



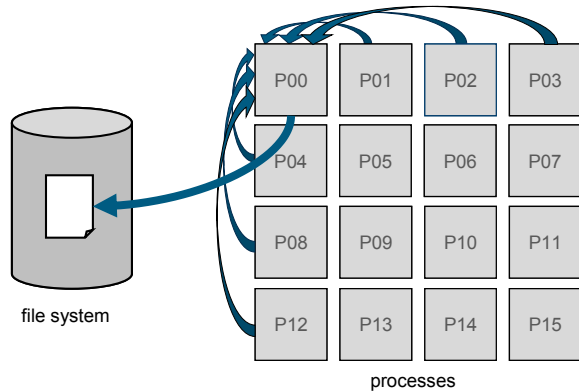
PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE



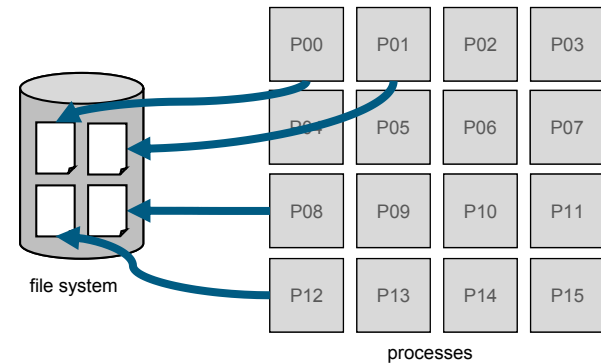
SCALABLE I/O FOR PARALLEL ACCESS TO TASK-LOCAL FILES WITH SIONLIB

23.03.2018 | SEBASTIAN LÜHRS
JÜLICH SUPERCOMPUTING CENTRE

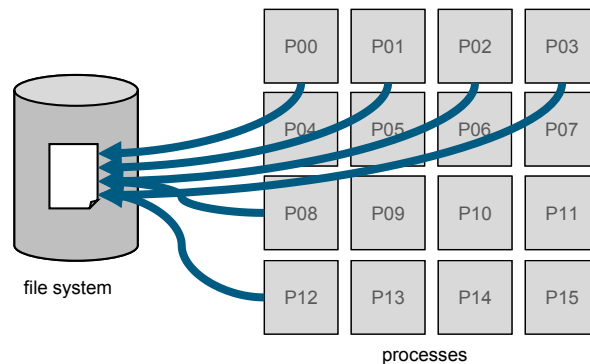
PARALLEL I/O STRATEGIES



One process performs I/O

