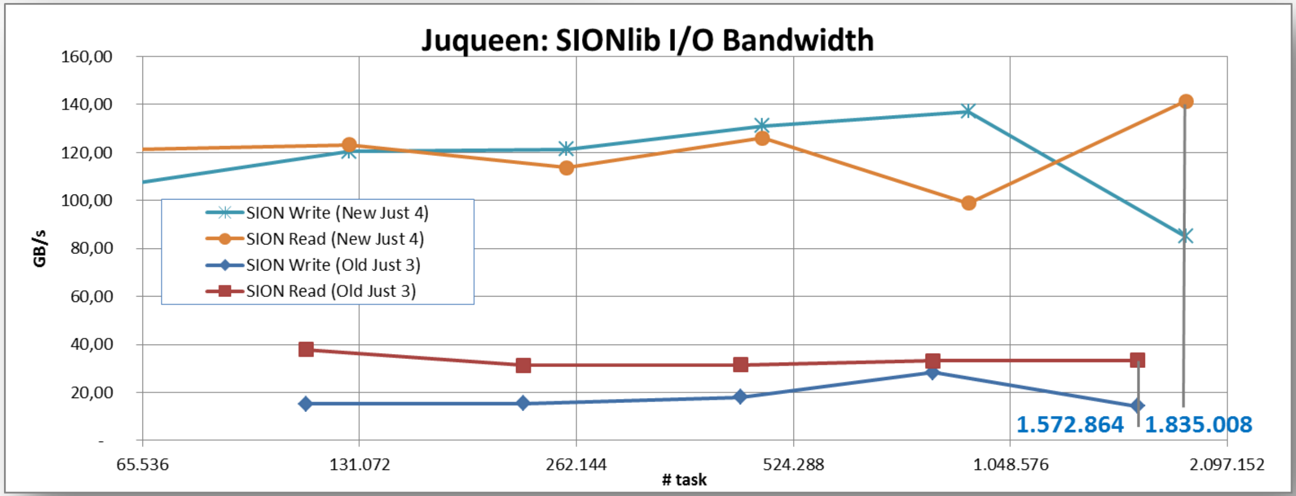
SIONlib: Scaling to Large # of Tasks



JUGENE: *Total bandwidth (write), one file per I/O-node (ION), varying the number of tasks doing the I/O*

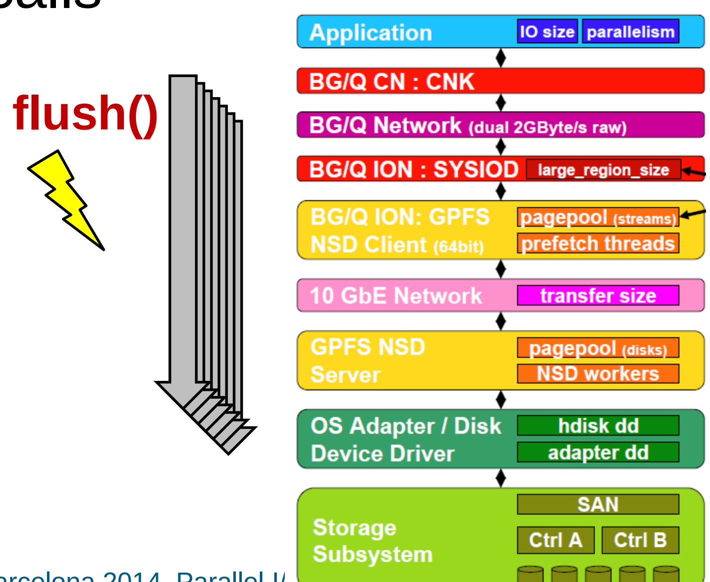
Preliminary Tests on JUQUEEN up to **1.8 Mio Tasks**

JUQUEEN: *Total bandwidth (write/read) , one file per I/O-bridge (IOB)*
Old (Just3) vs. New (Just4) GPFS file system



