

Parallel IO concepts (MPI-IO and pHDF5)

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Parallel filesystems and parallel IO libraries PATC@Mds



Outline Day 1

Morning:

- HDF5 in the context of Input/Output (IO)
- HDF5 Application Programming Interface (API)
- Playing with Dataspace
- Hands on session

Afternoon:

- Basics on HPC, MPI and parallel file systems
- Parallel IO with POSIX, MPI-IO and **Parallel HDF5**
- Hands on session (pHDF5)



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

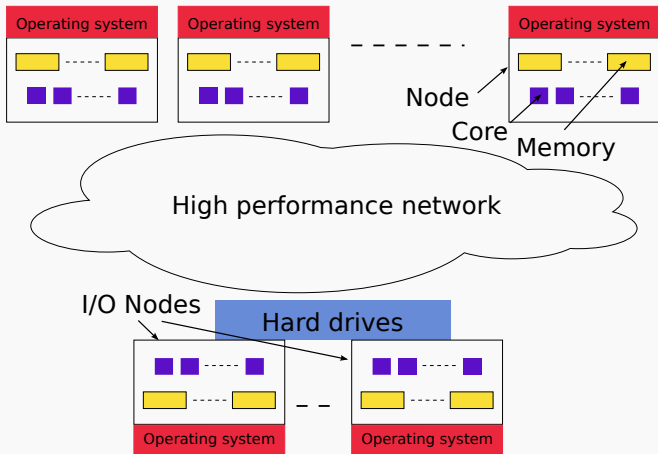
Until now, two major families of HPC machines existed:

- Shared memory machines
- Distributed memory machines

New architectures like GPGPUs, MIC, FPGAs, . . . are not covered here



Distributed memory machines





MPI: Message Passing Interface

MPI is an Application Programming Interface

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

It is composed of

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



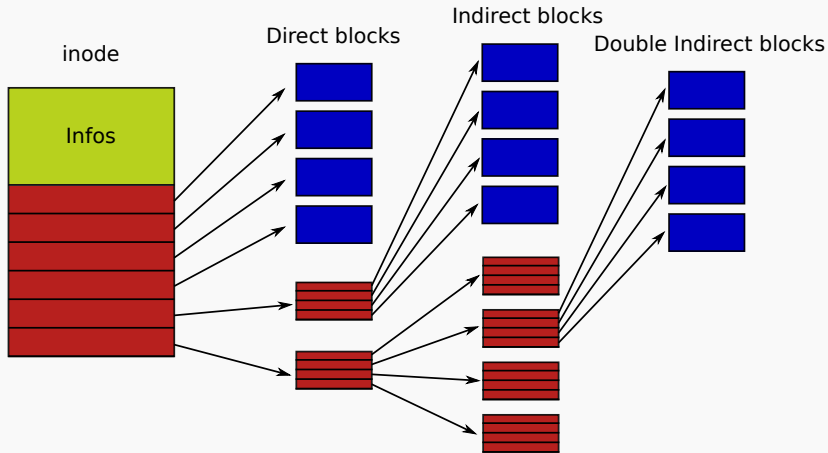
MPI communications

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

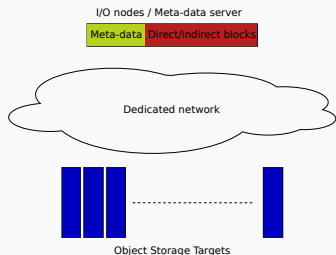
Meta-data, block address and file blocks are stored a single logical drive with a “serial” file system

Logical drive





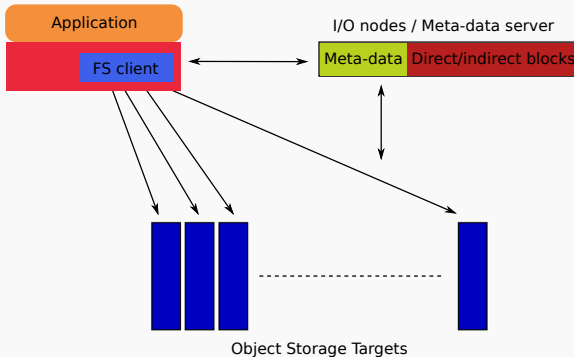
Parallel file system architecture



- 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.