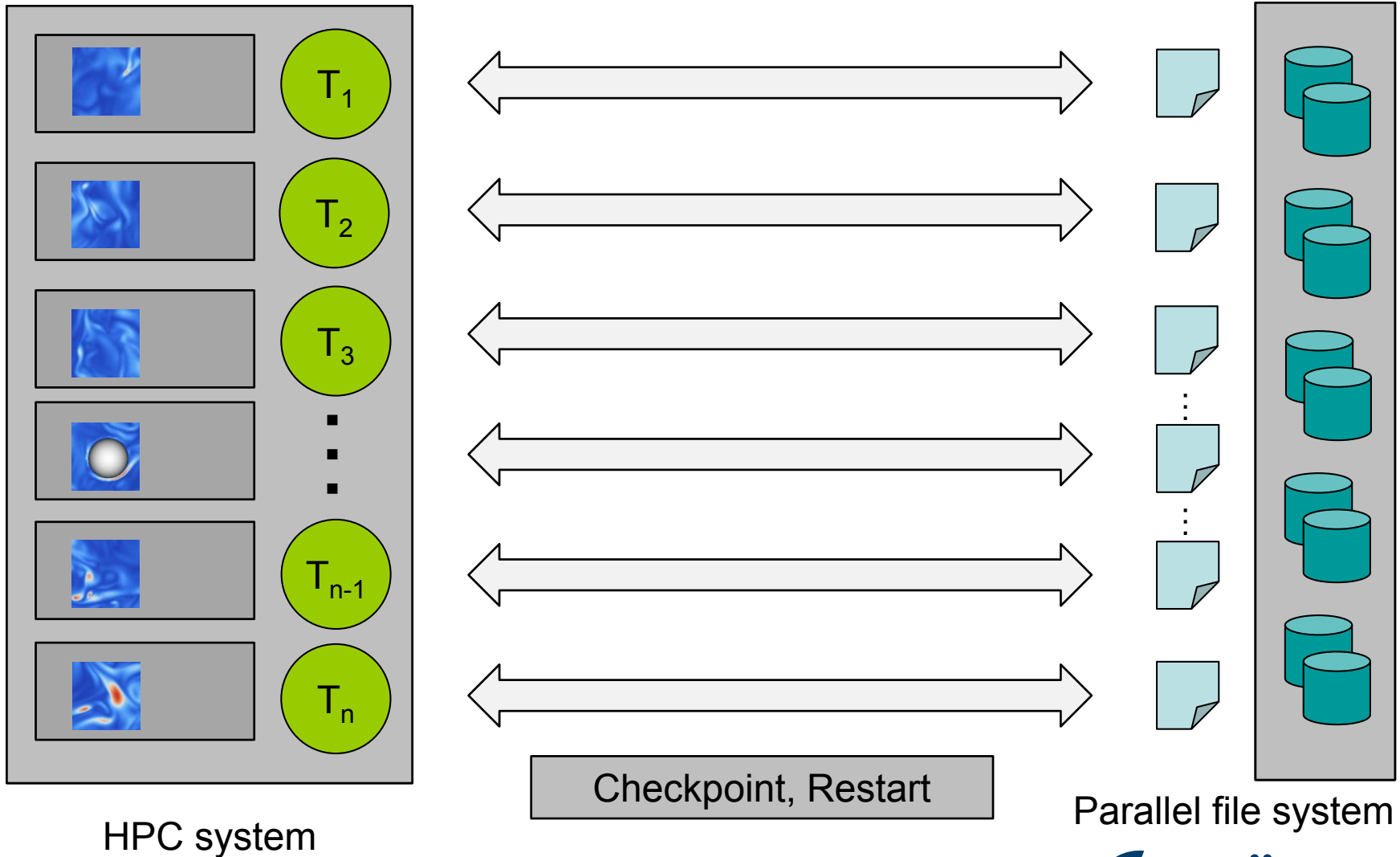


Task-local files

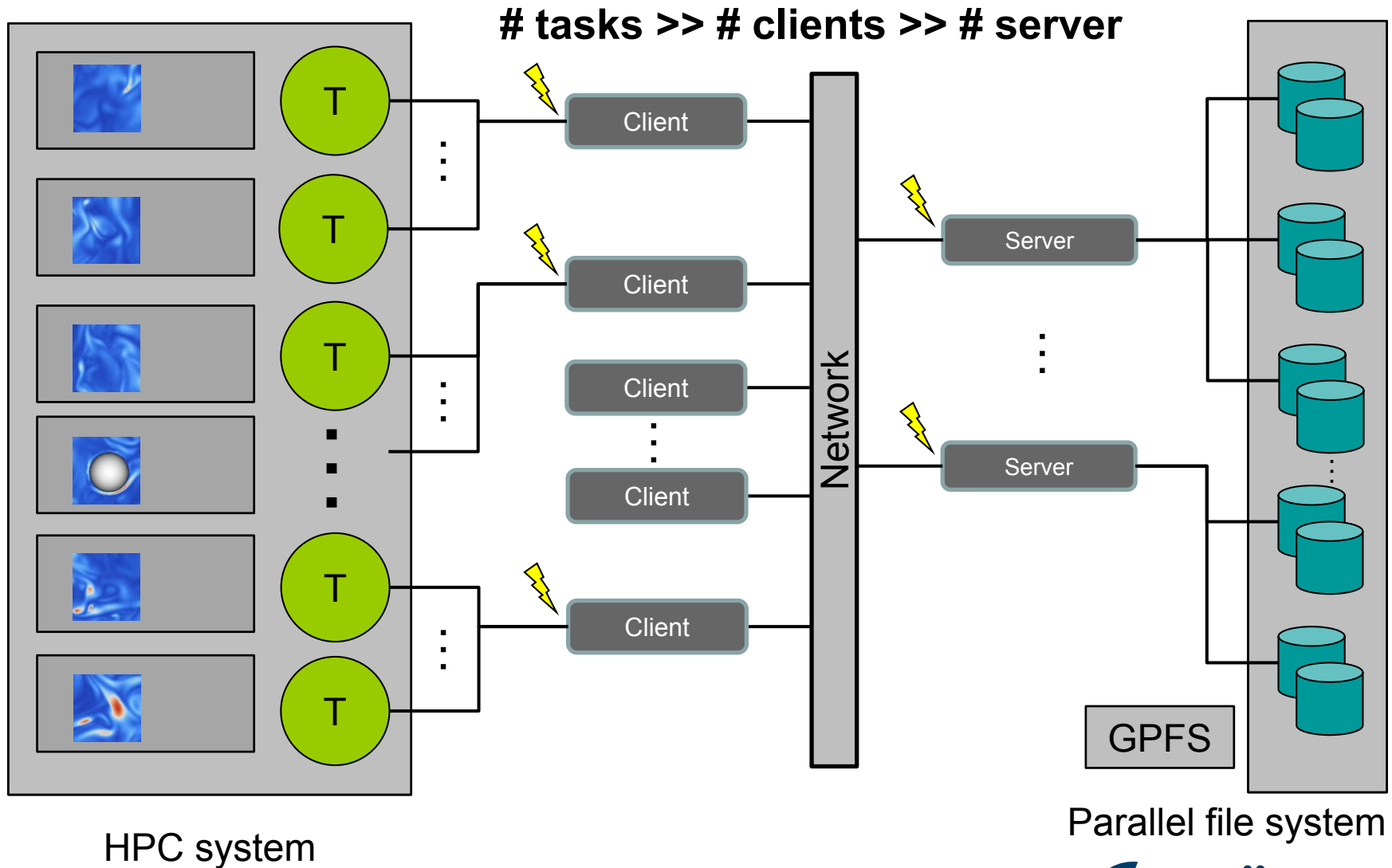


Shared files

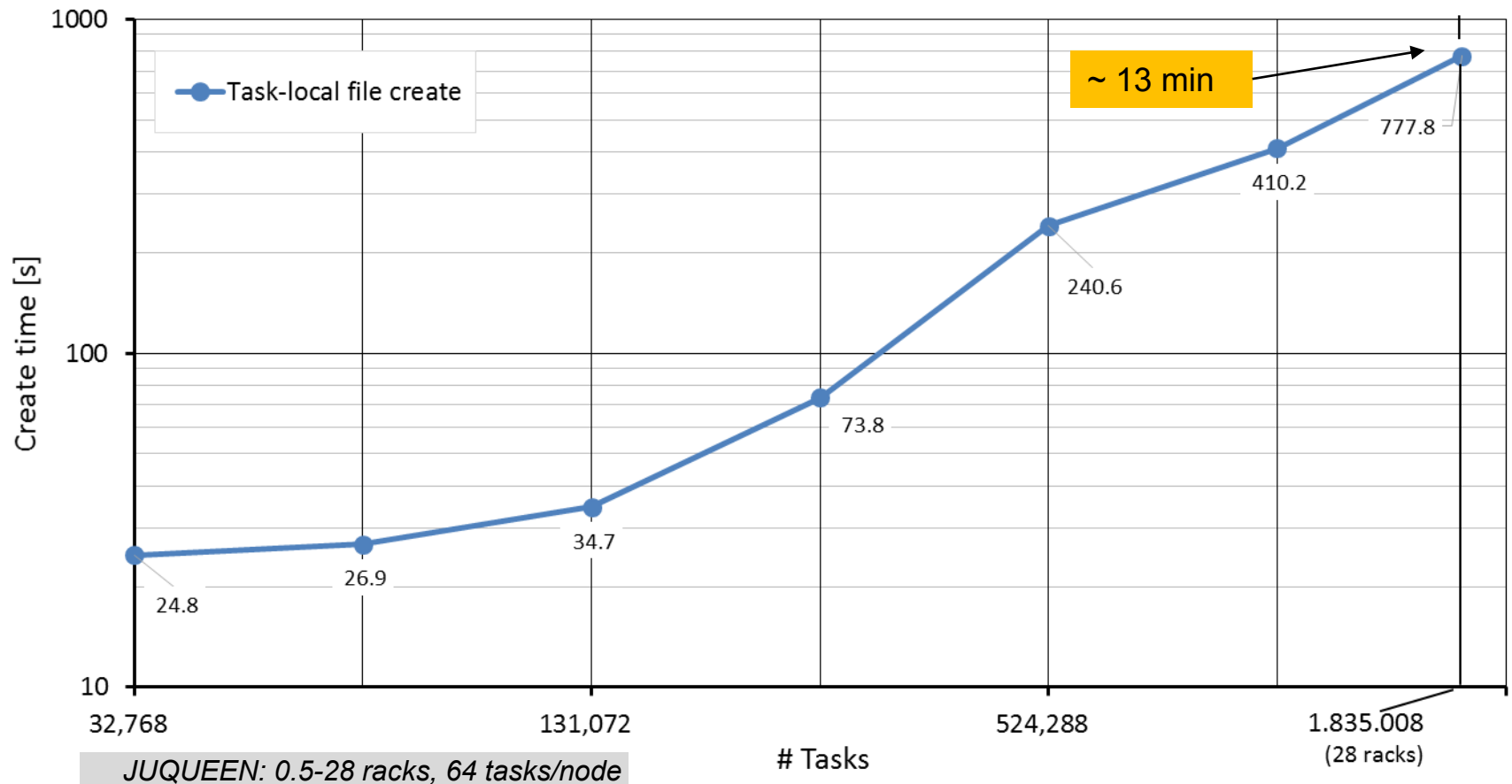
TASK-LOCAL I/O



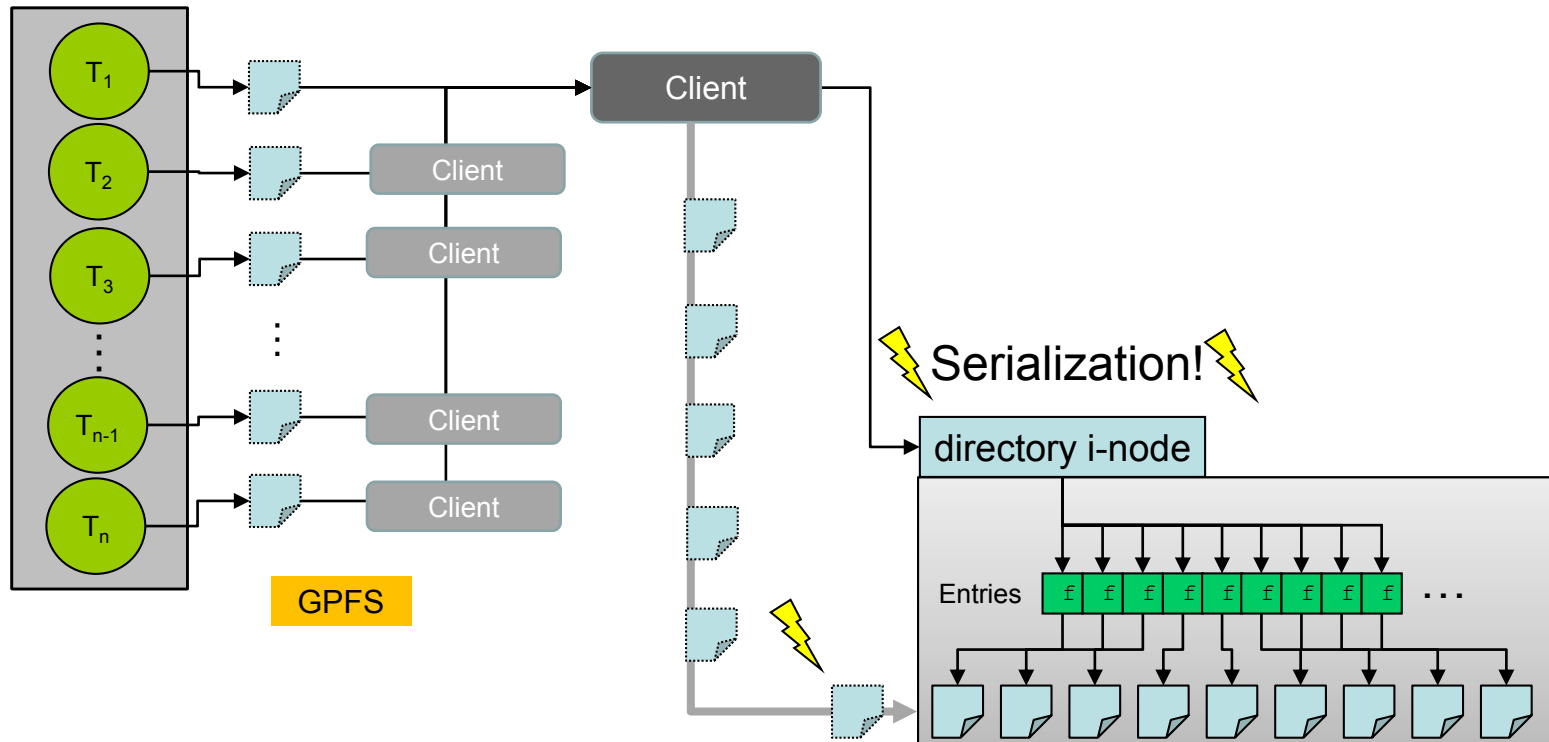
TASK-LOCAL I/O



I/O BOTTLENECK: PARALLEL FILE CREATION

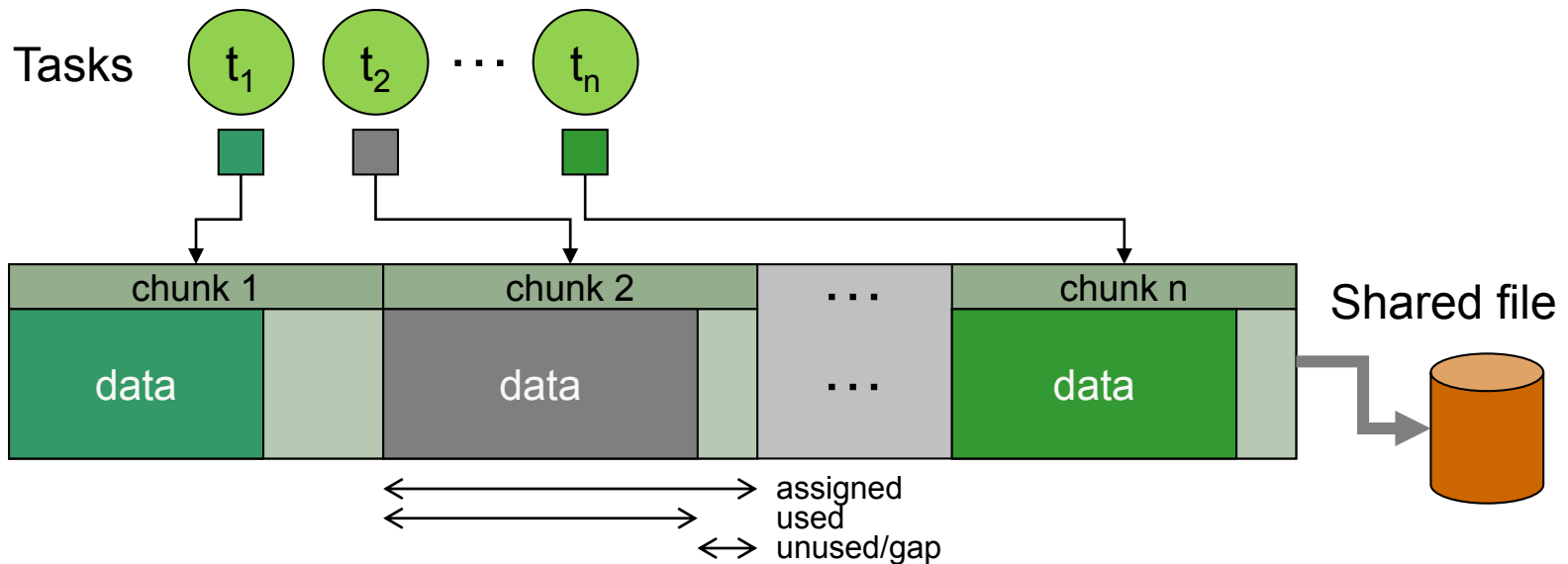
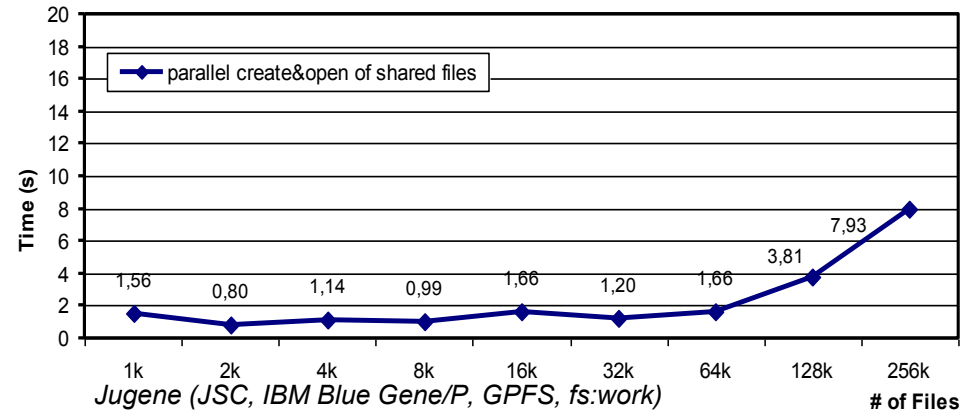


