



#### **MPI II**

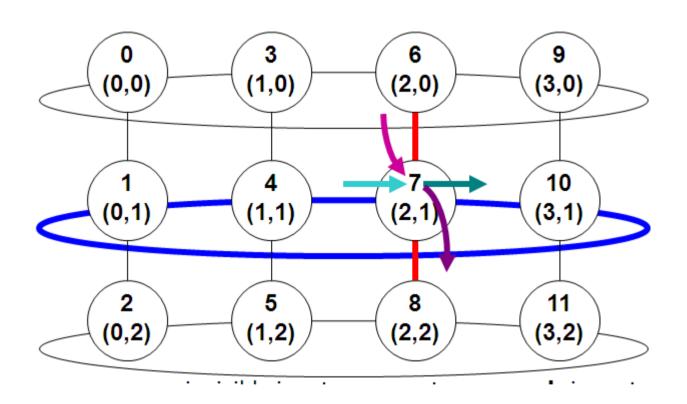
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Including adapted teaching material from books, lectures and presentations by B. Barney, G. Hager, M. Martinasso, R. Rabenseifner, O. Schenk, G. Wellein

#### **Outline**

- 1. Topology for managing rank numbering
- 2. User specific data type
- 3. Parallel I/O
- 4. Python & MPI

#### 1. Topology for managing rank numbering.



#### MPI\_Groups

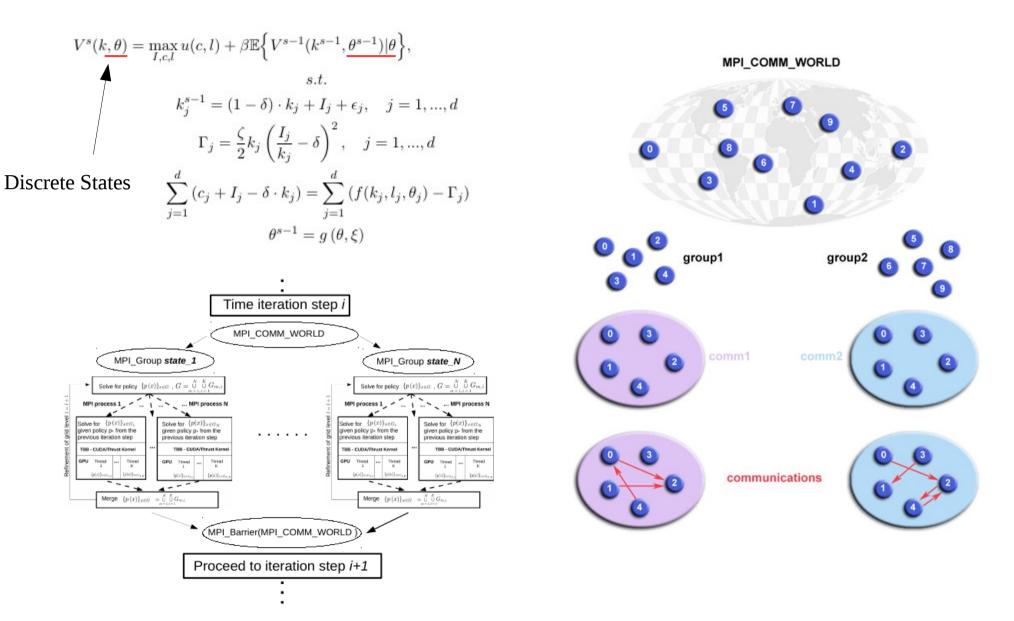


Fig. from https://computing.llnl.gov/tutorials/mpi/

1. Topology

# Group and Communicator Management Routines

- → A group is an ordered set of processes, each with a unique integer rank. In MPI, a group is represented within system memory as an object. It is accessible to the programmer only by a "handle". A group is always associated with a communicator object.
- → A communicator encompasses a group of processes that may communicate with each other. All MPI messages must specify a communicator. Like groups, communicators are accessible to the programmer only by "handles". The handle for the communicator that comprises all processes is MPI\_COMM\_WORLD.

From the programmer's perspective, a group and a communicator are one. The group routines are primarily used to specify which processes should be used to construct a communicator.

# Primary Purposes of Group and Communicator Objects

#### Goals:

- → Allow you to organize tasks, based upon function, into task groups.
- → Enable Collective Communications operations across a subset of related tasks.
- → Provide basis for implementing user defined virtual topology.

