HELP US ALL STAY HEALTHY

SIX SIMPLE TIPS

Maintain 1.5 metres distance between yourself and others where possible

Cough and sneeze into your elbow or a tissue (not your hands)

Avoid shaking hands

Put used tissues in the bin

Wash hands with soap and warm water or use an alcohol-based hand sanitiser after you cough or sneeze

Do not touch your face

IF YOU ARE UNWELL AND WORRIED ABOUT COVID-19:

- Call the National Coronavirus Helpline: 1800 020 080
- Call your usual GP for advice
- Call the UWA Medical Centre for advice: 6488 2118

UWA FAQs:
uwa.edu.au/coronavirus

Report COVID-19 hazards and suspected/confirmed cases via RiskWare:
uwa.edu.au/riskware

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High-Performance Computing

Lecture 8 MPI Parallel I/O and Process Topologies

CITS5507

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Acknowledgement: The lecture slides are based on many online sources.

Outline

- **Parallel File I/O**
  - ✓ Introduction
  - ✓ I/O strategy
  - ✓ Independent I/O
  - ✓ Collective I/O
  - ✓ I/O access pattern
- Process Topologies
  - ✓ Virtual topologies
  - ✓ Cartesian grid topology
  - ✓ Distributed graph topology
  - ✓ Summary

Introduction

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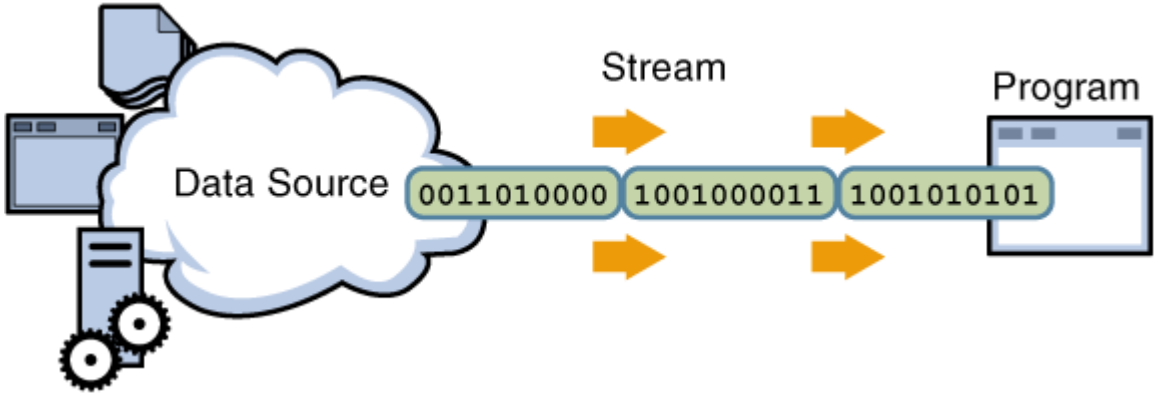
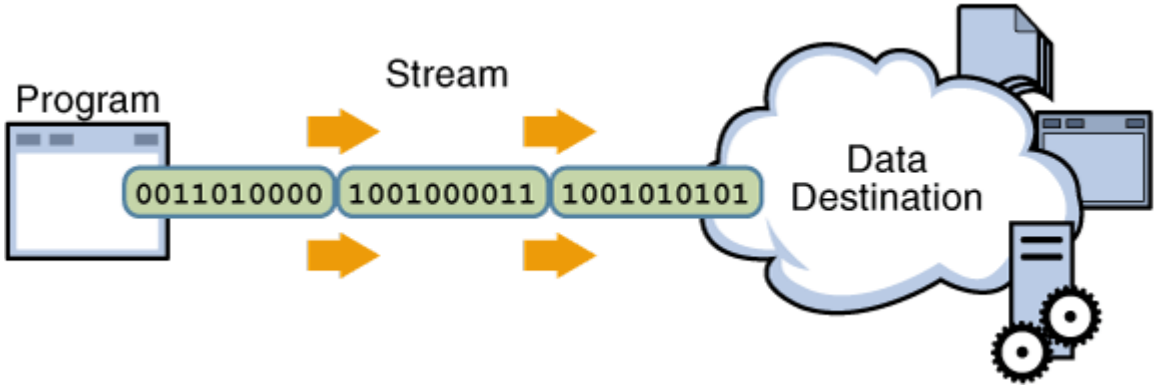
- We often use supercomputers to handle large datasets
- Reading in data takes a linear amount of time
- Reading/Writing to files can be parallelised
- Most supercomputers have a bespoke file-system designed for high performance and concurrent access
  - ✓ Your program should use this if possible
- Parallel I/O means concurrent reading/writing to the same file

File I/O

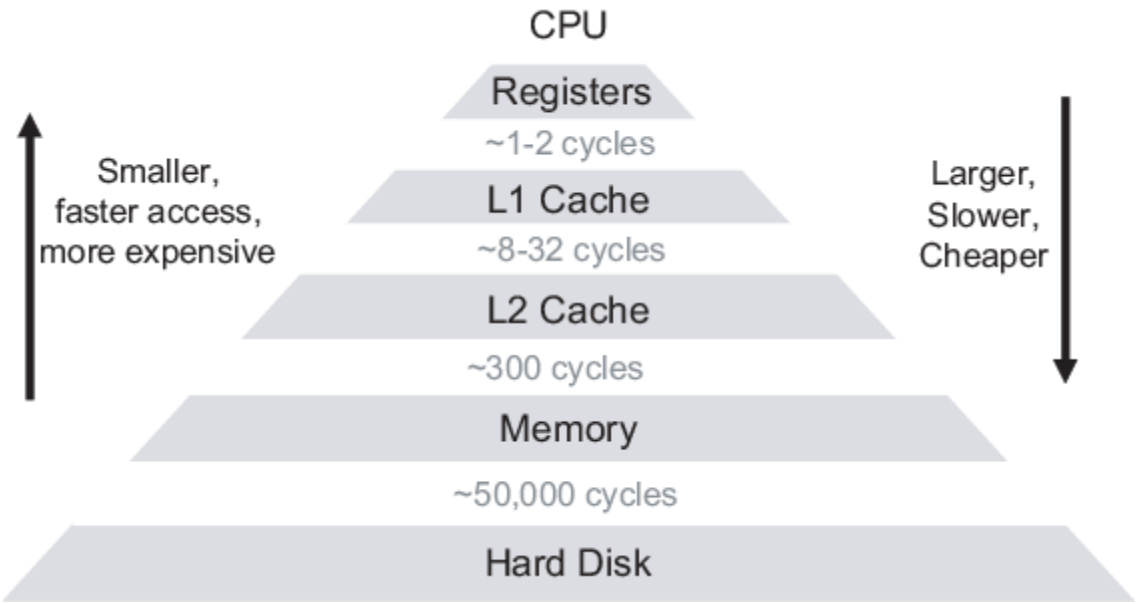
Data sources/destination may be files.



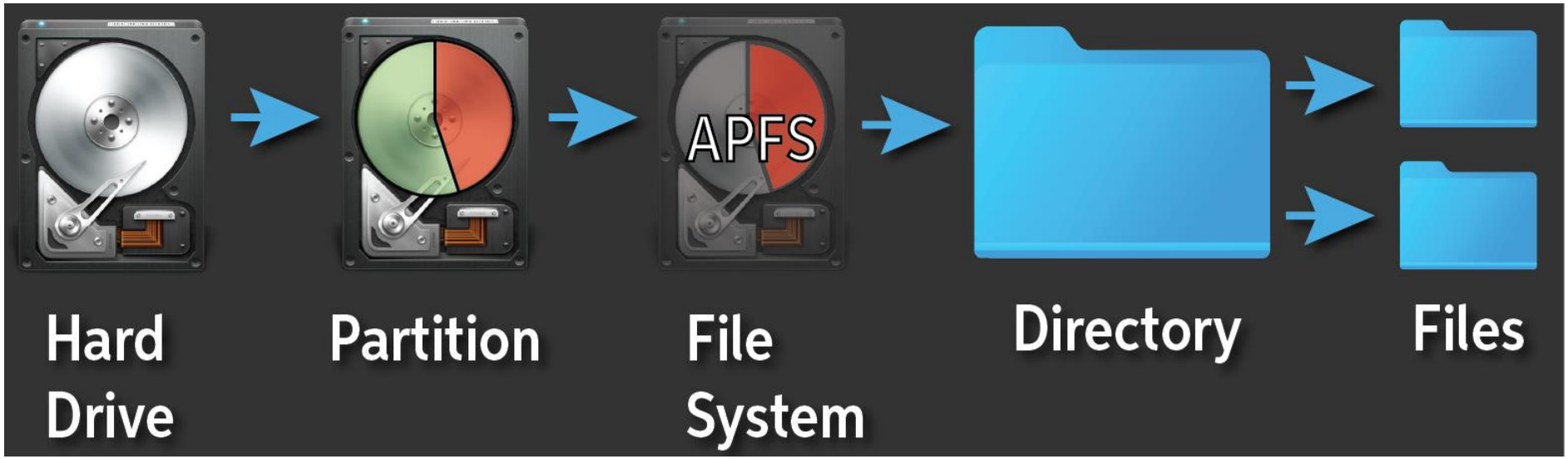


The Memory Hierarchy (Lecture 1)

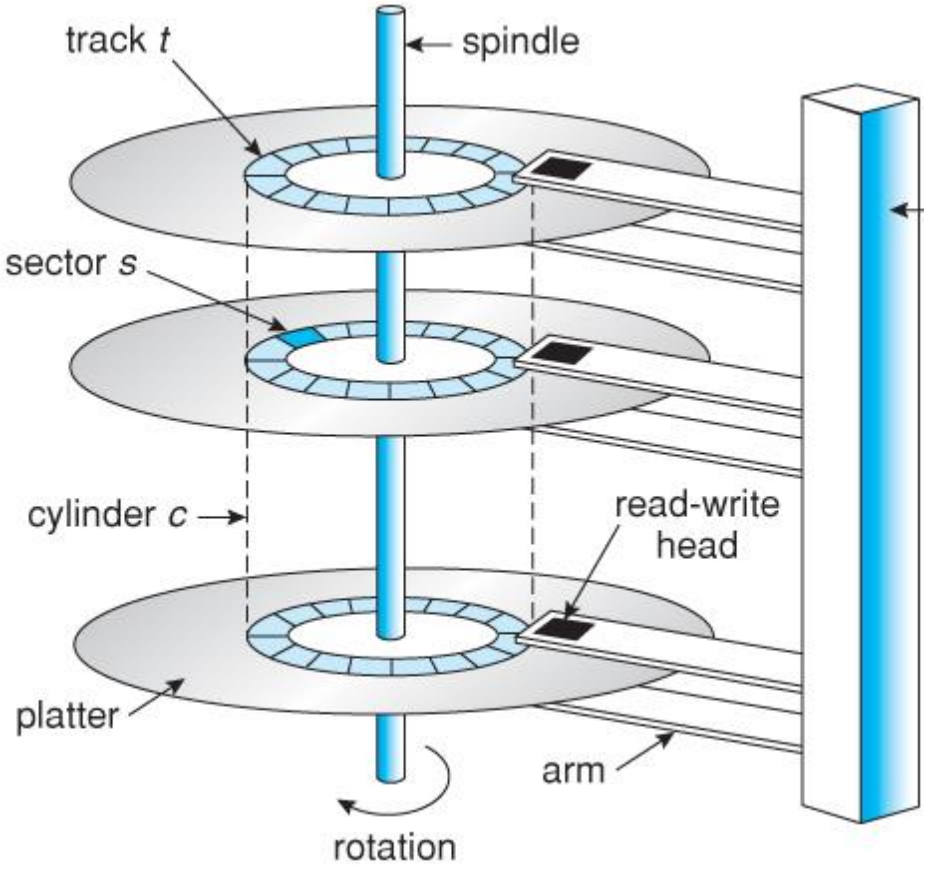
- Why not build computers entirely with fast memories like the cache?
  - ✓ The cost will be high, consumer hardware will not be competitively priced.
  - ✓ The cost is in manufacturing hardware, caches are usually "on-chip" with the processor.



