Parallel HDF5

Matthieu Haefele, CNRS/UPPA

Saclay, June 2024

HPC machine architecture

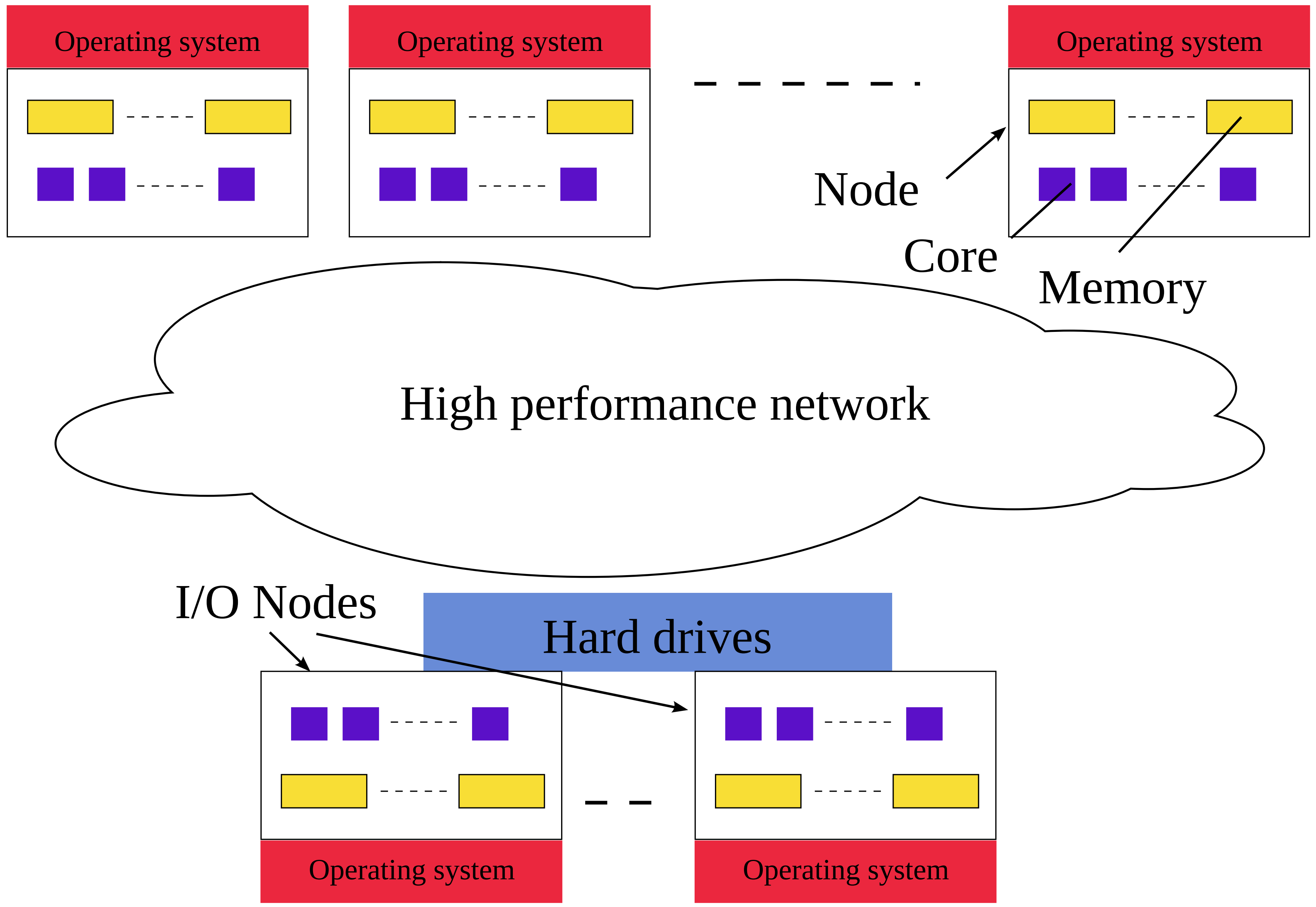
An HPC machine is composed of processing elements or cores which

- Can access a central memory
- Can communicate through a high performance network
- Are connected to a high performance storage system

Until now, two major families of HPC machines existed:

- Shared memory machines
- Distributed memory machines

Distributed memory machines



MPI: Message Passing Interface

MPI is an Application Programming Interface

- Defines a standard for developing parallel applications
- Several implementations exists (openmpi, mpich, IBM, Par-Tec…)

It is composed of

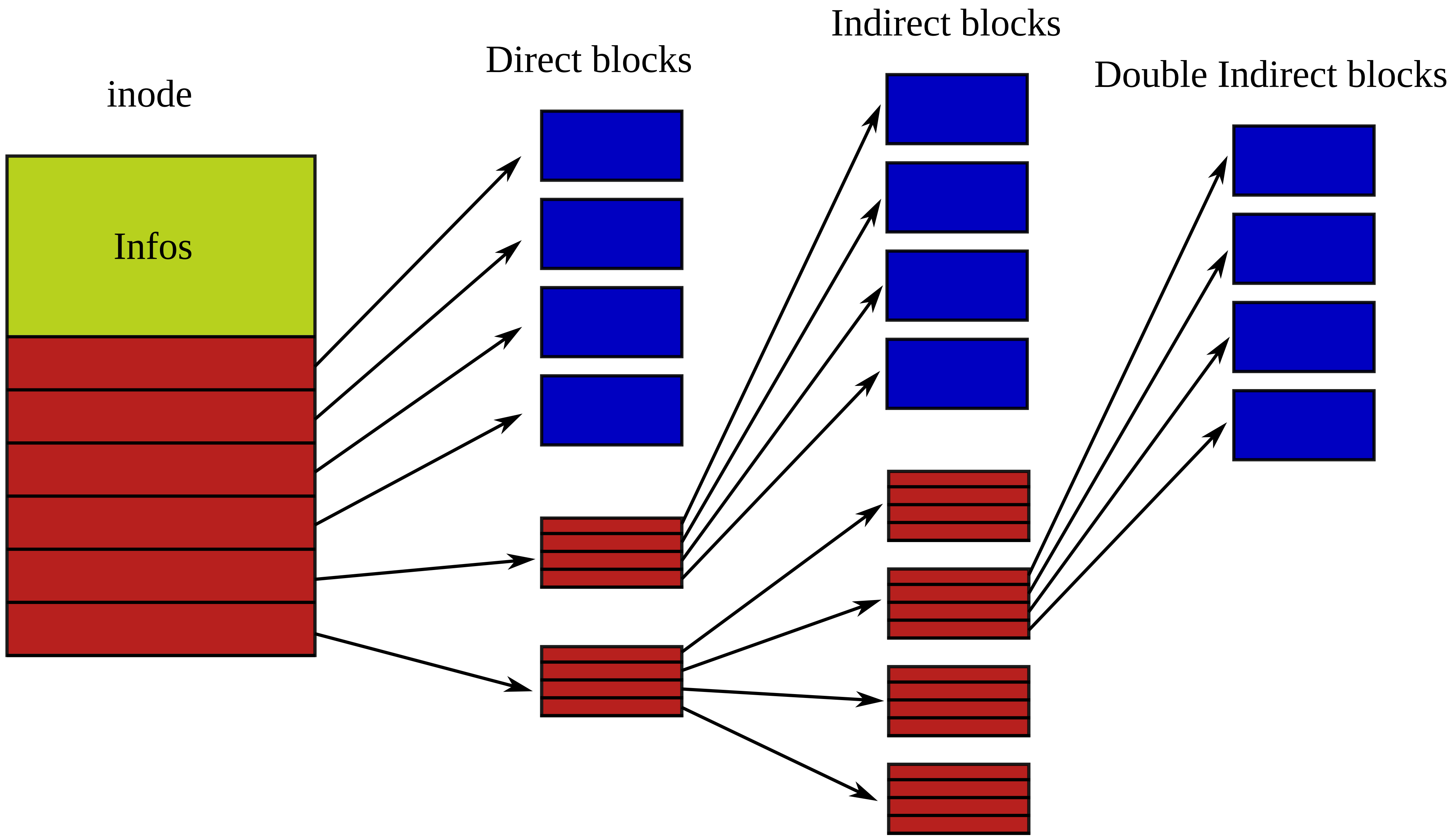
- A parallel execution environment
- A library to link the application with