#### **Remarks:**

- → Groups/communicators can be created and destroyed during program execution.
- → Processes may be in more than one group/communicator having a unique rank within each group/communicator.

## **Example**

Create two different process groups for separate collective communications exchange. → This requires creating new communicators.

- > cd OSM\_Lab/HPC\_day3/code\_day3/MPI
- 2. Have a look at the code
- >vi 4a.MPI\_group.cpp
- 3. compile by typing:
- > make
- 4. run the code

>mpiexec -np 8 ./4a.MPI\_group.exec

1. Topology

### Example (II)

```
#include <stdio.h>
#include <iostream>
#include "mpi.h"
#define NPROCS 8
using namespace std;
main(int argc, char *argv[]) {
int
           rank, new rank, sendbuf, recybuf, numtasks,
           ranks1[4]=\{0,1,2,3\}, ranks2[4]=\{4,5,6,7\};
MPI Group orig group, new group; // required variables
MPI Comm new comm; // required variable
MPI Init(&argc,&argv);
MPI Comm rank(MPI COMM WORLD, &rank);
MPI Comm size(MPI COMM WORLD, &numtasks);
if (numtasks != NPROCS) {
 cout << "Must specify 8 MPI processes = " << NPROCS << " !! Terminating "<< endl:
 MPI Finalize();
 return Θ;
sendbuf = rank;
// extract the original group handle
MPI Comm group(MPI COMM WORLD, &orig group);
// divide tasks into two distinct groups based upon rank
if (rank < NPROCS/2) {
 MPI Group incl(orig group, NPROCS/2, ranks1, &new group);
else {
 MPI Group incl(orig group, NPROCS/2, ranks2, &new group);
// create new new communicator and then perform collective communications
MPI Comm create(MPI COMM WORLD, new group, &new comm);
MPI Allreduce(&sendbuf, &recvbuf, 1, MPI INT, MPI SUM, new comm);
// get rank in new group
MPI Group rank (new group, &new rank);
cout << "rank= " << rank << " newrank= "<< new rank << " recvbuf= " <<recvbuf << endl;
MPI Finalize();
```

#### >mpiexec -np 8 ./4a.MPI\_group.exec

```
rank=
                 0 newrank=
                                        0 recvbuf=
rank=
                 1 newrank=
                                        1 recvbuf=
                                                               6
                                                               6
rank=
                 3 newrank=
                                        3 recvbuf=
rank=
                 4 newrank=
                                        0 recvbuf=
                                                              22
rank=
                                          recvbuf=
                                                              22
                 6 newrank=
rank=
                                          recvbuf=
                                                              22
                   newrank=
rank=
                 7 newrank=
                                        3 recvbuf=
                                                              22
                                        2 recvbuf=
                                                               6
rank=
                   newrank=
```

Reduction within group

$$0 + 1 + 2 + 3 = 6$$
  
 $4 + 5 + 6 + 7 = 22$ 

### Virtual topologies

- In terms of MPI, a virtual topology describes a mapping/ordering of MPI processes into a geometric "shape".
- The two main types of **topologies** supported by MPI are **Cartesian (grid) and Graph**.
- MPI topologies are virtual there may be no relation between the physical structure of the parallel machine and the process topology.
- Virtual topologies are built upon MPI communicators and groups.
- Must be "programmed" by the application developer.

#### Why Use Them?

→ Convenience:

Virtual topologies may be useful for applications with specific communication patterns - patterns that match an MPI topology structure.

For example, a Cartesian topology might prove convenient for an application that requires 4-way nearest neighbour communications for grid based data.

→ Communication Efficiency

Some hardware architectures may impose penalties for communications between successively distant "nodes". A particular implementation may optimize process mapping based upon the physical characteristics of a given parallel machine.

## **Domain Decomposition**

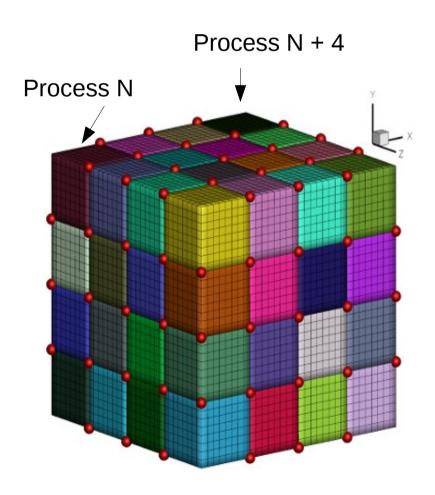
Cartesian distribution: data are distributed linearly between processors.

