Parallel I/O and Portable Data Formats

I/O strategies

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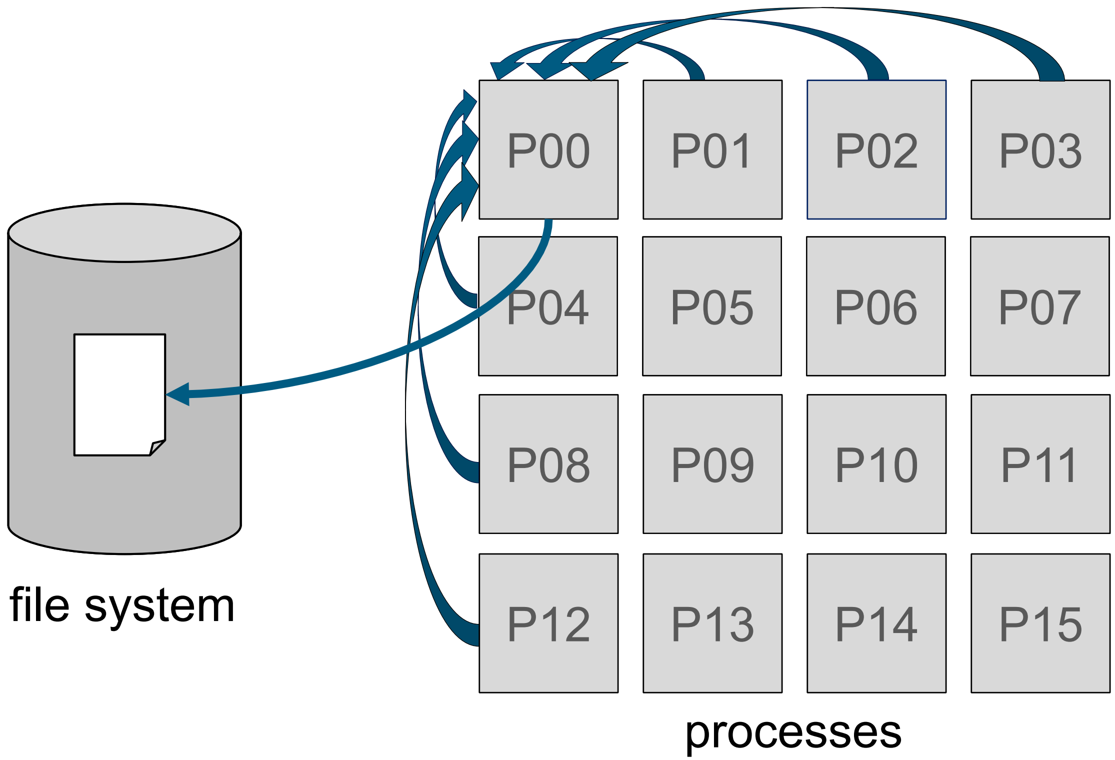
Jülich, March 12th, 2018

Outline

- Common I/O strategies
  - One process performs I/O
  - Task-local files
  - Shared files
- I/O workflow
- Pitfalls
- Parallel I/O software stack
- Course exercise description
  - General exercise workflow
  - Mandelbrot set description
  - Exercise API

One process performs I/O



One process performs I/O

+ Simple to implement

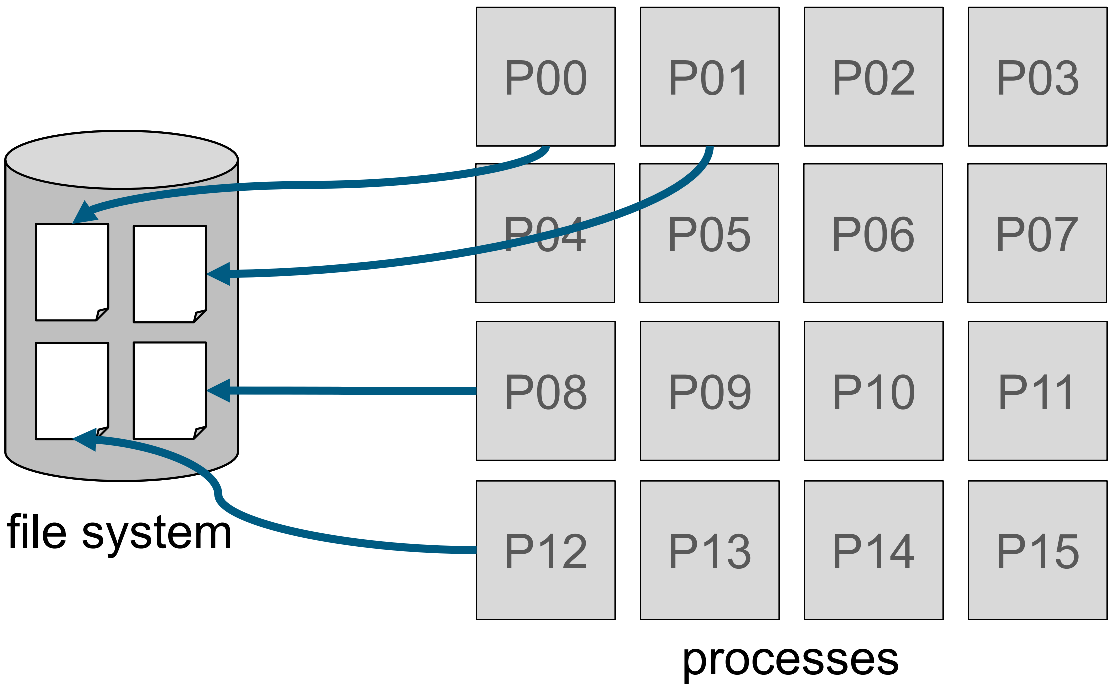
- I/O bandwidth is limited to the rate of this single process
- Additional communication might be necessary
- Other processes may idle and waste computing resources during I/O time