MPI communications

Four classes of communications

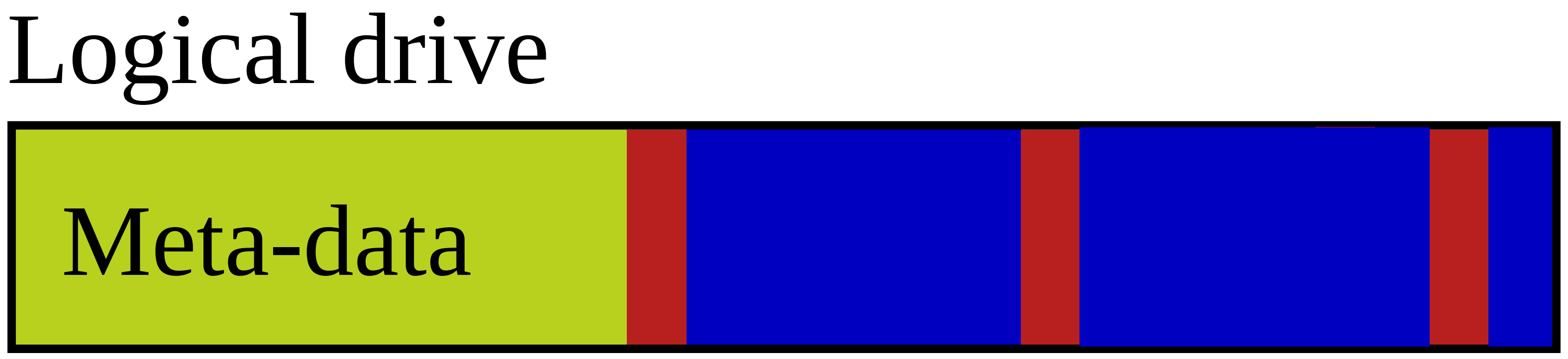
- **Collective**: all processes belonging to a same MPI communicator communicates together according to a defined pattern (scatter, gather, reduce, …)
- **Point-to-Point**: one process sends a message to another one (send, receive)
- For both Collective or Point-to-Point, **blocking and non-blocking** functions are available

inode pointer structure (ext3)

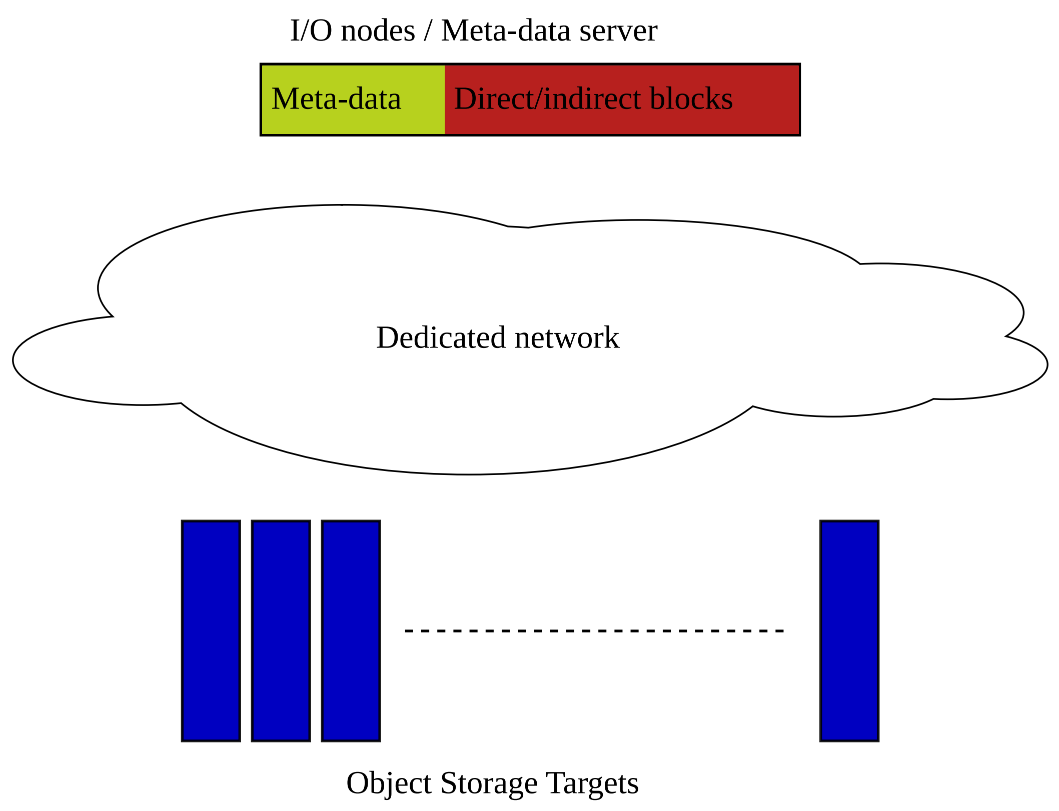


“Serial” file system

Meta-data, block address and file blocks are stored a single logical drive with a “serial” file system

