PARALLEL I/O AND PORTABLE DATA FORMATS

INTRODUCTION AND PARALLEL I/O STRATEGIES

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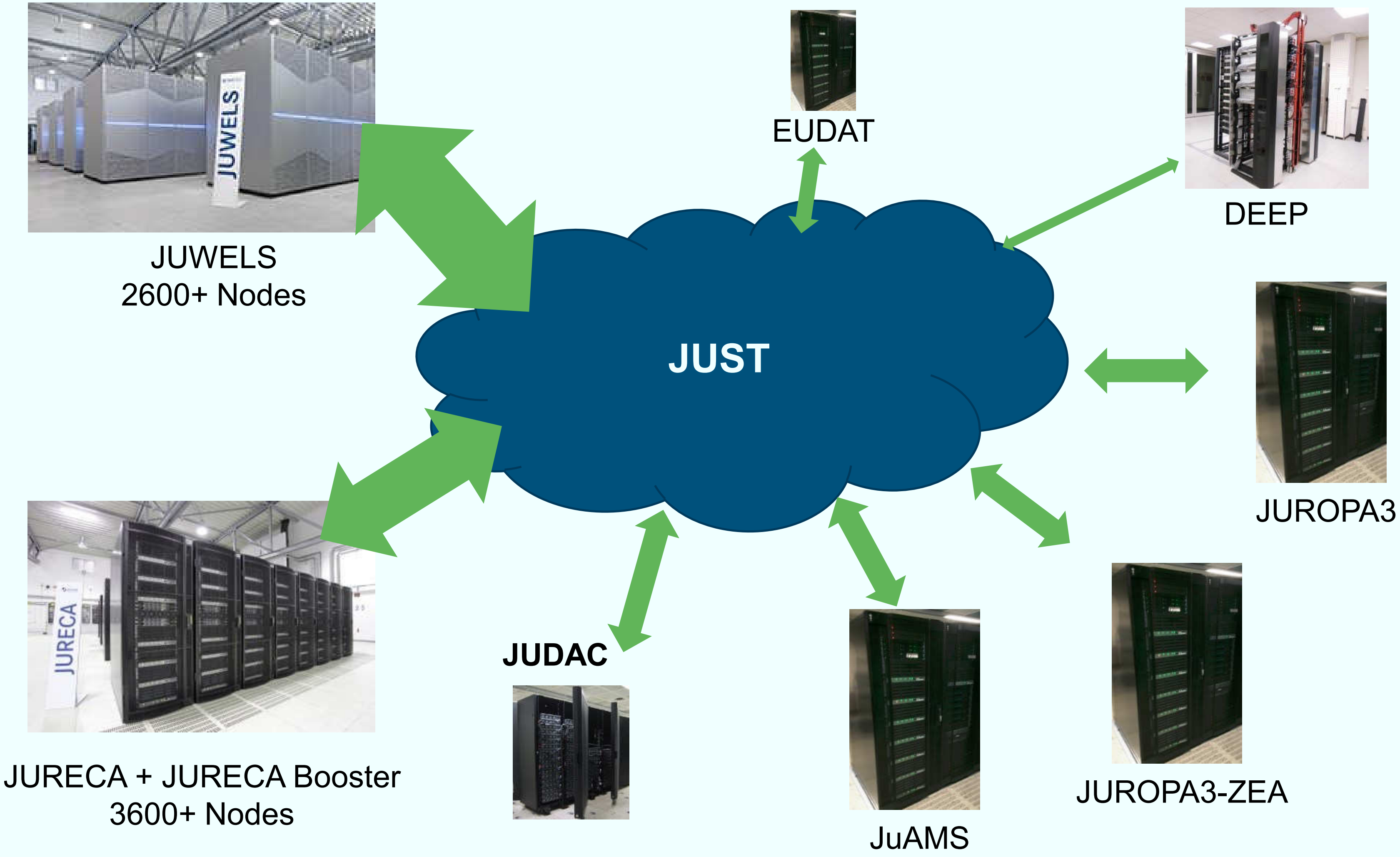
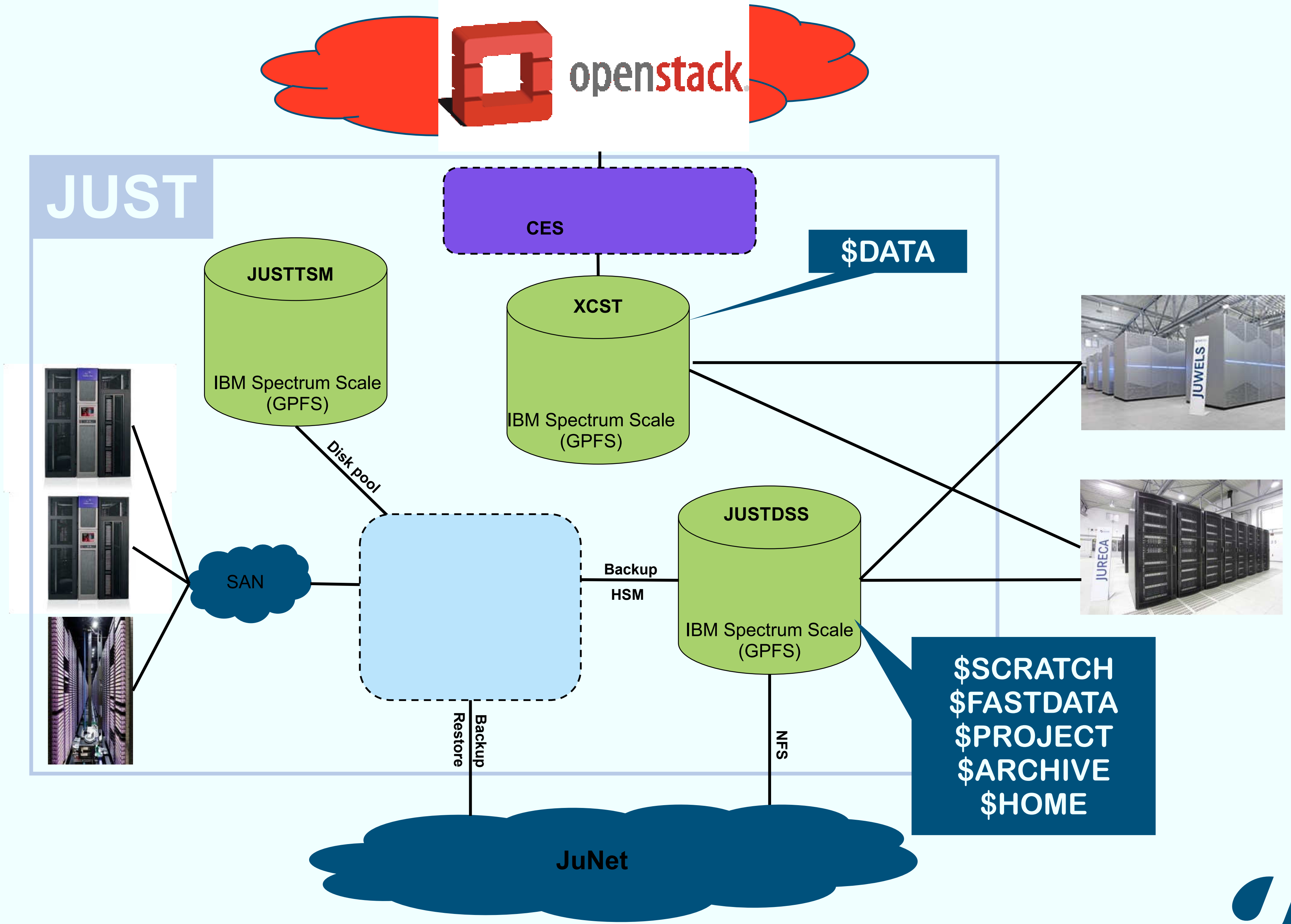
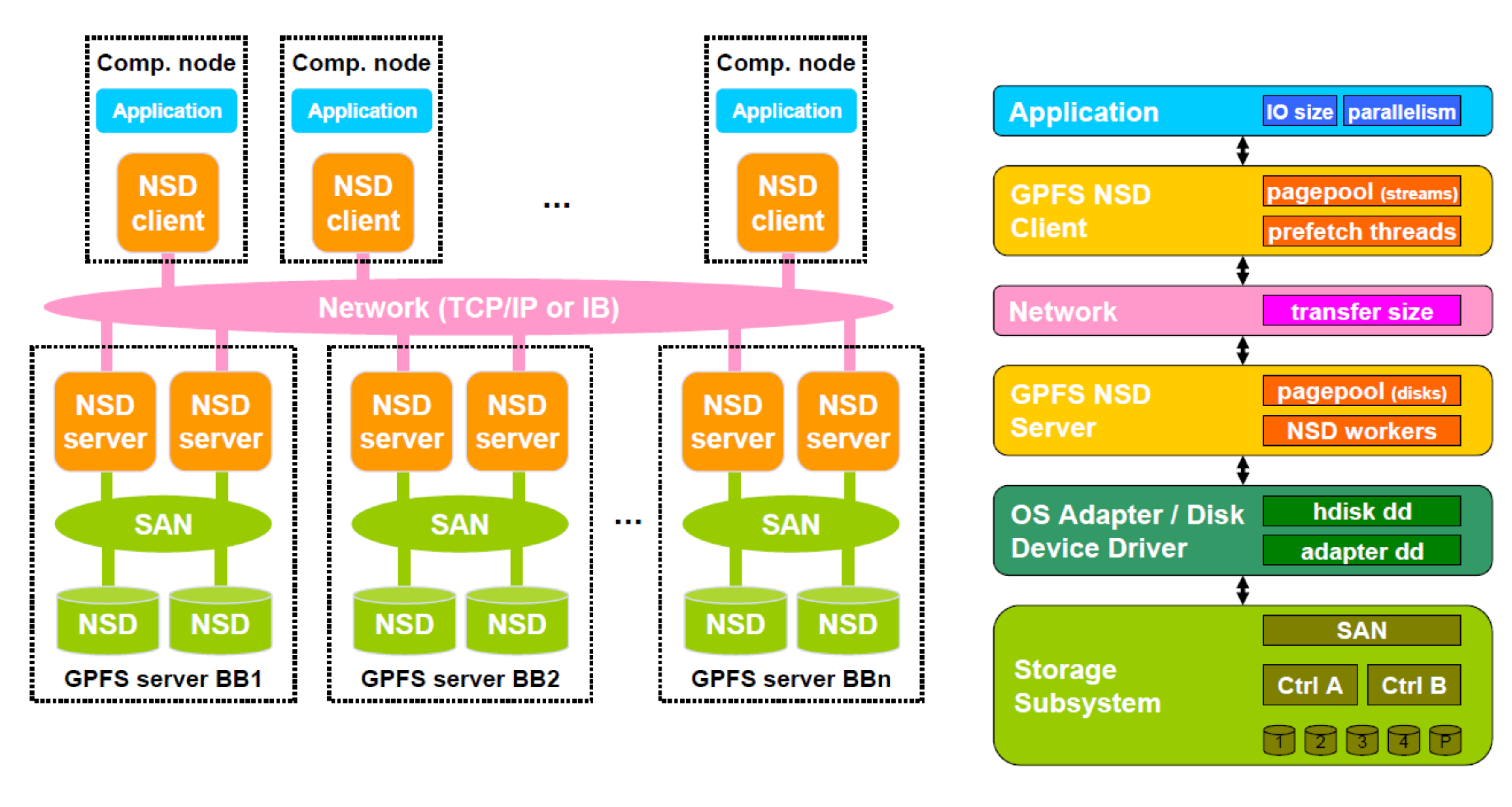
JUST STORAGE SYSTEM