I/O BOTTLENECK: PARALLEL FILE CREATION



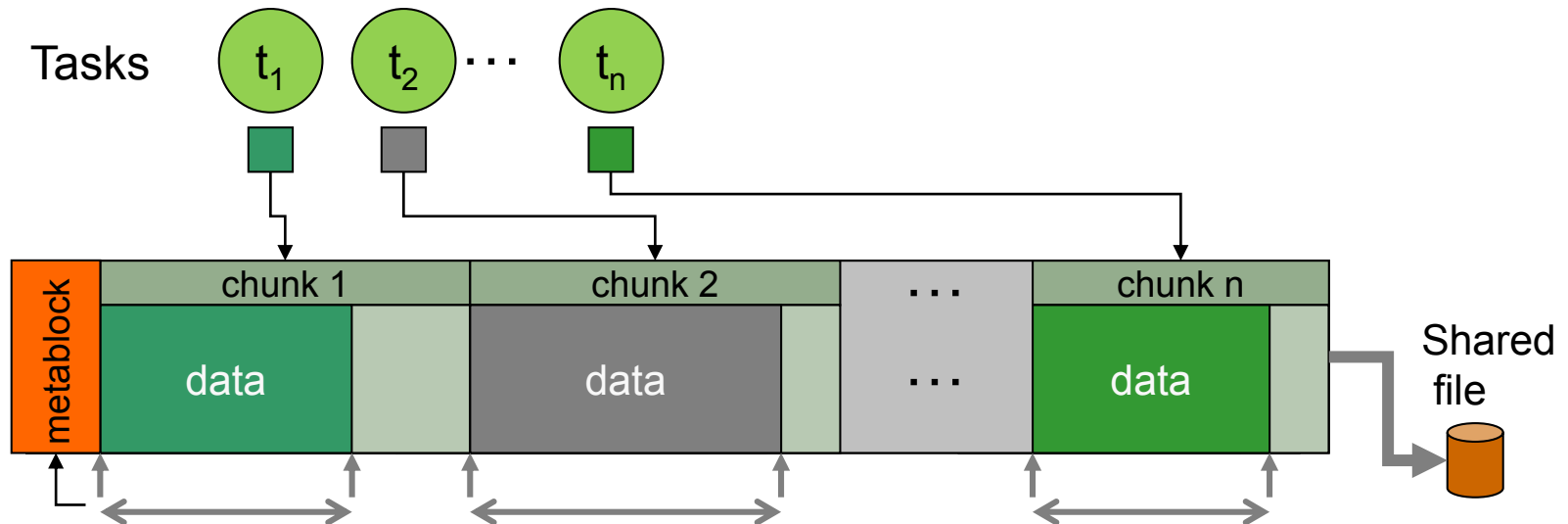
FILE FORMAT (1): A SINGLE SHARED FILE

- Create and open is fast
- Simplified file handling
- Only one big file
- Logical partitioning required



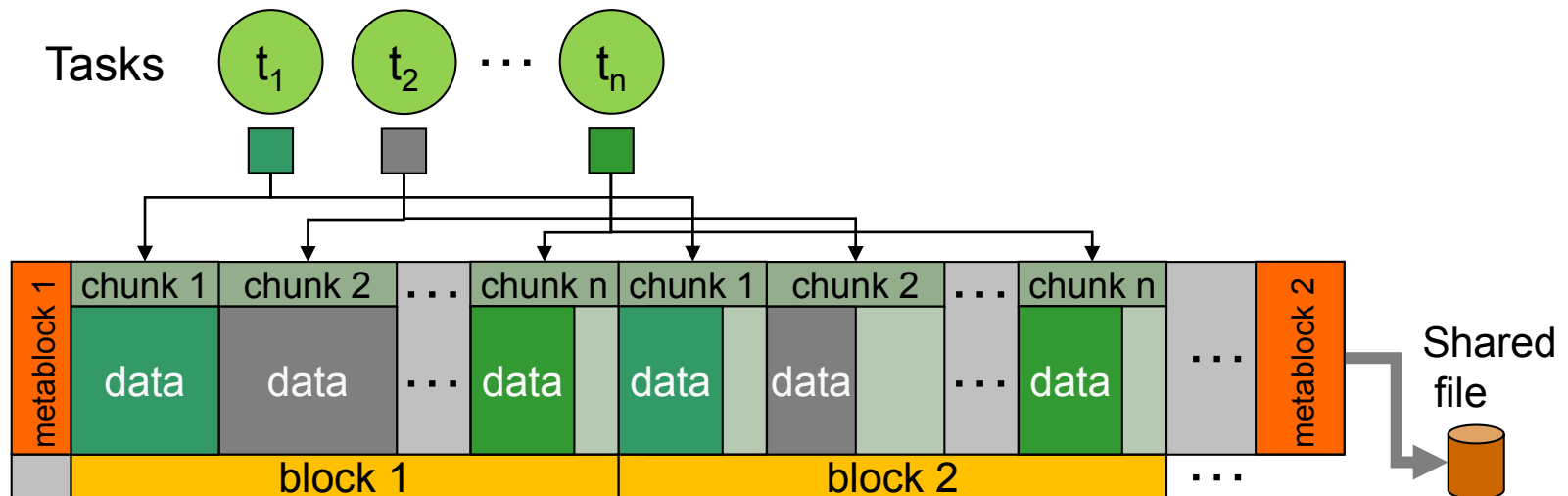
FILE FORMAT (2): METADATA

- Offset and data size per task
- Tasks have to specify chunk size in advance
- Data must not exceed chunk size



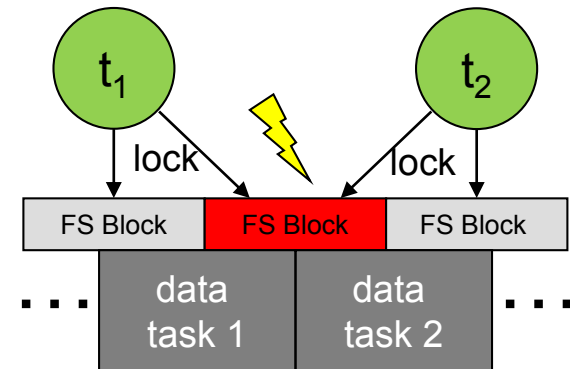
FILE FORMAT (3): MULTIPLE BLOCKS OF CHUNKS

- Enhancement: define blocks of chunks
- Metadata now with variable length ($\#tasks * \#blocks$)
- Second metadata block at the end
- Data of one block does not exceed chunk size



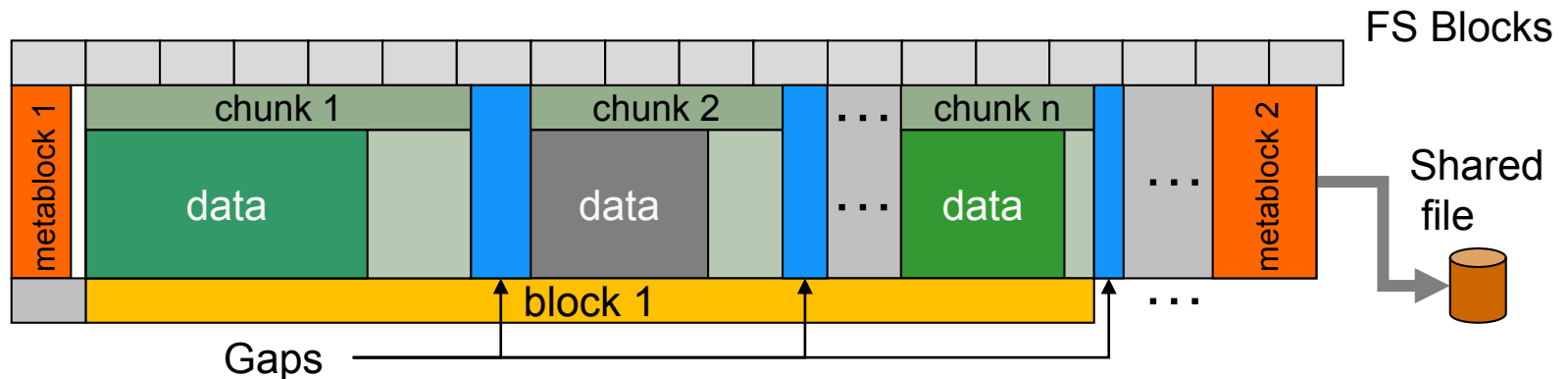
FILE FORMAT (4): ALIGNMENT TO BLOCK BOUNDARIES

- Contention when writing to same file-system block in parallel

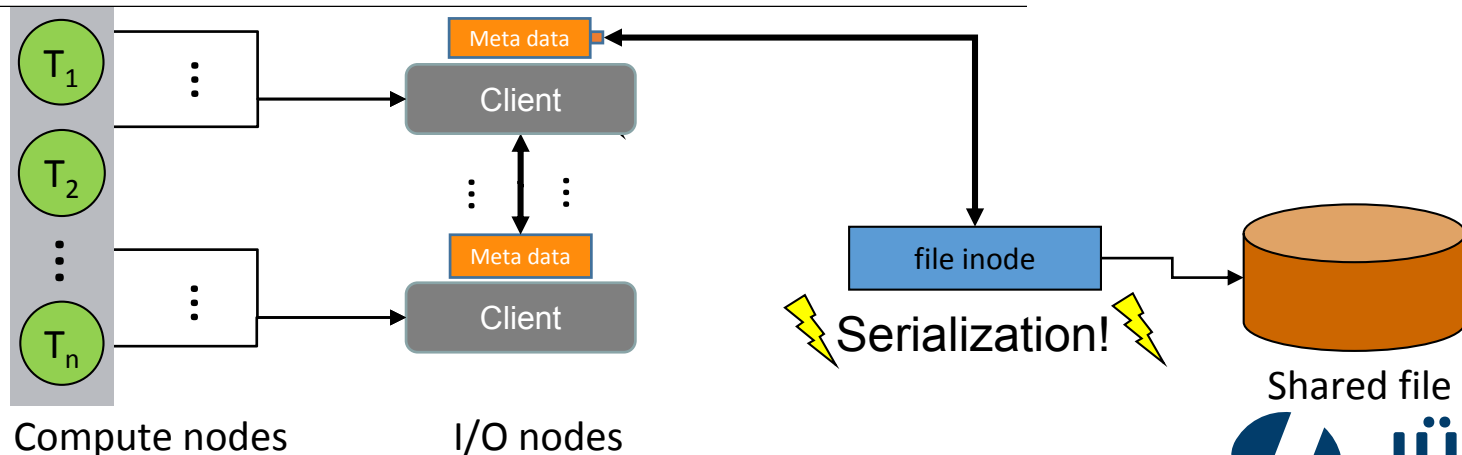
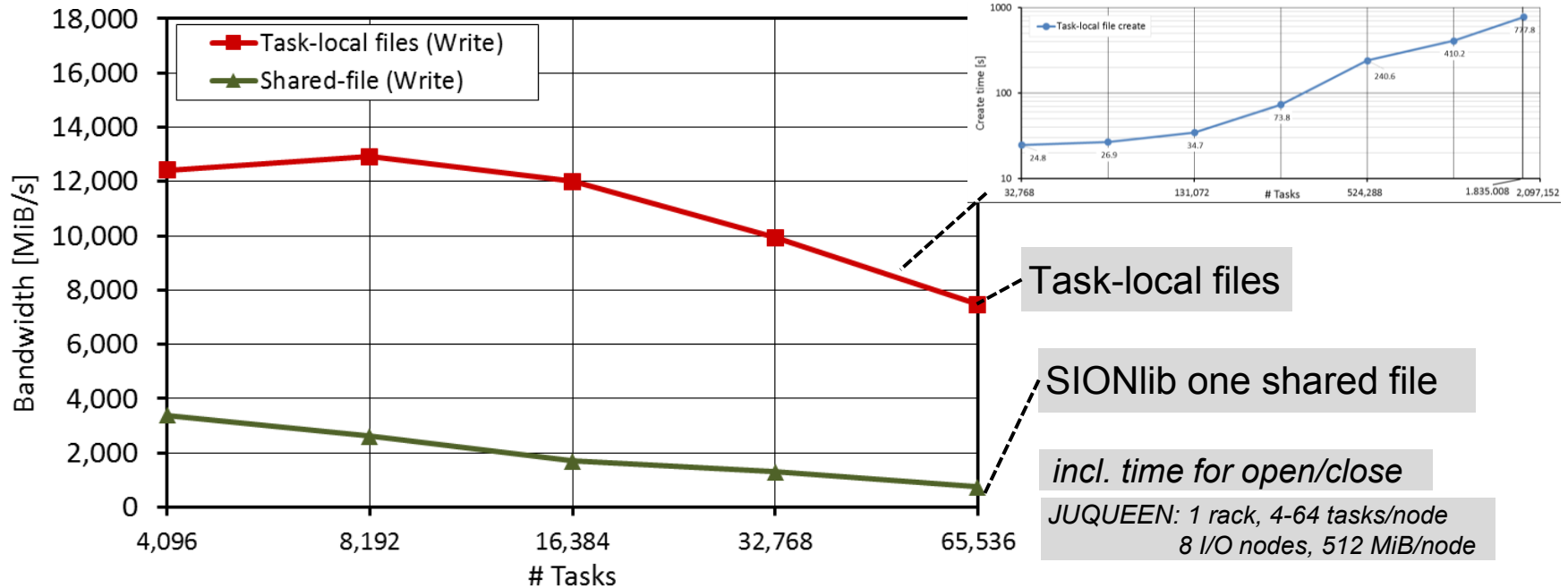