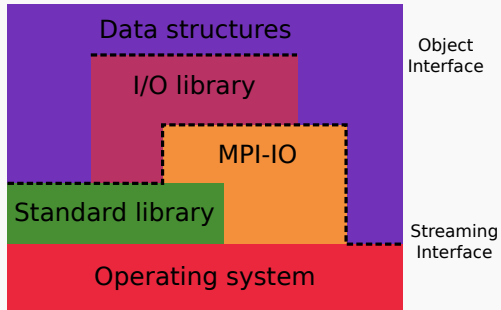
Parallel file system usage



The file system client gives to the application the view of a "serial" file system

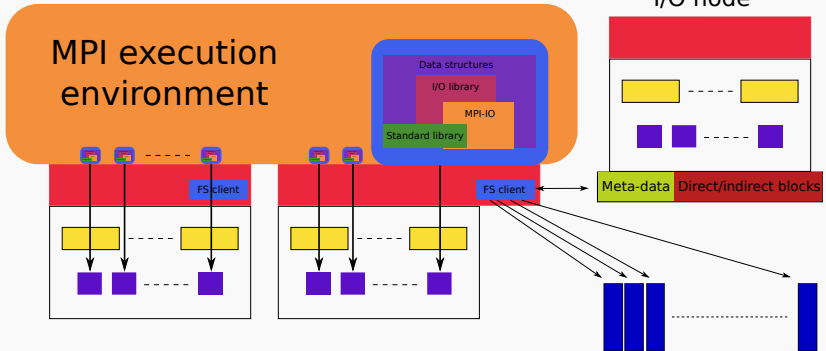


The software stack



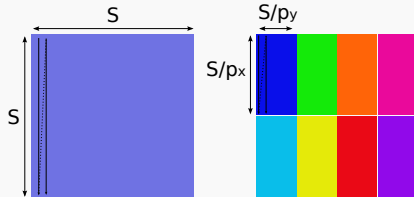


Let us put everything together





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

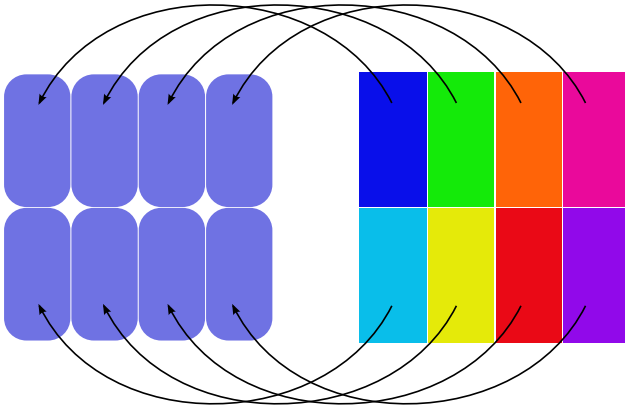
Each MPI process writes its own file

- A single distributed data is spread out in different files
- The way it is spread out depends on the number of MPI processes
- ⇒ More work at post-processing level
- ⇒ May lead to huge amount of files (forbidden)
- ⇒ Very easy to implement



Multiple files

POSIX IO operations





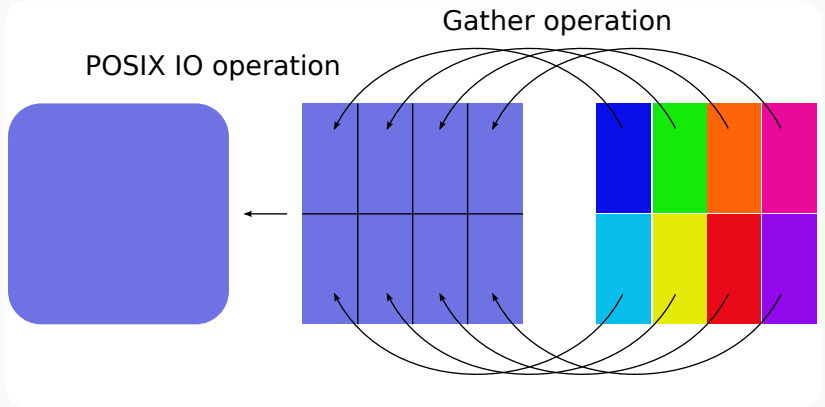
MPI gather + single file

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

- The memory of a single node can be a limitation
- ⇒ Single resulting 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 performs the gather operation within the MPI implementation