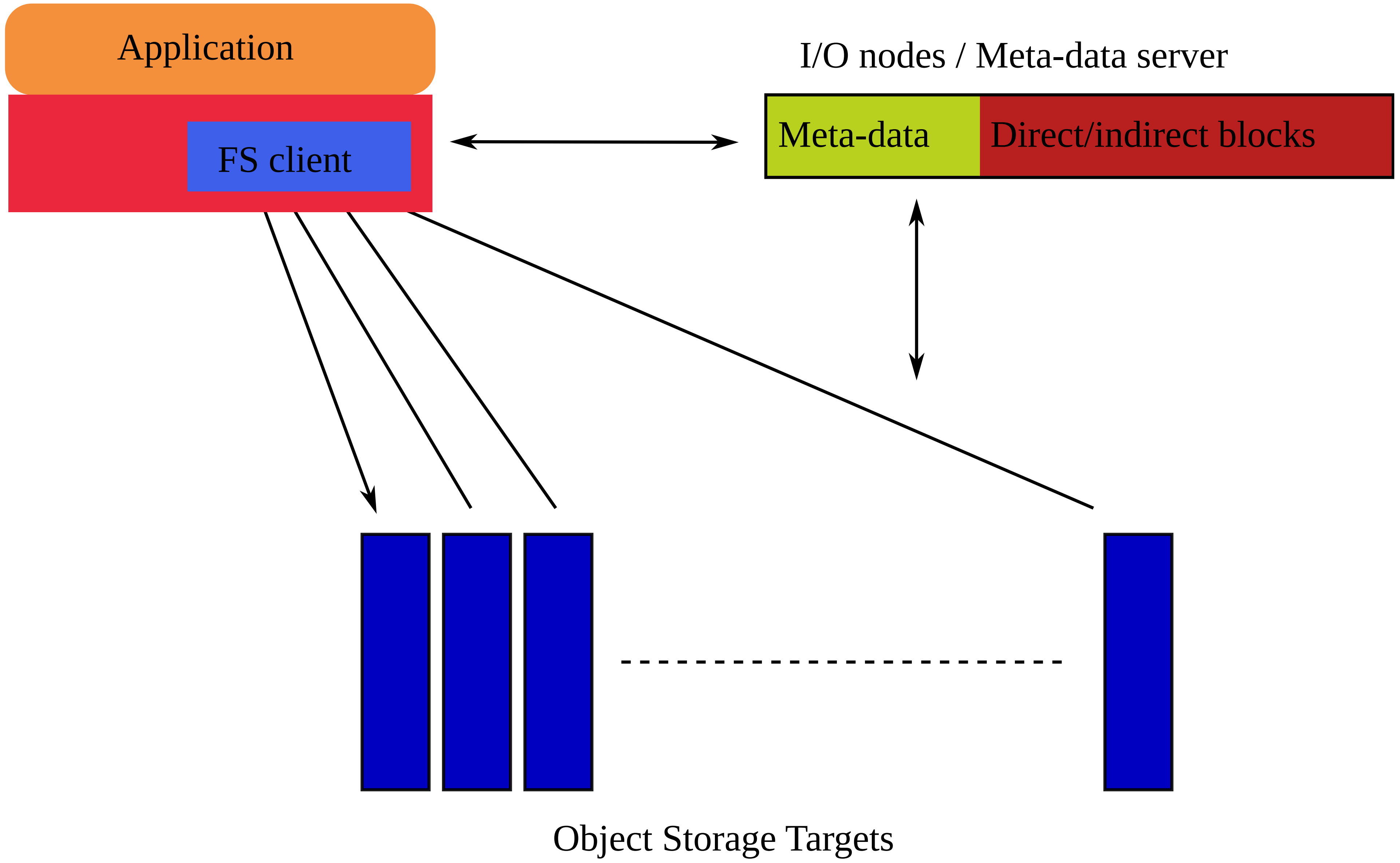


Parallel file system architecture

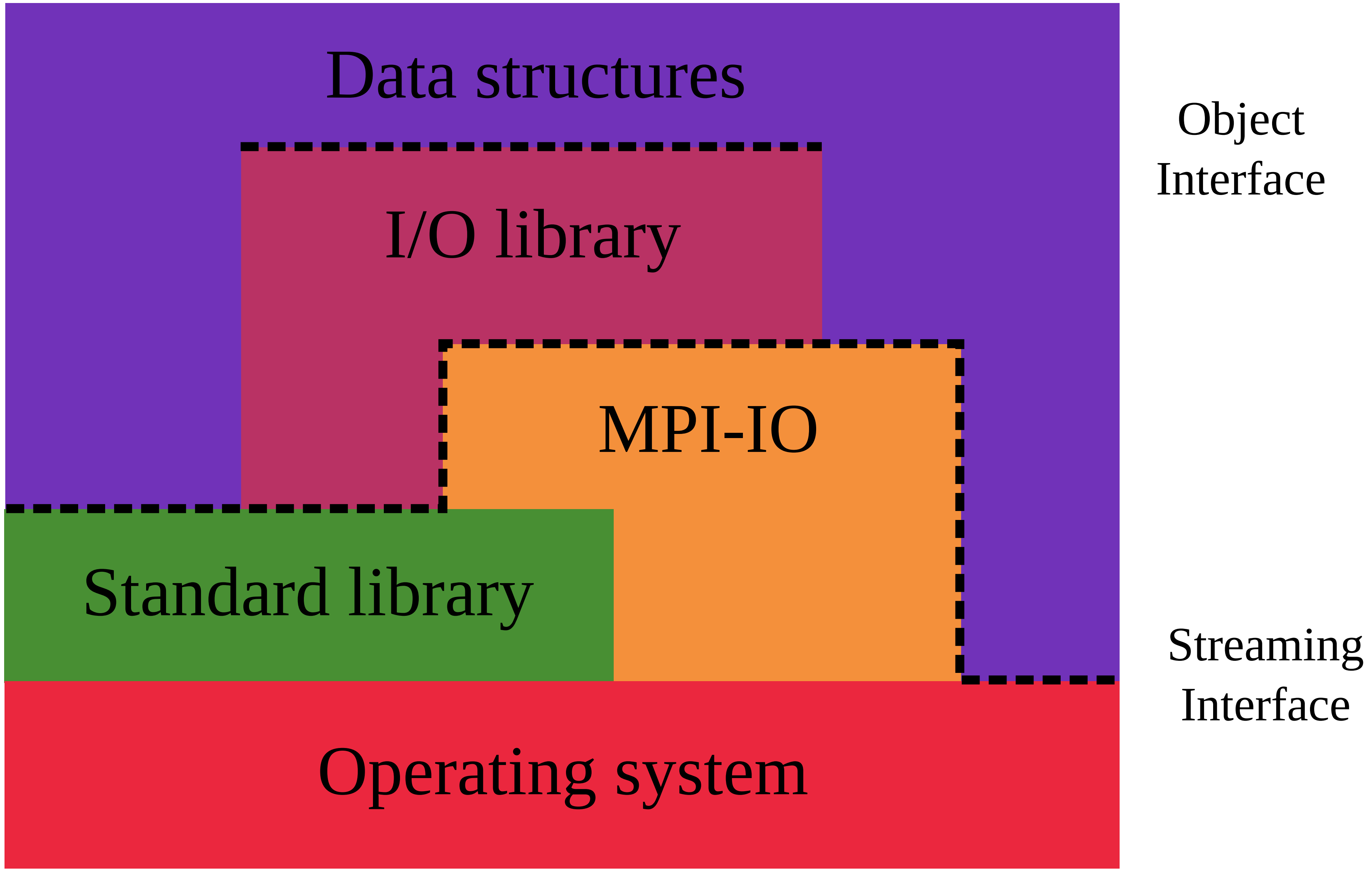


- Meta-data and file blocks are stored on separate devices
- Several devices are used
- Bandwidth is aggregated
- A file is **striped** across different object storage targets.