#tasks	data size	blksize	write bandwidth
32768	256 GB	aligned	3650.2 MB/s
32768	256 GB	not aligned	1863.8 MB/s

Jugene (JSC, IBM Blue Gene/P, GPFS, fs:work)

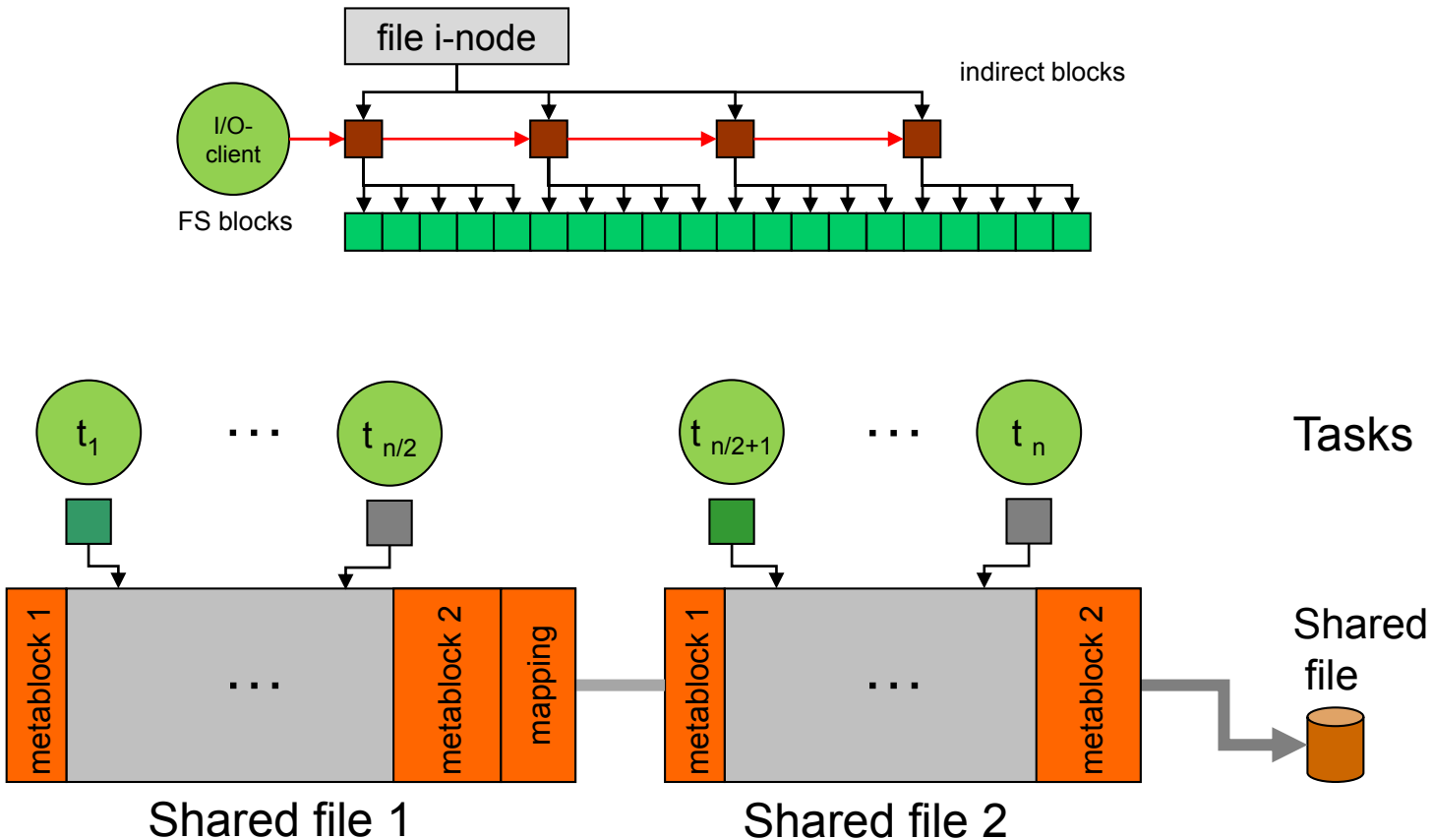


I/O BOTTLENECK: LARGE #TASKS & SHARED FILE

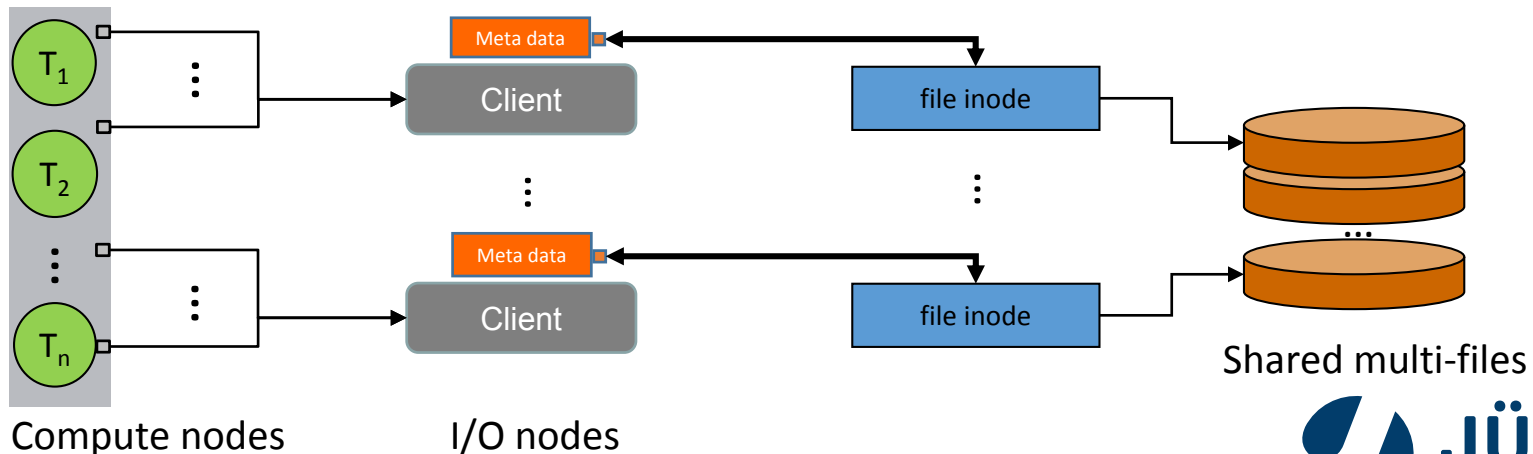
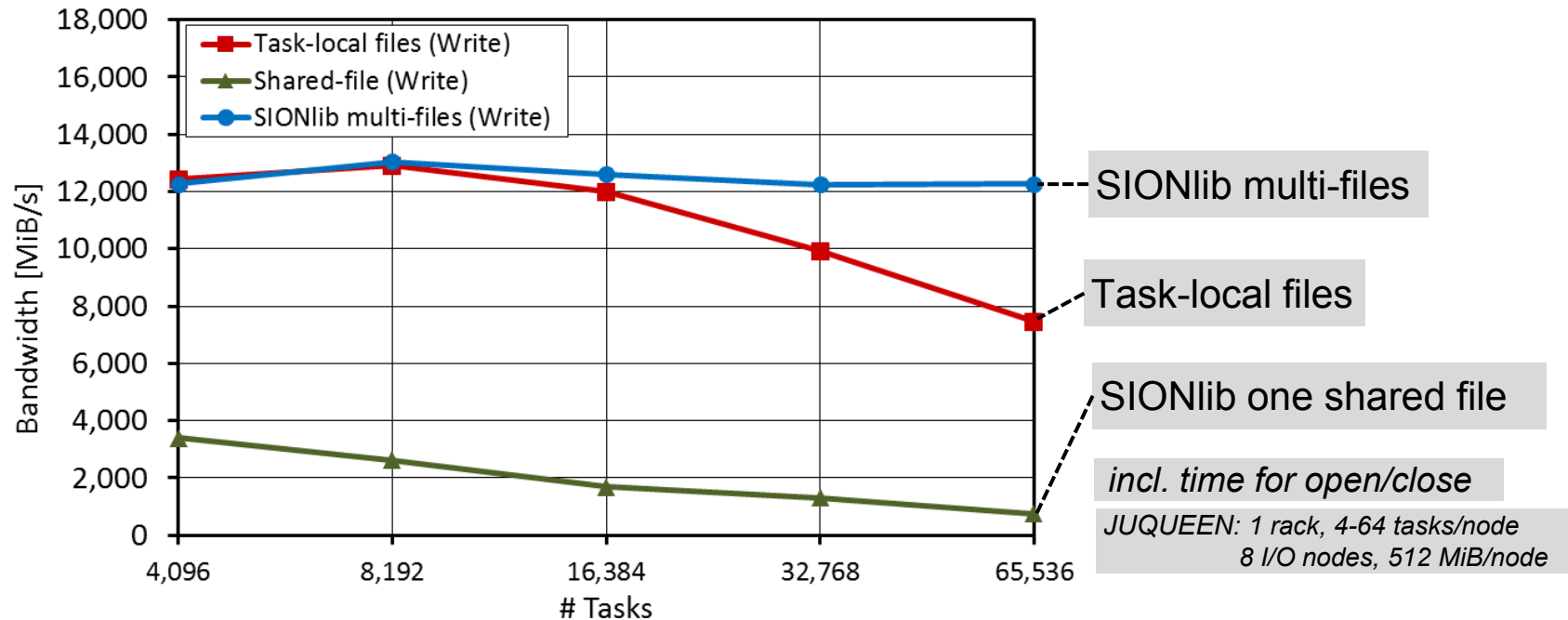