- No more memory limitation
- Single resulting file
- Definition of MPI derived types
- Performance linked to MPI library



MPI-IO API

Level 0

Level 1

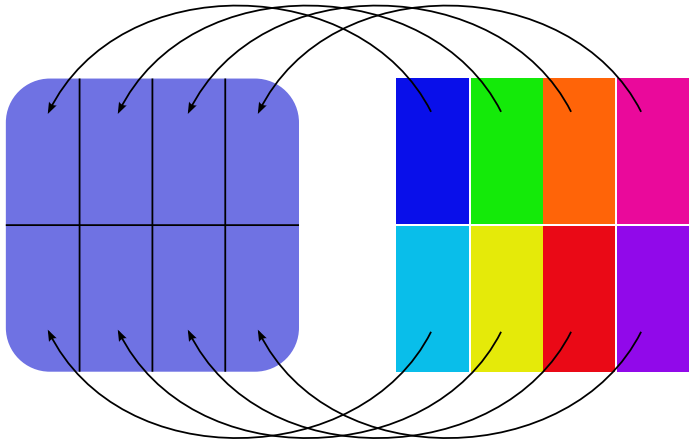
Positioning	Synchronism	Coordination	
		Non collective	Collective
Explicit offsets	Blocking	MPI_FILE_READ_AT MPI_FILE_WRITE_AT	MPI_FILE_READ_AT_ALL MPI_FILE_WRITE_AT_ALL
	Non blocking & Split call	MPI_FILE_IREAD_AT MPI_FILE_IWRITE_AT	MPI_FILE_READ_AT_ALL_BEGIN MPI_FILE_READ_AT_ALL_END MPI_FILE_WRITE_AT_ALL_BEGIN 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

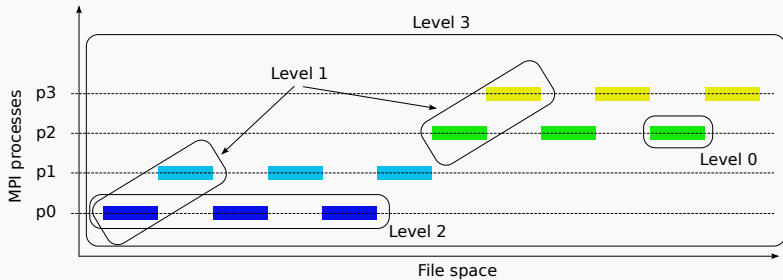


MPI-IO





MPI-IO level illustration





Parallel HDF5

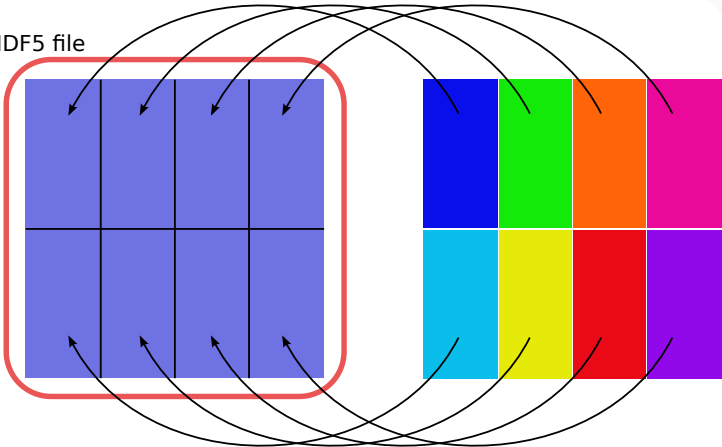
- Built on top of MPI-IO
- Must follow some restrictions to enable underlying collective calls of MPI-IO
- From the programming point of view, only few parameters have to be given to the HDF5 library
- Data distribution is described thanks to HDF5 hyper-slices
- Result is a single portable HDF5 file