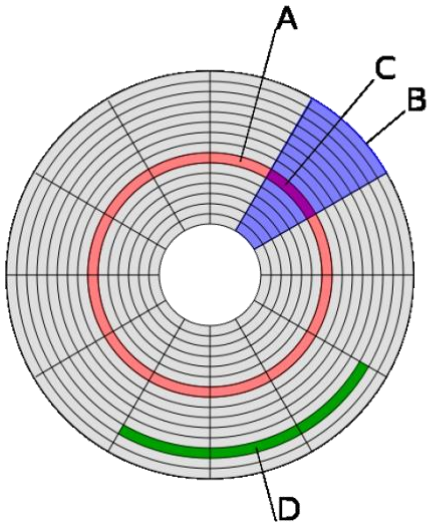
File System Workflow



Hard Drive Overview



A hard dirve



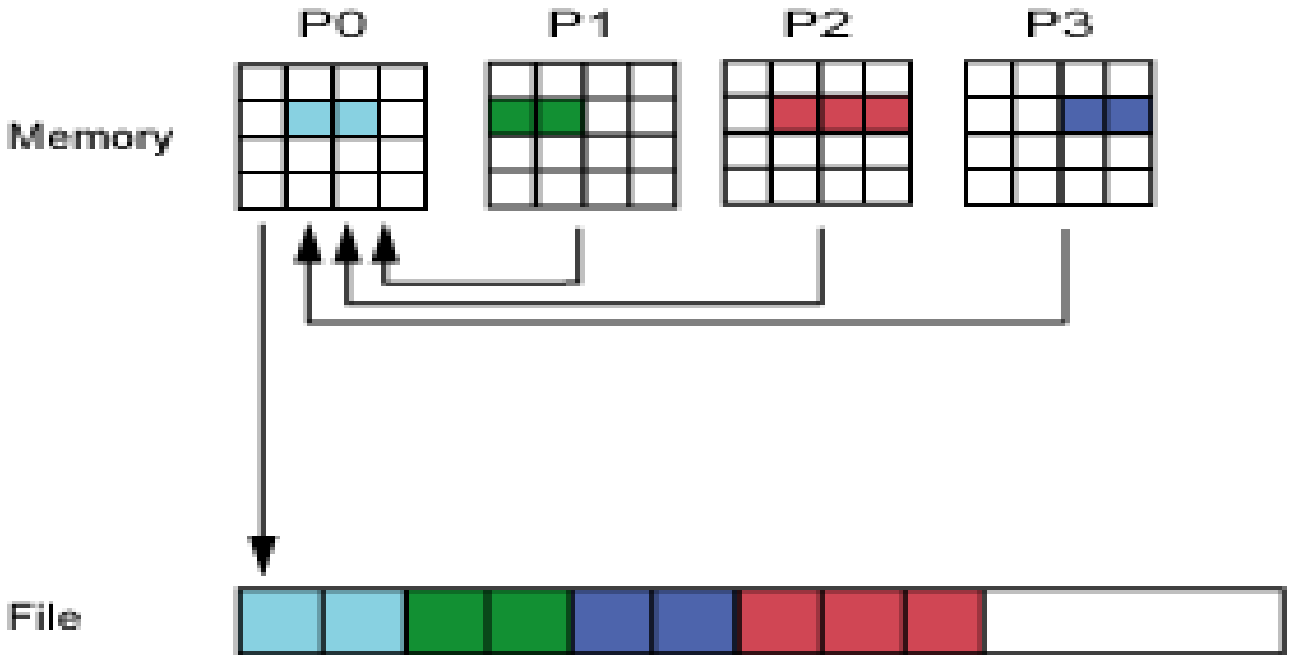
Hard Drive Structure:

A = track
B = sector
C = sector of a track
D = cluster

Single disk

Non-Parallel I/O

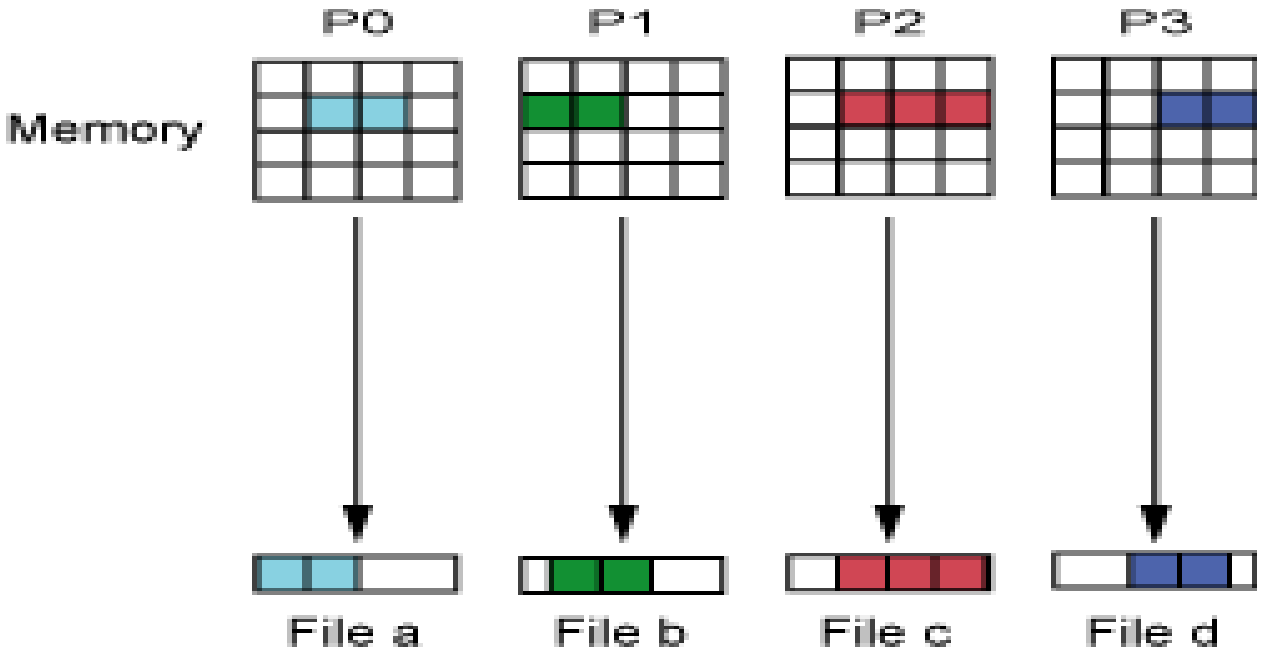
- All processes participating in I/O send write requests to a single process, which writes to the shared file **at once**.
  - ✓ **P1-P3** sends a write request to **P0** which writes the data of **P0-P3** to the shared file at once.
- Cons: Non-parallel; performance **worse** than sequential



Independent Parallel I/O

- Each process writes to a **separate** file

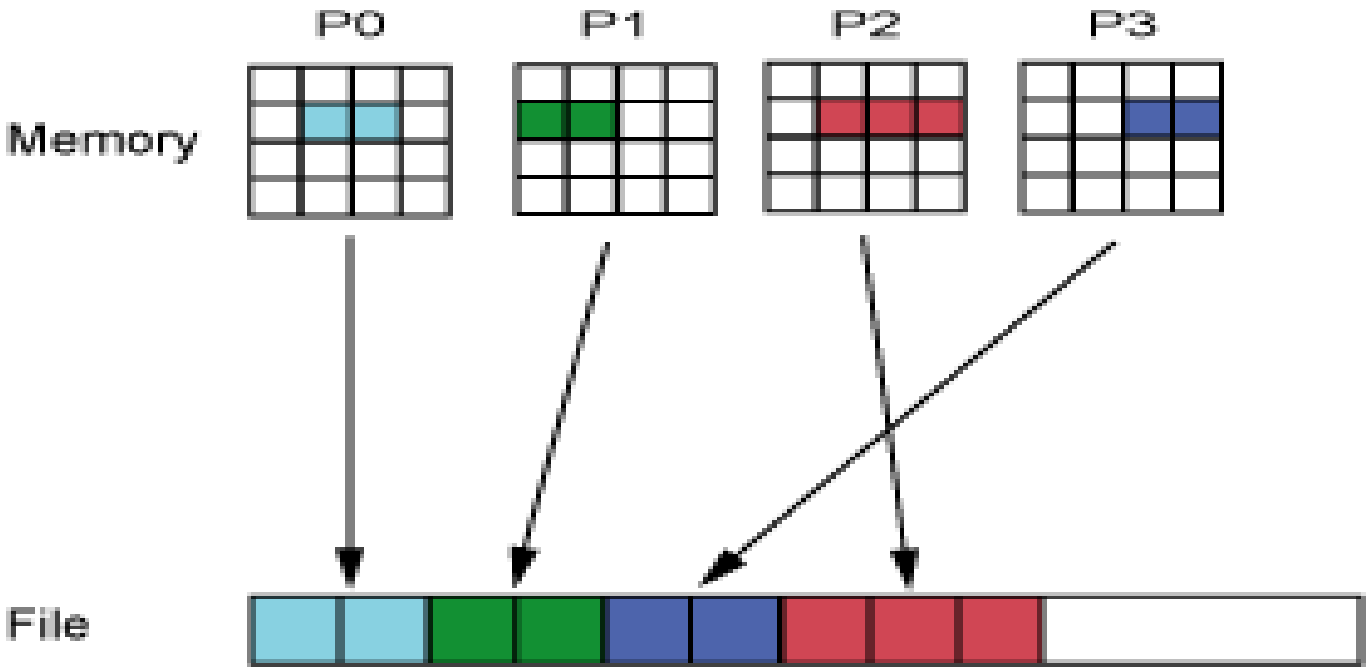
- Pro : Good parallelism
- Con: Lots of small files to manage



Cooperative Parallel I/O

- All processes write a **shared file** at the same time

- Pro: lots of parallelism
- Con: can only be expressed in MPI



Why use MPI for this?