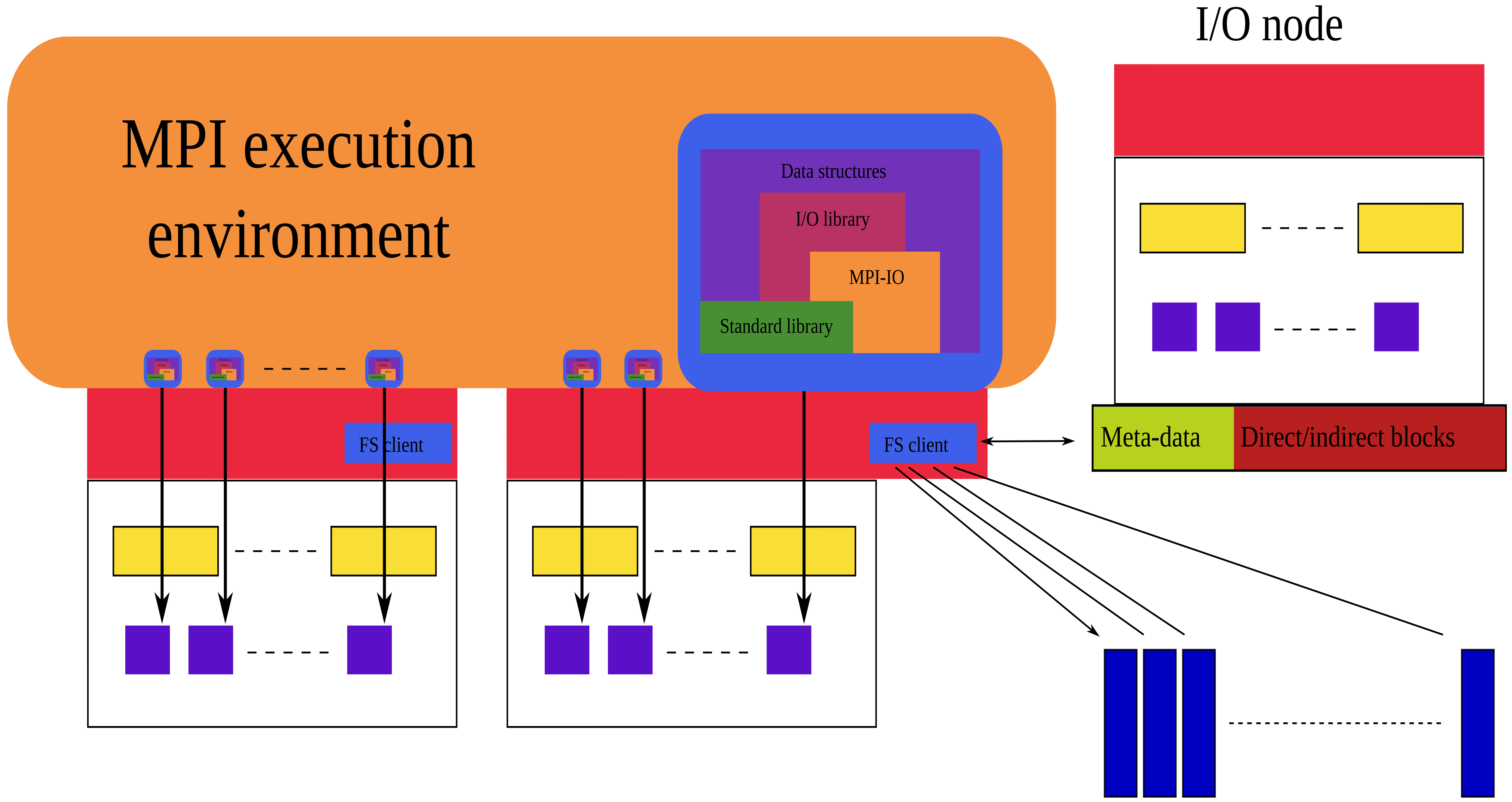
Parallel file system usage



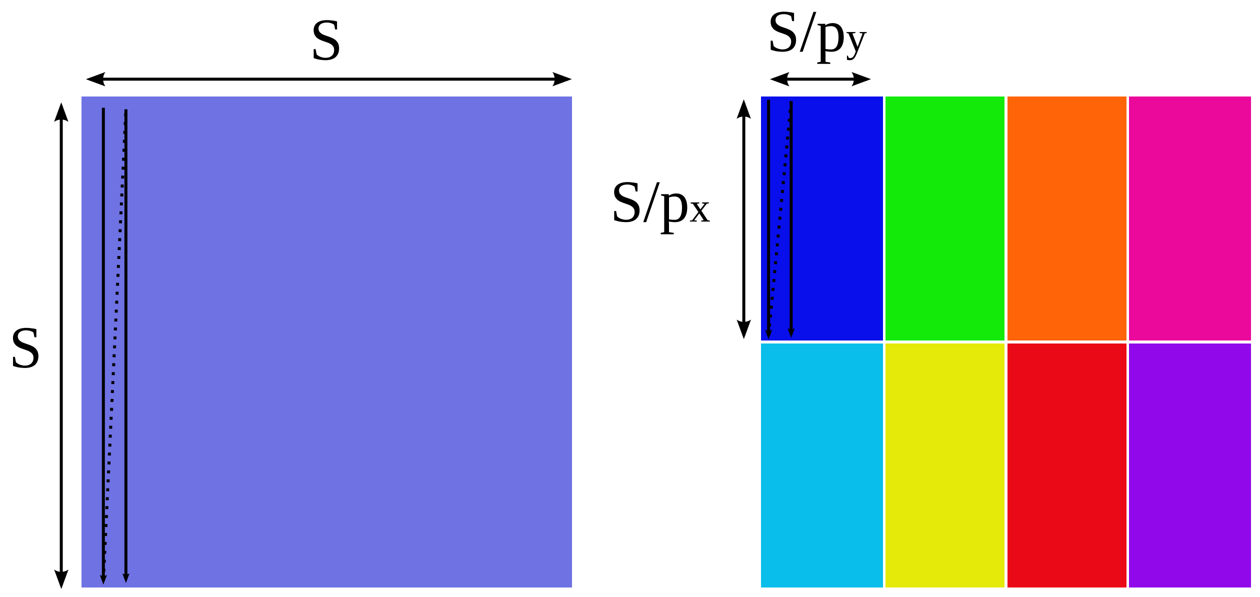
The software stack



Let us put everything together



Test case to illustrate strategies



Let us consider:

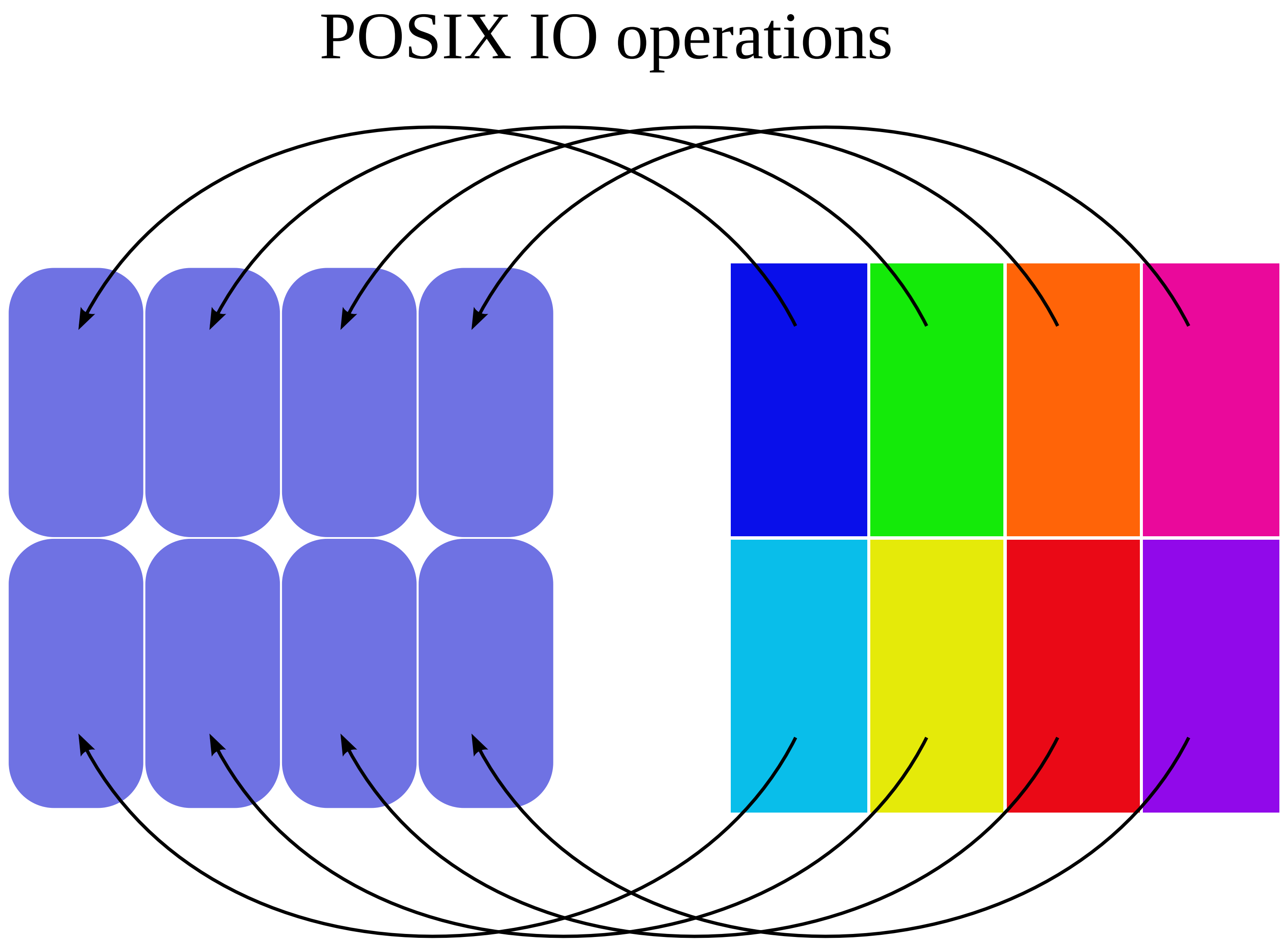
- A 2D structured array
- The array is of size $S \times S$
- A block-block distribution is used
- With $P = p_x p_y$ cores