Frequent flushing on small blocks

Pitfall 1

- 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

Task-local files



Task-local files

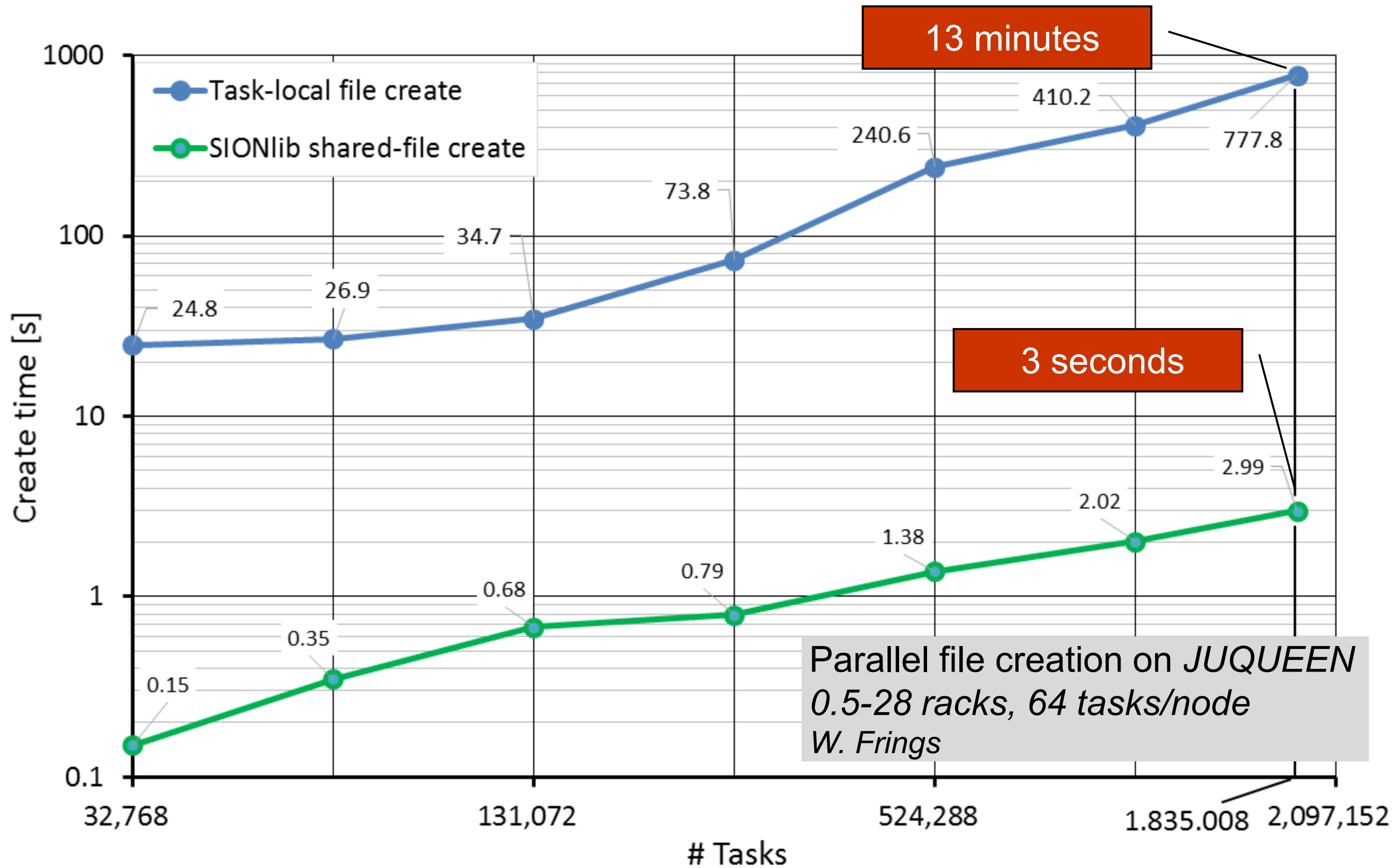
+ Simple to implement
+ No coordination between processes needed
+ No false sharing of file system blocks