FILE FORMAT (5): MULTIPLE PHYSICAL FILES

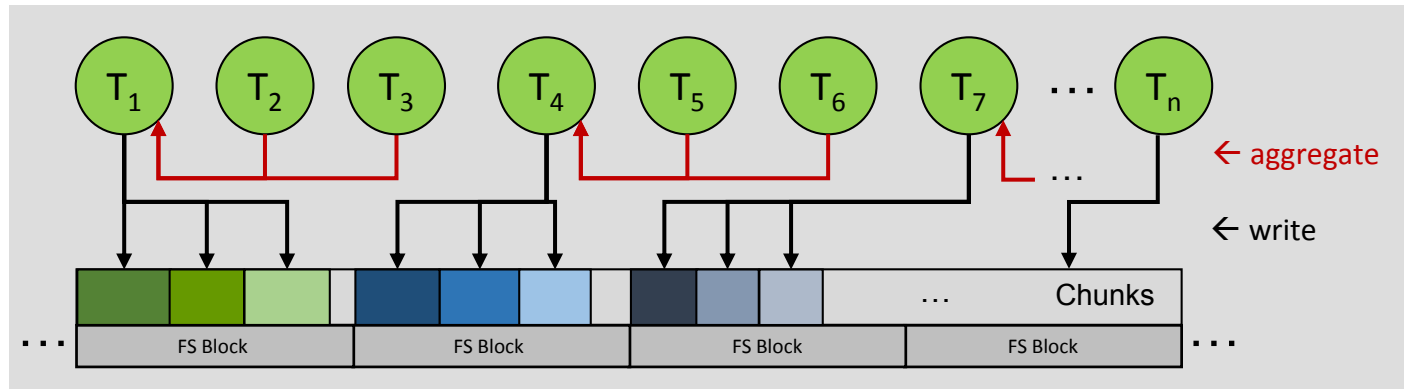
- Variable number of underlying physical files
- Bandwidth degradation on GPFS by using a single shared file



I/O BOTTLENECK: LARGE #TASKS & SHARED FILES



FILE FORMAT (6): COALESCING I/O



- data/task very small → sparse file container
- Coalescing I/O: **Aggregation of data among tasks**
- Variable number of senders/collectors
- Collective write/read operations required
- Advantages: No alignment between chunks of the same collector; less gaps, fewer data streams, less congestion in I/O infrastructure
- Reduced buffering on collector task (one file system block)

Optimization:

- Shared file container, non-collective write/read
- Multi-file approach
- Alignment to FS-blocks

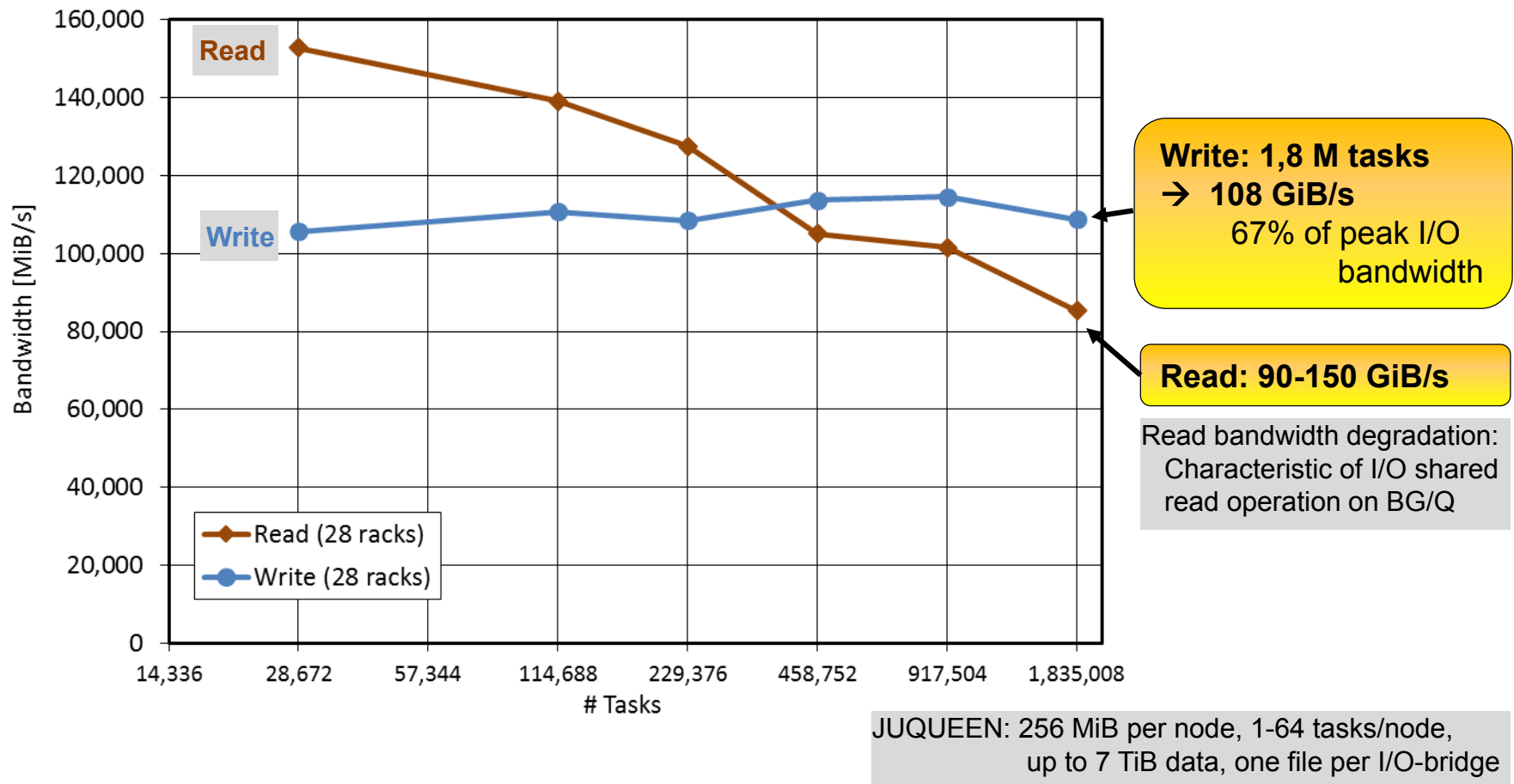
Additional features:

- *Coalescing I/O*
- *Generic interface*
- *Basic key-value stores*
- *Buddy checkpointing*

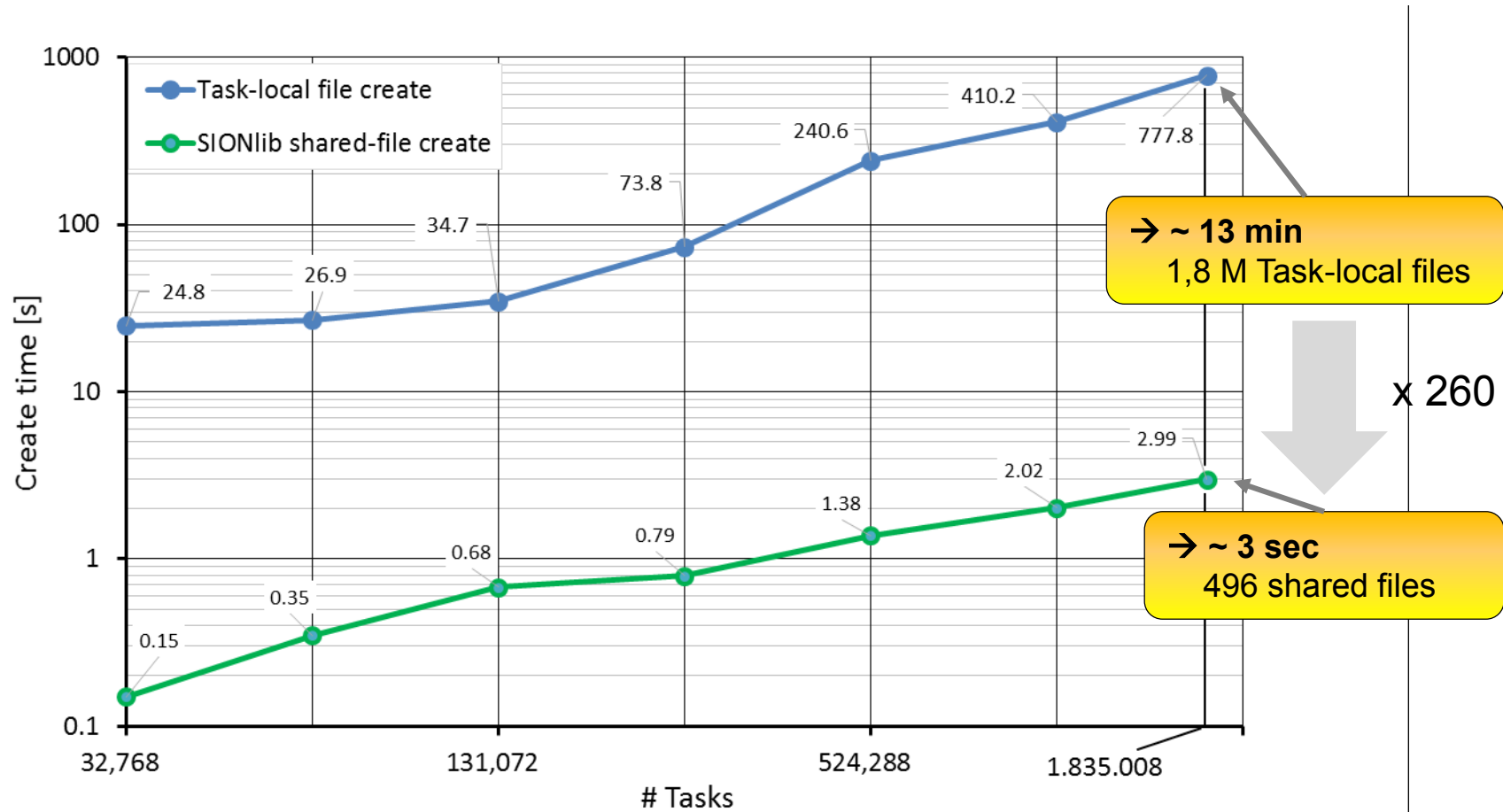
SIONlib: Library for efficient task-local I/O at large scale

- Easy-to-use interface
- Support for parallel and serial programs, parallel tools