- Easy to develop
- Single portable file
- Maybe some performance issues



Parallel HDF5

HDF5 file





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

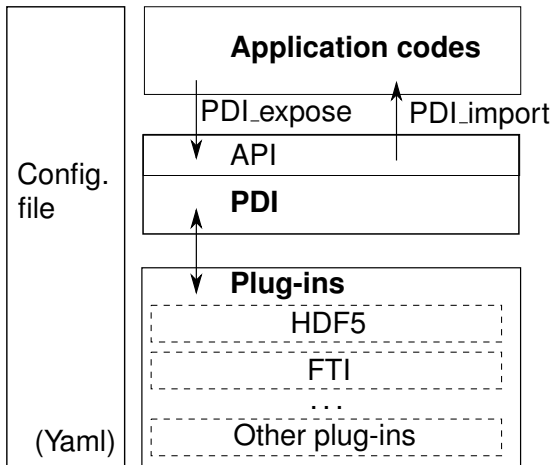
	Abstraction	API	Purpose	Hardware	Format	Single/multi File	Online Post-processing
POSIX	Stream	Imperative	General	No	Binary	Multi	No
MPI-IO	Stream	Imperative	General	No	Binary	Single	No
pHDF5	Object	Imperative	General	No	HDF5	Single/Multi	No
XIOS	Object	Declarative	General	No	NetCDF/HDF5	Single	Yes
SIONlib	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

PDI: the Approach

PDI: the Parallel Data Interface

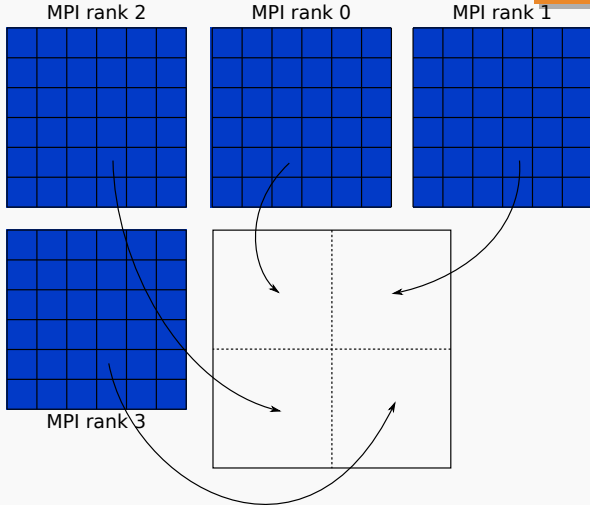
- PDI only provides a *declarative* API (no behavior)
 - `PDI_expose(name, data)`: data available for output
 - `PDI_import(name, data)`: imports data into application
- Behavior is provided by existing IO libraries
 - A plug-in system, event-based
 - HDF5, FTI (available), SION, XIOS, IME (planned), ...
- Behavior is selected through a configuration file
 - which & how plug-ins are used for which data & when
 - a simple yaml file-format

PDI: the Architecture





Hands-on parallel HDF5 objective 1/2



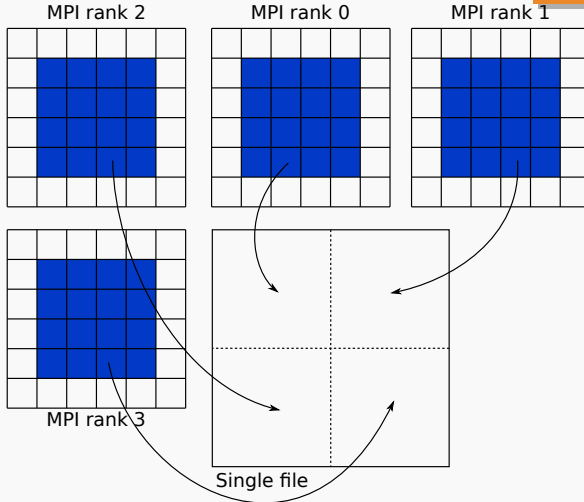


Hands-on parallel HDF5 1/2

1. `git clone https://github.com/mathaeefe/parallel_HDF5_hands-on.git`
2. **Parallel multi files:** all MPI ranks write their whole memory in separate file (provided in `phdf5-1`)
3. **Serialized:** each rank opens the file and writes its data one after the other
 - 3.1 Data written as separate datasets
 - 3.2 Data written in the same dataset
4. **Parallel single file:** specific HDF5 parameters given at open and write time to let MPI-IO manage the concurrent file access



Hands-on parallel HDF5 objective 2/2





Hands-on parallel HDF5 2/2

Same exercise 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