

Advanced Message-Passing Programming

Challenges of Parallel IO



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Overview

- Lecture will cover
 - Why is IO difficult
 - Why is parallel IO even worse
 - Straightforward solutions in parallel
 - What is parallel IO trying to achieve?
 - Files as arrays
 - MPI-IO and derived data types

Why is IO hard?

- Breaks out of the nice process/memory model
 - data in memory has to physically appear on an external device
- Files are very restrictive compared to data arrays
 - random access (fseek) very inefficient
 - linear access to file may require remapping of program data
- Many, many system-specific options to IO calls
- Different formats
 - text, binary, big/little endian, Fortran unformatted, HDF5, NetCDF, ...
- Disk systems are very complicated
 - RAID disks, many layers of caching on disk, in memory, ...
- IO is the HPC equivalent of printing!

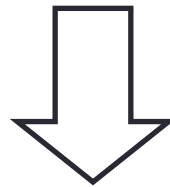
Serial IO of a 4x4 array

```
double x[4][4];  
fwrite(x, sizeof(double), 4*4, fp);
```

Serial data

4	8	12	16
3	7	11	15
2	6	10	14
1	5	9	13

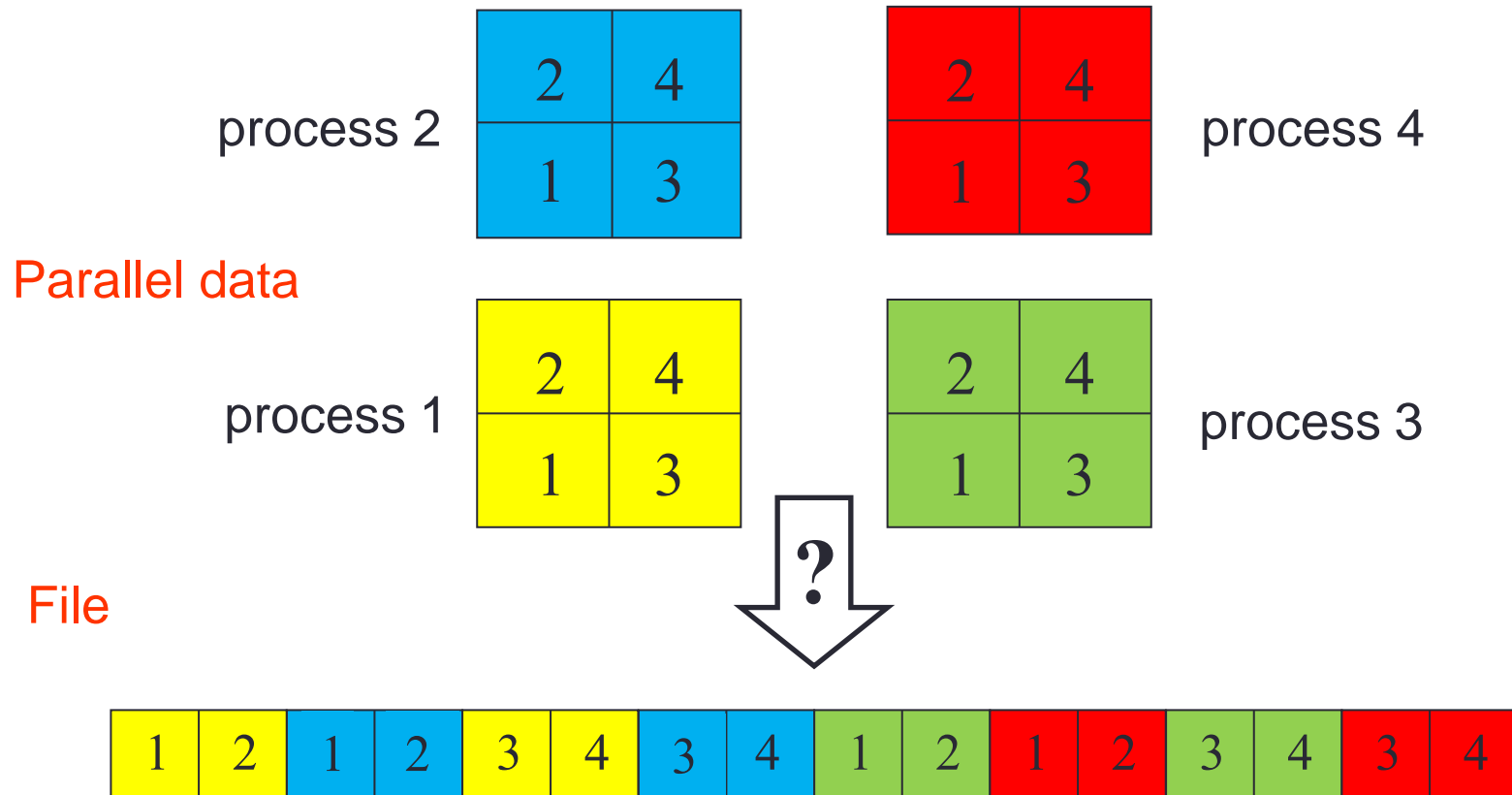
File



1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
---	---	---	---	---	---	---	---	---	----	----	----	----	----	----	----

Parallel IO of a 4x4 distributed array

```
double x[2][2]; // On each of 4 processes  
// Insert magic parallel IO call here!
```



Naive solution #1

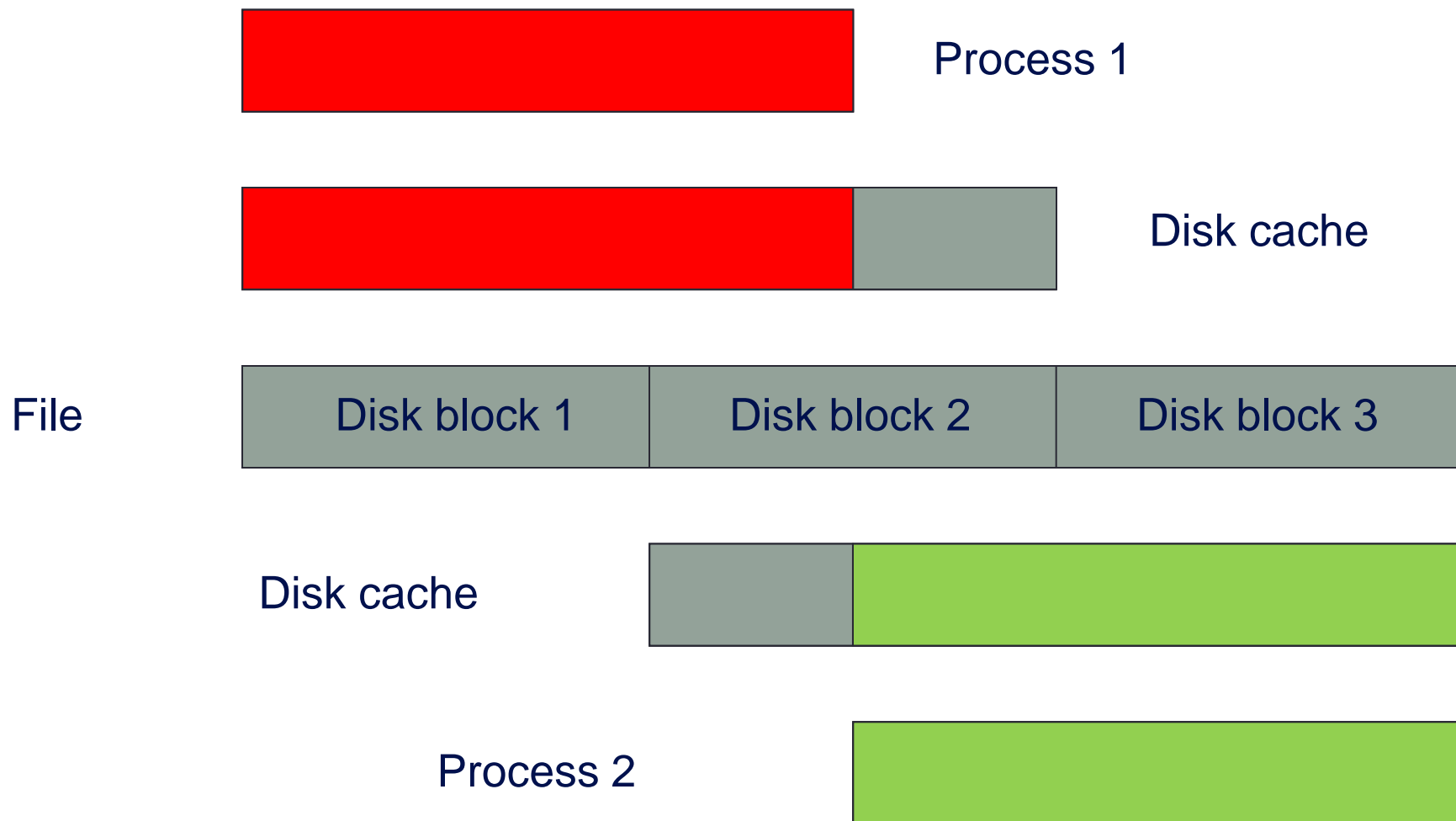
```
double x[2][2]; // On each of 4 MPI processes
FILE *fp;
fp = fopen("globalfile.dat", "w");
fseek(fp, process-specific-offset, SEEK_SET);
fwrite(...);
...
```