Useful e.g. when solving PDEs ("ghost zones").

This is in general a more effective way of distribute the domain, since:

- → It is much more scalable.
- → Communicated data volume can be smaller (especially when a large number of processors is used).
- → It can better map the geometry of the problem and of the Algorithm.

However, it is more difficult to handle: who are my neighbours?



#### Cartesian topology

```
comm_old input communicator
```

ndims number of dimensions of Cartesian grid

**dims** specifies the number of processes in each dimension

**periods** specifies whether the grid is periodic (true) or not (false)

in each dimension

reorder ranking may be reordered (true) or not (false)

comm\_cart communicator with new Cartesian topology

row-major ordering

0	1	2	3
(0,0)	(0,1)	(0,2)	(0,3)
4	5	6	7
(1,0)	(1,1)	(1,2)	(1,3)
8	9	10	11
(2,0)	(2,1)	(2,2)	(2,3)
12	13	14	15
(3,0)	(3,1)	(3,2)	(3,3)

# Example (run in break – is involved)

A simplified mapping of processes into a Cartesian virtual topology appears below.

Example: We want to create a 4 x 4 Cartesian topology from 16 processors and have each process exchange its rank with four neighbours.

0	1 (0,1)	2	3
(0,0)		(0,2)	(0,3)
4	5	6	7
(1,0)	(1,1)	(1,2)	(1,3)
8	9	10	11
(2,0)	(2,1)	(2,2)	(2,3)
12	13	14 (3,2)	15
(3,0)	(3,1)		(3,3)

- > cd OSM\_Lab/HPC\_day3/code\_day3/MPI
- 2. Have a look at the code
- >vi 5a.virtual\_topo.cpp
- 3. compile by typing:
- > make
- 4. run the code

>mpiexec -np 16 ./5a.virtual\_topo.exec

## **Example**

```
main(int argc, char *argv[]) {
int numtasks, rank, source, dest, outbuf, i, tag=1,
   inbuf[4]={MPI PROC NULL, MPI PROC NULL, MPI PROC NULL, MPI PROC NULL, },
   nbrs[4], dims[2]=\{4,4\}.
   periods[2]={0,0}, reorder=0, coords[2];
MPI Request regs[8]:
MPI Status stats[8]:
MPI Comm cartcomm; // required variable
MPI Init(&argc,&argv);
MPI Comm size(MPI COMM WORLD, &numtasks);
if (numtasks == SIZE) {
   // create cartesian virtual topology, get rank, coordinates, neighbor ranks
   MPI Cart create(MPI COMM WORLD, 2, dims, periods, reorder, &cartcomm);
   MPI Comm rank(cartcomm, &rank);
   MPI Cart coords(cartcomm, rank, 2, coords);
   MPI Cart shift(cartcomm, 0, 1, &nbrs[UP], &nbrs[DOWN]);
   MPI Cart shift(cartcomm, 1, 1, &nbrs[LEFT], &nbrs[RIGHT]);
   printf("rank= %d coords= %d %d neighbors(u,d,l,r)= %d %d %d %d %d\n",
          rank, coords [0], coords [1], nbrs [UP], nbrs [DOWN], nbrs [LEFT],
          nbrs[RIGHT]);
   outbuf = rank:
   // exchange data (rank) with 4 neighbors
   for (i=0; i<4; i++) {
      dest = nbrs[i];
      source = nbrs[i];
      MPI Isend(&outbuf, 1, MPI INT, dest, tag,
                MPI COMM WORLD, &reqs[i]);
      MPI Irecv(&inbuf[i], 1, MPI INT, source, tag,
                MPI COMM WORLD, &regs[i+4]);
   MPI Waitall(8, regs, stats);
                                     inbuf(u,d,l,r)= %d %d %d %d %d\n",
   printf("rank= %d
          rank,inbuf[UP],inbuf[DOWN],inbuf[LEFT],inbuf[RIGHT]); }
else
   printf("Must specify %d processors. Terminating.\n",SIZE);
MPI Finalize();
```