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

Serialization of meta data modification

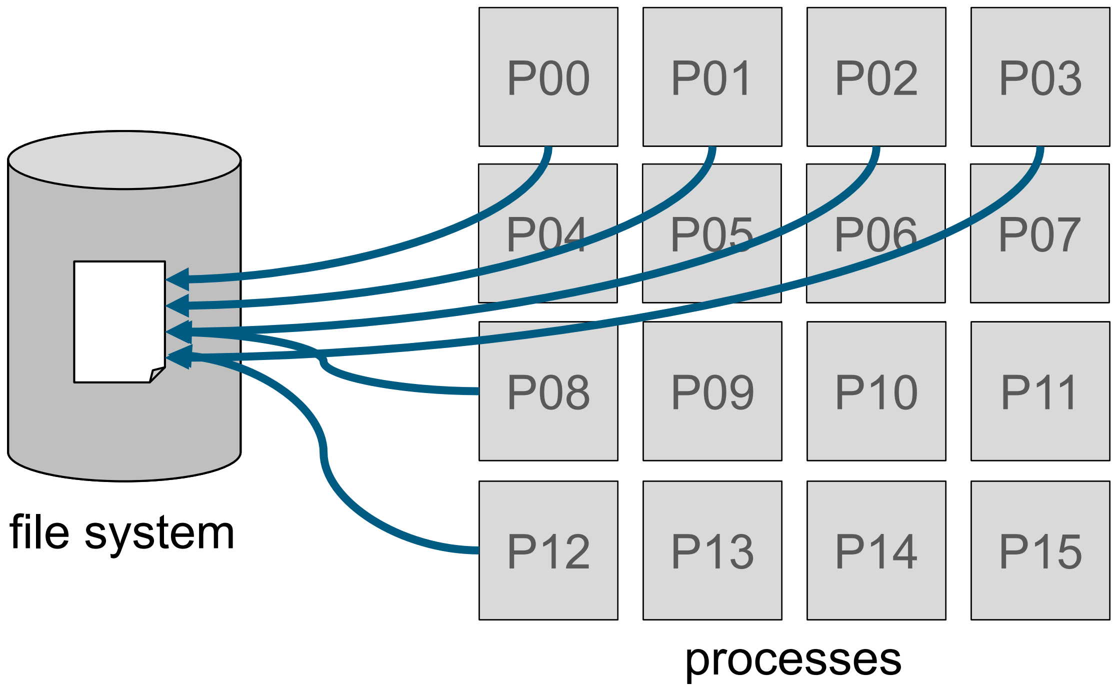
Pitfall 2

Example: Creating files in parallel in the same directory



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

Shared files

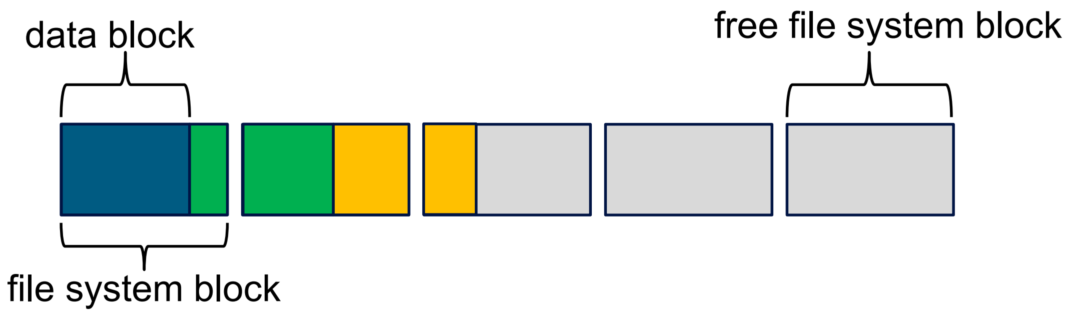


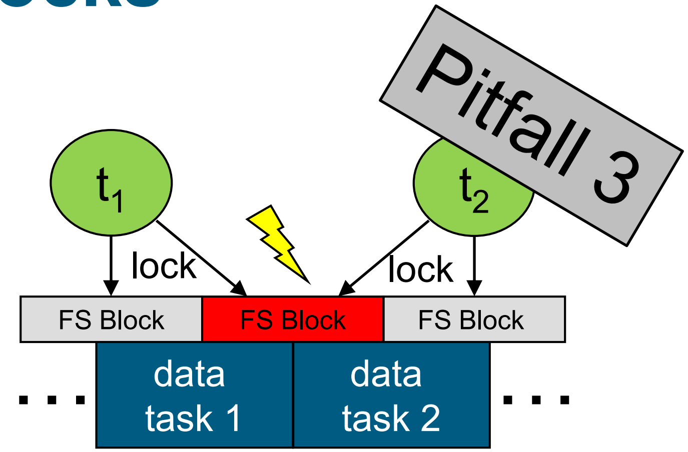
Shared files

+ 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

False sharing of file system blocks