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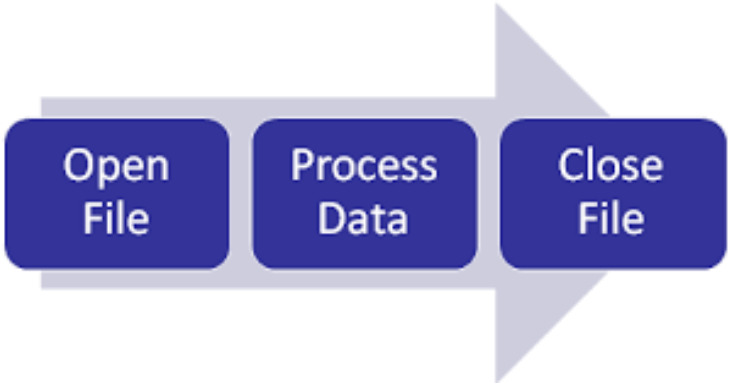
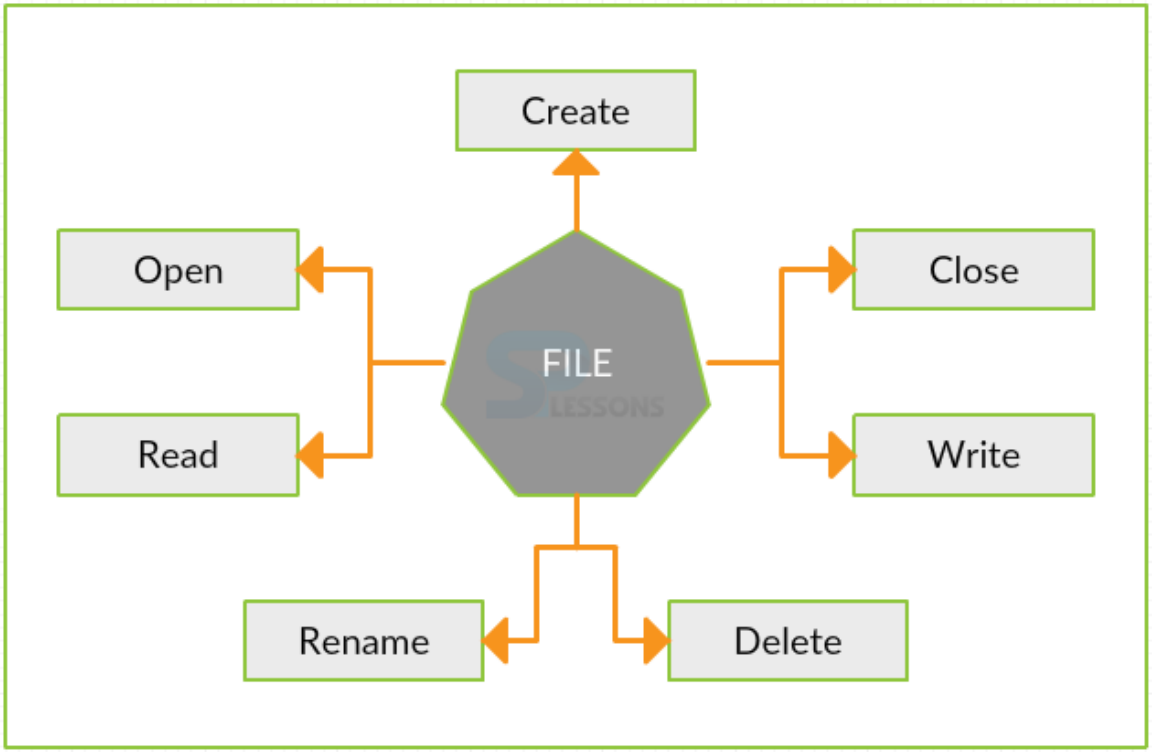
- Reading/Writing is similar to **sending**/**receiving**

- Allows developers to leverage MPI capabilities
  - ✓ Collective communicators
  - ✓ User-defined datatypes to describe file elements
  - ✓ Communicators allow separation from application messages and file messages
  - ✓ Non-blocking operations

- This lecture covers
  - ✓ **Independent I/O**
  - ✓ **Cooperative I/O**

Accessing Files and File Operations





File I/O – Rationale

- The idea is to have each process describe its part of the file
  - ✓ Provides a ‘view’ of the file
  - ✓ Achieves with ‘**offsets**’
  - ✓ Allows the MPI implementation to handle **non-contiguous** access and **shared access**

- Collective I/O combined with non-contiguous access is the key to the highest performance

Two Types of I/O

- MPI I/O supports **two** types of I/O
- Independent
  - ✓ Each process handles its **own** I/O
  - ✓ Supports derived datatypes (different to POSIX)

- Collective
  - ✓ I/O calls must be made by **all** processes
  - ✓ Used “shared file, all write”
  - ✓ Optimised by the MPI library

POSIX stands for Portable Operating System Interface, and is an IEEE standard designed to facilitate application portability.

Outline

- Parallel File I/O
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  - ✓ Collective I/O
  - ✓ I/O access pattern
- Process Topologies
  - ✓ Virtual topologies
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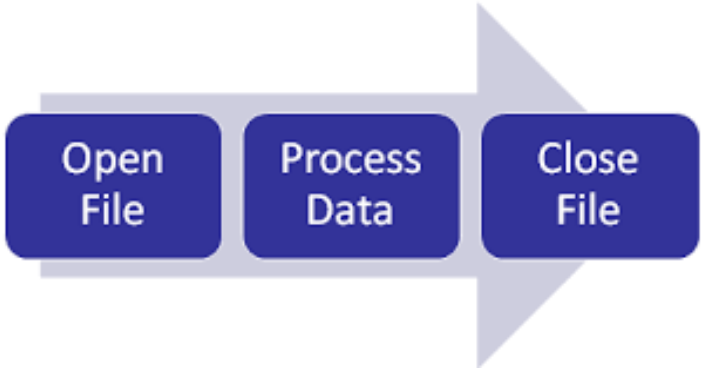
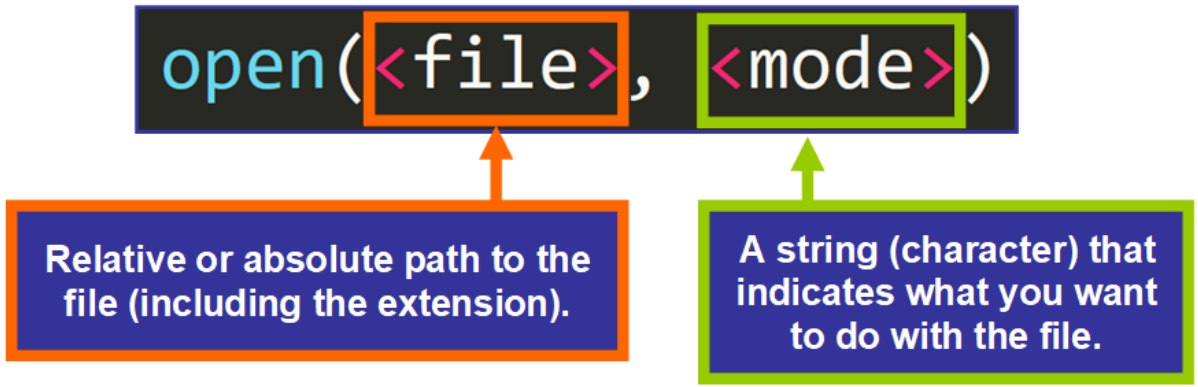
Independent I/O



- Just like C/C++ I/O you need to
  - ✓ Open the file
  - ✓ Read/Write data from/to the file
  - ✓ Close the file

- In MPI, these steps are almost the same:
  - ✓ Open the file: **MPI_File_open**
  - ✓ Write to the file: **MPI_File_write**
  - ✓ Close the file: **MPI_File_close**



MPI I/O Example

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```
#include <mpi.h>
#include <stdio.h>


int main(int argc, char *argv[])
{
    MPI_File fh;
    int buf[1000], rank;
    MPI_Init(0,0);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_File_open(MPI_COMM_WORLD, “test.out”,
                  MPI_MODE_CREATE|MPI_MODE_WRONLY,
                   MPI_INFO_NULL, &fh);
    if (rank == 0)
        MPI_File_write(fh, buf, 1000, MPI_INT, MPI_STATUS_IGNORE);
    MPI_File_close(&fh);
    MPI_Finalize();
    return 0;
}
```

MPI I/O Example (Cont'd): Comments

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- File Open is collective over the communicator
  - ✓ Can be used to support **collective I/O**, which is important for performance
  - ✓ Modes similar to Unix file open
  - ✓ **MPI_Info** provides additional hints for performance
- File Write is **independent** (hence choose the rank with **if**)
  - ✓ Many important variations covered in later slides
- File close is collective; similar in style to **MPI_Comm_free**

Independent I/O

- Also like C/C++ you need to provide file flags
  - ✓ **MPI_MODE_WRONLY** or **MPI_MODE_RDWR** (reading and writing)
  - ✓ **MPI_MODE_CREATE** also needed if the file may not exist
  - ✓ Can pass multiple flags with bitwise-or '|'

- When to use Independent I/O
  - ✓ Synchronisation of collective calls
  - ✓ Overhead of collective calls is too high
    - **E.g.** reading a very small proportion of a file

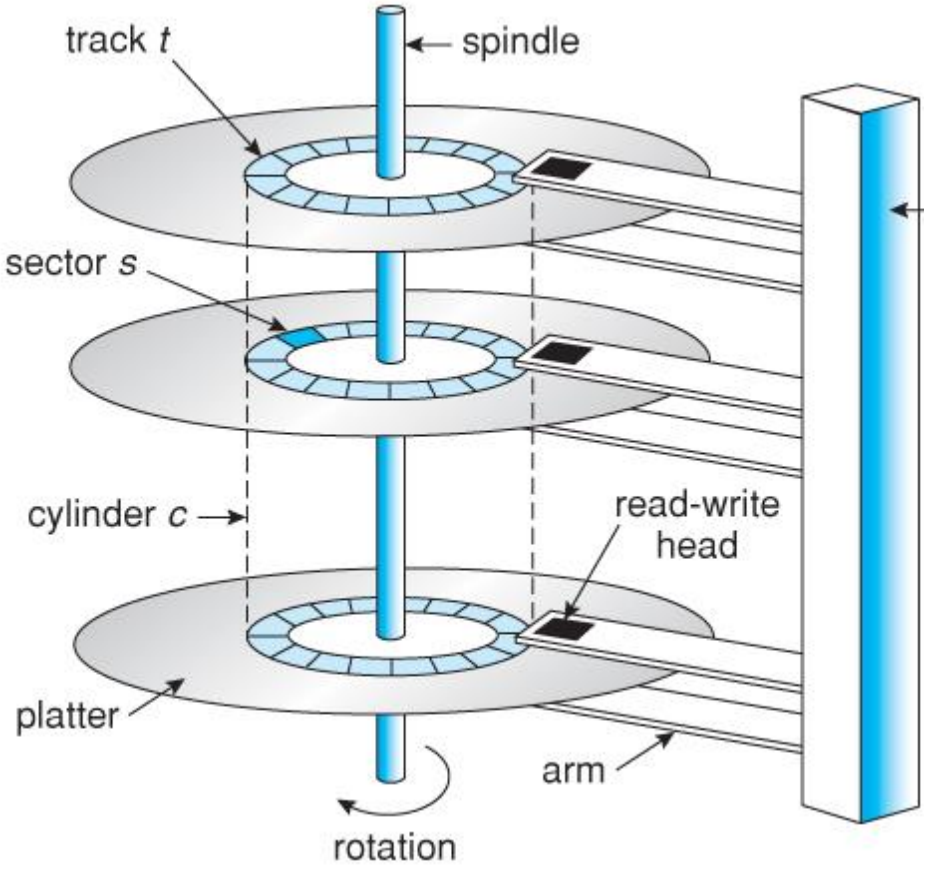
Accessing a Shared File

- MPI_File_open(comm, filename, flags, info, &file_handle)
- MPI_File_close(&file_handle)

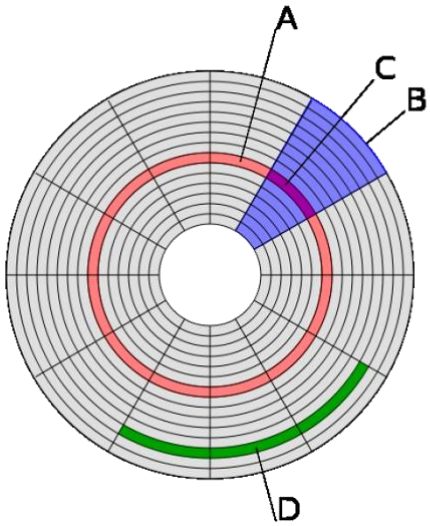
- MPI_File_seek(File_handle, offset, whence)
  - ✓ Updates the file pointer to 'whence' which can be one of
    - MPI_SEEK_SET – Set to the offset value
    - MPI_SEEK_CUR – Set to the current position + offset
    - MPI_SEEK_END – Set to the end of the file + offset

- MPI_File_read(file_handle, buffer, num_read, datatype, status)
- MPI_File_write(file_handle, size, datatype, status)

Hard Drive Overview (MPI_SEEK)



A hard dirve



Hard Drive Structure:

A = track
B = sector
C = sector of a track
D = cluster

Single disk

Accessing a Shared File (Continued)

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- MPI_File_read_at(file_handle, offset, buf, num_items, datatype, status)
- MPI_File_write_at(file_handle, offset, buf, count, datatype)

Example: Writing a File