- This will not work in general
 - multiple processes writing to the same file is problematic
- Performance will be poor
 - would require many cycles of seek, write, seek, write, ...

Why is Parallel IO Harder?

- Cannot have multiple processes writing to a single file
 - Unix generally cannot cope with this
 - data cached in units of disk blocks (eg 4K) and is *not coherent*
 - not even sufficient to have processes writing to distinct parts of file
 - parallel filesystem may get correct results by locking but serialises the IO
- Even reading can be difficult
 - 1024 processes opening a file can overload the filesystem,
- Data is distributed across different processes
 - processes do not in general own contiguous chunks of the file
 - cannot easily do linear writes
 - local data may have halos to be stripped off

Simultaneous Access to Files



Naive solution #2: Independent I/O

- Also called File-Per-Process
- Each process opens its own data file
 - writes local data
- Simple to implement but ...
 - a nightmare to cope with in practice (thousands of files)
 - often requires a lot of pre- and post-processing
- Data format depends on number of processes
 - completely different output from serial code
- I find this philosophically wrong!
 - parallel computing should get the **same result** but **faster**

Parallel IO of a 4x4 distributed array

```
double x[2][2]; // On each of 4 processes  
fp = fopen(localfile, "w");  
fwrite(x, sizeof(double), 2*2, fp);
```

1	2	3	4
---	---	---	---

data2.dat

1	2	3	4
---	---	---	---

data1.dat

2	4	2	4
1	3	1	3
2	4	2	4
1	3	1	3

1	2	3	4
---	---	---	---

data4.dat

1	2	3	4
---	---	---	---

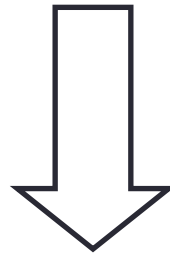
data3.dat

This is what we want to achieve

Parallel Data

2	4	2	4
1	3	1	3
2	4	2	4
1	3	1	3

File



1	2	1	2	3	4	3	4	1	2	1	2	3	4	3	4
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

Naive Solution #3: Controller IO

- Controller IO
 - send all data to/from single controller process
 - e.g. scatter/gather from/to other process from rank 0
 - write/read a single file
- Main advantage is that output is the same as serial
- Issues
 - quickly run out of memory on the controller
 - or have to write in many small chunks
- Performance is poor
 - only a single process is writing
 - a serial solution – no benefit from parallel filesystem (see later)

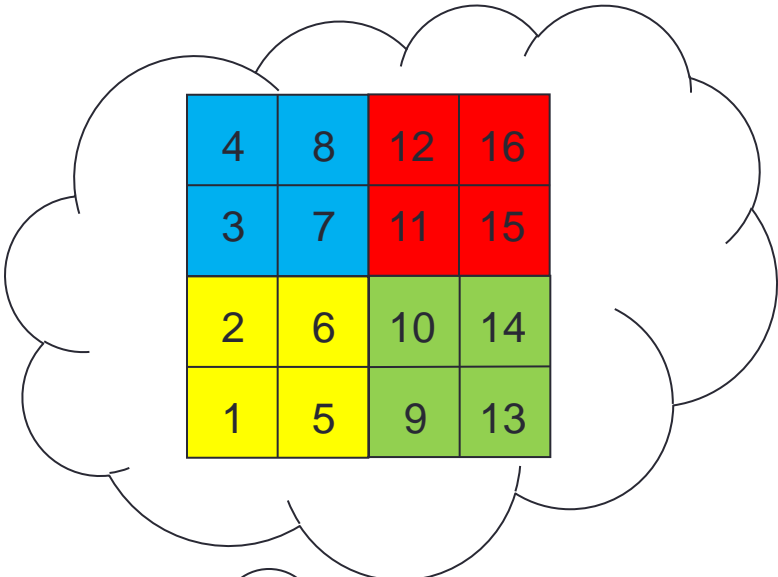
What do we Need?