JUelich STorage

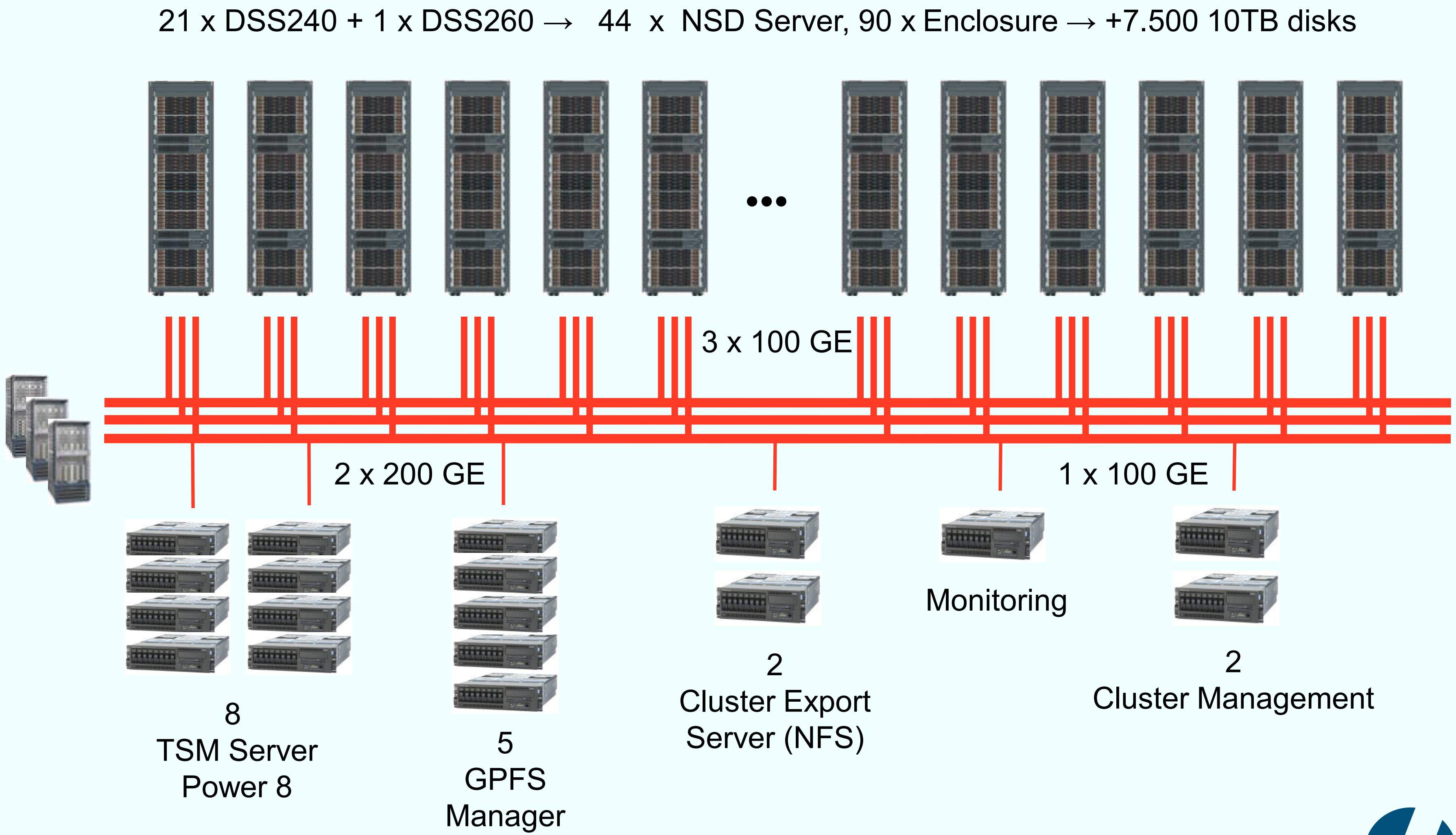



openstack
JUST
CES
$DATA
JUSTTSM
IBM Spectrum Scale (GPFS)
XCST
IBM Spectrum Scale (GPFS)
JUWELS
Disk pool
SAN
Backup
HSM
JUSTDSS
IBM Spectrum Scale (GPFS)
JURECA
Restore
Backup
NFS
$SCRATCH
$FASTDATA
$PROJECT
$ARCHIVE
$HOME
JuNet