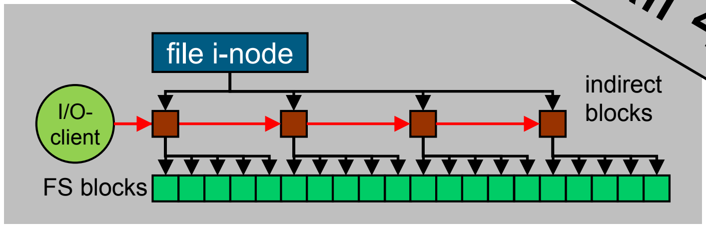


- Data blocks of individual processes **do not fill up a complete file system block**
- Several processes **share a file system block**
- Exclusive access (e.g. write) must be **serialized**
- The more processes have to synchronize the more waiting time will propagate

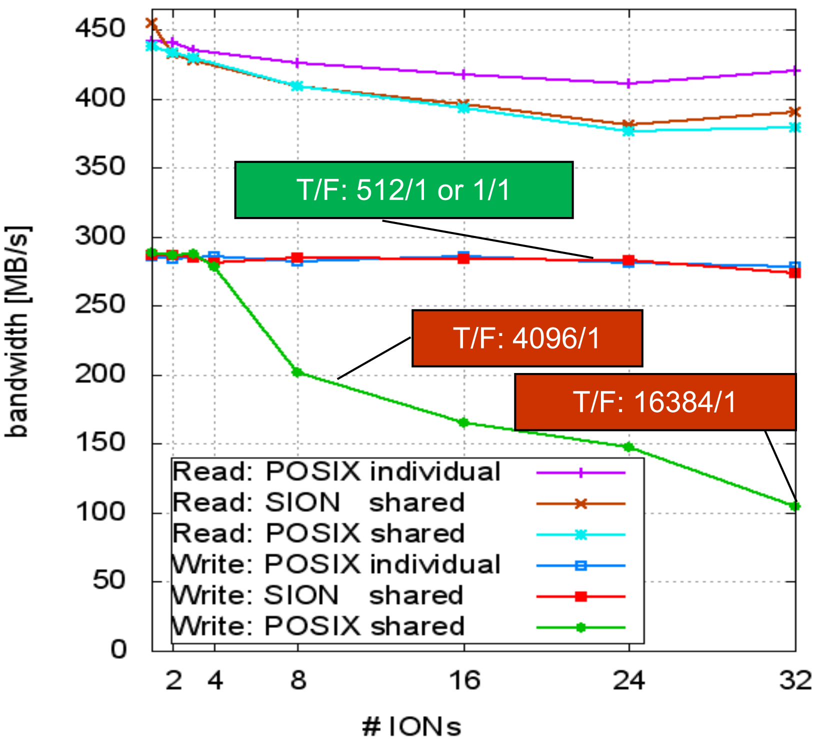
Number of Tasks per Shared File

Pitfall 4

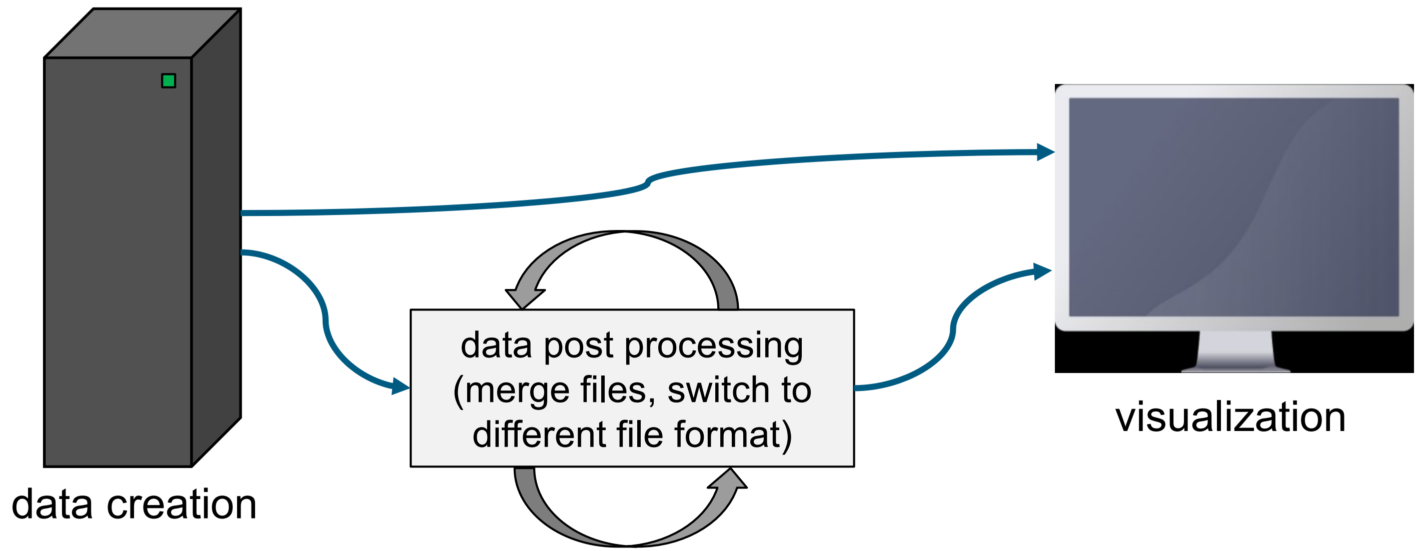
- Meta-data wall on file level
  - File meta-data management
  - Locking



