MPI More of the Story

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Slides at: https://github.com/timkphd/slides

Examples at

git clone https://github.com/timkphd/examples
cd examples/mpi4py

Goal for today: quickly go over things but leave you with many well commented examples and at least one useful full example program.

Outline

- Review
- Types
- Broadcast
- Wildcards
- Using Status and Probing
- Asynchronous Communication
- More Global communications
- Advanced topics
 - "V" operations
 - Communicators

Outline: Advance examples

- Finite difference code
- Mixing mpi4py and C or Fortran
- Bag of tasks
- Passing a token

Summary

- MPI is used to create parallel programs based on message passing
- Usually the same program is run on multiple processors
- The 6 basic calls in MPI are:

```
-INIT() "not required"
-comm=MPI.COMM WORLD
-comm.Get rank()
-comm.Get size()
-comm.Send(buf,dest, tag=0)
-comm.Recv(buf, source=ANY_SOURCE, tag=ANY_TAG, Status
 status=None)
-MPI.Finalize()
```

Basic Send and Receive

```
#!/usr/bin/env python
# numpy is required
import numpy
from numpy import *
# mpi4py module
from mpi4pv import MPI
# Initialize MPI and print out hello
comm=MPI.COMM WORLD
myid=comm.Get rank()
numprocs=comm.Get size()
print("hello from ",myid," of ",numprocs)
# Tag identifies a message
mytag=1234
# Process 0 is going to send the data
mvsource=0
# Process 1 is going to send the data
mvdestination=1
# Sending a single value each time
count=1
for k in range(1,4):
    if myid == mysource:
# For the upper case calls we need to send/recv numpy arrays
        buffer=array(k+5678,"i")
# We are sending a integer, size is optional, to mydestination
        comm.Send([buffer, MPI.INT], dest=mydestination, tag=mytag)
        print("Python processor ",myid," sent ",buffer)
    if myid == mydestination:
# We are receiving an integer, size is optional, from mysource
        if(k == 1) : buffer=empty((1),"i")
        comm.Recv([buffer, MPI.INT], source=mysource, tag=mytag)
        print("Python processor ",myid," got ",buffer)
MPI.Finalize()
```

P = ex01.py, f = ex01.f90

Blocking Send and Receive

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.Send()
- comm.Recv()
- MPI.Finalize

P_ex01b.py

Blocking Send and Receive Character Data

- MPI.COMM WORLD
- Get_rank()
- Get size()
- comm.Send()
- comm.Recv()
- MPI.Finalize

Skip to #18

<u>P_ex00.py</u>

Hello world

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- MPI.Finalize()

P = ex01.py, f = ex01.f90

Blocking Send and Receive

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.Send()
- comm.Recv()
- MPI.Finalize

<u>P_ex01b.py</u>

Blocking Send and Receive Character Data

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.Send()
- comm.Recv()
- MPI.Finalize

<u>P_ex02.py</u>

Blocking Send and Receive with probe to find size

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.Send()
- comm.probe()
- mystat.Get_count()
- comm.Recv()
- MPI Finalize

P_ex03.py

Nonblocking Send and Receive with wait

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.isend()
- comm.irecv()
- req.wait()
- MPI.Finalize

P_ex03I.py

Nonblocking Send and Receive with wait

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.Isend()
- comm.Irecv()
- req.wait()
- MPI.Finalize

P ex04.py

Broadcast of an array of integers and a string

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.bcast()
- comm.Bcast()
- MPI.Finalize

P_ex05.py

This program shows how to use MPI_Scatter and MPI_Gather. Each processor gets different data from the root processor by way of mpi_scatter. The data is summed and then sent back to the root processor using MPI_Gather. The root processor then prints the global sum.

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.bcast()
- comm.Scatter()
- comm.gather()
- comm.Gather()
- MPI.Finalize

<u>P_ex06.py</u>

This program shows how to use MPI_Scatter and MPI_Reduce Each processor gets different data from the root processor by way of mpi_scatter. The data is summed and then sent back to the root processor using MPI_Reduce. The root processor then prints the global sum.

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.bcast()
- comm.Scatter()
- comm.reduce()
- comm.Reduce()
- MPI.Finalize

P_ex07.py

This program shows how to use MPI_Alltoall. Each processor send/rec a different random number to/from other processors.

- MPI.COMM WORLD
- Get_rank()
- Get_size()
- comm.Alltoall()
- MPI.Finalize

P_ex08.py

This program shows how to use MPI_Gatherv. Each processor sends a different amount of data to the root processor. We use MPI_Gather first to tell the root how much data is going to be sent.