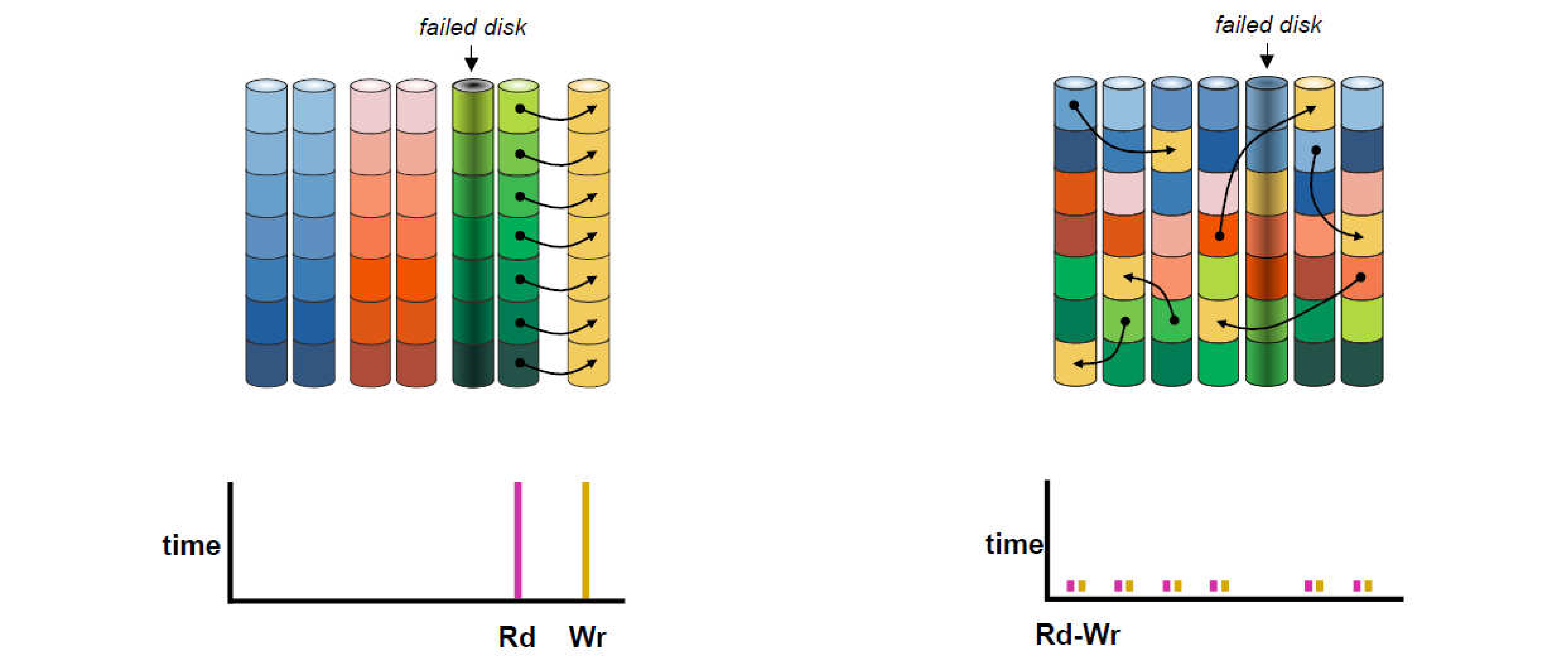
File I/O to GPFS



JUST – 5th generation



Declustered RAID



Disk failure causes disk rebuild

- Volume degraded for a long time
- performance impact for file system

Disk failure causes strips rebuild

- all disc involved
- Volume degraded for a short time
- minimized performance impact

JUST – Characteristics

Spectrum Scale (GPFS 5.0.1) + GNR (GPFS Native RAID)

- Declustered RAID technology
- End-to-End data integrity

Spectrum Protect (TSM) for Backup & HSM

Hardware:

- x86 based server + RHEL 7
- IBM Power 8 + AIX 7.2
- 100GE network fabric

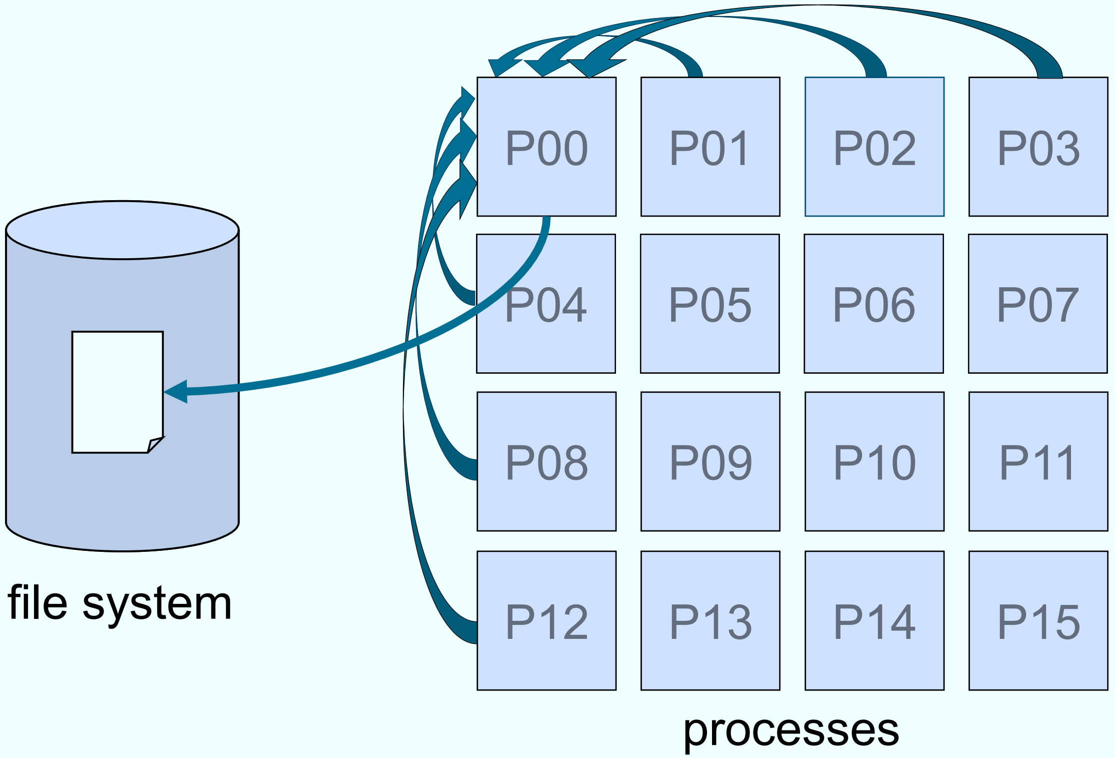
75 PB gross capacity

Bandwidth: **400 GB/s**

PARALLEL I/O STRATEGIES

Parallel I/O Strategies

One process performs I/O



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Parallel I/O Strategies

One process performs I/O

\+ Simple to implement

\- I/O bandwidth is limited to the rate of this single process

\- Additional communication might be necessary

\- Other processes may idle and waste computing resources during I/O time

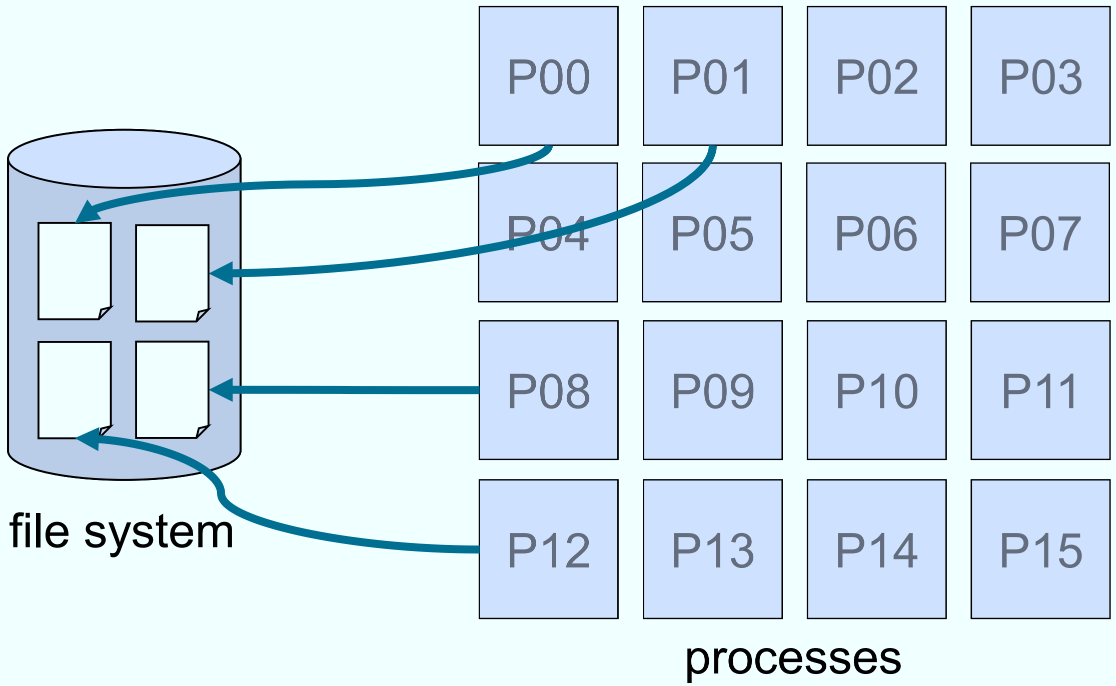
Parallel I/O Pitfalls

Frequent flushing on small blocks

- Modern file systems in HPC have **large file system blocks** (e.g. 4MB)
- 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

Parallel I/O Strategies

Task-local files



Parallel I/O Strategies

Task-local files

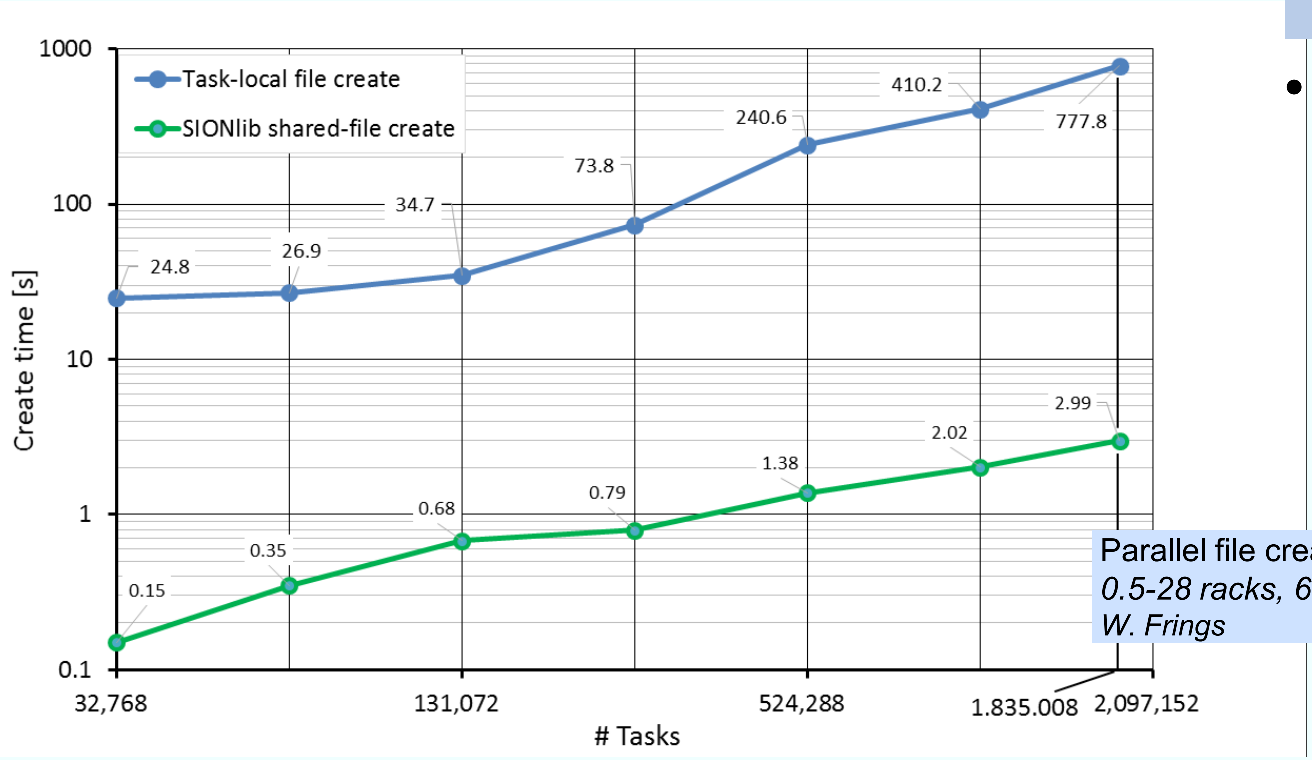
+ Simple to implement
+ No coordination between processes needed
+ No false sharing of file system blocks

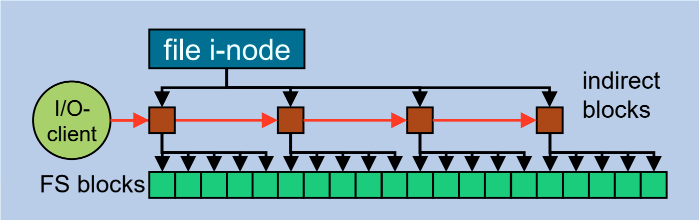
- Number of files quickly becomes unmanageable
- Files often need to be merged to create a canonical dataset
- File system might serialize meta data modification