```
#include<stdio.h>
#include "mpi.h"
#define N 16
int main(int argc, char **argv){
  int rank, num_of_process;
  MPI_File fhw;
  MPI_Status status;
  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Comm_size(MPI_COMM_WORLD, &num_of_process);
  int buf[N];
  for (int i=0;i<N;i++)
     buf[i] = i;
  int ave_num_of_ints = N / num_of_process;
  int offset = rank * ave_num_of_ints;
  MPI_File_open(MPI_COMM_WORLD, "dfile",
                MPI_MODE_CREATE|MPI_MODE_WRONLY, MPI_INFO_NULL, &fhw);
  printf("\nRank: %d, Offset: %d\n", rank, offset);
  MPI_File_write_at(fhw, offset * sizeof(int), buf+offset, ave_num_of_ints,
MPI_INT, &status);
  MPI_File_close(&fhw);
  MPI_Finalize();
  return 0;
}
```

using bytes

Note: try even number of processes (e.g. mpiexec –n 2 my_program)

Example: Reading a File (1)

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```
#include <mpi.h>
#include <stdio.h>
#define N 16
int main(int argc, char **argv){
  int rank, num_of_process;
  MPI_File fh; //Declaring a File Pointer
  MPI_Status status;
  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Comm_size(MPI_COMM_WORLD, &num_of_process);
  int ave_num_of_ints = N / num_of_process;
  int buf[ave_num_of_ints];
  int bufsize_byte = ave_num_of_ints * sizeof(int);

  MPI_File_open(MPI_COMM_WORLD,"dfile", MPI_MODE_RDONLY, MPI_INFO_NULL,&fh);
  MPI_File_seek(fh, rank * bufsize_byte, MPI_SEEK_SET); //File seek
  MPI_File_read(fh, buf, ave_num_of_ints, MPI_INT, &status); //File read
  printf("\nrank: %d, buf[%d]: %d", rank, rank*ave_num_of_ints, buf[0]);
  MPI_File_close(&fh); //Closing a File
  MPI_Finalize();
  return 0;
}
```

Example: Reading a File (2)

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```
#include <mpi.h>
#include <stdio.h>
#define N 16
int main(int argc, char **argv){
  int rank, num_of_process;
  MPI_File fh; //Declaring a File Pointer
  MPI_Status status;
  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Comm_size(MPI_COMM_WORLD, &num_of_process);
  int ave_num_of_ints = N / num_of_process;
  int buf[ave_num_of_ints];
  int bufsize_byte = ave_num_of_ints * sizeof(int);

  MPI_File_open(MPI_COMM_WORLD,"dfile", MPI_MODE_RDONLY, MPI_INFO_NULL,&fh);
//Combining File Seek & Read in One Step for Thread Safety
  MPI_File_read_at(fh, rank*bufsize_byte, buf, ave_num_of_ints, MPI_INT,
&status);
  printf("\nrank: %d, buf[%d]: %d", rank, rank*ave_num_of_ints, buf[0]);
  MPI_File_close(&fh); //Closing a File
  MPI_Finalize();
  return 0;
}
```

Non-contiguous I/O in File

- Each process describes the part of the file for which it is responsible
  - ✓ This is the "**file view**"
  - ✓ Described in MPI with an offset (useful for headers) and an **MPI_Datatype**
- Only the part of the file described by the file view is visible to the process; reads and writes access these locations
- This provides an efficient way to perform non-contiguous accesses

Non-contiguous Accesses

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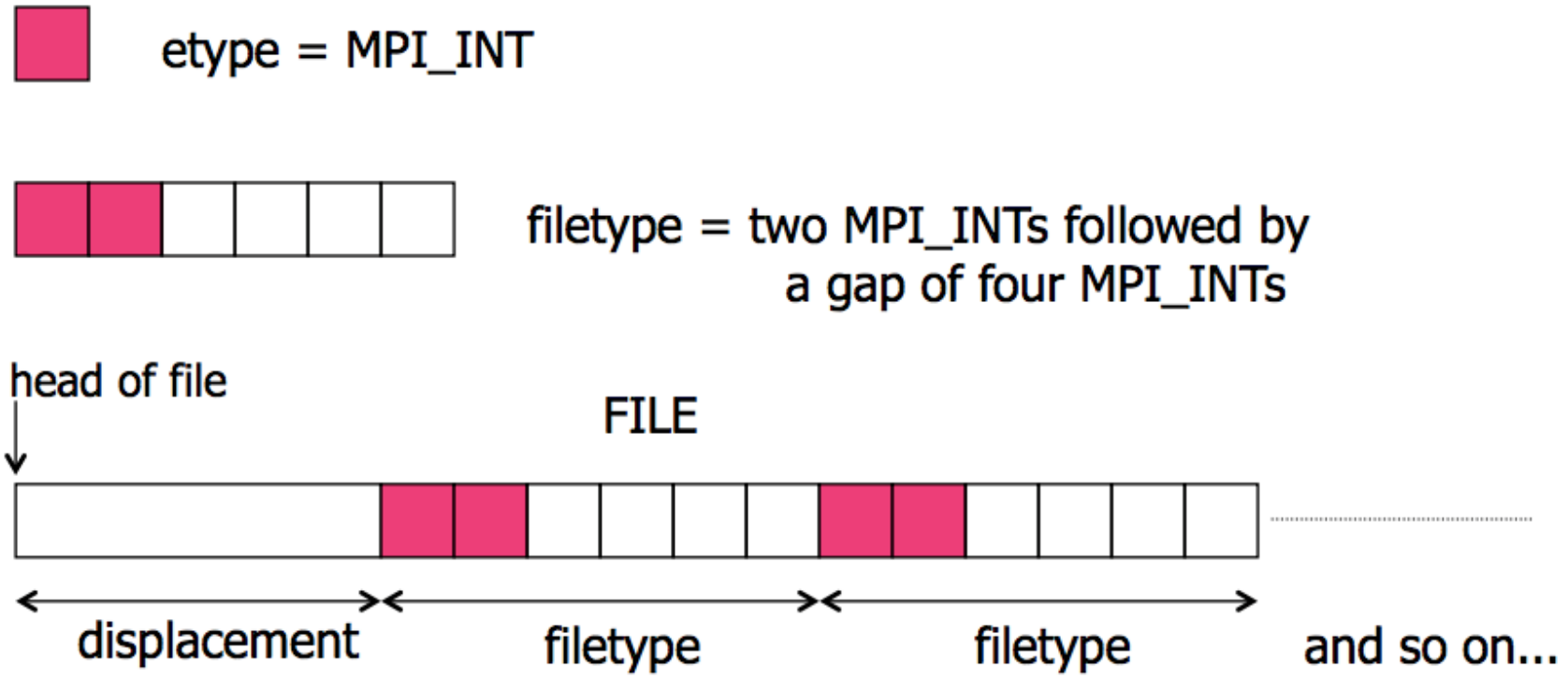
- Common in parallel applications
  - ✓ Example: distributed arrays stored in files
- A big advantage of MPI I/O over Unix I/O is the ability to specify non-contiguous accesses in memory and file within a single function call by using derived datatypes
- Allows MPI implementations to optimise the access
- Collective I/O combined with non-contiguous accesses yields the highest performance

File Views

- Specified by a triplet (displacement, etype, and filetype) passed to **MPI_File_set_view**

- displacement = number of bytes to be skipped from the start of the file
  - ✓ **e.g.** to skip a file header
- etype = basic unit of data access (can be any basic or derived datatype)
- filetype = specifies which portion of the file is visible to the process

A Non-contiguous Example



A Non-contiguous Example (Continued)

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```
#include <mpi.h>
#include <stdio.h>

int main(int argc, char *argv[])
{
    MPI_File fh;
    int buf[1000], rank;
    MPI_Init(0,0);
    MPI_Aint lb, extent;
    MPI_Datatype etype, filetype, contig;
    MPI_Offset disp;
    MPI_Type_contiguous(2, MPI_INT, &contig);
    lb = 0; extent = 6 * sizeof(int);
    MPI_Type_create_resized(contig, lb, extent, &filetype);
    MPI_Type_commit(&filetype);
    disp = 5 * sizeof(int);
    etype = MPI_INT;
    MPI_File_open(MPI_COMM_WORLD, "/pfs/datafile",
    MPI_MODE_CREATE | MPI_MODE_RDWR, MPI_INFO_NULL, &fh);
    MPI_File_set_view(fh, disp, etype, filetype, "native", MPI_INFO_NULL);
    MPI_File_write(fh, buf, 1000, MPI_INT, MPI_STATUS_IGNORE);
    MPI_Finalize();
}
```