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.gather
- comm.Gathery
- MPI.Finalize

P_ex09.py

This program shows how to use Alltoally Each processor gets amounts of data from each other processor. It is an extension to example P_ex07.py. In mpi4py the displacement array can be calculated automatically from the rounts array. We show how it would be done in "normal" MPI. See also P_ex08.py for how this can be done

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.Alltoall()
- comm.Alltoallv()
- MPI.Finalize

P_ex10.py, ex10.in

Pass a "token" from one task to the next with a single task reading token from a file.

An extensive program. We first create a new communicator that contains every task except the zeroth one. This is done by first defining a group, new_group. We define new_group based on the group associated with mpi_comm_world, old_group and an array, will_use. Will_use contains a list of tasks to be included in the new group. It does not contain the zeroth one. The new communicator is sub_comm_world.

There are other ways to create communicator but this is one of the more general methods.

Next, we have break of the task not in the communicator to call the routine get_input. This routine will do input from a file ex10.in. The file contains a list of integers. The task will send the integer to the first task in the new communicator.

The remaining tasks which are port of sub_comm_world call the routine pass_token. Pass_token "just" receives a value from the previous processor and passes it on to the next.

There is a minor subtlety in pass_token. We are using both our new communicator and MPI_COMM_WORLD. The tasks that are port of the new communicator use it to pass data. We note that the task that is injecting values into the stream is not part of the new communicator so it must use MPI_COMM_WORLD. Thus we do a probe on WORLD, which is actually MPI_COMM_WORLD looking for a message. When we get it we send it on using the new communicator.

- MPI.COMM WORLD
- Get_rank()
- Get_size()
- WORLD.Iprobe()
- comm.Get_group()
- old_group.Incl()
- comm.Create()
- new_group.Get_rank()
- MPI.Finalize

P_ex12.py

This program shows how to use mpi_comm_split

Split will create a set of communicators. All of the tasks with the same value of color will be in the same communicator. In this case we get two sets one for odd tasks and one for even tasks. Note they have the same name on all tasks, new_comm, but there are actually two different values (sets of tasks) in each one.

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.Split
- comm.bcast
- MPI.Finalize

P_ex13.py

This program shows how to use Scattery. Each processor gets a different amount of data from the root processor. We use MPI_Gather first to tell the root how much data is going to be sent.

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.gather
- comm.Scattery
- MPI.Finalize

simple.py , flist

This is a bag-of-tasks program. We define a manager task that distributes work to workers. Actually,

the workers request input data. The manager sits in a loop calling Iprobe waiting for requests for work.

In this case the manager reads input. The input is a list of file names. It will send a entry from the list as requested. When the worker is done processing it will request a new file name from the manager. This continues until the manager runs out of files to process. The manager subroutine is just "manager"

The worker subroutine is "worker". It receives file names form the manager.

The files in this case are outputs from an optics program tracking a laser beam as it propagates through the atmosphere. The workers read in the data and then create an image of the data by calling the routine mkview.plotit. This should worker with arbitrary 2d files except the size in mkview.plotit is currently hard coded to 64 x 64.

We use the call to "Split" to create a seperate communicator for the workers. This is not important in this example but could be if you wanted multiple workers to work together.

To get the data...

curl http://hpc.mines.edu/examples/laser.tgz | tar -xz

- MPI.COMM WORLD
- Get_rank()
- Get_size()
- · comm.gather
- comm.Send()
- comm.Recv()
- MPI.Status()
- comm.Iprobe()
- gotfrom=status.source
- MPI.Get_processor_name()
- MPI_COMM_WORLD.barrier()
- MPI.Finalize

File	Comment		
ccalc.c	parallel		
stc_03.c	parallel		
pcalc.py	parallel		
stp_00.py	serial		
stp.py	parallel		
tiny.in	tiny input file		
small.in	small input file		
<u>st.in</u>	regular input file		

We have a finite difference model that will serve to demonstrate what a computational scientist needs to do to take advantage of Distributed Memory computers using MPI.

The model we are using is a two dimensional solution to a model problem for Ocean Circulation, the Stommel Model. It has Wind-driven circulation in a homogeneous rectangular ocean under the influence of surface winds, linearized bottom friction, flat bottom and Coriolis force. Solution: intense crowding of streamlines towards the western boundary caused by the variation of the Coriolis parameter with latitude.

The python version, stp.py, follows this C version except it does a 1d decomposition.

The C version is 1500x faster than the python version.

pcalc.py and ccalc.c are similar except they create a new communicator that contains N-1 tasks. These tasks do the calculation and pass data to the remaining task to be plotted. Thus we can have "C" do the heavy calculation and python do plotting.

pwrite.py

pwrite.py is a small MPI program designed to be run in conjunction with either ccalc.c or pcalc.py. If you are using mpiexec to lanuch your programs these might be launched together using one of the commands:

```
mpiexec -n 5 ./ccalc : -n 1 ./pwrite.py < cut.in
mpiexec -n 5 ./pcalc.py : -n 1 ./pwrite.py < cut.in</pre>
```

pcalc.py and ccalc.c are versions of the finite difference program discussed above. pcalc.py and ccalc.c create a new communicator that contains N-1 tasks. These tasks do the calculation and pass data to the remaining task to be plotted. The remaining task is pwrite.py.