Parallel I/O Pitfalls

Serialization of meta data modification

Example: Creating files in parallel in the same directory





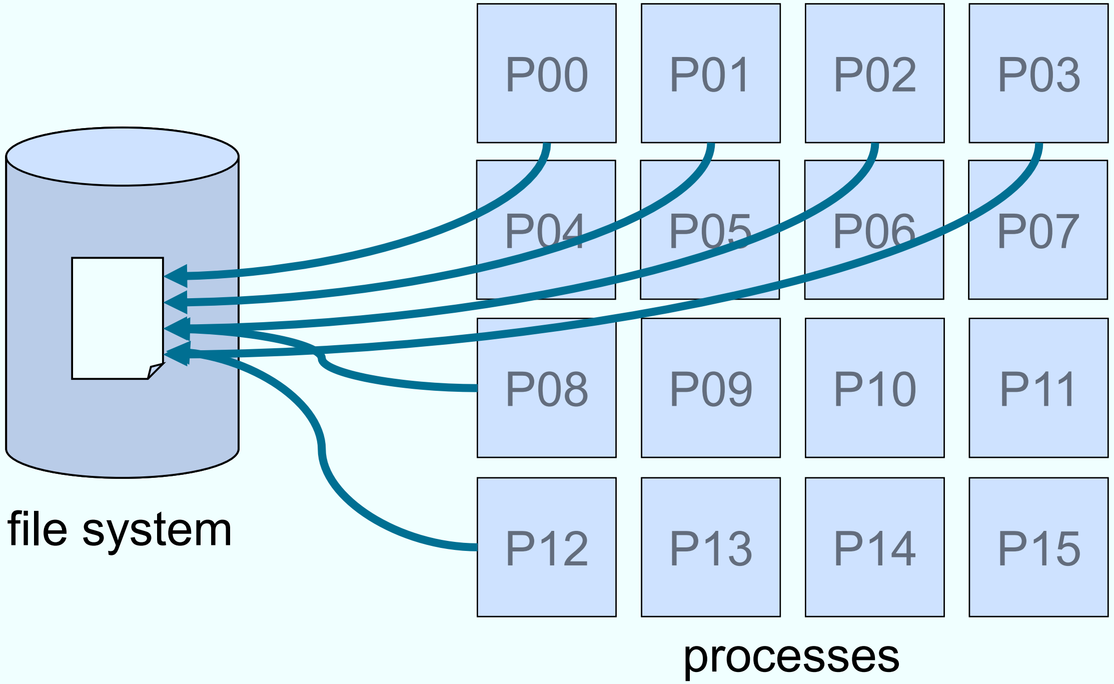
- Meta-data wall on file level
  - File changes by multiple processes can cause serialization
  - File meta-data management
  - Locking

Parallel file creation on *JUQUEEN*
0.5-28 racks, 64 tasks/node
W. Frings

The creation of 2.097.152 files costs 113.595 core hours on JUQUEEN!

Parallel I/O Strategies

Shared files



Parallel I/O Strategies

Shared files

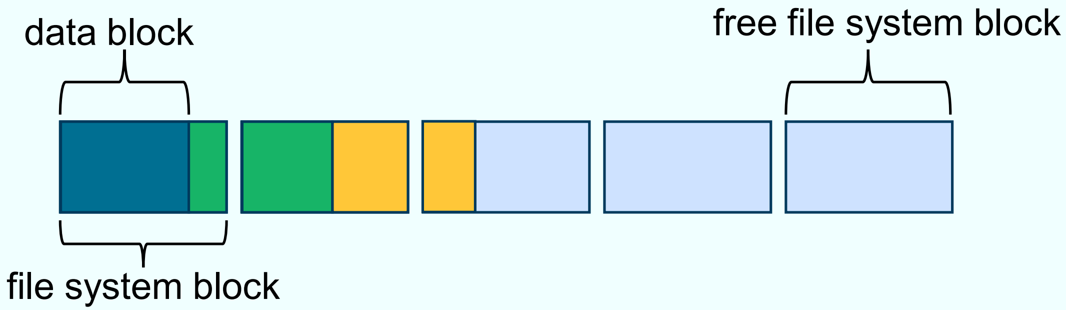
+ Number of files is independent of number of processes
+ File can be in canonical representation (no post-processing)

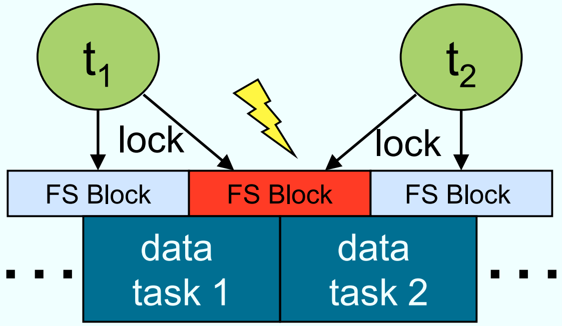
- Uncoordinated client requests might induce time penalties
- File layout may induce false sharing of file system blocks

Parallel I/O Pitfalls

False sharing of file system blocks

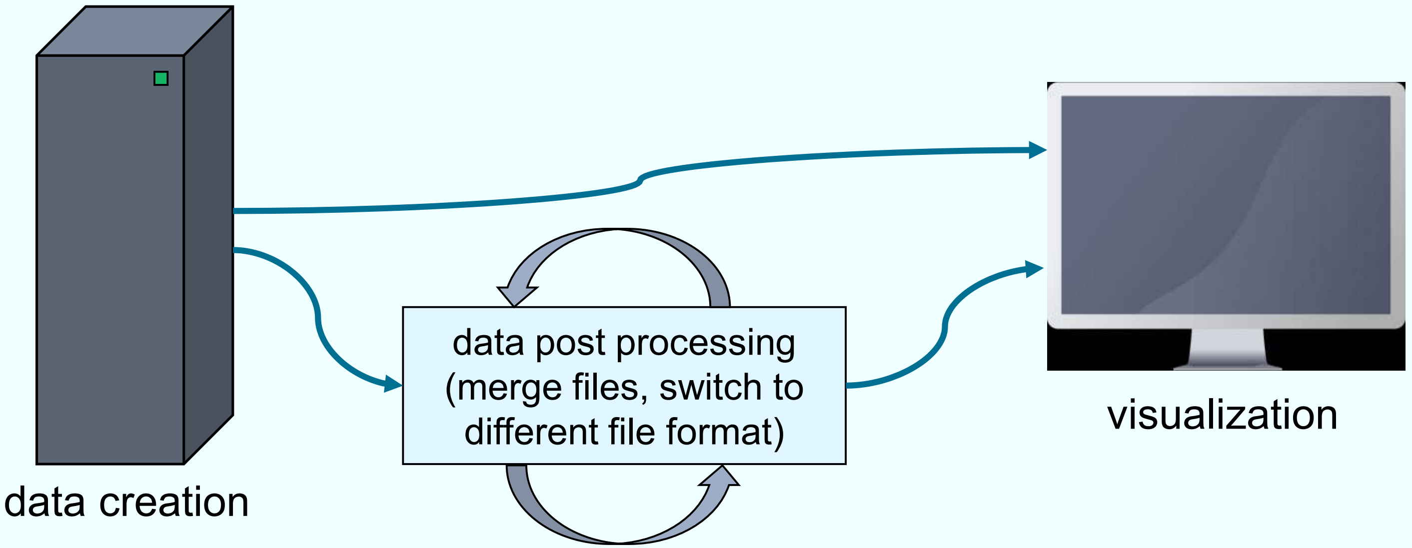
- Data blocks of individual processes do not fill up a complete file system block
- Several processes share a file system block
- Exclusive access (e.g. write) must be serialized
- The more processes have to synchronize the more waiting time will propagate





I/O Workflow

- Post processing can be very time-consuming (> data creation)
  - Widely used portable data formats avoid post processing
- Data transportation time can be long:
  - Use shared file system for file access, avoid raw data transport
  - Avoid renaming/moving of big files (can block backup)



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Parallel I/O Pitfalls

Portability

- Endianness (byte order) of binary data
- Conversion of files might be necessary and expensive

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

Parallel I/O Pitfalls

Portability

- Memory order depends on programming language
- Transpose of array might be necessary when using different programming languages in the same workflow
- Solution: Choosing a portable data format (HDF5, NetCDF)