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- Parallel File I/O
  - ✓ Introduction
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  - ✓ Independent I/O
  - ✓ **Collective I/O**
  - ✓ I/O access pattern
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  - ✓ Virtual topologies
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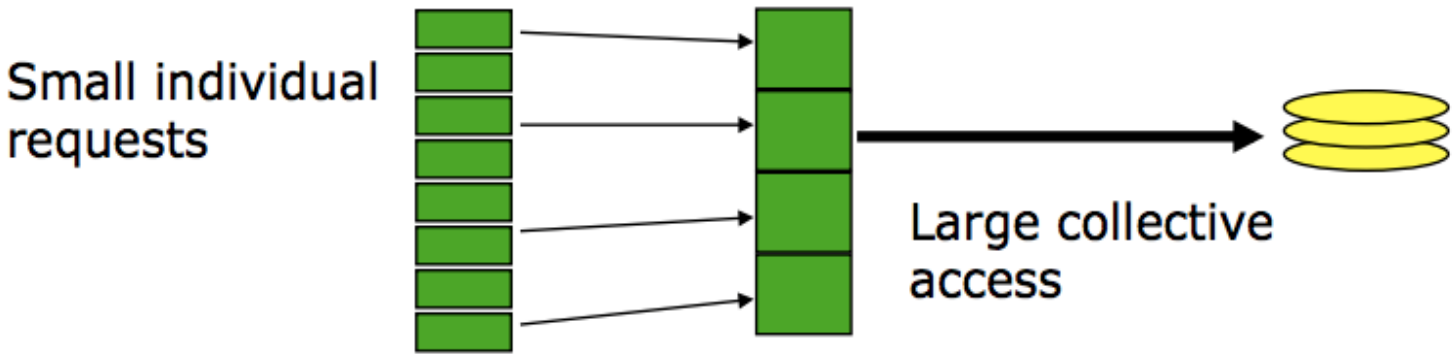
  - ✓ Distributed graph topology
  - ✓ Summary

Collective I/O

- Provides massive speedup
- Like communication, all processes (in a communicator) need to call the same function
- Allows implementation to make many optimisations
- Basic idea:
  - ✓ Build large blocks of data, so reads/writes to the I/O system can be large
  - ✓ Merging of requests from different processes
  - ✓ Particularly effective with very non-contiguous but overlapping requests are interleaved



Collective I/O Functions

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- MPI_File_write_at_all, etc.
  - ✓ **_all** indicates that all processes in the group specified by the communicator passed to **MPI_File_open** will call this function
  - ✓ **_at** indicates that the position in the file is specified as part of the call; this provides **thread-safety** and clearer code than using a separate “seek” call

- Each process specifies only its own access information—the argument list is the same as for the non-collective functions

The Other Collective I/O Calls

- MPI_File_seek
- MPI_File_read_all
- MPI_File_write_all
- MPI_File_read_at_all
- MPI_File_write_at_all
- MPI_File_read_ordered
- MPI_File_write_ordered

Using the Right MPI I/O Function

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- Any application as a particular “I/O access pattern” based on its I/O needs
- The same access pattern can be presented to the I/O system in different ways depending on what/how I/O functions are used
- We classify the different ways of expressing I/O access patterns in MPI I/O into four levels: **level 0 – level 3**

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Example

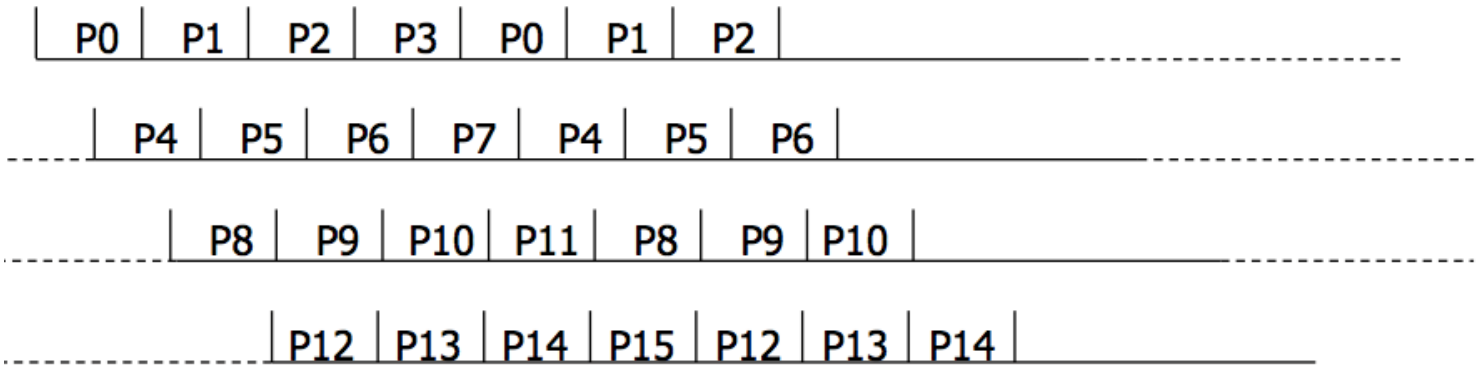
- **Distributed Array Access**

Large array distributed among 16 processes

P0	P1	P2	P3
P4	P5	P6	P7
P8	P9	P10	P11
P12	P13	P14	P15

Each square represents a subarray in the memory of a single process

Access Pattern in the file



Level-0 Access

- Each process makes one independent read request for each row in the local array (as in Unix)

```
MPI_File_open(..., file, ..., &fh);
for (i=0; i<n_local_rows; i++) {
  MPI_File_seek(fh, ...);
  MPI_File_read(fh, &(A[i][0]), ...);
}
MPI_File_close(&fh);
```

Level-1 Access

- Similar to level 0, but each process uses collective I/O functions

```
MPI_File_open(MPI_COMM_WORLD, file, ..., &fh);
for (i=0; i<n_local_rows; i++) {
  MPI_File_seek(fh, ...);
  MPI_File_read_all(fh, &(A[i][0]), ...);
}
MPI_File_close(&fh);
```

Level-2 Access

- Each process creates a derived datatype to describe the non-contiguous access pattern, defines a file view, and calls independent I/O functions

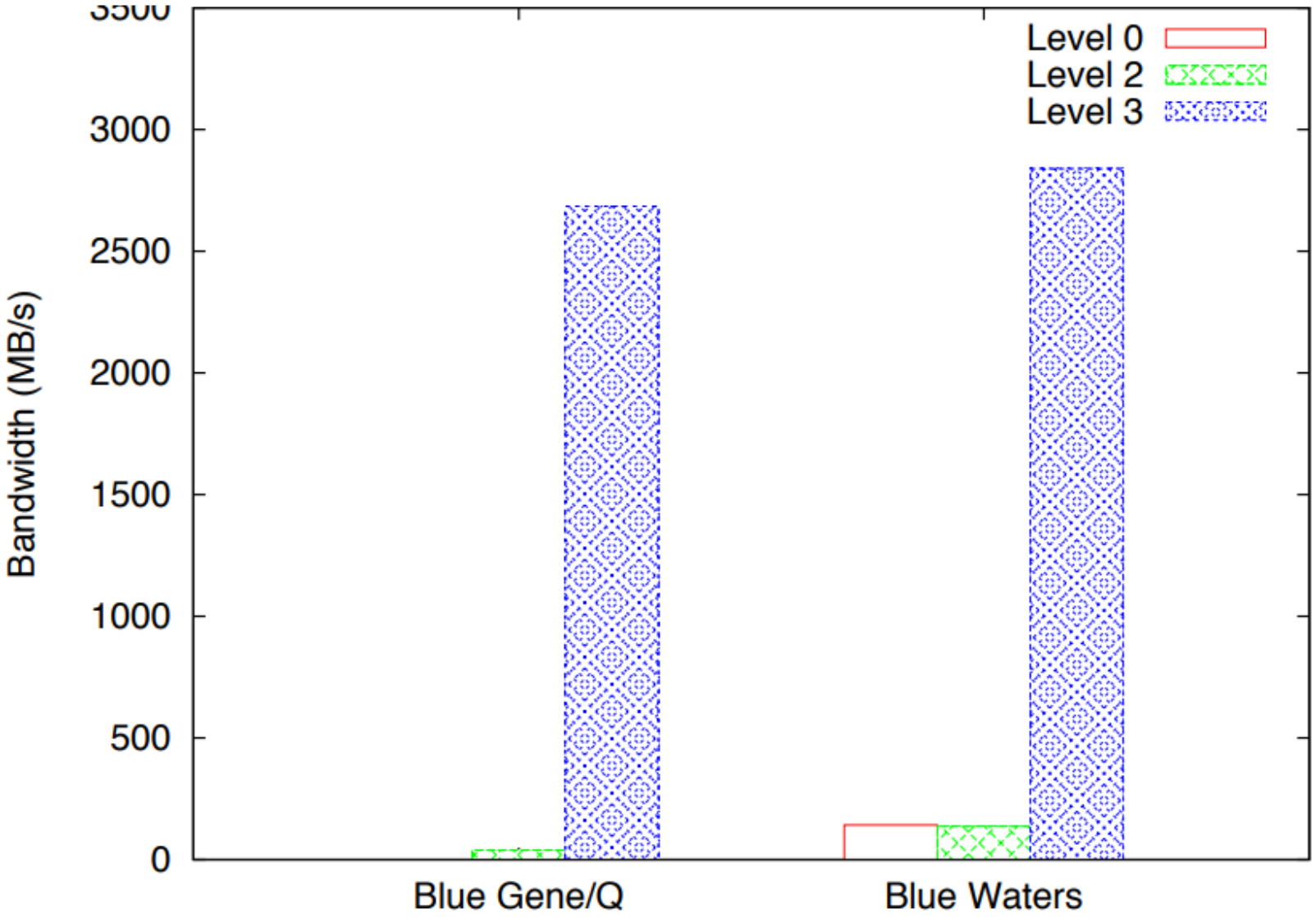
```
MPI_Type_create_subarray(..., &subarray, ...);
MPI_Type_commit(&subarray);
MPI_File_open(..., file, ..., &fh);
MPI_File_set_view(fh, ..., subarray, ...);
MPI_File_read(fh, A, ...);
MPI_File_close(&fh);
```

Level-3 Access

- Similar to level 2, except that each process uses collective I/O functions

```
MPI_Type_create_subarray(..., &subarray, ...);
MPI_Type_commit(&subarray);
MPI_File_open(MPI_COMM_WORLD, file,..., &fh);
MPI_File_set_view(fh, ..., subarray, ...);
MPI_File_read_all(fh, A, ...);
MPI_File_close(&fh);
```

Performance Comparison



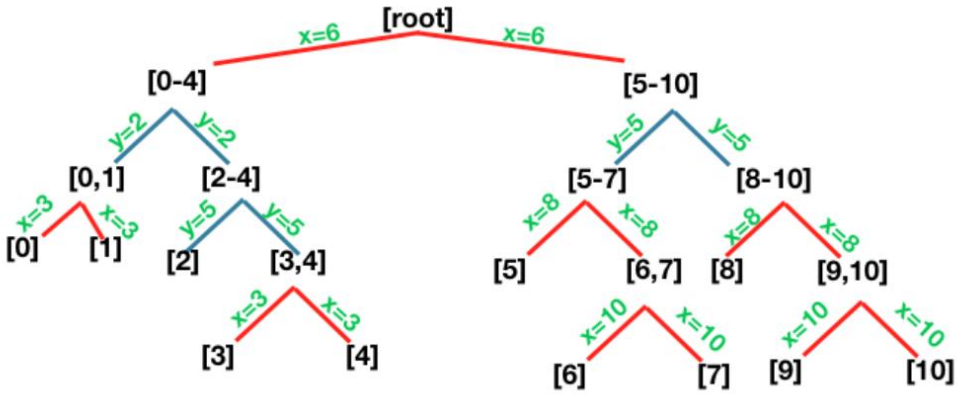
Outline

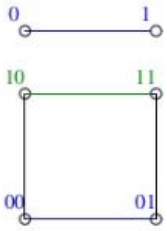
- Parallel File I/O
  - ✓ Introduction
  - ✓ I/O strategy
  - ✓ Independent I/O
  - ✓ Collective I/O
  - ✓ I/O access pattern
- **Process Topologies**
  - ✓ Virtual topologies
  - ✓ Cartesian grid topology
  - ✓ Distributed graph topology
  - ✓ Summary