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- world.Get_group()
- old_group.Incl()
- world.Create()
- world.barrier()
- MPI.Finalize

write grid.py

write_grid.py contains three procedures write_each, write_one, write_extra, plot_extra. These are different output routines for the finite difference code discussed above.

write each

Each MPI task writes its portion of the grid in a separate file. Could be called from stp.py

write_one

Each MPI task sends its portion of the grid to a single task and it is written as a single file. Could be called from stp.py

write_extra

This could be called from the "extra" MPI task pwrite.py. This routine collects the data from all other tasks and prints it.

plot_extra

This could be called from the "extra" MPI task pwrite.py. This routine collects the data from all other tasks and plots it using mkview.py

Write_one, write_extra, and plot_extra all work the same way. They collect data to a single task a line at a time using a combination of Gather and GatherV. For a give line, each processor tells the writing processor how much, if any of the line it holds using the Gather. The the Gatherv is used to actually transfer the data. For write_one and write_extra each line is printed as it is gathered. The routine plot_extra collects the whole grid before plotting it. Write_each opens a file with the name based on the task id. Each task writes its portion of the grid to its file.

- comm.Get_rank()
- comm.Get_size()
- comm.Gather()
- comm.Gatherv()

MPI Types

- MPI has many different predefined data types
- Can be used in any communication operation

Predefined types in C

C MPI Types				
MPI_CHAR	signed char			
MPI_SHORT	signed short int			
MPI_INT	signed int			
MPI_LONG	signed long int			
MPI_UNSIGNED_CHAR	unsigned char			
MPI_UNSIGNED_SHORT	unsigned short int			
MPI_UNSIGNED	unsigned int			
MPI_UNSIGNED_LONG	unsigned long int			
MPI_FLOAT	float			
MPI_DOUBLE	double			
MPI_LONG_DOUBLE	long double			
MPI_BYTE	-			
MPI_PACKED	-			

Predefined types in Fortran

Fortran	MPI	Types
---------	-----	-------

INTEGER
REAL
DOUBLE PRECISION
COMPLEX
LOGICAL
CHARACTER(1)
-

Predefined types in mpi4py (91)

SIGNED LONG

AINT BOOL BYTE CHAR CHARACTER COMPLEX COMPLEX16 COMPLEX32 COMPLEX4 COMPLEX8 COUNT CXX_BOOL CXX_DOUBLE_COMPLEX CXX_FLOAT_COMPLEX CXX_LONG_DOUBLE_COMPLEX C_BOOL C_COMPLEX C_BOOL C_COMPLEX C_BOOL C_COMPLEX C_BOOL C_COMPLEX C_BOOL C_COMPLEX C_BOOL C_COMPLEX C_DOUBLE_COMPLEX C_DOUBLE_COMPLEX C_DOUBLE_COMPLEX C_DOUBLE_COMPLEX C_LONG_DOUBLE_COMPLEX DATATYPE_NULL DOUBLE	DOUBLE_COMPLEX DOUBLE_INT DOUBLE_PRECISION FLOAT FLOAT_INT F_BOOL F_COMPLEX F_DOUBLE F_DOUBLE_COMPLEX F_FLOAT F_FLOAT INT INT INT INT16_T INT32_T INT64_T INT8_T INTEGER INTEGER INTEGER1 INTEGER2 INTEGER4 INTEGER8	INT_INT LB LOGICAL LOGICALI LOGICAL2 LOGICAL4 LOGICAL8 LONG LONG_DOUBLE LONG_DOUBLE_INT LONG_INT LONG_LONG OFFSET PACKED REAL REAL16 REAL2 REAL4 REAL8 SHORT SHORT_INT SIGNED_CHAR SIGNED_INT	SIGNED_LONG_LONG SIGNED_SHORT SINT16_T SINT32_T SINT64_T SINT8_T TWOINT UB UINT16_T UINT32_T UINT64_T UINT8_T UNSIGNED UNSIGNED_CHAR UNSIGNED_INT UNSIGNED_LONG UNSIGNED_LONG UNSIGNED_SHORT WCHAR _typedict _typedict_c _typedict_f
--	--	---	--

B.T.W. Rmpi has 3 normal types+ data frame

MPI Broadcast call: MPI_Bcast

- All nodes call MPI_Bcast
- One node (root) sends a message all others receive the message
- Bcast(self, buf, int root=0)
- bcast(self, obj, int root=0)

Broadcast

<u>P_ex04.py</u>

Broadcast of an array of integers and a string

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.bcast()
- comm.Bcast()
- MPI.Finalize