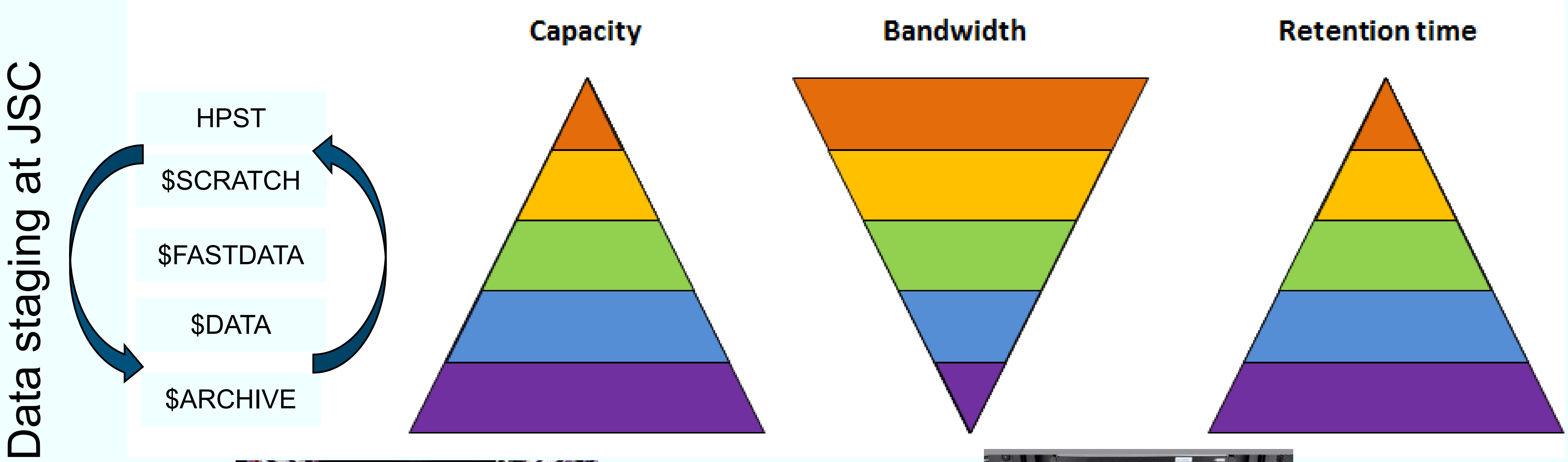
1	2	3
4	5	6
7	8	9

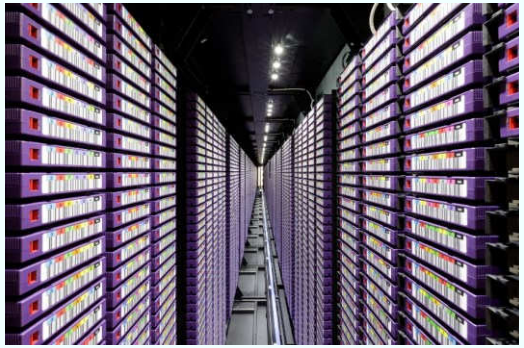
→

Address	row-major order (e.g. C/C++)	column-major order (e.g. Fortran)
1000	1	1
1001	2	4
1002	3	7
1003	4	2
1004	5	5
…	…	…

Storage Tiers

Different storage tiers with different optimization targets





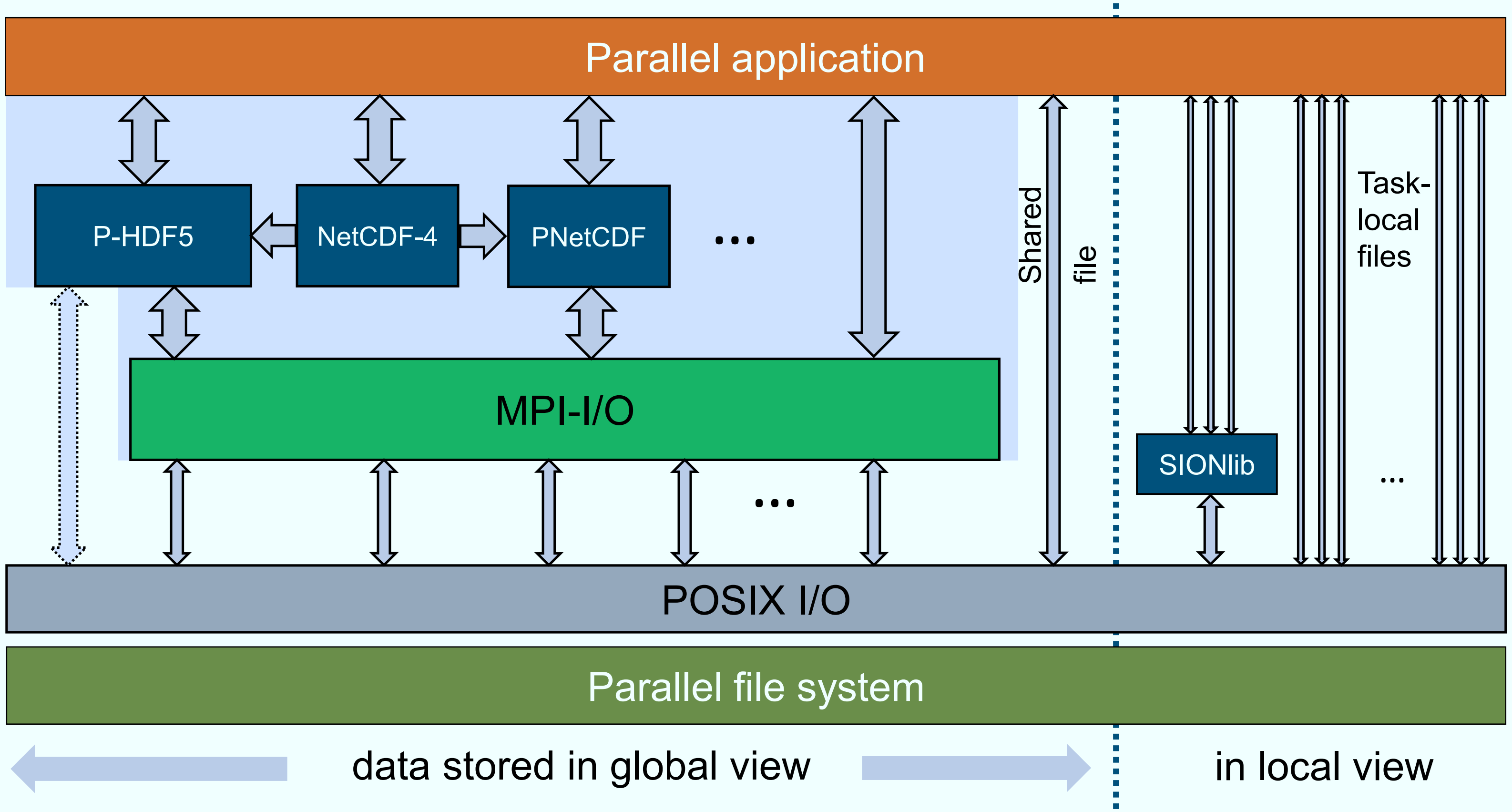
Tape Library

JUST 5

How to choose the 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”
  - External: Write/read data in non-decomposed format (portable, system-independent, self-describing)