JUQUEEN SIONLIB SCALING, BANDWIDTH



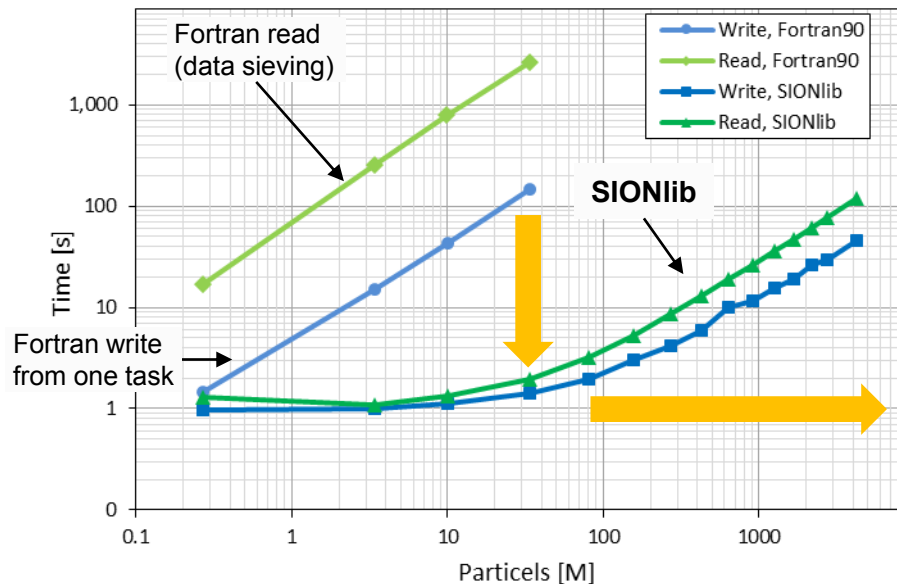
JUQUEEN SIONLIB SCALING, FILE CREATE



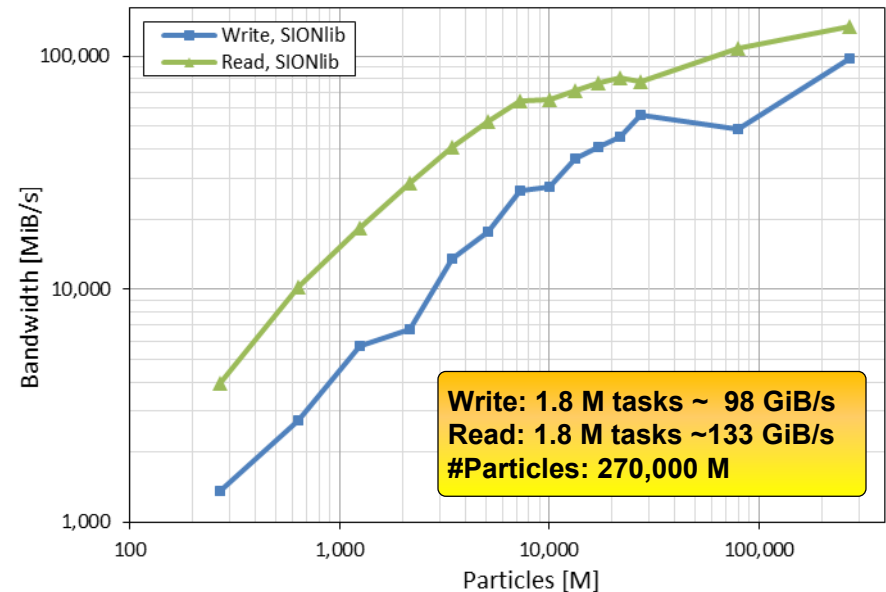
APPLICATION MP2C

MP2C: Massively Parallel Multi-Particle Collision Dynamics

Mesoscopic hydrodynamics + Molecular dynamics



JUQUEEN: 512 nodes, 16 tasks per node



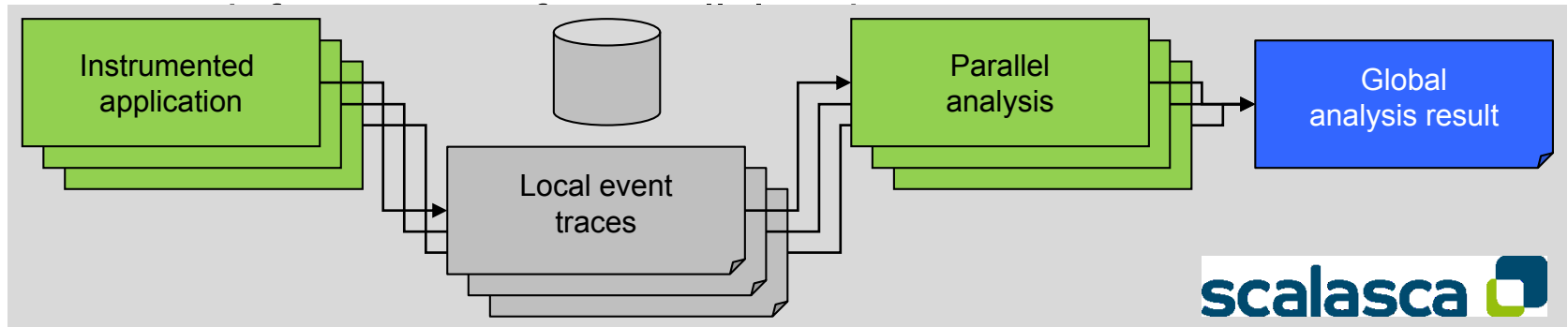
JUQUEEN: 28 racks, 64 tasks per node

WWW: <http://www.fz-juelich.de/ias/jsc/EN/Expertise/High-Q-Club/MP2C>

PARALLEL PERFORMANCE TOOLS

Scalasca Automatic parallel performance analysis

Score-P Scalable performance measurement

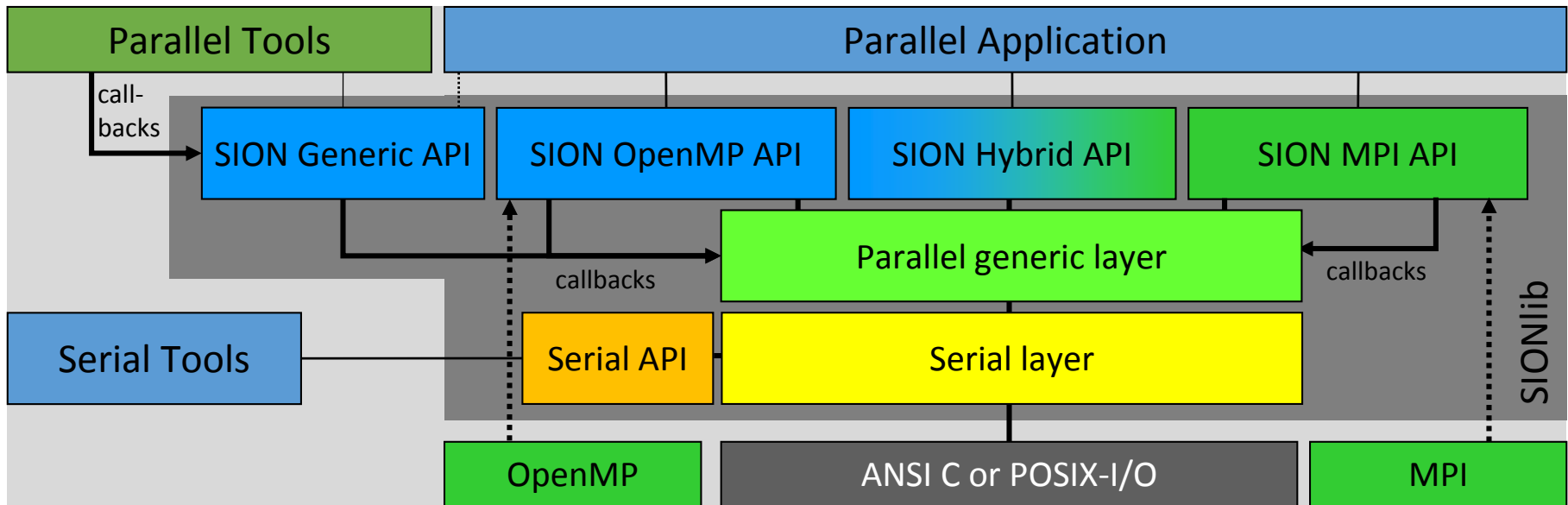


Results:

- Reduced number of event trace files
- Faster output of event trace files

Scalasca/ctest	# Tasks	I/O time / Write
Task-local I/O	131,072	151.0 s
SIONlib	131,072	89.6 s
JUQUEEN: 2048 nodes		x 1.69 faster

SOFTWARE LAYERS AND APIS



- Implementation in C,
- Language bindings for Fortran, C++, Python
- Designed as extension of ANSI C file I/O API
- Lightweight and easy-to-use library

VERSION, DOWNLOAD, INSTALLATION

- Version: 1.7.1 (November 2016)
- Version: file format: 5
- Open-source license

<http://www.juelich.de/jsc/sionlib>

- Installation (or `module load SIONlib/1.7.1-foss-2017a`)

Shell

```
configure -prefix=<INSTPATH> <--enable-debug> ...  
make  
make test  
make install
```

- Query version of SIONlib:

Shell

```
sionversion  
SIONlib Version 1.7.1 (svn_rev 2088), fileformat  
version 5 (./sionversion)
```

SIONLIB DATATYPES

- Only used for parameters for SIONlib function calls
- Data written to or read from file is a byte stream and does not need to be declared by special data types

C `sion_int32`

Fortran `INTEGER(kind=4)`

C `sion_int64`

Fortran `INTEGER(kind=8)`

- Typically used for all parameters that are used to describe or to compute file positions

HEADER FILE & RETURN CODES

```
C #include <sion.h>
```

```
Fortran use sion_f90  
use sion_f90_mpi
```

- **Important:** include MPI first
- C, C++: C-preprocessor directives, defined in `sion.h`

```
C #define SION_SUCCESS 1  
#define SION_NOT_SUCCESS 0
```

- Fortran: 1 → success, 0 → not success

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);
```

- No collective operation, no shared files
- Data: stream of bytes

SIONLIB: PARALLEL OPEN/CLOSE

- Parallel interface, using MPI

```
🔄 sion_paropen_mpi(), sion_parclose_mpi()
```

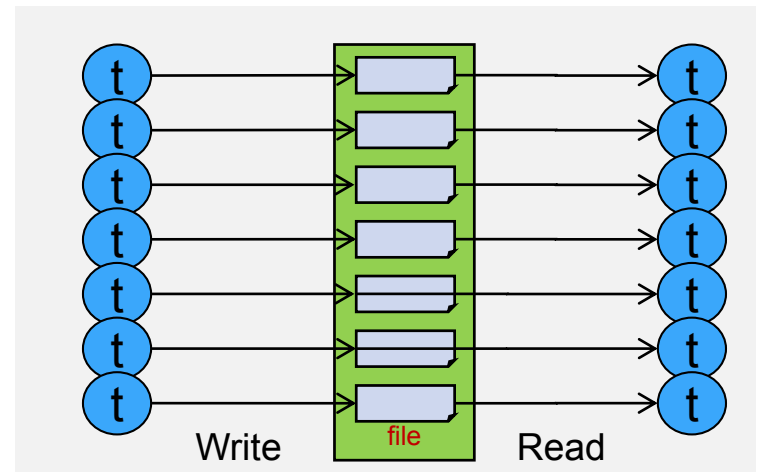
- Parallel interface, using OpenMP

```
🔄 sion_paropen_omp(), sion_parclose_omp()
```

- Parallel interface, using MPI+OpenMPI

```
🔄 sion_paropen_ompi(), sion_parclose_ompi()
```

- SIONlib data format does not distinguish data chunks of MPI tasks and OpenMP threads
→ *SIONlib task*



COLLECTIVE OPEN (MPI)

C

```
int sion_paropen_mpi (char *fname, const char *file_mode,  
                     int *numFiles,  
                     MPI_Comm gComm, MPI_Comm *lComm,  
                     sion_int64 *chunksize,  
                     sion_int32 *fsblksize,  
                     int *globalrank,  
                     FILE **fileptr, char **newfname);
```

Fortran