Other Pitfalls: 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



Other Pitfalls: 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**

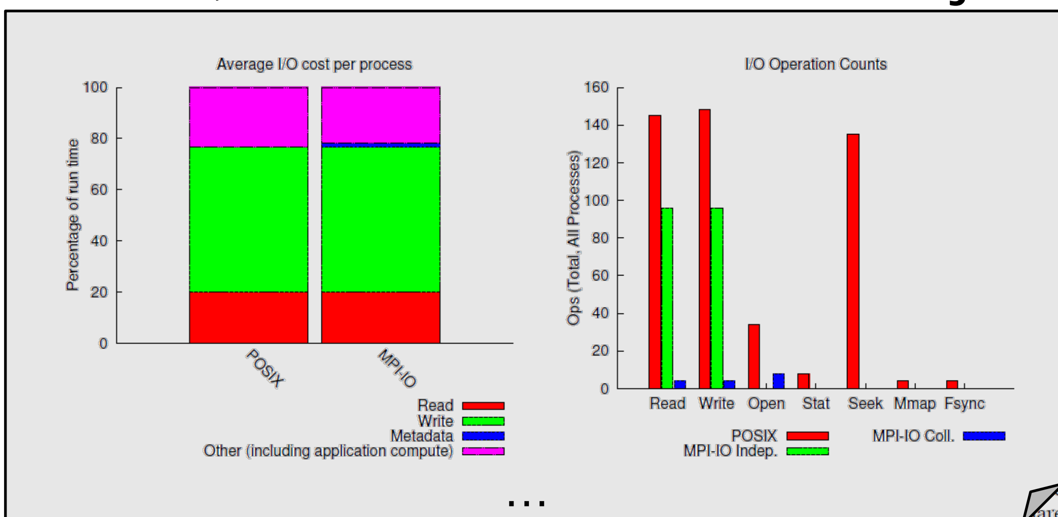
- Conversion of files might be necessary and expensive
- Solution: Choosing a portable data format (HDF5, NetCDF)

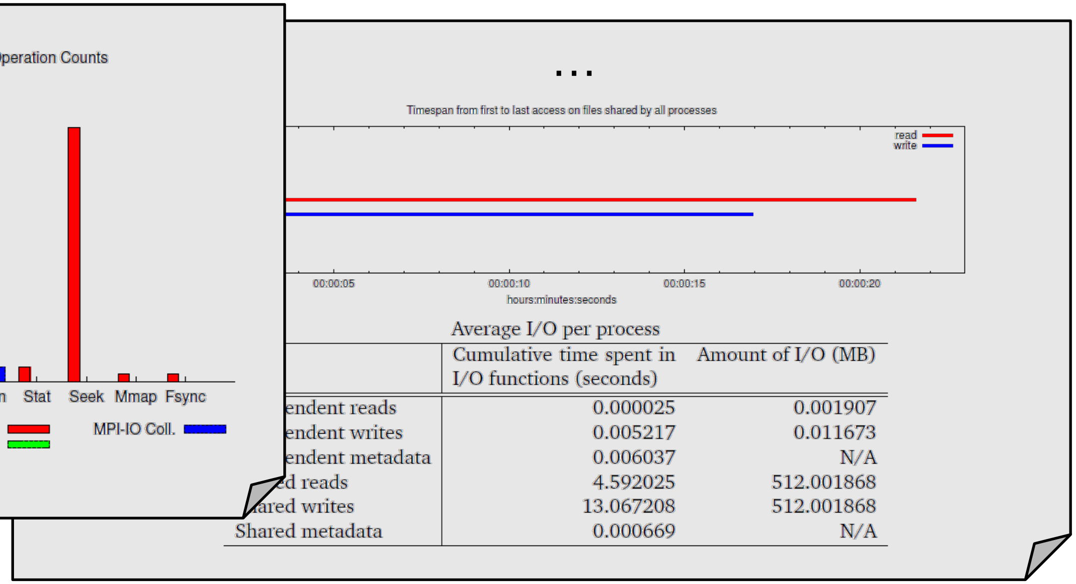
Darshan – I/O Characterization

- Darshan: Scalable HPC I/O characterization tool (ANL)
  - http://www.mcs.anl.gov/darshan (version 2.2.8)
- Profiling of I/O-Calls (POSIX, MPI-I/O, …) during runtime
- Instrumentation
  - *dynamic linked* binaries: **`LD_PRELOAD=<<path>libdarshan.so>`**
  - *static binaries*: Wrapper for compiler-calls for *static binaries*
- *Log-files:* ***`<uid><binname><jobid><ts>.darshan.gz`***
  - *Path: set by environment variable DARSHANLOGDIR*
    e.g. ***`mpirun … -x DARSHANLOGDIR=$HOME/darshanlog`***
- Reports: PDF-file or text files
  - *Extract information:*
    `darshan-parser <logfile>  > ~/job-characterization.txt`
  - *Generate PDF-report from logfile:*
    `darshan-job-summary.pl  <logfile>` → *PDF-file*

Darshan on MareNostrum-III

- Installation directory: **`DARSHANDIR=/gpfs/projects/nct00/nct00001/\`**
  `UNITE/packages/darshan/2.2.8-intel-openmpi`
- Program start: **`mpirun -x DARSHANLOGDIR=${HOME}/darshanlog \`**
  `-x LD_PRELOAD=${DARSHANDIR/lib/libdarshan.so…`
- Parser: ***`$DARSHANDIR/bin/darshan-parser <logfile>`***
  Output format: see documentation
  http://www.mcs.anl.gov/research/projects/darshan/docs/darshan-util.html
- Generate PDF-report: → on local system (needs pdflatex)
  `$LOCALDARSHANDIR/bin/darshan-job-summary.pl <logfile>`