Parallel I/O Software Stack



HANDS ON PREPARATION

HPC access

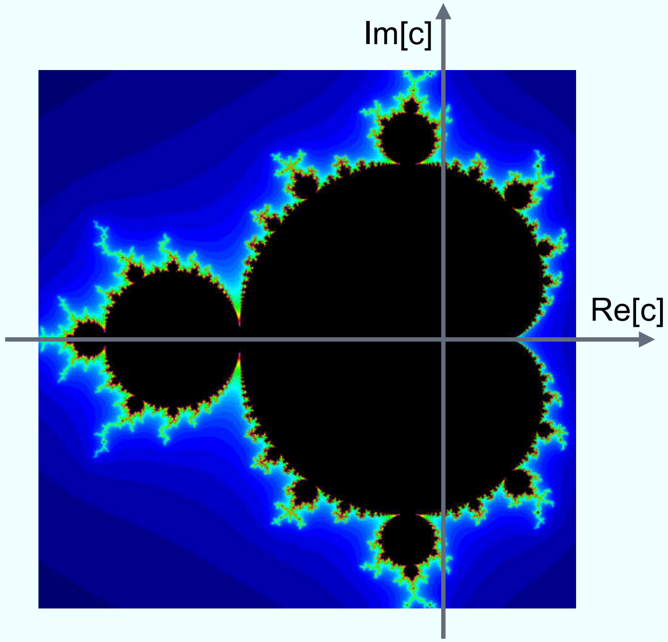
JUDOOR account and part of the training2000 project?	• Register and join the course project: **https://judoor.fz-juelich.de/projects/join/training2000**
Available SSH-Key?	• Create a new public/private Key-pair: `ssh-keygen` or use puttygen • Add the private key into your agent: ssh-add `<private_key>`
Public key on the system?	• Upload your public key via **https://judoor.fz-juelich.de** to the system
Login possible?	• Try to login: `ssh <userid>@jureca.fz-juelich.de`

Course exercise: 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



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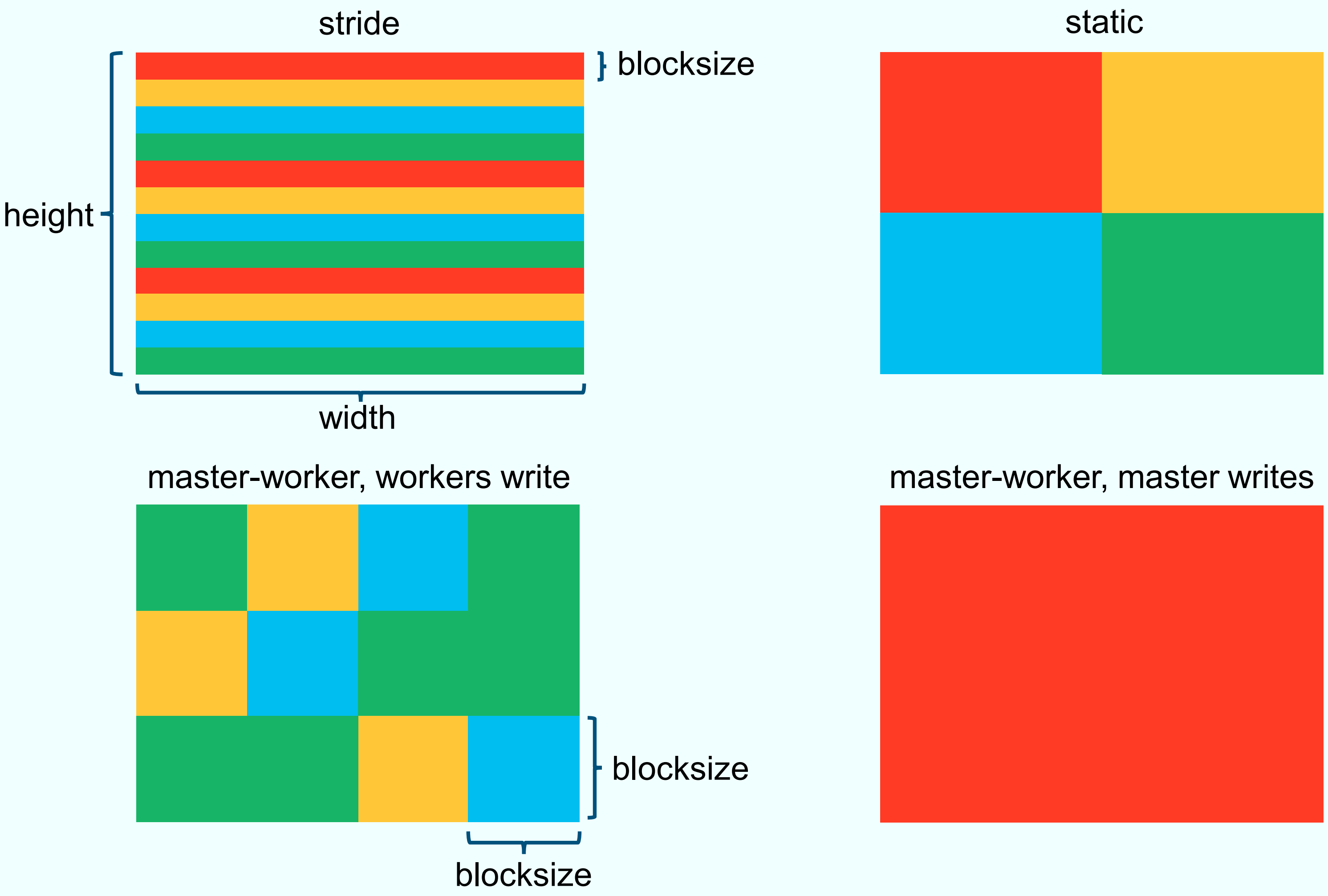
Course exercise: Mandelbrot set

- I/O comparison example
- Four different decomposition types
  - stride
  - static
  - master-worker (workers write)
  - master-worker (master writes)
- Five different output formats
  - SIONlib
  - HDF5
  - MPI-IO
  - parallel-netcdf
  - netcdf4

Decomposition types



mandelmpi

Command line options

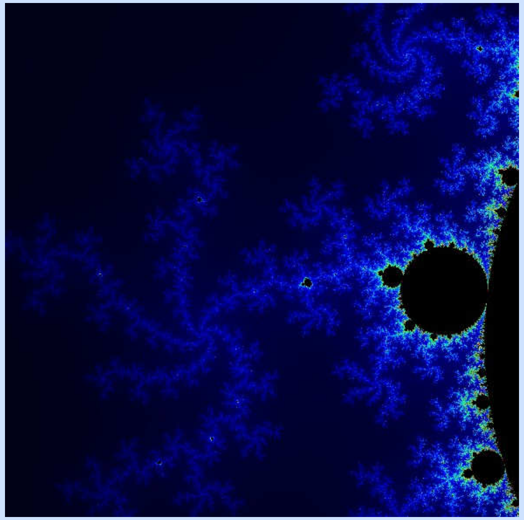
`-v`	use verbose mode
`-t`	decomposition type (`0`: stride, `1`: static, `2`: master-worker worker write, `3`: master-worker master write), default: `0`
`-w`	width, default: `256`
`-h`	height, default: `256`
`-b`	blocksize (not used for type = `1`), default: `64`
`-p`	number of procs in x-direction (only used for type = `1`)
`-q`	number of procs in y-direction (only used for type = `1`)
`-x`	coordinates of initial area: `x1 x2 y1 y2`, default: `-1.5 0.5 -1.0 1.0`
`-i`	max. iterations, default `256`
`-f`	output type (`0`: SIONlib, `1`: HDF5, `2`: MPI-IO, `3`: pnetcdf, `4`: netcdf4), default: `0`