- Example Blue Gene/P
  - Jugene (72 racks)
  - I/O forwarding nodes (ION)
  - GPFS client on ION
  - One file per ION



I/O Workflow

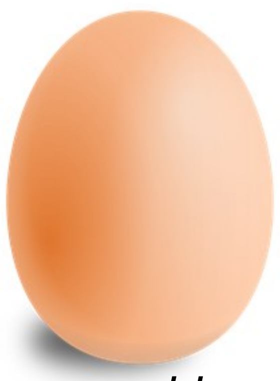


- Post processing can be very time-consuming (> data creation)
  - Widely used portable data formats avoid post processing
- Data transportation time can be long:
  - Use shared file system for file access, avoid raw data transport
  - Avoid renaming/moving of big files (can block backup)

Portability

Pitfall 5

- Endianness (byte order) of binary data



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

Portability

Pitfall 6

- Memory order depends on programming language

1	2	3
4	5	6
7	8	9

→

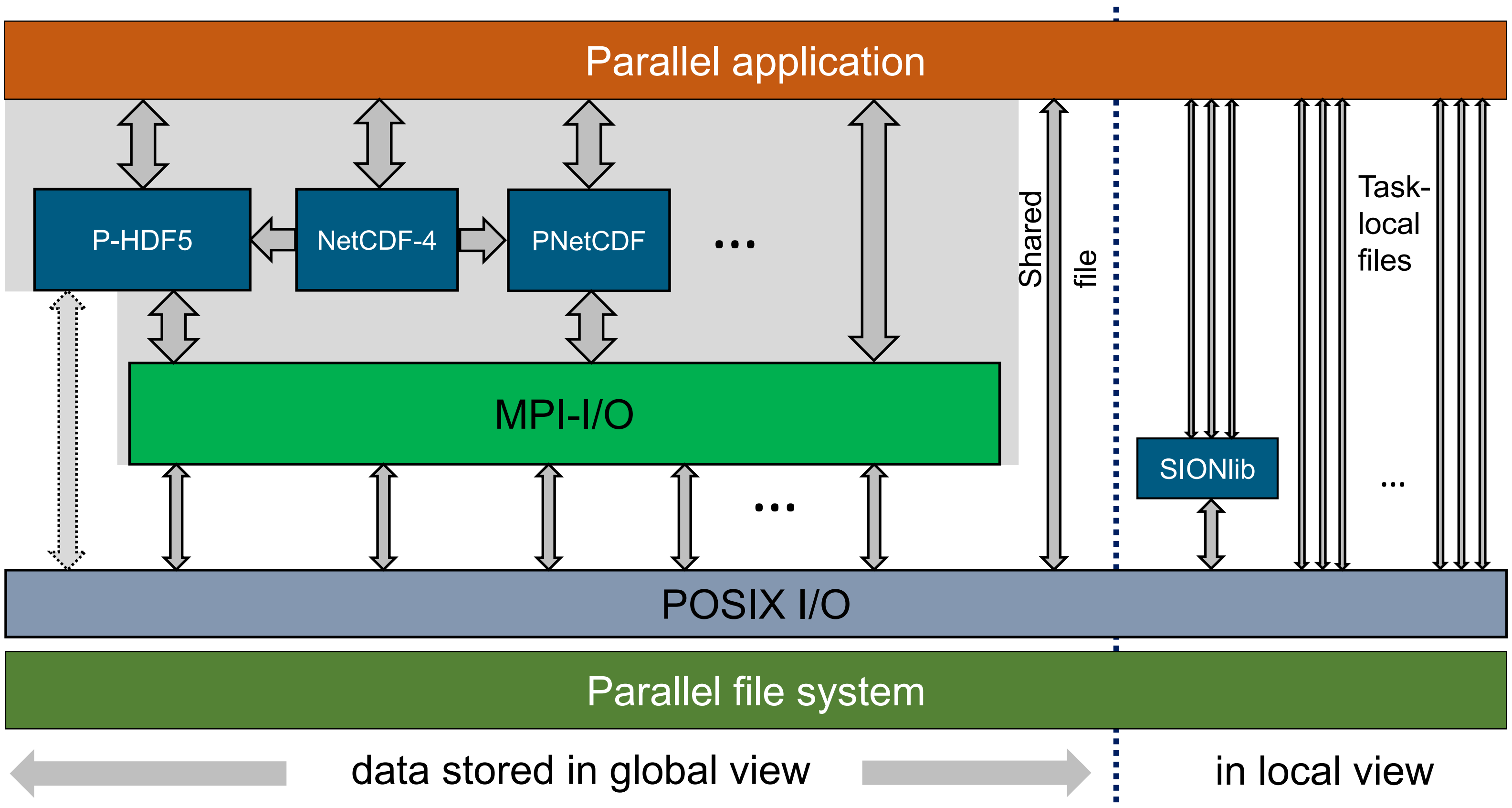
Address	row-major order (e.g. C/C++)	column-major order (e.g. Fortran)
1000	1	1
1001	2	4
1002	3	7
1003	4	2
1004	5	5
…	…	…