Wildcards

- Allow you to not necessarily specify a tag or source
- Example

- MPI_ANY_SOURCE and MPI_ANY_TAG are wild cards
- Status structure is used to get wildcard values

Wildcards

- Allow you to not necessarily specify a tag or source
- Example

```
status = MPI.Status()

comm.Recv([i, MPI.INT],
    source=MPI.ANY_SOURCE,
    tag=MPI.ANY_TAG,
    status=mystat)
```

- MPI_ANY_SOURCE and MPI_ANY_TAG are wild cards
- Status object is used to get wildcard values

Status

- The status parameter returns additional information for some MPI routines
 - Additional Error status information
 - Additional information with wildcard parameters
- C declaration : a predefined struct
 - MPI_Status status;
- Fortran declaration : an array is used instead
 - INTEGER STATUS(MPI_STATUS_SIZE)
- mpi4py: an class object
 - status=MPI.Status()

Accessing status information mpi4py

```
class Status(builtins.object)
    Status
    Methods defined here:
    Get count(...)
        Status.Get_count(self, Datatype datatype=BYTE)
        Get the number of *top level* elements
    Get_elements(...)
        Status.Get_elements(self, Datatype datatype)
        Get the number of basic elements in a datatype
    Get_error(...)
        Status.Get error(self)
        Get message error
    Get source(...)
        Status.Get source(self)
        Get message source
    Get_tag(...)
        Status.Get_tag(self)
        Get message tag
    Is_cancelled(...)
        Status.Is_cancelled(self
        Test to see if a request was cancelled
```

MPI_Probe

- MPI_Probe allows incoming messages to be checked without actually receiving.
 - The user can then decide how to receive the data.
 - Useful when different action needs to be taken depending on the "who, what, and how much" information of the message.

MPI4py "probe" part I

```
#!/usr/bin/env python3
# Program shows how to use probe and get_count to find the size
# of an incomming message
import numpy
from numpy import *
from mpi4py import MPI
import sys
# Initialize MPI and print out hello
comm=MPI.COMM WORLD
myid=comm.Get_rank()
numprocs=comm.Get_size()
print("hello from ",myid," of ",numprocs)
# Tag identifies a message
mytag=123
# Process 0 is going to send the data
if myid == 0:
    i=array(([1234,5678]),"i")
    icount=2
    comm.Send([i, MPI.INT], dest=1, tag=mytag)
```

MPI4py "probe" part 2

```
if myid == 1:
# We create a status to use int the probe command
    mystat=MPI.Status()
# Call probe to find out about the incoming message
    comm.probe(source=0, tag=mytag, status=mystat)
# We find out how big the incoming message is and allocate space
    icount=mystat.Get_count(MPI.INT)
    print("getting ", icount)
    i=empty((icount),"i")
# We are receiving an array of integers
    comm.Recv([i, MPI.INT], source=0, tag=mytag)
    print("i=",i)
MPI.Finalize()
```

MPI_Probe example

P_ex02.py

Blocking Send and Receive with probe to find size

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.Send()
- comm.probe()
- mystat.Get_count()
- comm.Recv()
- MPI.Finalize

MPI_BARRIER

- Blocks the caller until all members in the communicator have called it.
- Used as a synchronization tool.
- C
 - MPI_Barrier(comm)
- Fortran
 - Call MPI_BARRIER(COMM, IERROR)
- Parameter
 - Comm communicator (MPI_COMM_WORLD)

MPI_BARRIER

- Blocks the caller until all members in the communicator have called it.
- Used as a synchronization tool.
- mpi4py
 - Barrier(self)

Asynchronous Communication

- Asynchronous send: send call returns immediately, send actually occurs later
- Asynchronous receive: receive call returns immediately. When received data is needed, call a wait subroutine
- Asynchronous communication used in attempt to overlap communication with computation (usually doesn't work)
- Can help prevent deadlock (not advised)

Asynchronous Send with MPI_Isend

- C
 - MPI_Request request
 - int MPI_Isend(&buffer, count, datatype,
 dest,tag, comm, &request)
- Fortran
 - Integer REQUEST
 - MPI_ISEND(BUFFER, COUNT, DATATYPE, DEST, TAG,
 COMM, REQUEST, IERROR)
- Request is a new output Parameter
- Don't change data until communication is complete

Asynchronous Send with MPI_Isend

- mpi4py
 - isend(self, obj, int dest, int tag=0)
 - Isend(self, buf, int dest, int tag=0)
- They return a communication Request which is an object with various methods
- Don't change data until communication is complete

Asynchronous Receive with MPI_Irecv

- C
 - MPI_Request request;
- int MPI_Irecv(&buf, count, datatype, source, tag, comm, &request)
- Fortran
 - Integer request
 - MPI_IRECV(BUF, COUNT, DATATYPE, SOURCE, TAG, COMM, REQUEST, IERROR)
- Parameter Changes
 - Request: communication request
 - Status parameter is missing
- Don't use data until communication is complete