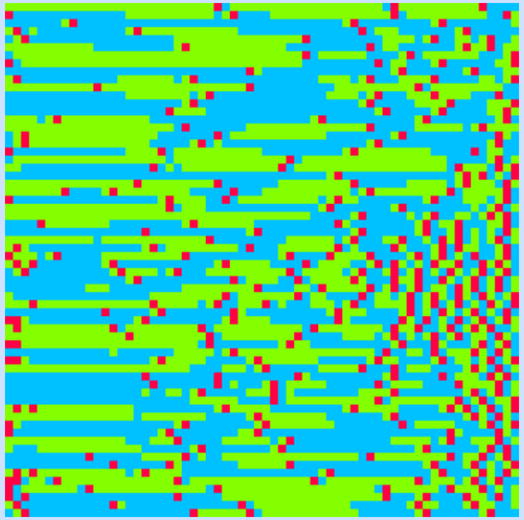
mandelseq

Command line options

`-f`	output type (`0`: SIONlib, `1`: HDF5, `2`: MPI-IO, `3`: pnetcdf, `4`: netcdf4), default: `0`

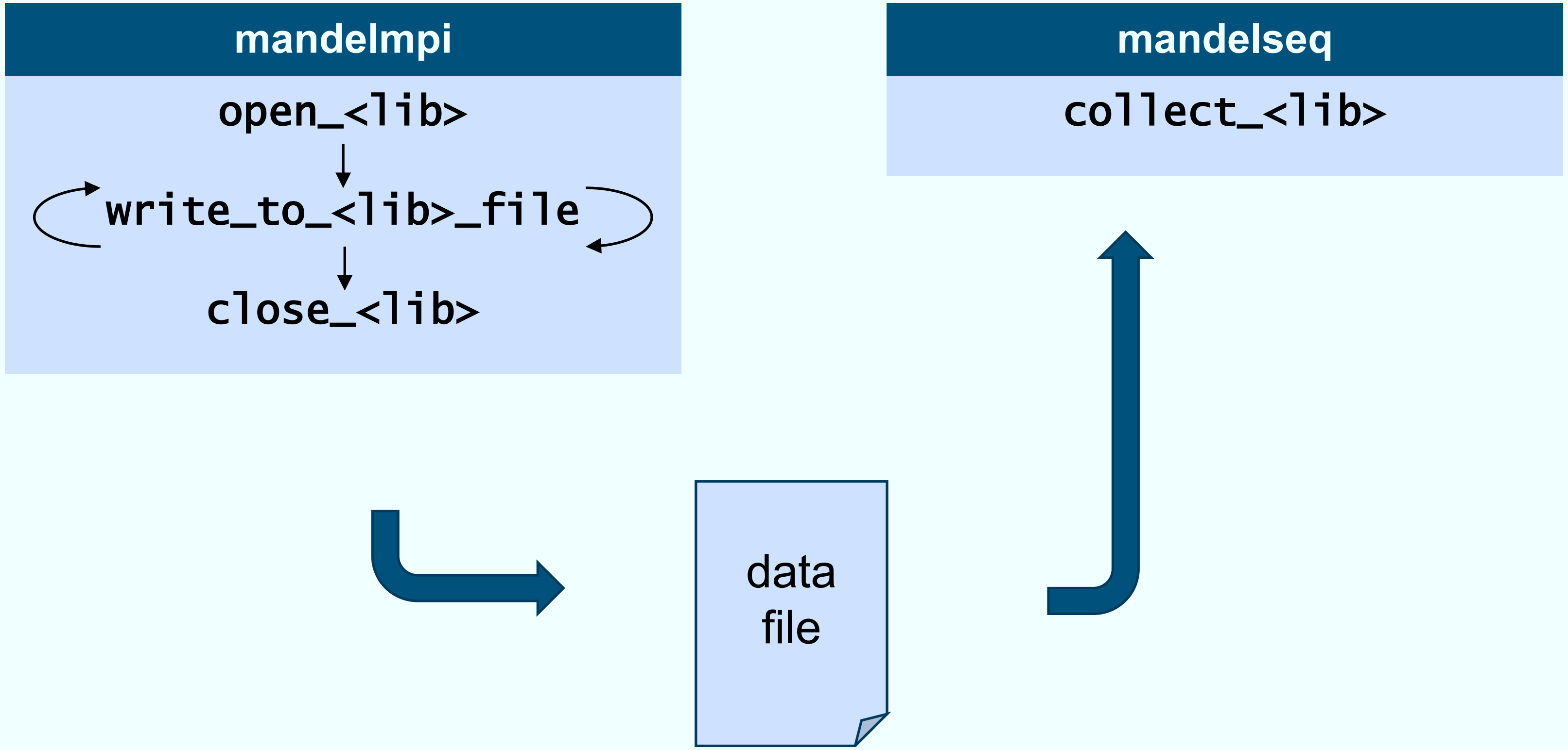
Output





process distribution image only available for SIONlib

Mandelbrot exercise workflow



Mandelbrot exercise workflow

1. Load modules

   `. load_modules_jureca.sh`

2. Run compilation

   `make`

3. Change runtime parameter in "run.job" file or use `srun`
4. Submit a job if not using `srun` directly

   `sbatch run.job`

5. Create result image

   `./mandelseq -f <format>`

6. View image (**not** in interactive session)

   `display mandelcol.ppm`

Mandelbrot exercise API

C

```c
typedef struct _infostruct
{
  int type; int width; int height;
  int numprocs;
  double xmin; double xmax; double ymin; double ymax;
  int maxiter;
} _infostruct;
```

Fortran

```fortran
type :: t_infostruct
  integer :: type, width, height
  integer :: numprocs
  real :: xmin, xmax, ymin, ymax
  integer :: maxiter
end type t_infostruct
```

Mandelbrot exercise API

C

```
void open_<lib>(<type> *fid, _infostruct *infostruct,
                int *blocksize, int *start, int rank)
```

Fortran

```
open_<lib>(fid, info, blocksize, start, rank)
  <type>, intent(out) :: fid
  type(t_infostruct), intent(in) :: info
  integer, dimension(2), intent(in) :: blocksize
  integer, dimension(2), intent(in) :: start
  integer, intent(in) :: rank
```

`fid`	lib specific file_id (can occurs twice if multiple ids needed)
`info`	global information structure
`blocksize`	chosen (or calculated) blocksizes (C: [y,x], Fortran: [x,y])
`start`	calculated start point (C: [y,x], Fortran: [x,y], starting at `0`)
`rank`	process MPI rank

Mandelbrot exercise API

C

```
void close_<lib>(<type> *fid, _infostruct *infostruct,
                 int rank)
```

Fortran

```
close_<lib>(fid, info, rank)
  <type>, intent(inout) :: fid
  type(t_infostruct), intent(in) :: info
  integer, intent(in) :: rank
```

`fid`	lib specific file_id (can occurs twice if multiple ids needed)
`info`	global information structure
`rank`	process MPI rank

Mandelbrot exercise API

C

```c
void write_to_<lib>_file(
  <type> *fid, _infostruct *infostruct, int *iterations,
  int width, int height, int xpos, int ypos)
```

Fortran

```fortran
write_to_<lib>_file(fid, info, iterations, width, height,
                    xpos, ypos)
  <type>, intent(in) :: fid
  type(t_infostruct), intent(in) :: info
  integer, dimension(:), intent(in) :: iterations
  integer, intent(in) :: width
  integer, intent(in) :: height
  integer, intent(in) :: xpos
  integer, intent(in) :: ypos
```

`iterations`	data array
`width, height`	size of current data block (pixel coordinates)
`xpos, ypos`	position of current data block (pixel coordinates starting at `0`)

Mandelbrot exercise API

C

```c
void collect_<lib>(
  int **iterations, int **proc_distribution,
  _infostruct *infostruct)
```

Fortran

```fortran
collect_<lib>(iterations, proc_distribution, info)
  integer, dimension(:), pointer :: iterations
  integer, dimension(:), pointer :: proc_distribution
  type(t_infostruct), intent(inout) :: info
```

`iterations`	data array
`proc_distribution`	process distribution array (only in Sionlib)
`info`	global information structure