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

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”
    → Restart/checkpoint files
  - External: Write/read data in non-decomposed format
    (portable, system-independent, self-describing)
    → Workflows, Pre-, Post-processing, Data exchange

Parallel I/O Software Stack



General exercise workflow

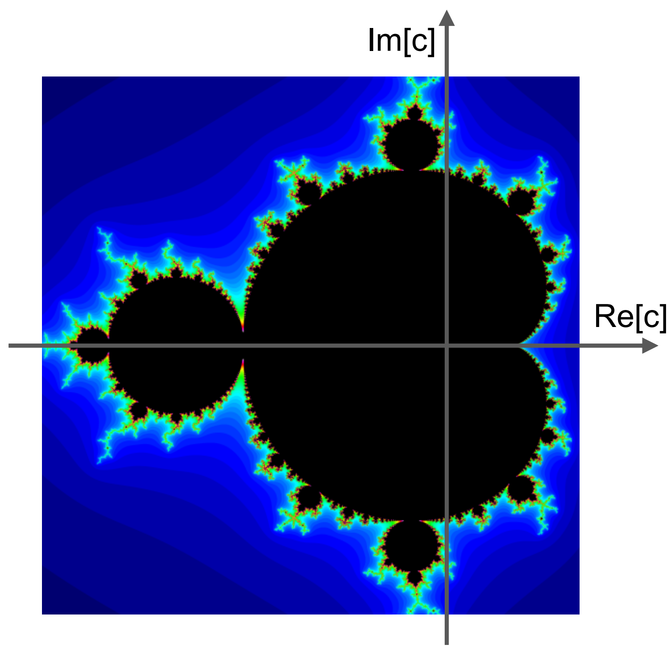
- Login to your workstation using `trainXXX` and the given password
- SSH passphrase is the same password
- Start a terminal session and login to the JURECA Cluster:
  `ssh -X jureca.fz-juelich.de`
- Use emacs or vim directly on the JURECA system to avoid copying exercise files from/to the workstation system
- Open another terminal window also connected to the JURECA system
- Start an interactive computing session:
  `salloc --reservation=parallel-io-1 --nodes=1 --time=06:00:00`
- Use the interactive session to execute jobs (using `srun`) and your first SSH session to manipulate your files
- You will find exercise and solution files in:
  `/work/hpclab/train112`