Asynchronous Receive with MPI_Irecv

- mpi4y
 - Irecv(self, buf, int source=ANY_SOURCE, int tag=ANY_TAG)
 - irecv(self, buf=None, int source=ANY_SOURCE, int tag=ANY_TAG)

- Parameter Changes
 - They return a communication Request which is an object with various methods
 - Status parameter is missing
- Don't use data until communication is complete

MPI_Wait used to complete communication

- Request from Isend or Irecv is input
- The completion of a send operation indicates that the sender is now free to update the data in the send buffer
- The completion of a receive operation indicates that the receive buffer contains the received message
- MPI_Wait blocks until message specified by "request" completes

MPI_Wait used to complete communication

C

```
- MPI Request request;
- MPI Status status;
- MPI_Wait(&request, &status)
Fortran
- Integer request
- Integer status(MPI_STATUS SIZE)
- MPI WAIT (REQUEST, STATUS, IERROR)
```

MPI_Wait blocks until message specified by "request" completes

MPI_Wait used to complete communication

- Very different in mpi4py
- Wait is a method of the class object "Request"
- Where req is the Request returned by the Isend/Irecv the call is:
 - Irecv
 - req.wait()
 - req.Wait()
 - irecv()
 - buffer=req.wait()

Asynchronous Send and Receive with MPI_Wait used to complete communication

<u>P_ex03.py</u>

Nonblocking Send and Receive with wait

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.isend()
- comm.irecv()
- req.wait()
- MPI.Finalize

P_ex03I.py

Nonblocking Send and Receive with wait

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.Isend()
- comm.Irecv()
- req.wait()
- MPI.Finalize

MPI_Test

- Similar to MPI_Wait, but does not block
- Value of flags signifies whether a message has been delivered
- C
 - int flag
 - int MPI_Test(&request,&flag, &status)
- Fortran
 - LOGICAL FLAG
 - MPI_TEST(REQUEST, FLAG, STATUS, IER)

Non blocking send example

```
call MPI_Isend (buffer,count,datatype,dest,tag,comm, request, ierr)

10 continue

Do other work ...
```

call MPI_Test (request, flag, status, ierr)
if (.not. flag) goto 10

MPI_Test

- Very different in mpi4py
- req.test returns a tuple (flag, buffer), works with both irecv and Irecv
- req.Test just returns a flag, works only with Irecv

Irecv

```
while (not req.Test()) :
    time.sleep(0.5)
    print("dest", req.Test(), req.test()[0])

print("processor ", destination," got ", buffer)
```

```
dest False (False, None)
dest False (False, None)
source True (True, None)
dest True (True, None)
processor 1 got [5678]
```

irecv

```
buffer=(False, None)
while buffer == (False, None):
    buffer=req.test()
    print("dest", req.Test(), buffer)
    time.sleep(0.5)
buffer=buffer[1]

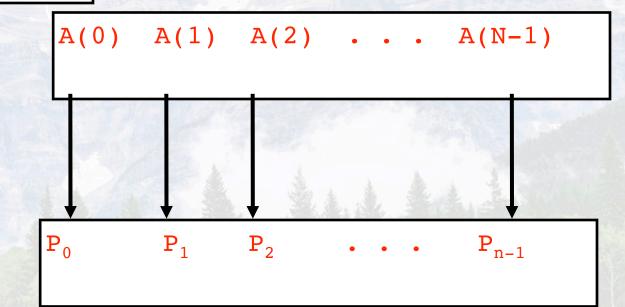
print("processor ", destination," got ", buffer)

    dest False (False, None)
    dest False (False, None)
    source True (True, None)
    processor 0 sent 5678
    dest True (True, 5678)
    processor 1 got 5678
```

Scatter Operation using MPI_Scatter

 Similar to Broadcast but sends a section of an array to each processors

Data in an array on root node:



Goes to processors:

MPI Scatter

• (

- int MPI_Scatter(&sendbuf, sendcnts, sendtype,
&recvbuf, recvcnts, recvtype, root, comm);

Fortran

- MPI_Scatter(sendbuf, sendcnts, sendtype,
 recvbuf, recvcnts, recvtype, root, comm, ierror)

Parameters

- Sendbuf is an array of size (number processors*sendcnts)
- Sendents number of elements sent to each processor
- Recvents number of elements obtained from the root processor
- Recvbuf elements obtained from the root processor, may be an array

MPI_Scatter

- mpi4py
 - scatter(self, sendobj, int root=0)
 - Scatter(self, sendbuf, recvbuf, int root=0)