#### >mpiexec -np 16 ./5.virtual\_topo.exec

```
2 coords= \theta 2 neighbors(u,d,l,r)= -2 6 1 3
rank= 3 \operatorname{coords} = 0 \operatorname{3} \operatorname{neighbors}(u,d,l,r) = -2 \operatorname{7} 2 -2
rank= 10 coords= 2 2 neighbors(u,d,l,r)= 6 14 9 11
rank= 6 coords= 1 2 neighbors(u,d,l,r)= 2 10 5 7
rank= 7 coords= 1 3 neighbors(u,d,l,r)= 3 11 6 -2
rank= 15 coords= 3 3 neighbors(u,d,l,r)= 11 -2 14 -2
rank= 14 coords= 3 2 neighbors(u,d,l,r)= 10 -2 13 15
rank= 11 coords= 2 3 neighbors(u,d,l,r)= 7 15 10 -2
rank= 13 coords= 3 1 neighbors(u,d,l,r)= 9 -2 12 14
rank= 5 \text{ coords} = 1 \text{ 1 neighbors}(u,d,l,r) = 1 9 4 6
rank= 0 coords= 0 0 neighbors(u,d,l,r)= -2 4 -2 1
rank= 4 coords= 1 0 neighbors(u,d,l,r)= 0 8 -2 5
rank= 8 coords= 2 0 neighbors(u,d,l,r)= 4 12 -2 9
rank= 12 coords= 3 0 neighbors(u,d,l,r)= 8 -2 -2 13
                          inbuf(u,d,l,r) = -2 7 2 -2
rank=
rank= 9 coords= 2 1 neighbors(u,d,l,r)= 5 13 8 10
rank= 11
                          inbuf(u,d,l,r) = 7 15 10 -2
rank=
                          inbuf(u,d,l,r)=3116-2
rank= 15
                          inbuf(u,d,l,r) = 11 - 2 14 - 2
rank=
                          inbuf(u,d,l,r) = 2 10 5 7
rank= 12
                          inbuf(u,d,l,r) = 8 -2 -2 13
                          inbuf(u,d,l,r) = 4 12 -2 9
rank=
      8
rank=
      13
                          inbuf(u,d,l,r) = 9 -2 12 14
rank=
      1 coords= 0 1 neighbors(u,d,l,r)= -2 5 0 2
rank=
                          inbuf(u,d,l,r) = 5 13 8 10
rank= 14
                          inbuf(u,d,l,r) = 10 -2 13 15
rank= 5
                          inbuf(u,d,l,r) = 1 9 4 6
rank=
                          inbuf(u,d,l,r) = -2 6 1 3
rank= 0
                          inbuf(u,d,l,r) = -2 \ 4 \ -2 \ 1
rank=
      4
                          inbuf(u,d,l,r) = 0 8 - 2 5
rank= 10
                          inbuf(u,d,l,r) = 6 14 9 11
rank=
                          inbuf(u,d,l,r) = -2 5 0 2
```

# 2. User specific data type

MPI predefines its primitive data types:

	C Data Types	Fortran Data Types
MPI_CHAR	MPI_C_COMPLEX	MPI_CHARACTER
MPI_WCHAR	MPI_C_FLOAT_COMPLEX	MPI_INTEGER
MPI_SHORT	MPI_C_DOUBLE_COMPLEX	MPI_INTEGER1
MPI_INT	MPI_C_LONG_DOUBLE_COMPLEX	MPI_INTEGER2
MPI_LONG	MPI_C_BOOL	MPI_INTEGER4
MPI_LONG_LONG_INT	MPI_LOGICAL	MPI_REAL
MPI_LONG_LONG	MPI_C_LONG_DOUBLE_COMPLEX	MPI_REAL2
MPI_SIGNED_CHAR	MPI_INT8_T	MPI_REAL4
MPI_UNSIGNED_CHAR	MPI_INT16_T	MPI_REAL8
MPI_UNSIGNED_SHORT	MPI_INT32_T	MPI_DOUBLE_PRECISION
MPI_UNSIGNED_LONG	MPI_INT64_T	MPI_COMPLEX
MPI_UNSIGNED	MPI_UINT8_T	MPI_DOUBLE_COMPLEX
MPI_FLOAT	MPI_UINT16_T	MPI_LOGICAL
MPI_DOUBLE	MPI_UINT32_T	MPI_BYTE
MPI_LONG_DOUBLE	MPI_UINT64_T	MPI_PACKED
	MPI_BYTE	
	MPI_PACKED	

## **Derived Data Types**

MPI also provides facilities for you to **define your own data structures** based upon sequences of the MPI primitive data types.