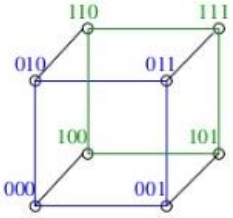
Why we need virtual topologies

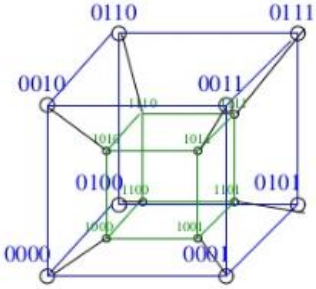
- So far, we deal with MPI processes as a linear range
- The processes needs to be mapped onto the hardware
  - ✓ Which is probably not a line of machines
  - ✓ Many different architectures

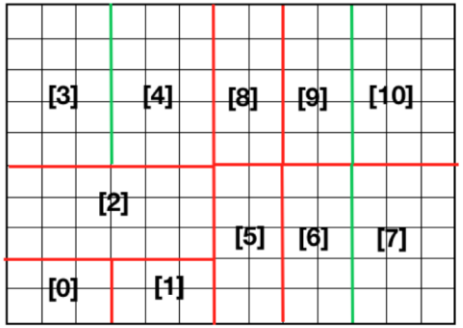
- Most numerical algorithms have some structure to their communication











Why we need virtual topologies (cont'd)

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- If we don't exploit the structure in an algorithm
  - ✓ Could get 'random' process assignment
  - ✓ Extra communication overhead

- Virtual topologies allow you to specify communication patterns, allowing MPI to make smarter mapping choices no matter what machine you use

Outline

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- Parallel File I/O
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  - ✓ Distributed graph topology
  - ✓ Summary

Virtual and Physical Topologies

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- A **virtual topology** represents the way that MPI processes communicate.
  - ✓ Communication patterns between processes can be represented as a graph
  - ✓ **Nodes == Processes**
  - ✓ **Edges == Communication**
  - ✓ This definition will work for any possible topology, but many are common, like Grids (2D, 3D, *n*D), Rings and Tori

- A **physical topology** represents that connections between the cores, chips, and nodes in the hardware.

- Issue is mapping of the **virtual topology** onto the **physical topology**

Virtual Topologies

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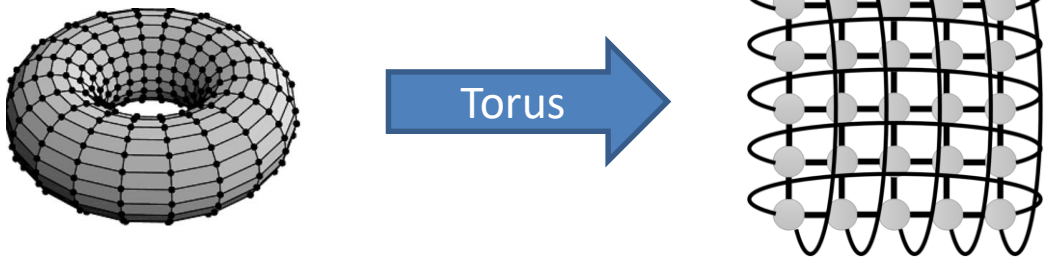
Two types of virtual topologies supported:

- **Cartesian**
  - ✓ *MPI_CART:* This value holds for Cartesian topologies, where processes act as if they are ordered in a multi-dimensional `brick';
- **Graph** (different graph types in MPI)
  - ✓ ~~*MPI_GRAPH*~~: this value describes the graph topology that was defined in MPI; It is unnecessarily burdensome, since each process needs to know the total graph, and should therefore be considered obsolete.
  - ✓ *MPI_DIST_GRAPH*: this value describes the distributed graph topology where each process only describes the edges in the process graph that touch itself.

Cartesian Topologies

- Concept
  - ✓ Any decomposition in natural coordinates
  - ✓ Indexing starts from 0
  - ✓ MPI_COMM_WORLD is a 1D Cartesian topology.

- Can be non-periodic or periodic
  - ✓ Periodic 1D == Ring
  - ✓ Non-Periodic 2D == Rectangle
  - ✓ Periodic 2D (in one dimension)==Cylinder
  - ✓ Full Periodic 2D == Torus



MPI_CART_CREATE

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- The cartesian topology is specified by giving *MPI_Cart_create* the sizes of the processor grid along each axis, and whether the grid is periodic along that axis.

```
MPI_CART_CREATE(comm_old, ndims, dims, periods, reorder, comm_cart)
```

- comm_old (IN) Input communicator
- ndims (IN) Number of dimensions
- dims (IN) Array of integers specifying number of processes in each dimension
- periods (IN) Logical array of size ndims specifying if each dimension is periodic (true) or not (false)
- reorder (IN) *Whether the ranks can be re-order from the old communicator*
- comm_cart (OUT) Communicator with new Cartesian topology

MPI_CART_CREATE

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- Returns a handle to a new communicator with the topology specified
- As always, all processes need to call the same function with the same arguments for success
- If the total Cartesian grid is smaller than the number of processes you have, some will receive MPI_COMM_NULL
- This call returns errors if the grid is larger than the number of processes you have

Cartesian Topology: Rank and Coordinate

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- Communication speed may increase if process addressing reordered by system. Therefore, each point in this new communicator has a coordinate and a rank.

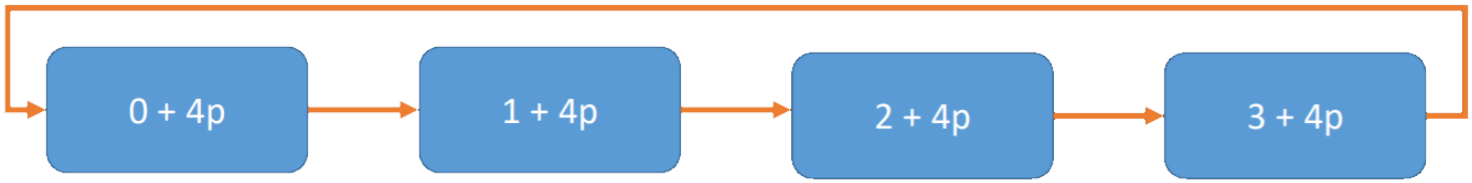
- They can be queried with MPI_Cart_coords and MPI_Cart_rank respectively.

```
int MPI_Cart_coords(MPI_Comm comm, int rank, int maxdims, int *coords);

int MPI_Cart_rank(MPI_Comm comm, init *coords, int *rank);
```

Cartesian Example 1: Ring

```
MPI_CART_CREATE(comm_old, ndims, dims, periods, reorder, comm_cart)
```



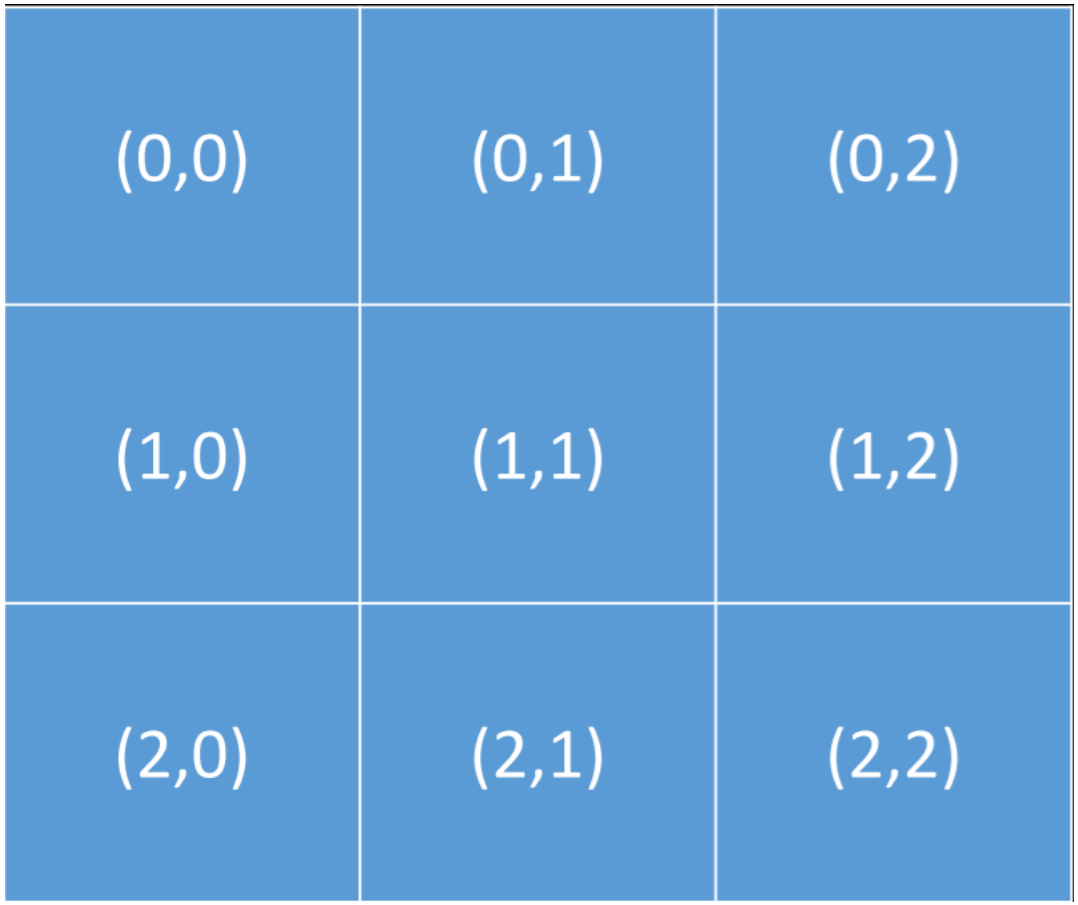
Assume we have access to:

- comm_size – Size of MPI_COMM_WORLD (4)
- rank – Rank of the calling process

```
MPI_Cart_Create(MPI_COMM_WORLD, 1, comm_size, true, true, NEW_COMM);
```