Multiple files

Each MPI process writes its own file

- A single distributed data is spread out in different files
- The way it is spread out depends on the number of MPI processes

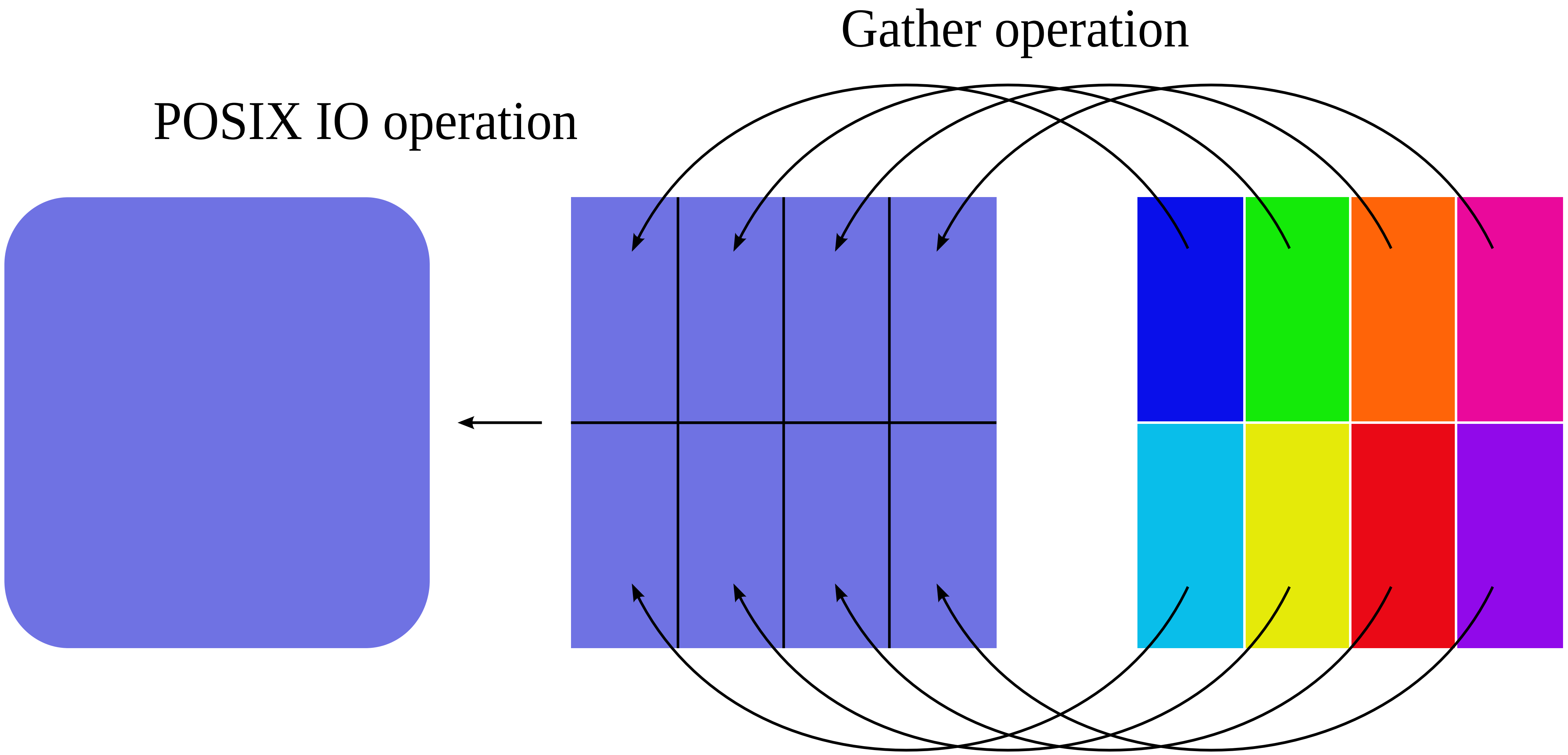
Multiple files



MPI gather + single file

A collective MPI call is first performed to gather the data on one MPI process. Then, this process writes a single file

MPI Gather + single file



MPI-IO concept

- I/O part of the MPI specification
- Provide a set of read/write methods
- Allow one to describe how a data is distributed among the processes (thanks to MPI derived types)
- MPI implementation takes care of actually writing a single contiguous file on disk from the distributed data
- Result is identical as the gather + POSIX file