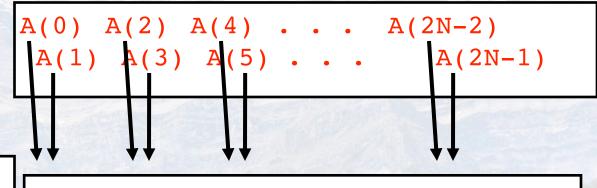
Parameters

- Sendbuf is an array of size (number processors*sendcnts)
- Sendents number of elements sent to each processor (not needed)
- Recvents number of elements obtained from the root processor (not needed)
- Recvbuf elements obtained from the root processor, may be an array

Scatter Operation using MPI_Scatter

Scatter with Sendents = 2

Data in an array on root node:



Goes to processors:

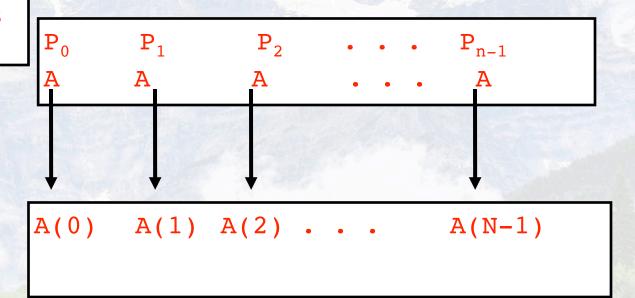
\mathbf{P}_0	\mathtt{P}_1	P_2	• • •	P_{n-1}	
B(0)	B(O)	B(0)		B(0)	
B(1)	B(1)	B(1)		B(1)	

Gather Operation using MPI_Gather

- Used to collect data from all processors to the root, inverse of scatter
- Data is collected into an array on root processor

Data from various Processors:

Goes to an array on root node:



MPI Gather

- int MPI_Gather(&sendbuf, sendcnts, sendtype, &recvbuf,
 recvcnts, recvtype, root, comm);

Fortran

- MPI_Gather(sendbuf, sendcnts, sendtype,
 recvbuf, recvcnts, recvtype, root, comm, ierror)

Parameters

- Sendents # of elements sent from each processor
- Sendbuf is an array of size sendents
- Recvents # of elements obtained from each processor
- Recvbuf of size Recvcnts*number of processors

MPI_Gather

- mpi4py
 - gather(self, sendobj, int root=0)
 - Gather(self, sendbuf, recvbuf, int root=0)
- Parameters
 - Sendbuf is an array can be size I
 - Recvbuf elements obtained at the root processor an array

Scatter and Gather

<u>P_ex05.py</u>

This program shows how to use MPI_Scatter and MPI_Gather. Each processor gets different data from the root processor by way of mpi_scatter. The data is summed and then sent back to the root processor using MPI_Gather. The root processor then prints the global sum.

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.bcast()
- comm.Scatter()
- comm.gather()
- comm.Gather()
- MPI.Finalize

Reduction Operations

- Used to combine partial results from all processors
- Result returned to root processor
- Several types of operations available
- Works on single elements and arrays

MPI_Reduce

- mpi4py
 - reduce(self, sendobj, op=SUM, int root=0)
 - Reduce(self, sendbuf, recvbuf, Op op=SUM, int root=0)
- Parameters
 - Like MPI_Bcast, a root is specified.
 - Operation is a type of mathematical operation

Operations for MPI_Reduce

MPI MAX Maximum

MPI MIN Minimum

MPI PROD Product

MPI SUM Sum

MPI_LAND Logical and

MPI_LOR Logical or

MPI_LXOR Logical exclusive or

MPI_BAND Bitwise and

MPI BOR Bitwise or

MPI BXOR Bitwise exclusive or

MPI MAXLOC Maximum value and location

MPI_MINLOC Minimum value and location

Global Sum with MPI_Reduce

mpi4py

```
#each processor does a local sum
total=0
for i in range(0, count):
   total=total+myray[i]
print("myid=", myid, "total=", total)
#reduce back to the root and print
#reduce(self, sendobj, op=SUM, int root=0)
#Reduce(self, sendbuf, recvbuf, Op op=SUM, int root=0)
if lower:
   back_ray=comm.reduce(total)
else:
   back ray=empty(2,"i")
                         # Why does this need to be 2?
                          # Maybe to support the max_loc operation?
                          # However, MAXLOC does not work?
   comm.Reduce(total,back ray,op=MPI.SUM,root=mpi root)
if myid == mpi root:
    print("results from all processors=",back ray)
```

Global Sum with MPI_Reduce

P ex06.py

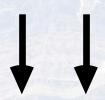
This program shows how to use MPI_Scatter and MPI_Reduce Each processor gets different data from the root processor by way of mpi_scatter. The data is summed and then sent back to the root processor using MPI_Reduce. The root processor then prints the global sum.