Cartesian Example 2: Square Grid

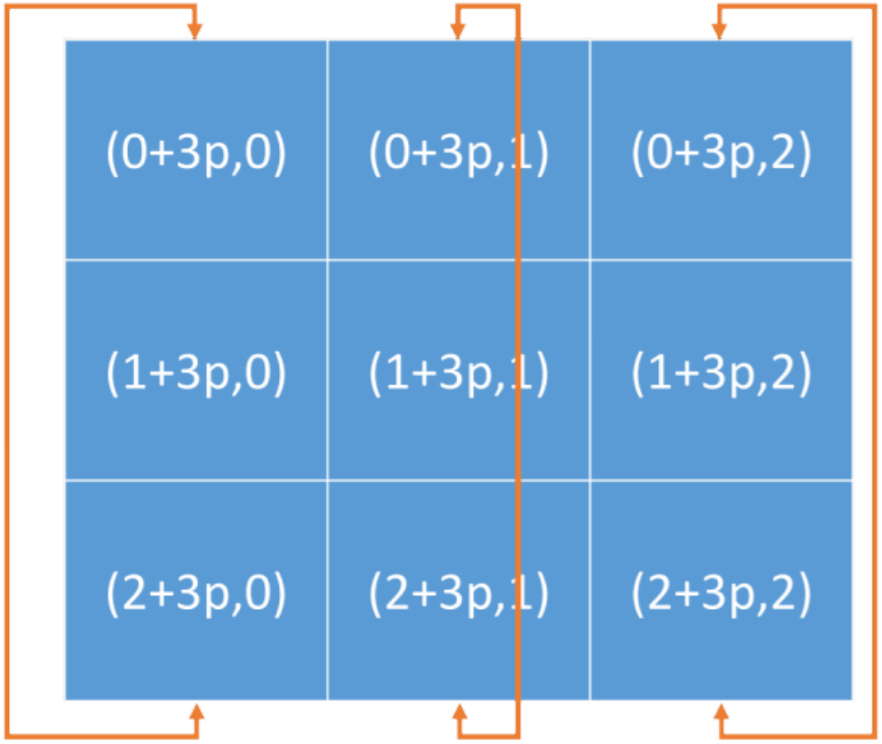
```
MPI_CART_CREATE(comm_old, ndims, dims, periods, reorder, comm_cart)
```




```
MPI_Cart_Create
(
    MPI_COMM_WORLD,
    2,
    {3,3},
    {False, False},
    True,
    NEW_COMM
);
```

Cartesian Example 3a: Cylinder

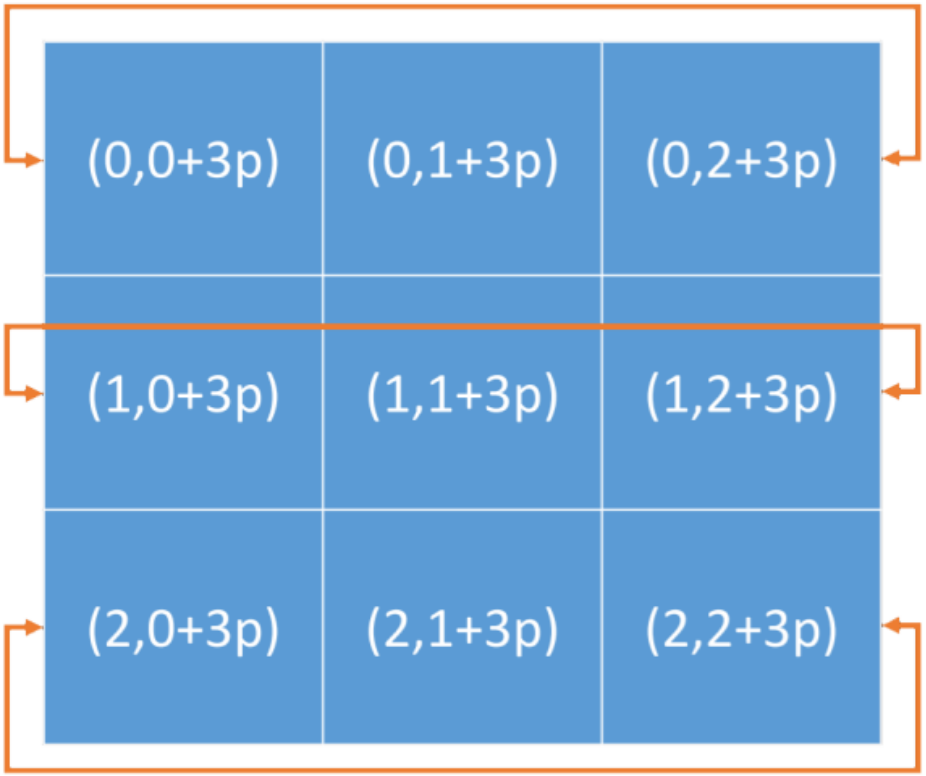
```
MPI_CART_CREATE(comm_old, ndims, dims, periods, reorder, comm_cart)
```




```
MPI_Cart_Create
(
MPI_COMM_WORLD,
2,
{3,3},
{True, False},
True,
NEW_COMM
);
```

Cartesian Example 3b: Cylinder

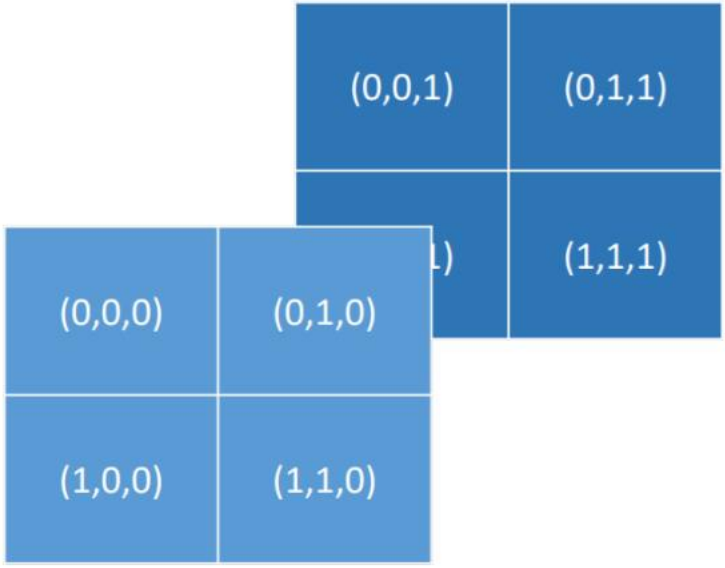
```
MPI_CART_CREATE(comm_old, ndims, dims, periods, reorder, comm_cart)
```




```
MPI_Cart_Create
(
MPI_COMM_WORLD,
2,
{3,3},
{False, True},
True,
NEW_COMM
);
```

Cartesian Example 4a: 3D Torus

```
MPI_CART_CREATE(comm_old, ndims, dims, periods, reorder, comm_cart)
```




```
MPI_Cart_Create
(
MPI_COMM_WORLD,
3,
{2,2,2},
{True, True, True},
True,
NEW_COMM
);
```

Cartesian Example 4b: 2D Torus

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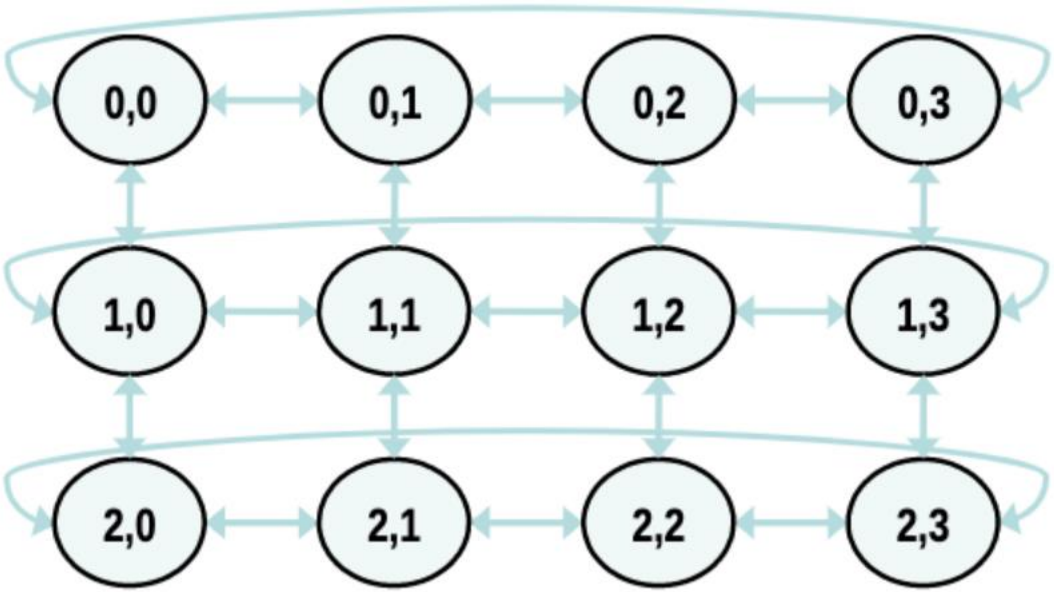
```
#include<mpi.h> #include<stdio.h>
/* A two-dimensional torus of 12 processes in a 4x3 grid */
int main(int argc, char *argv[]) {
int rank, size; MPI_Comm comm;
int dim[2], period[2], reorder;
int coord[2], id;

MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &size);

dim[0]=4;  dim[1]=3;
period[0]=1; period[1]=0; reorder=1;
MPI_Cart_create(MPI_COMM_WORLD, 2, dim, period, reorder, &comm);
if (rank == 5) {
      MPI_Cart_coords(comm, rank, 2, coord);
      printf("Rank %d coordinates are %d %d\n",
      rank, coord[0], coord[1]);fflush(stdout);
      }
if(rank==0) {
      coord[0]=3;
      coord[1]=1;
      MPI_Cart_rank(comm, coord, &id);
      printf("The processor at position (%d, %d) has rank %d\n",
      coord[0], coord[1], id);fflush(stdout);
      }
MPI_Finalize();
return 0;
}
```

Cartesian Example 4b: 2D Torus (Cont'd)



Cartesian Conveniences

```
MPI_DIMS_CREATE(nnodes, ndims, dims)
```

- Suggests the most balanced division of n-nodes into an n-dimensional grid
- Result is stored in the integer array dims
- If dims[i] is set to a positive number, the routine will not modify the number of nodes in dimension i;

dims before call	function call	dims on return
(0,0)	MPI_DIMS_CREATE(6, 2, dims)	(3,2)
(0,0)	MPI_DIMS_CREATE(7, 2, dims)	(7,1)
(0,3,0)	MPI_DIMS_CREATE(6, 3, dims)	(2,3,1)
(0,3,0)	MPI_DIMS_CREATE(7, 3, dims)	erroneous call

Cartesian Conveniences

```
int MPI_Cart_shift(MPI_Comm comm, int direction, int displ, int
*source, int *dest)
```

- Returns the shifted source and destination ranks, given a shift direction and amount
- The direction argument is in the range [0,n-1] for an n-dimensional Cartesian mesh

• Comm	(in)	communicator with cartesian structure	(handle)
• direction	(in)	coordinate dimension of shift	(integer)
• displacement	(in)	(> 0: upwards shift, < 0: downwards shift)	(integer)
• rank_source	(out)	rank of source process	(integer)
• rank_dest	(out)	rank of destination process	(integer)

MPI_Cart_shift Example (aside)