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

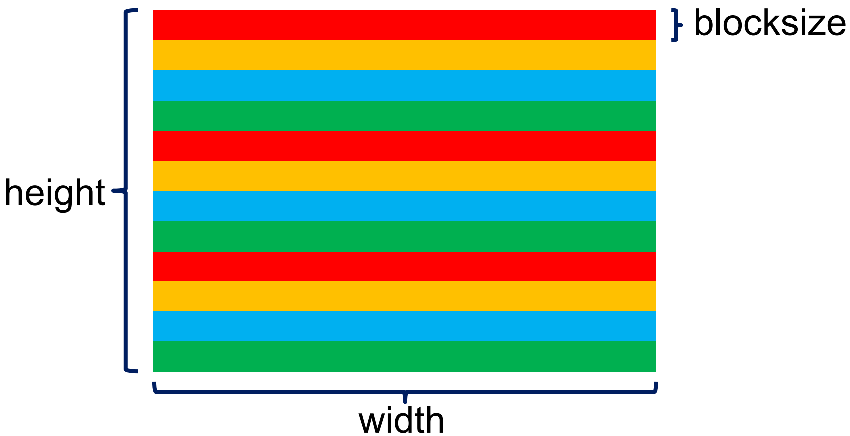


Course exercise: Mandelbrot set

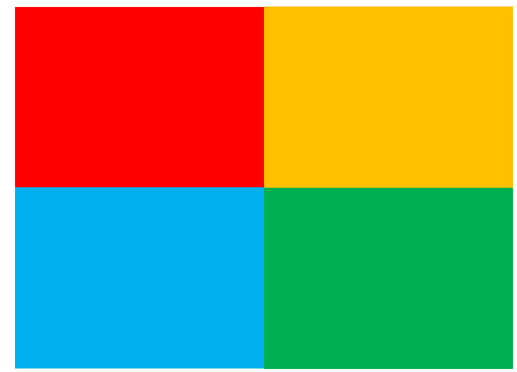
- I/O comparison example
- Four different decomposition types
  - stride
  - static
  - master-worker (workers write)
  - master-worker (master writes)
- Five different output formats
  - SIONlib
  - HDF5
  - MPI-IO
  - parallel-netcdf
  - netcdf4
- Two different programs
  - `mandelmpi`: parallel Mandelbrot calculation
  - `mandelseq`: serial output picture generation

Decomposition types

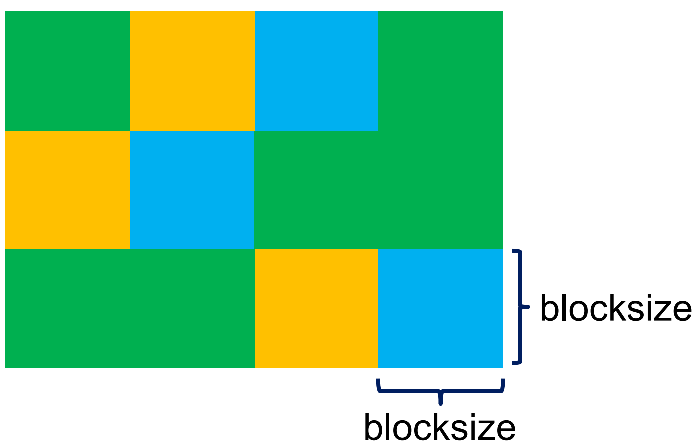
stride



static



master-worker, workers write



master-worker, master writes

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`

mandelmpi

Example output

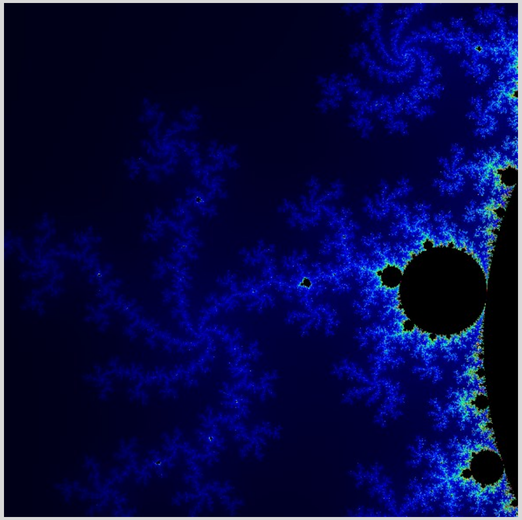
```
using SIONlib
start calculation (x= -0.59 .. -0.54,y= -0.58 .. -0.53)
calc_master[00]: 4096x4096
calc_worker[01]: 64x64
calc_worker[02]: 64x64
calc_worker[03]: 64x64

PE 00 of 04: t= 2 4096 x 4096 bs= 64 calc=   50.859, wait= 26.326,
        io= 716.462, mpi= 7893.249, runtime= 8687.163 (ms)

PE 01 of 04: t= 2 4096 x 4096 bs= 64 calc= 5749.752, wait= 25.301,
        io= 805.705, mpi= 2047.276, runtime= 8688.862 (ms)

PE 02 of 04: t= 2 4096 x 4096 bs= 64 calc= 2651.758, wait= 28.214,
        io= 744.241, mpi= 5258.484, runtime= 8693.876 (ms)

PE 03 of 04: t= 2 4096 x 4096 bs= 64 calc= 4631.728, wait= 42.970,
        io= 793.272, mpi= 3196.786, runtime= 8695.410 (ms)
```