- A way to do parallel IO properly
 - where the IO system deals with all the system specifics
- Want a single file format
 - We already have one: the serial format
- All files should have same format as a serial file
 - entries stored according to position in global array
 - not dependent on which process owns them
 - order should always be 1, 2, 3, 4,, 15, 16
- A number of libraries exist
 - we will consider MPI-IO first

Information on Data Layout

- What does the IO system need to know about the data?
 - how the local arrays should be stitched together to form the file
- But ...
 - mapping from local data to the global file is only in the mind of the programmer!
 - the program does not know that we imagine the processes to be arranged in a 2D grid
- How do we describe data layout to the IO system?
- Crucial extra step in all parallel IO:
 - tell the IO library what portion(s) of the global file each process owns

Programmer View vs Machine View



4	8	12	16
3	7	11	15
2	6	10	14
1	5	9	13



1	2	3	4
---	---	---	---

Process 4

1	2	3	4
---	---	---	---

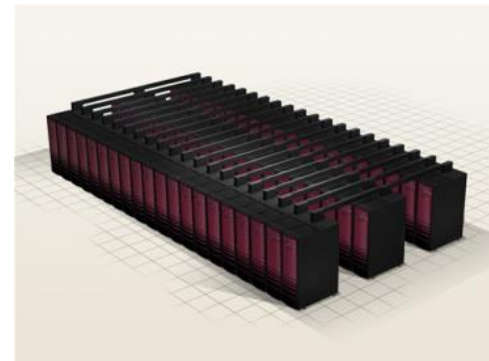
Process 2

1	2	3	4
---	---	---	---

Process 3

1	2	3	4
---	---	---	---

Process 1



Files vs Arrays

- Think of the file as a large array
 - forget that IO actually goes to disk
 - imagine we are recreating a single large array on a controller process
- The IO system must create this array and save to disk
 - without running out of memory
 - never actually creating the entire array
 - i.e. without doing naive controller IO
 - and by doing a small number of large IO operations
 - merge data to write large contiguous sections at a time
 - utilising any parallel features
 - doing multiple simultaneous writes if there are multiple IO nodes
 - managing any coherency issues re file blocks

MPI-IO Approach

- MPI-IO is part of the MPI standard
 - <http://www.mpi-forum.org/docs/docs.html>
- Each process needs to describe what subsection of the global array it holds
 - it is entirely up to the programmer to ensure that these do not overlap for write operations!

Data Sections

4	8	12	16
3	7	11	15
2	6	10	14
1	5	9	13

on process 3

4	8	12	16
3	7	11	15
2	6	10	14
1	5	9	13

- Describe 2x2 subsection of 4x4 array
- Using standard MPI derived datatypes
- A number of different ways to do this

Other Parallel IO Libraries

- MPI-IO is usually the lowest level
 - you may never call it directly
- Higher level libraries exist
 - HDF5
 - NetCDF
 - ADIOS2
- Approach is the same
 - some way of describing what portion(s) of file each process owns
 - these libraries usually use MPI-IO to do their reads and writes

Summary

- Parallel IO is difficult
 - in theory and in practice
- MPI-IO provides a higher-level abstraction
 - user describes global data layout using derived datatypes
 - MPI-IO hides all the system specific filesystem details ...
 - ... but (hopefully) takes advantage of them for performance
- More flexible formats exist, e.g. NetCDF, HDF5 and ADIOS2
 - they gain performance by layering on top of MPI-IO
- MPI-IO requires a good understanding of derived datatypes