Such user defined structures are called **derived data** types.

Primitive data types are contiguous.

Derived data types allow you to specify non-contiguous data in a convenient manner and to treat it as though it was contiguous.

MPI provides several methods for constructing derived data types:

- Contiguous (we will below only consider this one as an example)
- Vector
- Indexed
- Struct
- MPI derived data types (differently from C or Fortran) are created (and destroyed) at run-time through calls to MPI library routines.
   Implementation steps:
- 1. Construct the data type
- 2. Allocate the data type
- 3. Use the data type
- 4. Deallocate the data type

## Allocate and destroy the data type

A constructed data type must be committed to the system before it can be used in a communication.

```
MPI_TYPE_COMMIT(DATATYPE, IERR)
MPI_TYPE_FREE(DATATYPE, IERR)
```

#### e.g. Contiguous Datatype

MPI\_TYPE\_CONTIGOUS constructs a type-map consisting of the replication of a data type into contiguous locations.

```
count number of BLOCKs to be added
oldtype oldtype Datatype of each element
newtype new derived datatype
```

## **Example**

Create a data type representing a row of an array and distribute a different row to all processes.

> cd OSM\_Lab/HPC\_day3/code\_day3/MPI

2. Have a look at the code

>vi 6a.derived\_data.cpp

3. compile by typing:

> make

4. run the code

/1.0, 2.0, 3.0, 4.0, & 5.0, 6.0, 7.0, 8.0, & 9.0, 10.0, 11.0, 12.0, & 13.0, 14.0, 15.0, 16.0 /

Rank 0 /1.0, 2.0, 3.0, 4.0,

Rank 1 5.0, 6.0, 7.0, 8.0,

Rank 2 9.0, 10.0, 11.0, 12.0,

Rank 3 13.0, 14.0, 15.0, 16.0

>mpiexec -np 4 ./6a.derived\_data.exec

### Example data type

```
main(int argc, char *argv[]) {
int numtasks, rank, source=0, dest, tag=1, i;
float a[SIZE][SIZE] =
 {1.0, 2.0, 3.0, 4.0,
  5.0, 6.0, 7.0, 8.0,
  9.0, 10.0, 11.0, 12.0,
   13.0, 14.0, 15.0, 16.0};
float b[SIZE];
MPI Status stat:
                                                                   >mpiexec -np 4 ./6.derived_data.exec
MPI Datatype rowtype;
                       // required variable
MPI Init(&argc,&argv);
MPI Comm rank(MPI COMM WORLD, &rank);
MPI Comm size(MPI COMM WORLD, &numtasks);
// create contiguous derived data type
MPI Type contiguous(SIZE, MPI FLOAT, &rowtype);
MPI Type commit(&rowtype);
if (numtasks == SIZE) {
   // task 0 sends one element of rowtype to all tasks
  if (rank == 0) {
      for (i=0; i<numtasks; i++)
       MPI_Send(&a[i][0], 1, rowtype, i, tag, MPI_COMM_WORLD);
                                                   send one of those elements, not 4
  // all tasks receive rowtype data from task 0
  MPI Recv(b, SIZE, MPI FLOAT, source, tag, MPI COMM WORLD, &stat);
  printf("rank= %d b= %3.1f %3.1f %3.1f %3.1f\n",
          rank, b[0], b[1], b[2], b[3]);
else
   printf("Must specify %d processors. Terminating.\n",SIZE);
// free datatype when done using it
                                                        rank=
                                                                                1.00000000
                                                                                                 2.00000000
                                                                                                                 3.00000000
                                                                                                                                 4.00000000
                                                                        0 b=
MPI Type free(&rowtype);
                                                        rank=
                                                                        1 b=
                                                                                5.00000000
                                                                                                6.00000000
                                                                                                                 7.00000000
                                                                                                                                 8.00000000
MPI Finalize();
                                                                        2 b=
                                                                                9.00000000
                                                                                                10.0000000
                                                         rank=
                                                                                                                 11.0000000
                                                                                                                                 12.0000000
                                                                        3 b=
                                                                                13.0000000
                                                                                                 14.0000000
                                                                                                                 15.0000000
                                                                                                                                 16,0000000
                                                         ank=
```