```
FSION_PAROPEN_MPI (FNAME, FILE_MODE, NUMFILES,  
                   GCOMM, LCOMM, CHUNKSIZE, FSBLKSIZE,  
                   GLOBALRANK, NEWFNAME, SID)  
CHARACTER* (*) FNAME, FILE_MODE, NEWFNAME  
INTEGER        NUMFILES, FSBLKSIZE, GLOBALRANK, SID  
INTEGER        GCOMM, LCOMM  
INTEGER*8      CHUNKSIZE
```

- Open a SION file in parallel for reading or writing data
- Collective call, called by each task at the same time
- Accesses one or more physical files of a logical SION file
- Parameters are passed “by reference” to pass back information in read open mode

PARAMETERS OF OPEN CALLS I

fname: file name

- Character string describing path and file name
- Will not be extended by SION-specific suffix
- In general multiple physical files are generated
- First file: ***filename***
- All other files: **filename** + “.” + 6-digit-number (000001 ...)
- All commands and function calls use the base name

fmode: file mode

- Must specify at least one of the following

r,rb,br	(read block), open existing SION file for reading
w,wb,bw	(write block), create a new SION file, open for write; overwrite if existing
posix	use internally POSIX interface for file access, otherwise ANSI-C

PARAMETERS OF OPEN CALLS II

sid: SIONlib file descriptor

- Unique integer value, referring internally to data structure
- Associated to SION file (internal file handle)
- Allows multiple simultaneously opened files
- C: return code, Fortran: last parameter of open call
- Integer file handle for Fortran necessary

chunksize: size of data per task

- Pointer of type: `sion_int64*` (C), `Integer*8` (Fortran)
- Size of data in bytes written by this tasks (maximum size of single `sion_fwrite` call)
- May be different for each task and must be set if open for writing
- Will be increased internally to the next multiple of the file system block size

PARAMETERS OF OPEN CALLS III

fsblksize: file system block size

- Size of file system block in bytes
- Read-mode: file system block size at write time
- Write-mode: automatically detected by SIONlib if set to -1

fileptr: ANSI-C file pointer

- Can be replaced by NULL pointer if not needed (recommended)
- Will be removed in future versions
- Only needed if wrapper functions for writing and reading are not used
- Not available in Fortran

newfname:

- File name of physical file assigned to this task

PARAMETERS OF SION_PAROPEN_MPI

gComm: MPI Communicator

- Call is collective over all tasks of this communicator
- Each task gets assigned one chunk of SION file
- Read: number of tasks must be equivalent to number tasks written to SION file

lComm: MPI Communicator

- Tasks of the same communicator are writing to the same physical file
- `MPI_Comm_null` if not specified

numfiles: Number of physical files

- If using lComm: set numfiles=-1
- Read-mode: parameters will be set by open call

globalrank:

- Rank of task in global communicator gComm

SERIAL OPEN/CLOSE

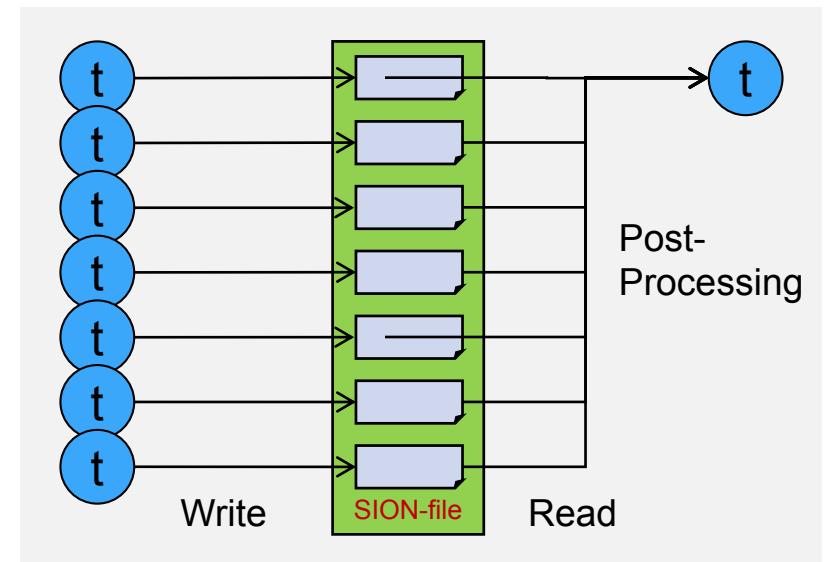
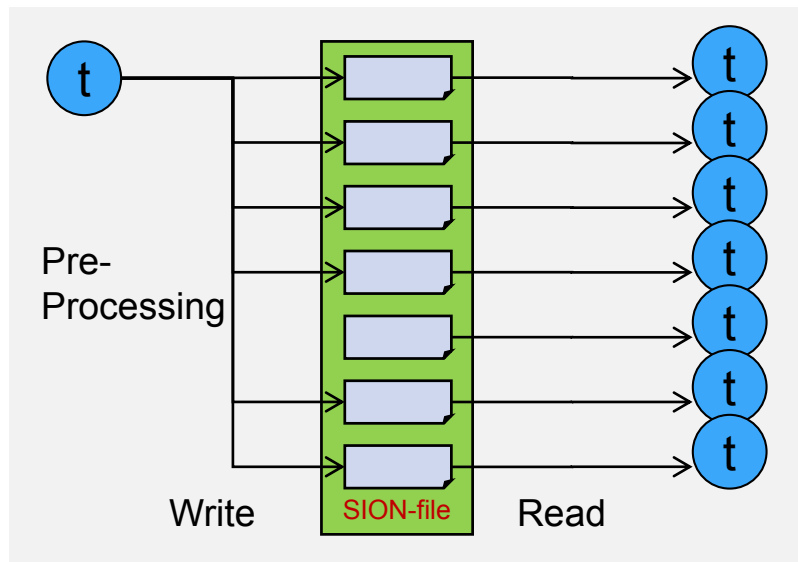
- Serial interface, accessing data of all SIONlib tasks in container

```
🔄 sion_open(), sion_close()
```

- Serial interface, accessing data of one SIONlib task

```
🔄 sion_open_rank(), sion_close()
```

Use case: pre- and post-processing tools, converters



SERIAL OPEN

C

```
int sion_open (char          *fname,  
               const char   *file_mode,  
               int          *ntasks,   int *nfiles,  
               sion_int64   **chunksizes,  
               sion_int32   *fsblksize,  
               int **globalranks, FILE **fileptr);
```

Fortran

```
FSION_OPEN (FNAME, FILE_MODE, NTASKS, NUMFILES,  
             CHUNKSIZES, FSBLKSIZE, GLOBALRANKS, SID)  
CHARACTER* (*) FNAME, FILE_MODE  
INTEGER       NUMFILES, NTASKS, FSBLKSIZE, SID  
INTEGER       GLOBALRANKS (NTASKS)  
INTEGER*8     CHUNKSIZES (NTASKS)
```

- Open a SION file in serial mode
- All chunks of all tasks can be selected, via `sion_seek`
- Multiple physical files can be handled
- Designed for serial pre- and post-processing tools
- Reads all metadata of all tasks into memory

COLLECTIVE CLOSE

C `int sion_parclose_mpi(int sid)`

Fortran `FSION_PARCLOSE_MPI (SID, IERR)`
`INTEGER SID, IERR`

- Closes a SION file in parallel on all tasks/threads
- Collective call, called by each task/thread at the same time
- Metadata will be collected from each tasks
- Metadata blocks of SION file will be written in this call
- Currently no fault tolerant handling of the metadata, call has to executed successfully

SERIAL CLOSE

C `int sion_close(int sid)`

Fortran `FSION_CLOSE(SID, IERR)`
`INTEGER SID, IERR`

- Closes a SION file in serial mode
- Metadata blocks of SION file will be written in this call
- Currently no fault tolerant handling of the metadata, call has to be executed successfully

EXERCISE

Exercise 1 – SIONlib hello world

- Write a parallel program in C or Fortran which creates and closes an empty SIONlib file
- Use a chunksize to store 1000 Integer

Check the resulting file using:

`siondump`

```
module load SIONlib/1.7.1-foss-2017a
```

```
mpicc file.c `sionconfig --libs --mpi --c --64`
```

```
mpif90 `sionconfig --cflags --mpi --f90 --64` file.f90  
`sionconfig --libs --mpi --f90 --64`
```

WRITE DATA

C

```
size_t sion_fwrite (void *data,  
                    size_t size,  
                    size_t nmemb,  
                    int      sid);
```

Fortran

```
FSION_WRITE (DATA, SIZE, NMEMB, SID, RC)  
INTEGER SID  
INTEGER*8 SIZE, NMEMB, RC
```

- Write `size*nmemb` chunk, beginning from current position
 - This size must not exceed the chunksize defined in open call
- Internally this function uses `sion_ensure_free` space to check whether there is enough space is available
- Returns number of elements written

ENSURE FREE SPACE IN CHUNK

C

```
int sion_ensure_free_space (int sid,  
                             sion_int64 bytes);
```

Fortran

```
FSION_ENSURE_FREE_SPACE (SID, BYTES, IERR)  
INTEGER SID, IERR  
INTEGER*8 BYTES
```

- Ensures that there is enough space available for writing
- A new chunk will be allocated if not enough space is left in the current chunk
- The function is a task-local function, which can be called independently from other MPI tasks
- The function moves the file pointer to a new position in some cases and flushes also the local file pointer
- Returns 1 if space could be ensured, there is currently no indicator if a new chunk was allocated

EXERCISE

Exercise 2 – SIONlib write

- Extend your parallel program in C or Fortran
- Each task should fill a array with 1000 elements using its unique rank
- Each task should write the array into the prepared SIONlib file

Check the resulting file using:

`siondump`

```
module load SIONlib/1.7.1-foss-2017a
```

```
mpicc file.c `sionconfig --libs --mpi --c --64`
```

```
mpif90 `sionconfig --cflags --mpi --f90 --64` file.f90  
`sionconfig --libs --mpi --f90 --64`
```

READ DATA

C

```
size_t sion_fread (void *data,  
                  size_t size,  
                  size_t nmemb,  
                  int sid);
```

Fortran

```
FSION_READ (DATA, SIZE, NMEMB, SID, IERR)  
INTEGER SIZE, NMEMB, SID, IERR
```

- Read `size*nmemb` bytes from current position in chunk
- Internally this function reads in a while loop until all data is read from file
- Reading more data than stored in one chunk is possible with this wrapper
- Returns number of elements read
- `sion_bytes_avail_in_block` can be used to get all available data

END OF FILE

```
 int SION_feof(int sid);
```

```
 FSION_FEOF (SID, IERR)  
INTEGER SID, IERR
```

- Equivalent to POSIX feof which cannot be used for shared SION files
- Internally this function flushes all buffer and checks current positions against chunk boundaries
- Moves file pointer to next chunk if end of current chunk is reached
- The function is a task-local function, which can be called independently from other MPI tasks.
- Returns 1 if pointer is behind last byte of data for this task

SEEK: CHANGE FILE POSITION

C	<pre>int sion_seek (int sid, int rank, int chunknr, sion_int64 posinchunk);</pre>
Fortran	<pre>FSION_SEEK (SID, RANK, CHUNKNUM, POSINCHUNK, IERR) INTEGER SID, RANK, CHUNKNUM, IERR INTEGER*8 POSINCHUNK</pre>

- Sets the file pointer to a new position
- Seek parameters:
 - rank: rank number (0,...), or SION_CURRENT_RANK
 - chunknum: chunk number (0,...), or SION_CURRENT_BLK
 - posinchunk: position (0,...), or SION_CURRENT_POS
- In parallel write mode seeking is currently not supported

EXERCISE

Exercise 3 – SIONlib read

- Write a serial program in C or Fortran
- Read all elements of your created files and print them to the screen