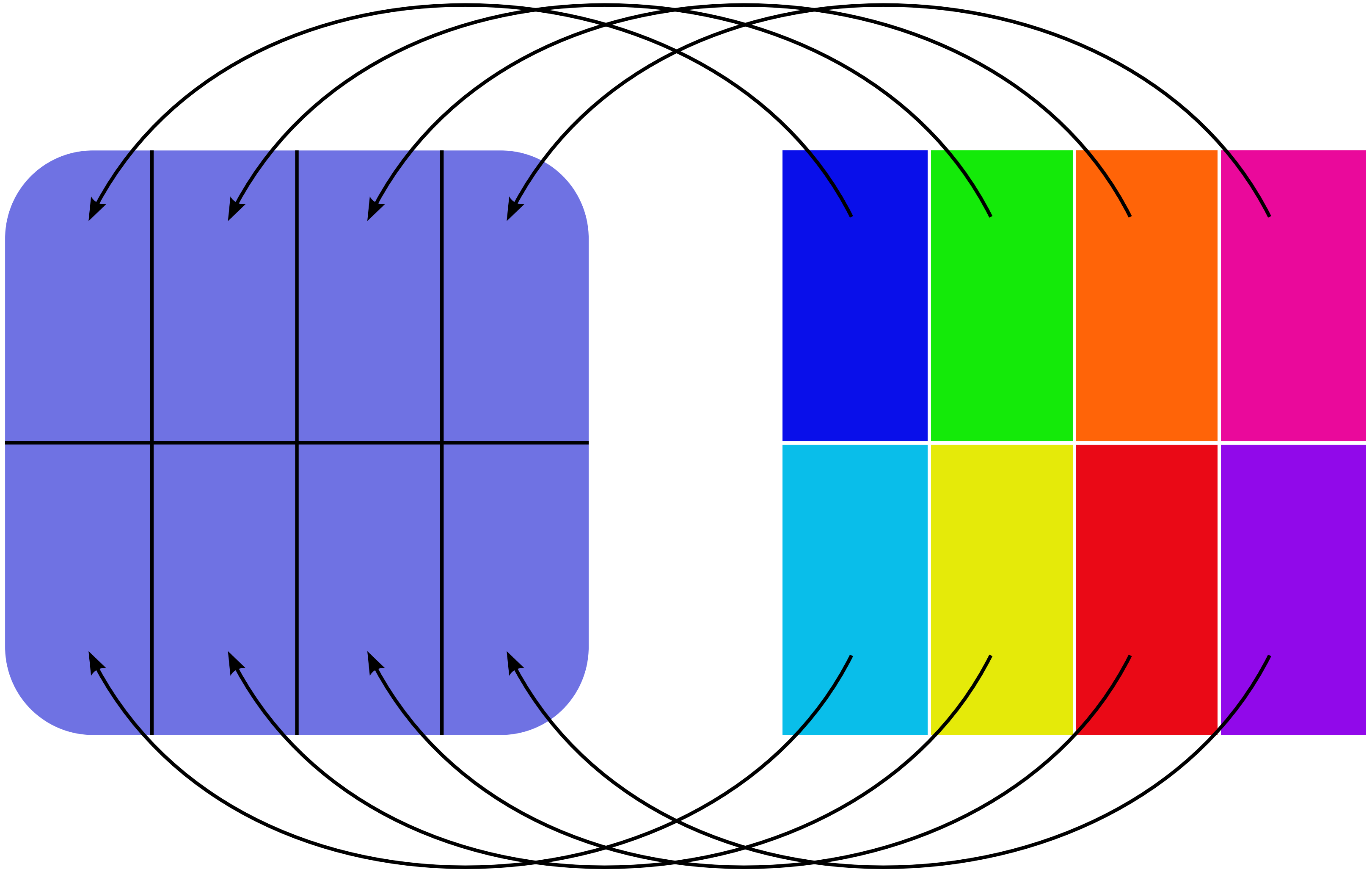
MPI-IO API

Level 0 Level 1

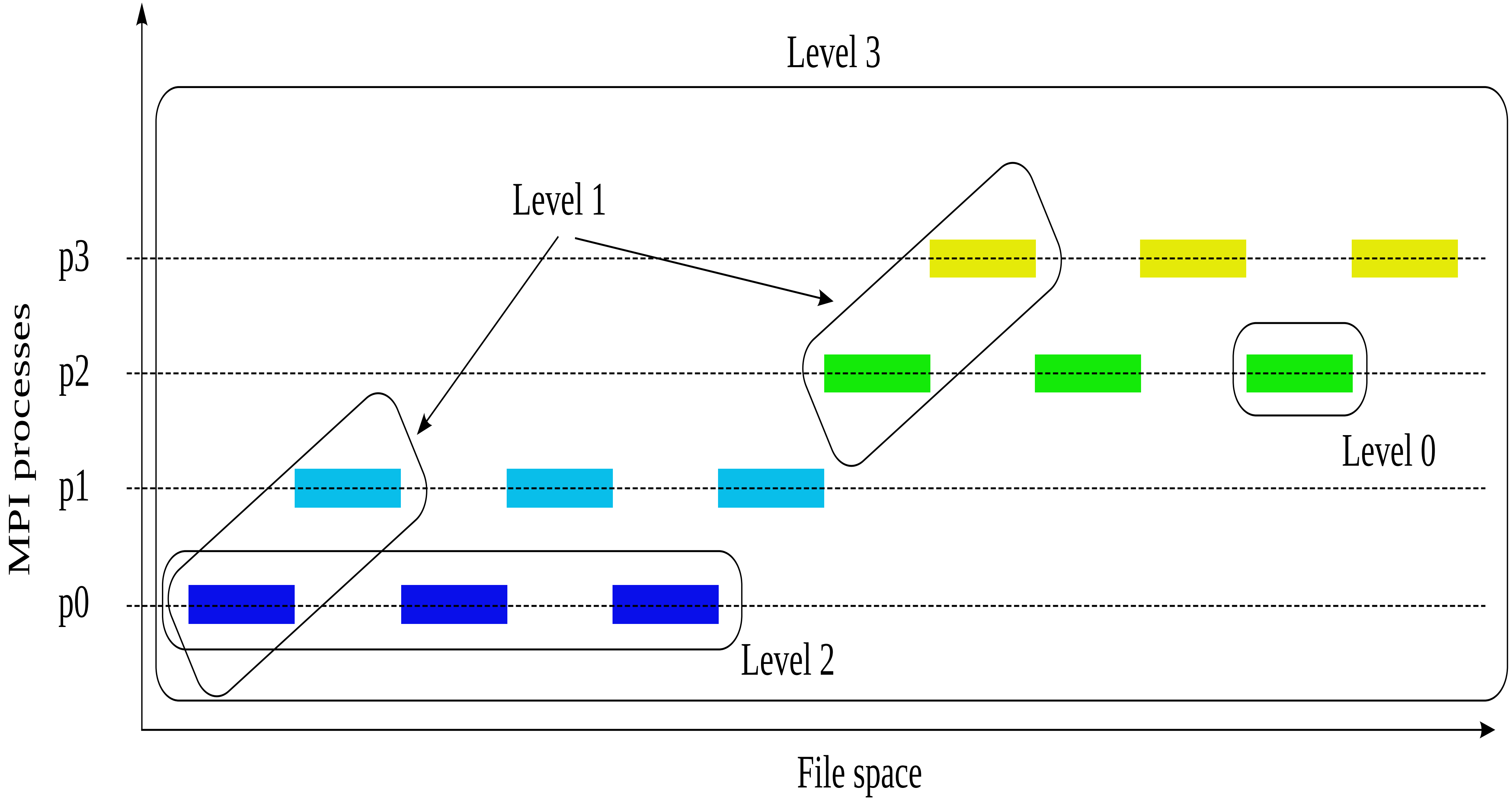
Positioning	Synchronism	Coordination	
		Non collective	Collective
Explicit offsets	Blocking	MPI_FILE_READ_AT MPI_FILE_WRITE_AT	MPI_FILE_READ_AT_ALL MPI_FILE_WRITE_AT_ALL
	Non blocking & Split call	MPI_FILE_IREAD_AT MPI_FILE_IWRITE_AT	MPI_FILE_READ_AT_ALL_BEGIN MPI_FILE_READ_AT_ALL_END MPI_FILE_WRITE_AT_ALL_BEGIN MPI_FILE_WRITE_AT_ALL_END
Individual file pointers	Blocking	MPI_FILE_READ MPI_FILE_WRITE	MPI_FILE_READ_ALL MPI_FILE_WRITE_ALL
	Non blocking & Split call	MPI_FILE_IREAD MPI_FILE_IWRITE	MPI_FILE_READ_ALL_BEGIN MPI_FILE_READ_ALL_END MPI_FILE_WRITE_ALL_BEGIN MPI_FILE_WRITE_ALL_END
Shared file pointers	Blocking	MPI_FILE_READ_SHARED MPI_FILE_WRITE_SHARED	MPI_FILE_READ_ORDERED MPI_FILE_WRITE_ORDERED
	Non blocking & Split call	MPI_FILE_IREAD_SHARED MPI_FILE_IWRITE_SHARED	MPI_FILE_READ_ORDERED_BEGIN MPI_FILE_READ_ORDERED_END MPI_FILE_WRITE_ORDERED_BEGIN MPI_FILE_WRITE_ORDERED_END