#### 3. Parallel I/O

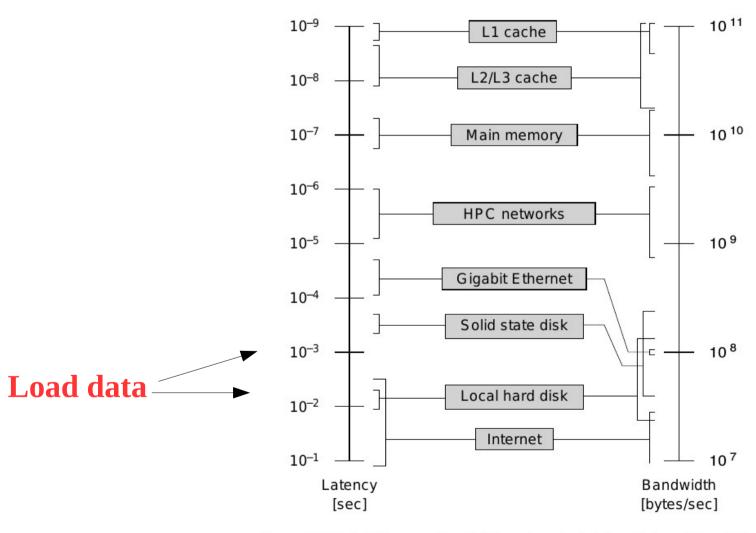
High Performance Computing (HPC) applications often do I/O for:

- Reading initial conditions or datasets for processing.
- Writing numerical data from simulations
  - → Parallel applications commonly need to write distributed arrays to disk.
  - → Saving application-level checkpoints.
- Application state is written to a file for restarting the application in case of a system failure.

#### Efficient I/O without stressing out the HPC system is challenging:

- Load and store operations are more time-consuming than multiply operations.
- Total Execution Time = Computation Time + Communication Time + I/O time.
- Optimize all the components of the equation above to get best performance.

#### Recall: data access speed



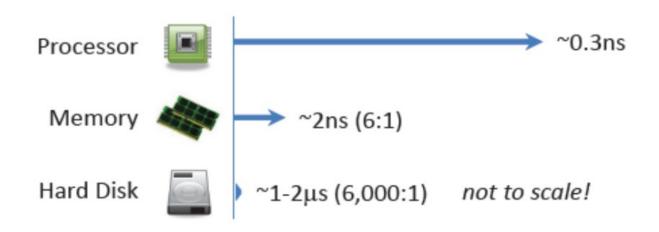
**Figure 3.1:** Typical latency and bandwidth numbers for data transfer to and from different devices in computer systems. Registers have been omitted because their "bandwidth" usually matches the computational capabilities of the compute core, and their latency is part of the pipelined execution.

Fig. from Hager & Wellein

## Relative Speed of Components in HPC Platform

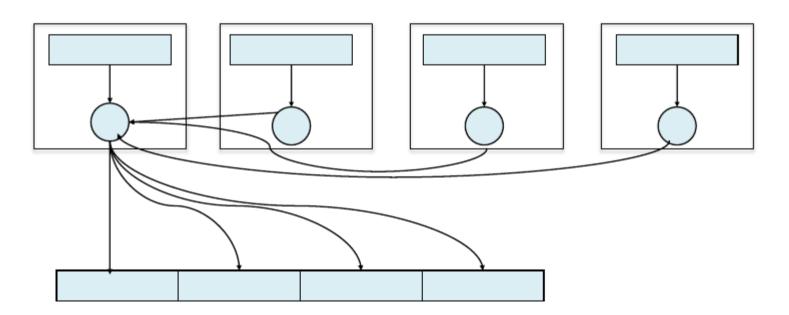
An HPC platform's I/O subsystems are typically slow as compared to its other parts.