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.bcast()
- comm.Scatter()
- comm.reduce()
- comm.Reduce()
- MPI.Finalize

Global Sum with MPI_Reduce

2d array spread across processors

	X(0)	X(1)	X(2)
NODE 0	A0	B0	C0
NODE 1	A1	B1	C1
NODE 2	A2	B2	C2



	X(0)	X(1)	X(2)
NODE 0	A0+A1+A2	B0+B1+B2	C0+C1+C2
NODE 1			
NODE 2			
•	•		

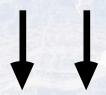
All Gather and All Reduce

- Gather and Reduce come in an "ALL" variation
- Results are returned to all processors
- The root parameter is missing from the call
- Similar to a gather or reduce followed by a broadcast

Global Sum with MPI_AllReduce

2d array spread across processors

	X(0)	X(1)	X(2)
NODE 0	A0	B0	C0
NODE 1	A1	B1	C1
NODE 2	A2	B2	C2



	Y(0)	Y(I)	Y(2)
NODE 0	A0+A1+A2	B0+B1+B2	C0+C1+C2
NODE 1	A0+A1+A2	B0+B1+B2	C0+C1+C2
NODE 2	A0+A1+A2	B0+B1+B2	C0+C1+C2

All to All communication with MPI_Alltoall

- mpi4py
 - alltoall(self, sendobj)
 - Alltoall(self, sendbuf, recvbuf)
 - Parameters
- Each processor sends and receives the same amount of data to/from all others

All to All with MPI_Alltoall

- Parameters
 - Sendents # of elements sent to each processor
 - Sendbuf is an array of size sendents
 - Recvents # of elements obtained from each processor
 - Recvbuf of size Recvcnts*number of processors
- Note that both send buffer and receive buffer must be an array of (size of the number of processors)*N

All to All with MPI_Alltoall

P_ex07.py

This program shows how to use MPI_Alltoall. Each processor send/rec a different random number to/from other processors.

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.Alltoall()
- MPI.Finalize

Things Left

- "V" operations (Skipping for today)
- Communicators
- Derived types (Not as important in Python)
- Parallel IO
 - See simple example
 - http://mpi4py.scipy.org/docs/usrman/tutorial.html#mpi-io
 - Also there are hdf5 examples in the same repository in the pandas directory
- Real life examples
 - Finite Difference Code
 - Bag of tasks

Communicators

- In "normal" MPI a communicator is a parameter in all MPI message passing routines
- In mpi4py a communicator is a class object that has message passing routines as methods
- A communicator is a collection of processors that can engage in communication
- MPI_COMM_WORLD is the default communicator that consists of all processors
- MPI allows you to create subsets of communicators

Why Communicators?

- Isolate communication to a small number of processors
- Useful for creating libraries
- Different processors can work on different parts of the problem
- Useful for communicating with "nearest neighbors"

MPI_Comm_create

- MPI_Comm_create creates a new communicator newcomm with group members defined by a group data structure.
- C
 - int MPI_Comm_create(comm, group, &newcomm)
- Fortran
 - Call MPI_COMM_CREATE(comm, GROUP, NEWCOMM, IERROR)
- mpi4py
 - newcom=comm.Create(group)
- How do you define a group?

MPI_Comm_group

- Given a communicator, MPI_Comm_group returns in group associated with the input communicator
- C
 - int MPI_Comm_group(comm, &group)
- Fortran
 - Call MPI_COMM_GROUP(COMM, GROUP, IERROR)

MPI_Comm_group

- Given a communicator, MPI_Comm_group returns in group associated with the input communicator
- mpi4py
 - old_group=comm.Get_group()
- As we have seen comm is an object. Get_group is a method
- Groups "old_group" is also an object with a collection of methods

MPI_Group_incl

- MPI_Group_incl creates a group new_group that consists of the n processes in old_group with ranks rank[0],..., rank[n-1]
- C
- int MPI_Group_incl(group,n,&ranks,&new_group)
- Fortran

MPI_Group_incl

- Fortran
 - Call MPI_GROUP_INCL(old_GROUP, N,
 RANKS, NEW_GROUP, IERROR)
- Parameters
 - old_group: your old group
 - N: number of elements in array ranks (and size of new_group) (integer)
 - Ranks: ranks of processes in group to appear in new_group (array of integers)
 - New_group:new group derived from above, in the order defined by ranks

MPI_Group_incl

- MPI_Group_incl creates a group new_group that consists of the n processes in old_group with ranks rank[0],..., rank[n-1]
- mpi4py
- new_group=old_group.Incl(ranks)

Create communicator...

```
# get our old group from MPI_COMM_WORLD
old_group=comm_Get_group()
# create a new group from the old group
# containing a subset of the processors
num_used=. . .
will_use=zeros(num_used,"i")
for ijk in range(0, num_used):
  will_use[ijk]=. . .
new_group=old_group.Incl(will_use)
# create the new communicator
sub_comm_world=comm.Create(new_group)
```

Create communicator Example

P_ex10.py, ex10.in

Pass a "token" from one task to the next with a single task reading token from a file.