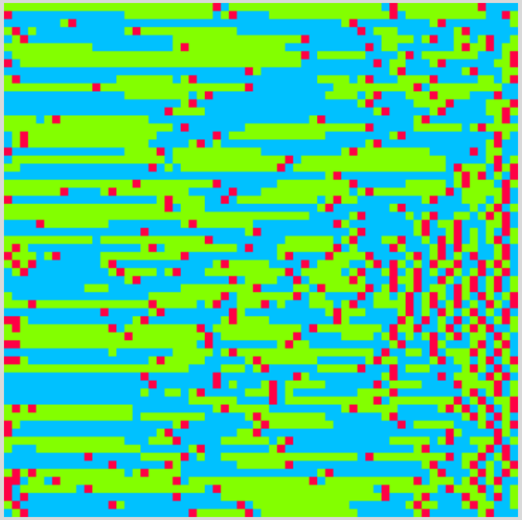
mandelseq

Command line options

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

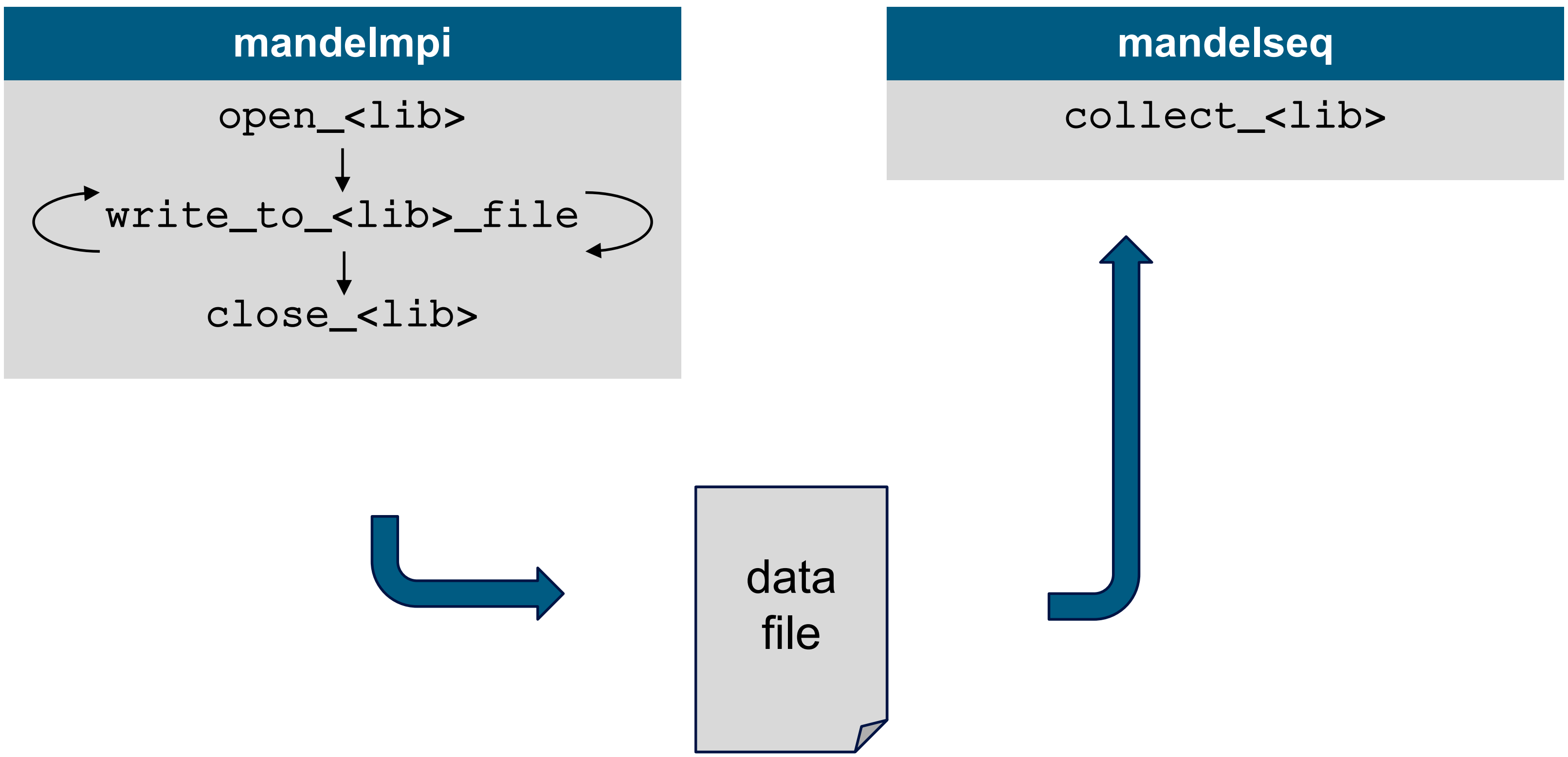
Output





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` directly in your interactive session
4. Submit a job if not using an interactive session
   `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

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

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

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

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

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