The I/O gap between memory speed and average disk access stands at roughly 10<sup>-3</sup>



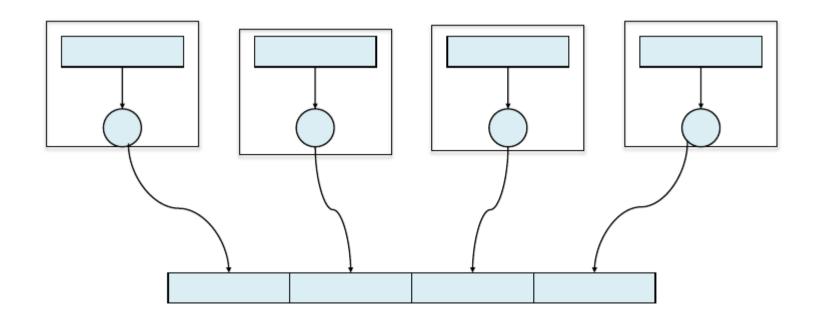
## Typical I/O pattern

- All processes send data to master process, and then the process designated as master writes the collected data to the file.
- This sequential nature of I/O can limit performance and scalability of many applications.

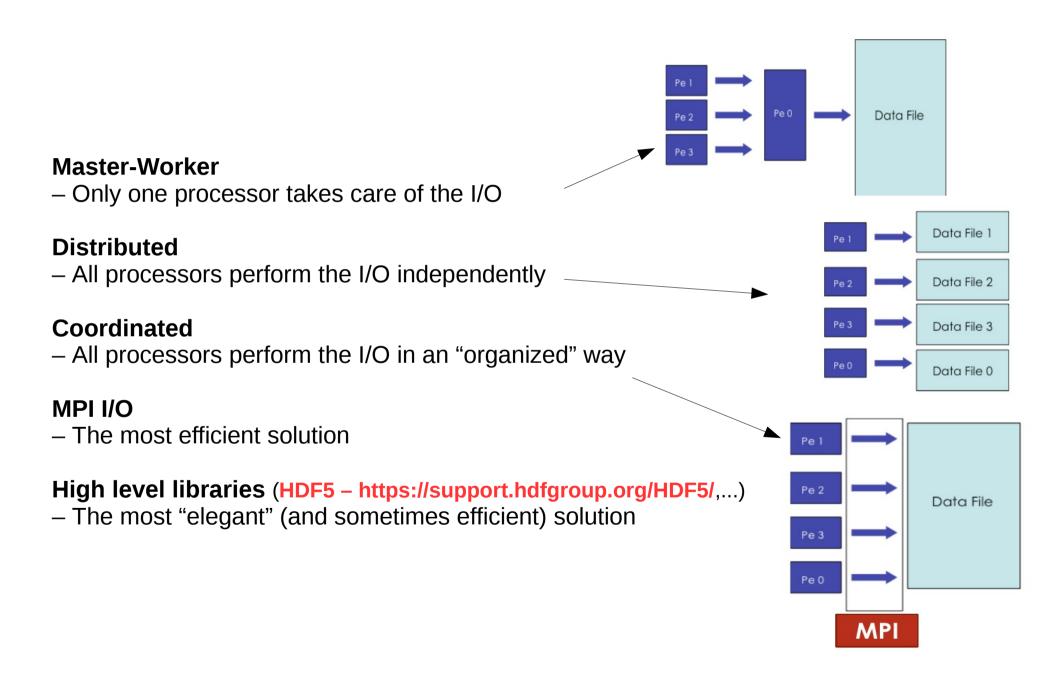


## Desired pattern

- Multiple processes participating in reading data from or writing data to a common file in parallel.
- This strategy improves performance and provides a single file for storage and transfer purposes.



## Parallel I/O: possible strategies



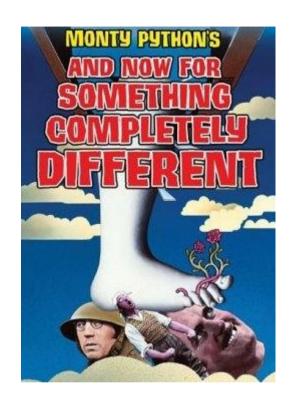
#### MPI I/O & Files\*

#### MPI I/O:

- MPI extends the same concepts introduced for parallelizing an algorithm to I/O.
- MPI I/O can be interpreted as message passing to (write) or from (read) a disk.
- A file written with MPI I/O has NOTHING special. It can be read by a sequential (non MPI) code.

#### **MPI Files:**

- An MPI file is an ordered collection of data items.
- MPI supports random or sequential access to any set of these items.
- A file is opened collectively by a group of processes (communicator).







## 4. MPI in Python

#### See https://mpi4py.scipy.org

→ **MPI for Python** supports convenient, pickle-based communication of generic Python object as well as fast, near C-speed, direct array data communication of buffer-provider objects (e.g., NumPy arrays).