```
module load SIONlib/1.7.1-foss-2017a  
mpicc file.c `sionconfig --libs --c --64`
```

```
mpif90 `sionconfig --cflags --f90 --64` file.f90  
`sionconfig --libs --f90 --64`
```

COMMAND LINE TOOLS

- **siondump:** Show metadata of file
- **sionsplit:** Split SIONlib file into task-local files
- **sioncat:** Extract data from file
- **siondefrag:** Contracting all of the chunks of a task, which are spread in the file over multiple blocks, into a single chunk
- **sionconfig:** Get compile and link options

TOOLS: SIONSPLIT

Command

```
sionsplit [options] sionfile prefix
```

Parameters & Options:

<i>sionfile</i>	Input file in SIONlib format
<i>prefix</i>	directory and/or filename-prefix for task-local files
<i>[-v]</i>	verbose mode
<i>[-g]</i>	use global rank for numbering files
<i>[-d <num>]</i>	number of digits for filename generation (default 5)

- Generates task-local files from SION-file

TOOLS: SIONCAT

Command

```
sioncat [options] sionfile
```

Parameters & Options:

<i>sionfile</i>	Input file in SIONlib format
<code>[-v]</code>	verbose mode
<code>[-t <tasknum>]</code>	write only data of task <tasknum>
<code>[-b <chnknum>]</code>	write only data of chunk <chnknum>
<code>[-o <outfile>]</code>	file data will be written to, if not specified stdout will used

- Extract all or selected data from a SION file

TOOLS: SIONDUMP

siondump [options] *sionfile*

Parameters & Options:

Command

<i>sionfile</i>	Input file in SIONlib format
[-a]	print all information about all blocks
[-m]	print all mapping information
[-l]	print all sizes in number of bytes
[-k]	print key-value statistic for each task
[-K]	print key-value list for each task
[-S]	print size of internal data structure in memory
[-V]	show version number of SIONlib
[-v]	verbose mode

- Print metadata information of a SION file

TOOLS: SIONDEFrag

siondefrag [options] *sionfile new_sionfile*

Parameters & Options:

Command

<i>sionfile</i>	Input file in SIONlib format
<i>new_sionfile</i>	Output file in SIONlib format
<code>[-Q <fsblksize>]</code>	filesystem blocksize for new sion file in MB (default: input file)
<code>[-q <fsblksize>]</code>	filesystem blocksize for new sion file in bytes
<code>[-V]</code>	show version number of SIONlib
<code>[-v]</code>	verbose mode

- Generates new SION file from existing one
- Changes the underlying file system block size
- Can be used to remove empty gaps, caused by
 - Not completely filled chunks
 - Alignment to file system blocks

TOOLS: SIONCONFIG

sionconfig [options]

Options:

Command

(--com --ser --omp --mpi --ompi --gen)	select SIONlib API
(--cflags --libs --path)	select output of sionconfig
[--32 --64]	Precision
[--be] [--fe] [--mic]	Cross compile
[--gcc]	for GCC Compiler
[--c --f77 --f90 --cxx]	Language selection
[-V]	show version number
[-v]	verbose mode

- Returns flags and options for compiler and cinker on stdout

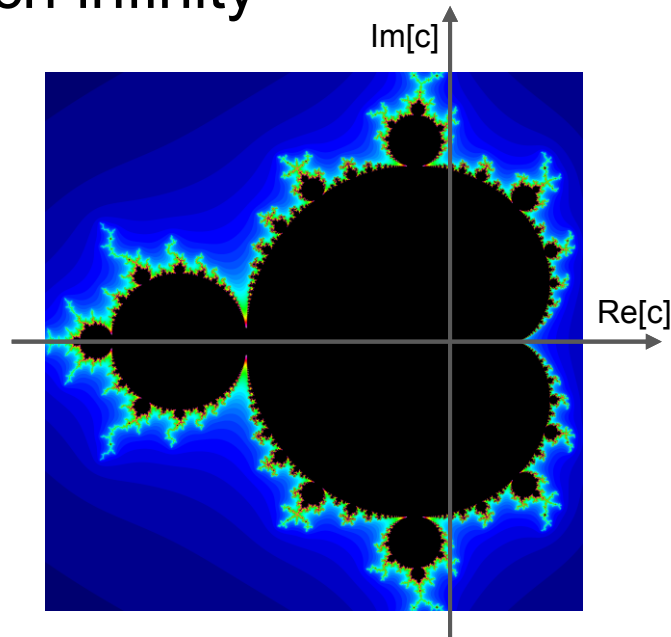
EXAMPLE: MANDELBROT SET

Set of all complex numbers c in the complex plane for which

$$z_{n+1} = z_n^2 + c$$

$$z_0 = 0$$

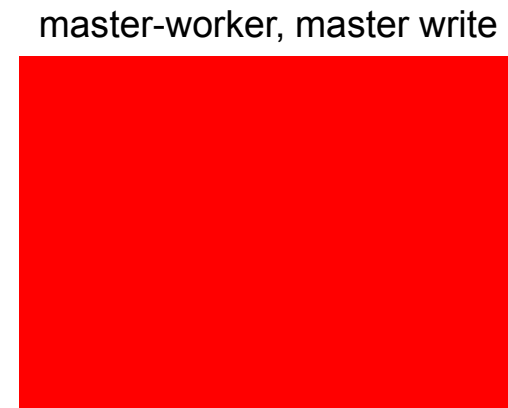
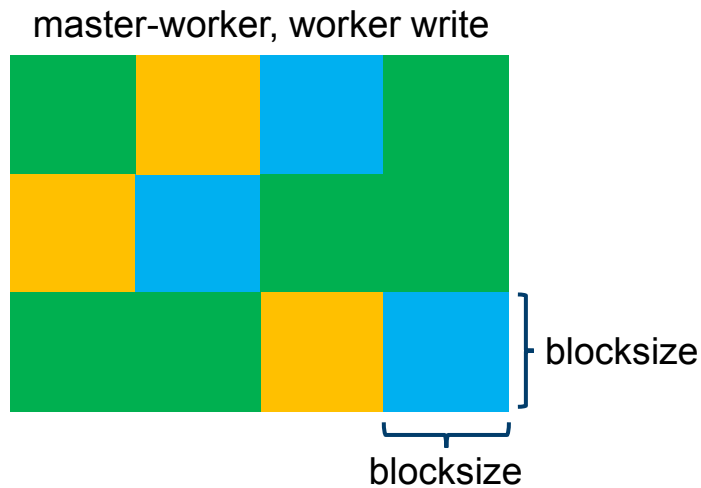
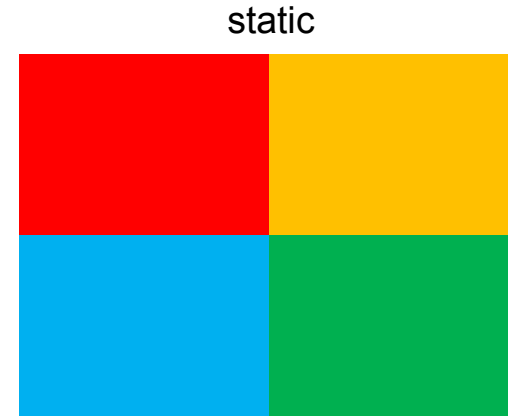
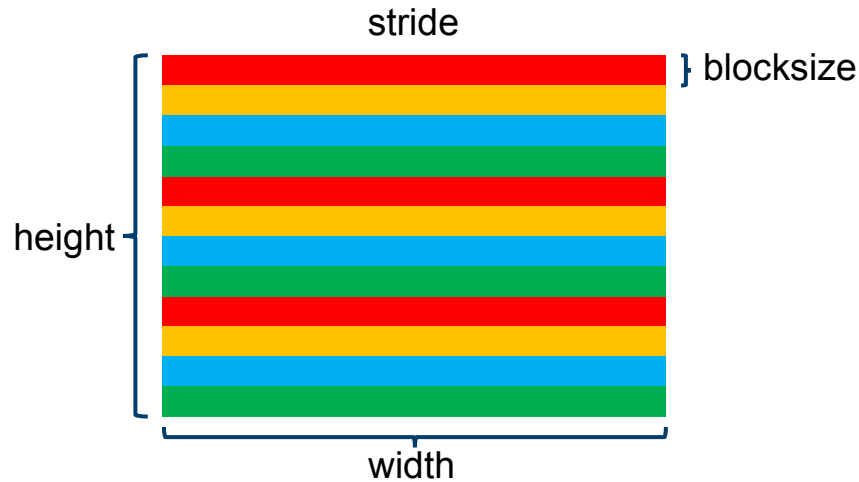
does not approach infinity



EXAMPLE: MANDELBROT SET

- I/O comparison example
- four different decomposition types
 - stride
 - static
 - master-worker (worker write)
 - master-worker (master write)
- two different programs
 - `mandelmpi`: parallel Mandelbrot calculation
 - `mandelseq`: serial output picture generation

EXAMPLE: MANDELBROT SET



IMPACT

SIONlib application integration

DUNE-ISTL (Multigrid solver)	NEST (Human Brain Simulation)
ITM (Fusion-community)	OSIRIS (Fully-explicit particle-in-cell code)
LBM (Fluid flow/mass transport)	PEPC (Pretty Efficient Parallel C. Solver)
KKRnano (Korringa-Kohn-Rostoker Green Fct.)	Profasi (Protein folding and aggr. simulator)
MAXW-DGTD (Human exposure to em. fields)	PSC (Particle-in-cell code)
MP2C (Mesoscopic hydrodynamics + MD)	TurboRVB (High temp. superconductivity)
muPhi (Flow and Transport in Porous Media)	MPAS (Model for prediction across scales)

SIONlib in parallel performance tools

Scalasca	Automatic parallel performance analysis
Score-P	Scalable performance measurement
	Infrastructure for parallel codes (BMBF-project Score-E)

SIONlib in EU funded projects

DEEP-ER	Adaption to new platform, resiliency (buddy checkpointing)
DEEP-EST	Adaption to new platform
EoCoE	Integration into applications

- *<http://www.fz-juelich.de/jsc/sionlib>*
- Open source license
- *sionlib_jsc@fz-juelich.de*

References:

- Wolfgang Frings, Felix Wolf, Ventsislav Petkov, **Scalable Massively Parallel I/O to Task-Local File**, Proceedings of the Conference on High Performance Computing Networking, Storage and Analysis, Portland, Oregon, November 14-20, 2009, SC'09, New York, ACM, ISBN 978-1-60558-744-8.
- Wolfgang Frings, **Efficient Task-Local I/O Operations of Massively Parallel Applications**, Schriften des Forschungszentrums Jülich, IAS Series, 30, 2016, ISBN 978-3-95806-152-1