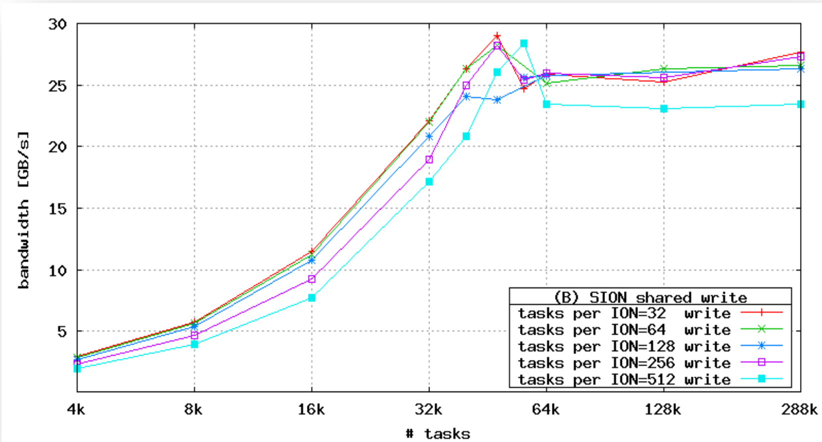


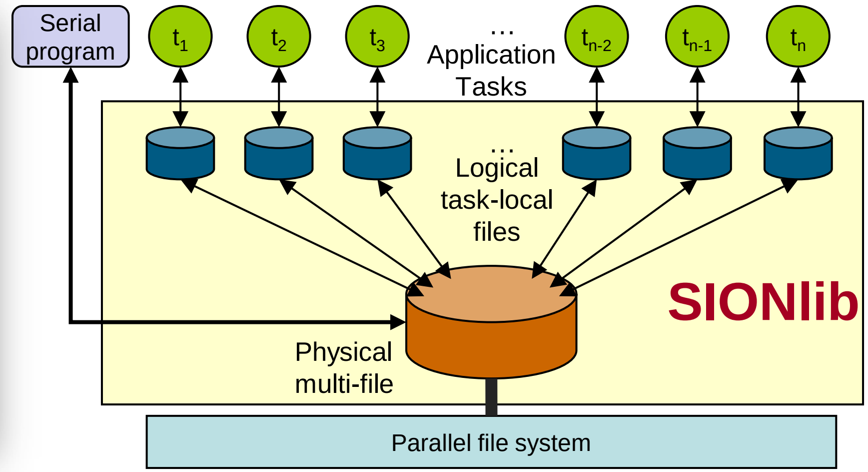


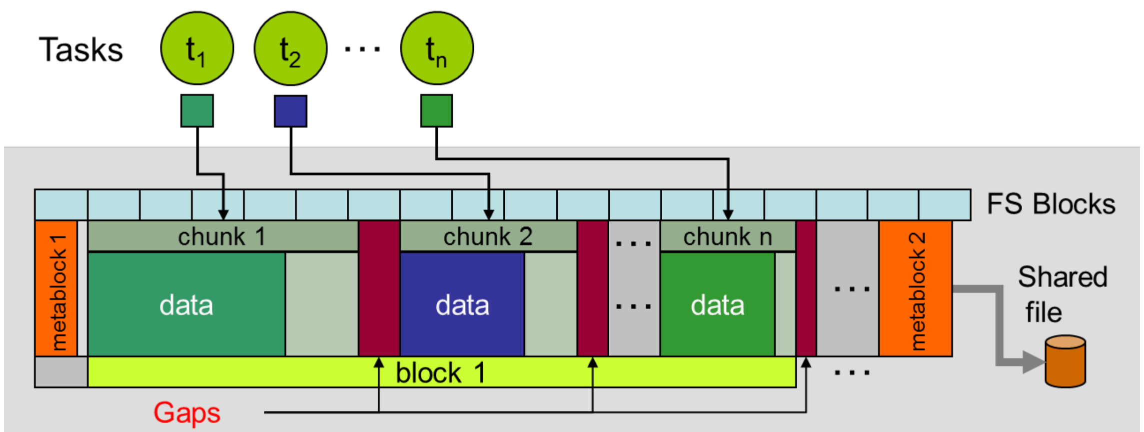
How to choose an I/O strategy?

- 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, …*

Questions ?







Thank You !