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```
#include <stdio.h>
#include <mpi.h>
int main(int argc; char **argv; )
{
     int rank, value, size, false=0;
     int right_nbr, left_nbr;
     MPI_Comm one_dim_comm;
     MPI_Status status;
     MPI_Init( &argc, &argv );
     MPI_Comm_size( MPI_COMM_WORLD, &size );
     MPI_Cart_create( MPI_COMM_WORLD, 1, &size, 1, 1, &one_dim_comm );

     /*   create a one-dimensional grid.
          False means that there is no periodicity
     (the process outside the two ends is identified as MPI_PROC_NULL),
          1 means that it can be reordered,
          and the obtained topological coordinate adjacency relation is:
            MPI_PROC_NULL, 0, 1, ... , size-1 , MPI_PROC_NULL
     */
     MPI_Cart_shift( one_dim_comm, 0, 1, &left_nbr, &right_nbr );
     /*The identity of the left and right processes
     is obtained by shifting over the defined grid*/
     MPI_Comm_rank( one_dim_comm, &rank );
     MPI_Comm_size( one_dim_comm, &size );
```

MPI_Cart_shift Example

```
    do
    {
        if (rank == 0) {
        /*Process 0 is responsible for reading in
         the data and passing it on to the next process*/
        scanf( "%d", &value );
        MPI_Send( &value, 1, MPI_INT, right_nbr, 0, one_dim_comm );
        /*Sends data to the process on the right*/
        }
        else {
        MPI_Recv( &value, 1, MPI_INT, left_nbr, 0, one_dim_comm,
        &status );
        /*The next process receives data from the left process*/
        MPI_Send( &value, 1, MPI_INT, right_nbr, 0, one_dim_comm );
        /*Sends data to the process on the right*/
        }
        printf( "Process %d got %d\n", rank, value );
    } while (value >= 0);
    /*If the scanned data is non-negative,
    continue reading and passing*/
    MPI_Finalize( );
}
```

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  - ✓ Virtual topologies
  - ✓ Cartesian grid topology
  - ✓ **Distributed graph topology**
  - ✓ Summary

Distributed Graph Topology

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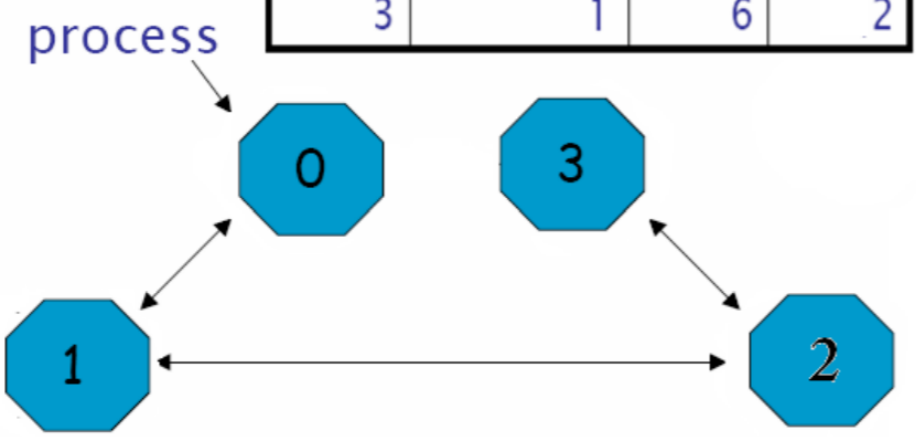
Elements of Graph Topology

- Nodes: Processors
- Lines: Communicators between nodes
- Arrows: Show origins and destinations of links
- Index: array of integers describing node degrees

Node	Nneighbors	index	edges
0	1	1	1
1	2	3	0,2
2	2	5	1,3
3	1	6	2



MPI_GRAPH_CREATE

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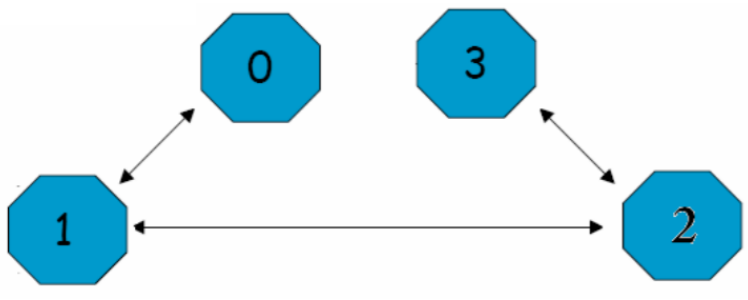
```
int MPI_Graph_create(MPI_Comm comm_old, int nnodes, int *index, int *edges,
        int reorder, MPI_Comm *comm_graph)
```

- comm_old [in] input communicator without topology (handle)
- nnodes [in] number of nodes in graph (integer)
- index [in] array of integers describing node degrees
- edges [in] array of integers describing graph edges
- reorder [in] ranking may be reordered (true) or not (false) (logical)
- comm_graph [out] communicator with graph topology added (handle)

MPI_GRAPH_CREATE - Example



Node	Nneighbors	index	edges
0	1	1	1
1	2	3	0,2
2	2	5	1,3
3	1	6	2

```
#include "mpi.h"
MPI_Comm graph_comm;
int nnodes = 4; /* number of nodes */
int index[4] = {1, 3, 5, 6}; /* index definition */
int edges[6] = {1, 0, 2, 1, 3, 2}; /* edges definition */
int reorder = 1; /* allows processes reordered for efficiency */
MPI_Graph_create(MPI_COMM_WORLD, nnodes, index, edges, reorder, graph_comm);
```

**In C, index[0] is the degree of node zero, and index[i] - index[i-1] is the degree of node i where i=1, ..., nnodes-1;*

Graph Neighbors

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- The number of the neighboring processes may be obtained by the following function:

```
int MPI_Graph_neighbors_count(MPI_Comm comm, int rank, int *mneighbors);
```

- Obtaining **the ranks of the neighboring** vertices is provided by the following function:

```
int MPI_Graph_neighbors(MPI_Comm comm,int rank, int mneighbors, int *neighbors);
```

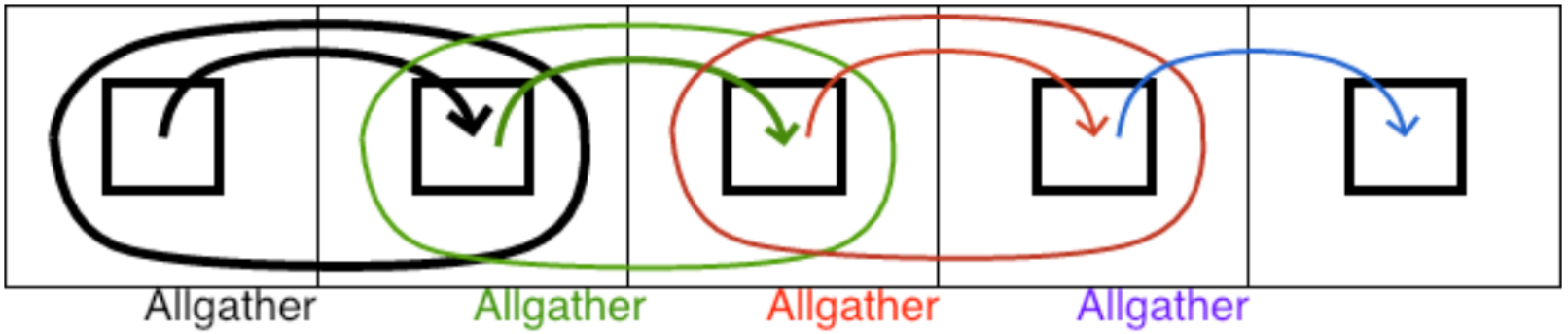
- (where mneighbors is the size of the array neighbors)

Neighbor Collectives

- MPI's notion of neighborhood collectives, offer an elegant way of expressing such communication structures.

- The neighbor collectives have the same argument list as the regular collectives, but they apply to a graph communicator.

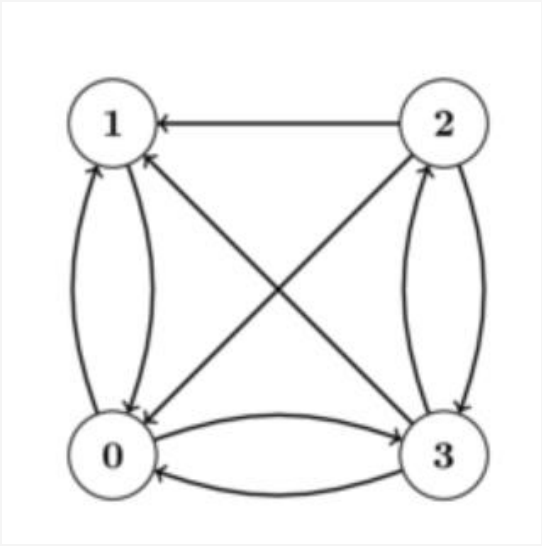
```
int MPI_Neighbor_allgather(const void *sendbuf, int sendcount,
MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype,
MPI_Comm comm)
```



Graph Example

```
#include <mpi.h>
#include <stdio.h>
#define nnode 4
int main() {
MPI_Init(NULL, NULL);
int rank;
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
int source = rank;
int degree;
int dest[nnode];
int weight[nnode] = {1, 1, 1, 1};
int recv[nnode] = {-1, -1, -1, -1};
int send = rank; // set dest and degree.

if (rank == 0) { dest[0] = 1; dest[1] = 3; degree = 2; }
else if(rank == 1) { dest[0] = 0; degree = 1; }
else if(rank == 2) { dest[0] = 3; dest[1] = 0; dest[2] = 1; degree = 3; }
else if(rank == 3) { dest[0] = 0; dest[1] = 2; dest[2] = 1; degree = 3; }
```



Graph Example (continue)

```
    // create graph.
    MPI_Comm graph;
    MPI_Dist_graph_create(MPI_COMM_WORLD, 1, &source,
    &degree, dest, weight, MPI_INFO_NULL, 1, &graph);

    // send and gather rank to/from neighbors.
    MPI_Neighbor_allgather(&send, 1, MPI_INT, recv, 1, MPI_INT, graph);
    printf("Rank: %i, recv[0] = %i, recv[1] = %i, recv[2] = %i,
    recv[3] = %i\n", rank, recv[0], recv[1], recv[2], recv[3]);
    MPI_Finalize();
    return 0;
}
```

In this function, each process i gathers data items from each process j if an edge (j,i) exists in the topology graph, and each process i sends the same data items to all processes j where an edge (i,j) exists. The send buffer is sent to each neighboring process and the i-th block in the receive buffer is received from the i-th neighbor.

Summary

- I/O can destroy performance if handled poorly
- MPI I/O offers many ways to access files in parallel
  - ✓ Independent file access
  - ✓ Non-contiguous access to shared files
  - ✓ Collective calls to shared files

- Virtual topologies allows for the user to develop simpler communication calls and hence higher performance
  - ✓ Cartesian grids are flexible and common
  - ✓ Particular useful for numerical routines
  - ✓ Graph topologies

References

- Readings
  - Introduction to Parallel I/O
  - Advanced MPI: Parallel I/O
  - An Article on MPI Process Topologies
  - MPI Topologies
  - MPI_Cart_shift

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