Level 2 Level 3

MPI-IO



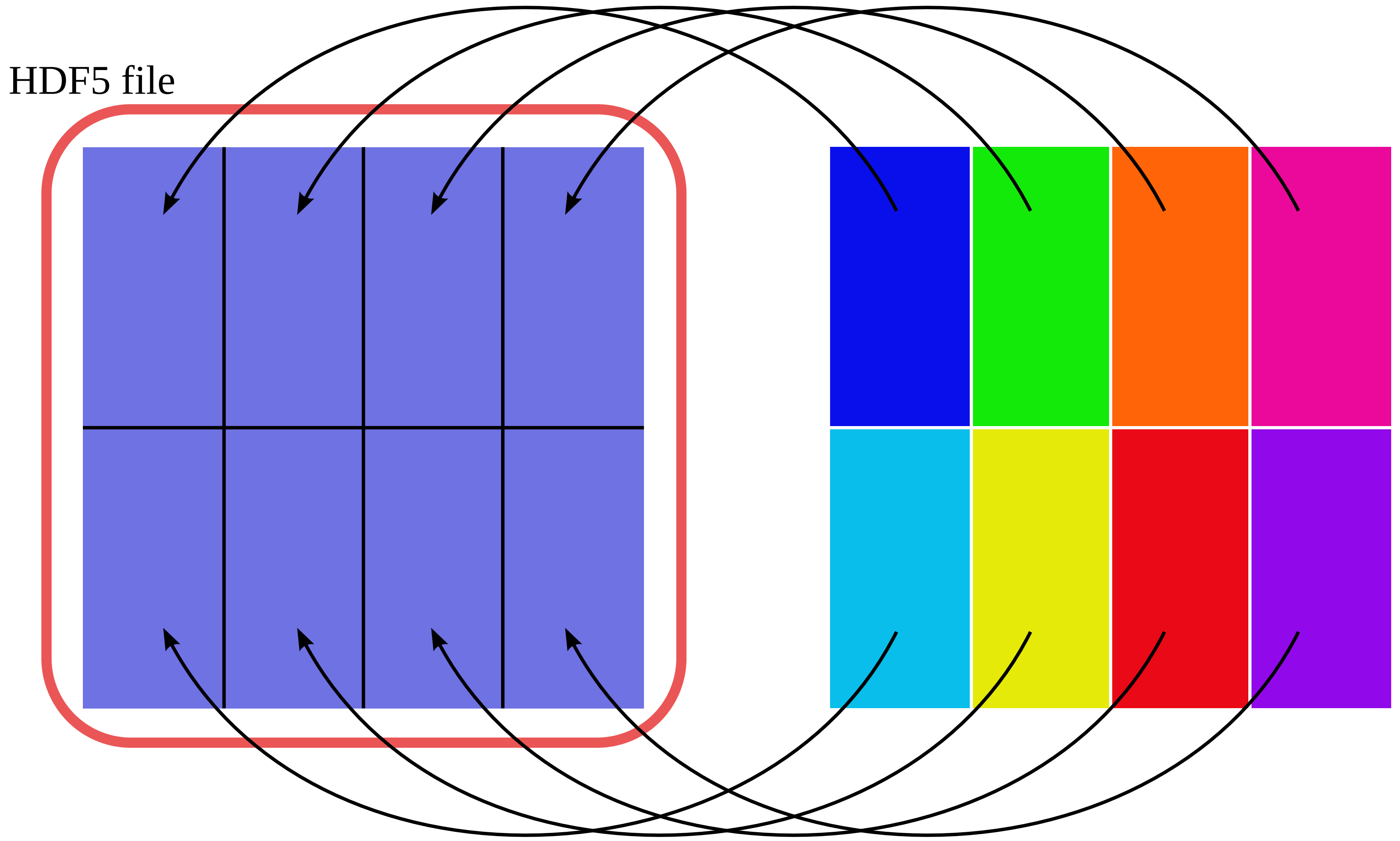
MPI-IO level illustration



Parallel HDF5

- Built on top of MPI-IO
- Must follow some restrictions to enable underlying collective calls of MPI-IO
- From the programming point of view, only few parameters have to be given to the HDF5 library
- Data distribution is described thanks to HDF5 hyper-slices
- Result is a single portable HDF5 file

Parallel HDF5



Parallel HDF5 implementation

```
INTEGER(HSIZE_T) :: array_size(2), array_subsize(2), array_start(2)
INTEGER(HID_T) :: plist_id1, plist_id2, file_id, filespace, dset_id, memspace
array_size(1) = S
array_size(2) = S
array_subsize(1) = local_nx
array_subsize(2) = local_ny
array_start(1) = proc_x * array_subsize(1)
array_start(2) = proc_y * array_subsize(2)

!Allocate and fill the tab array

CALL h5open_f(ierr)
CALL h5pcreate_f(H5P_FILE_ACCESS_F, plist_id1, ierr)
CALL h5pset_fapl_mpio_f(plist_id1, MPI_COMM_WORLD, MPI_INFO_NULL, ierr)
CALL h5fcreate_f('res.h5', H5F_ACC_TRUNC_F, file_id, ierr, access_prp = plist_id1)

! Set collective call
CALL h5pcreate_f(H5P_DATASET_XFER_F, plist_id2, ierr)
CALL h5pset_dxpl_mpio_f(plist_id2, H5FD_MPIO_COLLECTIVE_F, ierr)

CALL h5screate_simple_f(2, array_size, filespace, ierr)
CALL h5screate_simple_f(2, array_subsize, memspace, ierr)

CALL h5dcreate_f(file_id, 'pi_array', H5T_NATIVE_REAL, filespace, dset_id, ierr)
CALL h5sselect_hyperslab_f (filespace, H5S_SELECT_SET_F, array_start, array_subsize, ierr)
CALL h5dwrite_f(dset_id, H5T_NATIVE_REAL, tab, array_subsize, ierr, memspace, filespace, plist_id2)

! Close HDF5 objects
```

IO technology comparison

Scientific results / diagnostics

- Multiple POSIX files in ASCII or binary
- MPI-IO
- pHDF5
- XIOS

Restart files

- SIONlib
- ADIOS

IO technology comparison

	Abstraction	API	Purpose	Hardware	Format	Single/multi File	Online Post-processing
POSIX	Stream	Imperative	General	No	Binary	Multi	No
MPI-IO	Stream	Imperative	General	No	Binary	Single	No
pHDF5	Object	Imperative	General	No	HDF5	Single/Multi	No
XIOS	Object	Declarative	General	No	NetCDF/HDF5	Single	Yes
SIONlib	Stream	Imperative	General	No	Binary	Multi++	No
ADIOS	Object	Decl./Imp	General	Yes	NetCDF/HDF5	Single/Multi	Yes
FTI	Object	Declarative	Specific	Yes	Binary	N.A	No