#### **Communication of generic Python objects:**

You have to use **all-lowercase methods** (of the Comm class), like send(), recv(), bcast(). Note that isend() is available, but irecv() is not.

Collective calls like scatter(), gather(), allgather(), alltoall() expect/return a sequence of Comm.size elements at the root or all process. They return a single value, a list of Comm.size elements, or None.

Global reduction operations reduce() and allreduce() are naively implemented, the reduction is actually done at the designated root process or all processes.

## "Hello World" in Python

Go to OSM\_Lab/HPC\_day3/code\_day3/MPI4PY

Run with

> mpiexec -np 4 python hello.py

#hello.py
from mpi4py import MPI
comm = MPI.COMM\_WORLD
rank = comm.Get\_rank()
size = MPI.COMM\_WORLD.Get\_size()
print "hello world from process ", rank, " from total ", size , "processes"

#### Point-to-Point Communication

Go to OSM\_Lab/HPC\_day3/code\_day3/MPI4PY/pointtopoint.py

```
#passRandomDraw.py
import numpy
from mpi4py import MPI
comm = MPI.COMM_WORLD
rank = comm.Get_rank()

randNum = numpy.zeros(1)

if rank == 1:
    randNum = numpy.random.random_sample(1)
    print "Process", rank, "drew the number", randNum[0]
    comm.Send(randNum, dest=0)

if rank == 0:
    print "Process", rank, "before receiving has the number", randNum[0]
    comm.Recv(randNum, source=1)
    print "Process", rank, "received the number", randNum[0]
```

### MPI Broadcast in Python

Go to OSM\_Lab/HPC\_day3/code\_day3/MPI4PY/bcast.py

### MPI Reductions in Python

- Estimate integrals using the trapezoid rule.
- A range to be integrated is divided into many vertical slivers, and each sliver is approximated with a trapezoid.

$$area \approx \sum_{i=0}^{n} \frac{[f(a) + f(b)]}{2} \cdot \Delta x = \left[ \frac{f(a) + f(b)}{2} + \sum_{i=0}^{n} f(a + i\Delta x) + f(a + (i+1)\Delta x) \right] \cdot \Delta x$$

, a, "to", b, "is", total

### <u>MPI Reductions in Python</u>

```
import numpy
import sys
                                                        Go to
from mpi4py import MPI
from mpi4py.MPI import ANY SOURCE
                                                        OSM_Lab/HPC_day3/code_day3/MPI4PY/reduction.py
comm = MPI.COMM WORLD
rank = comm.Get rank()
size = comm.Get size()
                                                        Run with
#takes in command-line arguments [a,b,n]
a = float(sys.argv[1])
                                                        > mpiexec -n 4 python reduction.py a b N
b = float(sys.argv[2])
n = int(sys.argv[3])
                                                        → integration range [a,b], discretization N
#we arbitrarily define a function to integrate
def f(x):
       return x*x
                                                        > mpiexec -n 4 python reduction.py 0.0 1.0 1000
#this is the serial version of the trapezoidal rule
#parallelization occurs by dividing the range among processes
def integrateRange(a, b, n):
       integral = -(f(a) + f(b))/2.0
                                                        OUTPUT = ???
       # n+1 endpoints, but n trapazoids
       for x in numpy.linspace(a,b,n+1):
                                                                          f(x) = x^2
                      integral = integral + f(x)
       integral = integral* (b-a)/n
       return integral
#h is the step size. n is the total number of trapezoids
#local n is the number of trapezoids each process will calculate
#note that size must divide n
local n = n/size
#we calculate the interval that each process handles
#local a is the starting point and local b is the endpoint
local a = a + rank*local n*h
local b = local a + local n*h
#initializing variables. mpi4py requires that we pass numpy objects.
integral = numpy.zeros(1)
total = numpy.zeros(1)
                                                                                            Reduction
# perform local computation. Each process integrates its own interval
integral[0] = integrateRange(local a, local b, local n)
# communication
# root node receives results with a collective "reduce"
comm.Reduce(integral, total, op=MPI.SUM, root=0)
# root process prints results
if comm.rank == 0:
       print "With n =", n, "trapezoids, our estimate of the integral from"\
```

### **Questions?**

1. Advice – RTFM https://en.wikipedia.org/wiki/RTFM

2. Advice — http://lmgtfy.com/ http://lmgtfy.com/?q=message+passing+interface