Performance with parallel HDF5

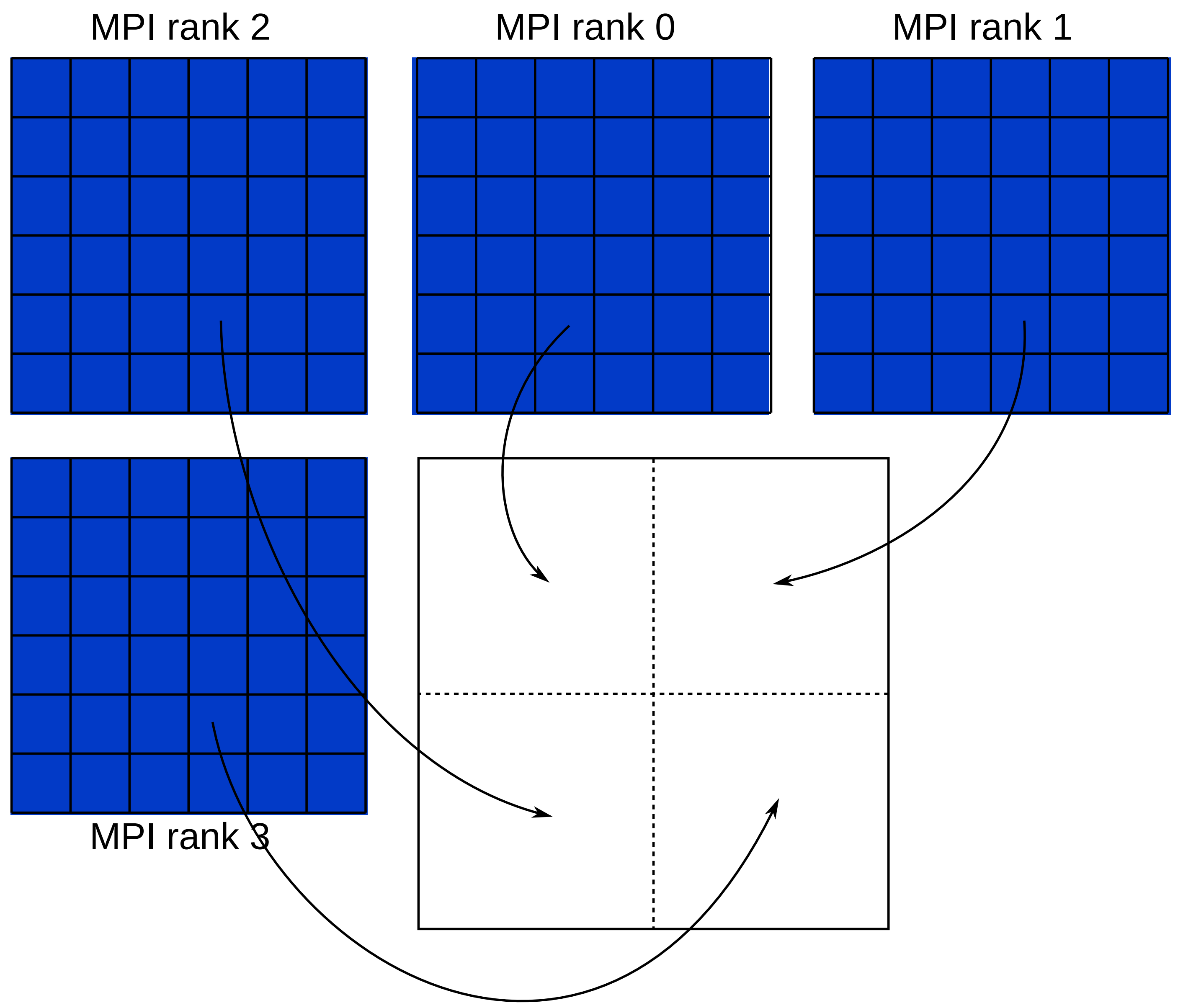
- Relies strongly on MPI-IO performance
- Translates HDF5 hyperslab into MPI derived types
- Performance degradation can come from bad interaction between HDF5, MPI-IO and File system

Performance with parallel HDF5, still some hints

- For contiguous storage, regular hyperslab can enable the usage of collective IO
- For chunk storage, collective IO can be enabled under two constraints
- Increasing cache size for meta-data operations is a good idea
- Aligning dataset to file system block size is a good idea

More information on the HDF5 webiste in this note and this page

Hands-on parallel HDF5 objective 1/2



Hands-on parallel HDF5 1/2

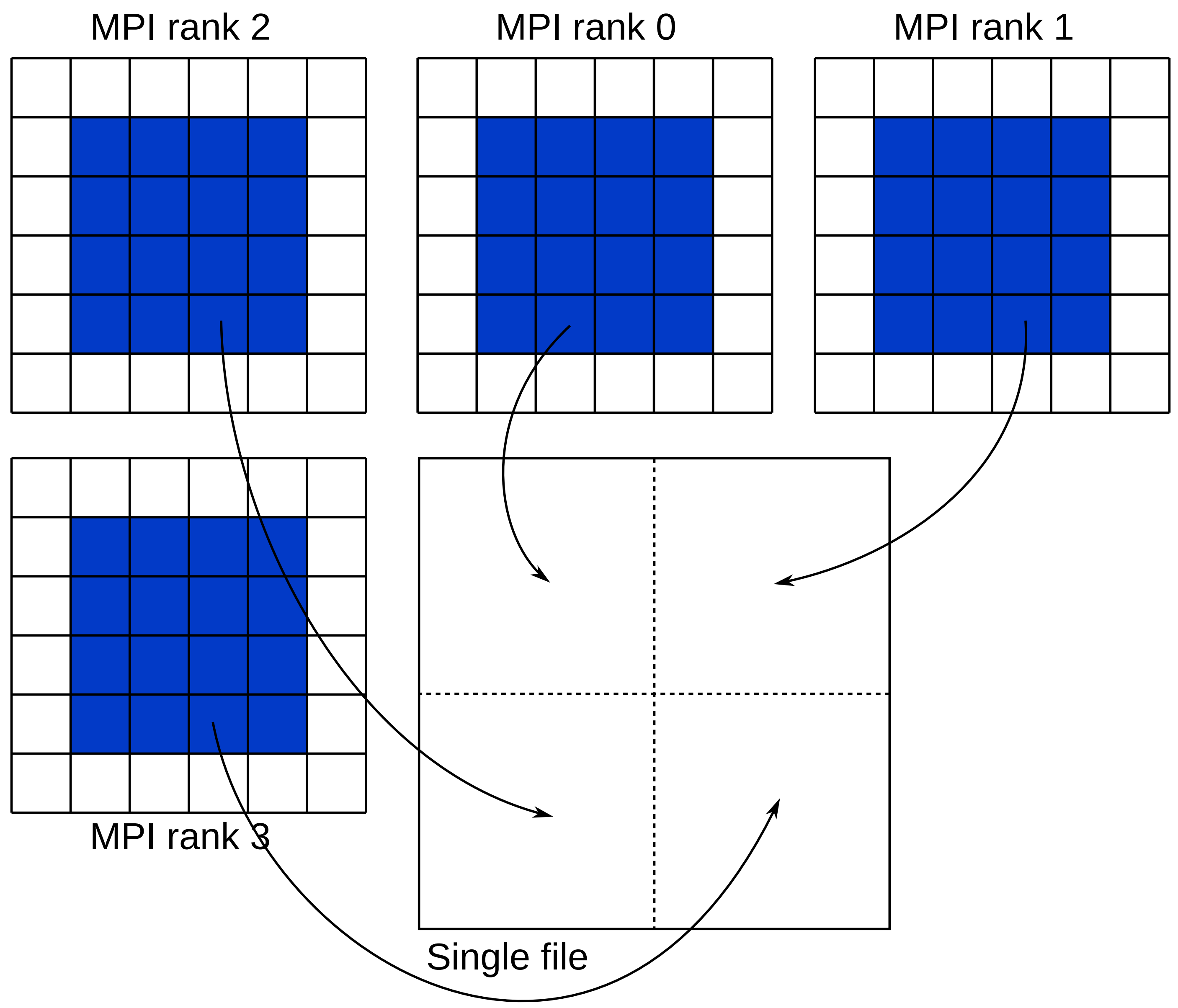
- hands-on on github
- Just use the one prepared for this training by

```
cp -r /home/prace/parallel_HDF5_hands-on .
```

Starting point: **Parallel multi files**. All MPI ranks write their whole memory in separate files

1. **Serialized:** each rank opens the file and writes its data one after the other
   i. Data written in the same file as separate datasets (phdf5-1)
   ii. Data written in the same file and in the same dataset (phdf5-2)
2. **Parallel single file:** specific HDF5 parameters given at open and write time to let MPI-IO manage the concurrent file access (phdf5-3)

Hands-on parallel HDF5 objective 2/2



Hands-on parallel HDF5 2/2

Same exercice as the previous one, but now each rank has ghost cells that should not be written.

1. **Parallel multi files:** all MPI ranks write their whole memory in separate file (provided in phdf5-4)
2. **Parallel single file:** specific HDF5 parameters given at open and write time to let MPI-IO manage the concurrent file access that write the good portion of memory