An extensive program. We first create a new communicator that contains every task except the zeroth one. This is done by first defining a group, new_group. We define new_group based on the group associated with mpi_comm_world, old_group and an array, will_use. Will_use contains a list of tasks to be included in the new group. It does not contain the zeroth one. The new communicator is sub_comm_world.

There are other ways to create communicator but this is one of the more general methods.

Next, we have break of the task not in the communicator to call the routine get_input. This routine will do input from a file ex10.in. The file contains a list of integers. The task will send the integer to the first task in the new communicator.

The remaining tasks which are port of sub_comm_world call the routine pass_token. Pass_token "just" receives a value from the previous processor and passes it on to the next.

There is a minor subtlety in pass_token. We are using both our new communicator and MPI_COMM_WORLD. The tasks that are port of the new communicator use it to pass data. We note that the task that is injecting values into the stream is not part of the new communicator so it must use MPI_COMM_WORLD. Thus we do a probe on WORLD, which is actually MPI_COMM_WORLD looking for a message. When we get it we send it on using the new communicator.

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- WORLD.Iprobe()
- comm.Get_group()
- old_group.Incl()
- comm.Create()
- new_group.Get_rank()
- MPI.Finalize

MPI_Group_excl

 MPI_Group_excl creates a group of processes new_group that is obtained by deleting from old_group those processes with ranks ranks[0], ..., ranks[n-1]

- Provides a short cut method to create a collection of communicators
- All processors with the "same color" will be in the same communicator
- Index gives rank in new communicator
- Fortran
 - call MPI_COMM_SPLIT(OLD_COMM, color, index, NEW_COMM, mpi_err)
- C
 - MPI_Comm_split(OLD_COMM, color, index, &NEW_COMM)

- Provides a short cut method to create a collection of communicators
- All processors with the "same color" will be in the same communicator
- Index gives rank in new communicator
- mpi4py
 - new_comm=old_comm.Split(color,index)

Split odd and even processors into 2 communicators

```
Program comm_split
include "mpif.h"
Integer color, zero one
call MPI_INIT( mpi_err )
call MPI_COMM_SIZE( MPI_COMM_WORLD, numnodes, mpi_err )
call MPI COMM RANK( MPI COMM WORLD, myid, mpi err )
color=mod(myid,2) !color is either 1 or 0
call MPI_COMM_SPLIT(MPI_COMM_WORLD, color, myid, NEW_COMM, mpi_err)
call MPI COMM RANK( NEW COMM, new id, mpi err )
call MPI COMM SIZE( NEW COMM, new nodes, mpi err )
Zero one = -1
If(new id==0)Zero one = color
Call MPI_Bcast(Zero_one,1,MPI_INTEGER,0, NEW_COMM,mpi_err)
If(zero_one==0)write(*,*)"part of even processor communicator"
If(zero_one==1)write(*,*)"part of odd processor communicator"
Write(*,*) "old_id=", myid, "new id=", new id
Call MPI_FINALIZE(mpi_error)
End program
```

Split odd and even processors into 2 communicators

P_ex12.py

This program shows how to use mpi_comm_split Split will create a set of communicators. All of the tasks with the same value of color will be in the same communicator. In this case we get two sets one for odd tasks and one for even tasks. Note they have the same name on all tasks, new_comm, but there are actually two different values (sets of tasks) in each one.

- MPI.COMM_WORLD
- Get_rank()
- Get_size()
- comm.Split
- comm.bcast
- MPI.Finalize

```
#!/usr/bin/env python3
 This program shows how to use mpi_comm_split
                                                            Mpi4py
import numpy
                                                color/com.Split example
from numpy import *
from mpi4py import MPI
import sys
# Get an integer representation of our color Note: this will be the same at select_val
color=col to int[color str]
print("myid= %d color integer = %d color name = %s" %(myid,color,color_str))
new comm=comm.Split(color,myid)
# Get the new id and number of tasks in the communicator
new id=new comm.Get rank()
new nodes=new comm.Get size()
```

Sorry - I went a bit hog wild on this example here we just show the important parts

```
# Here we do a bcast from the new roots to show we can use the communicator
bcast_val=None
if new_id == 0 : bcast_val=myid
bcast_val=new_comm.bcast(bcast_val)
# Iterate through the colors and each processor will print its information
for k in col_to_int.keys():
    if( k == color str):
         print("new id is %d in the %s communicator or %d.%s \
original id is %d \
id bcast from root %d" %(new_id,k,new_id,k,myid,bcast_val))
MPI.Finalize()
```

MPI_Comm_split example output

Note, I have sorted the output

```
osage:mpi4py tkaiser$ mpiexec -n 6 ./P ex12.py | sort
color to integer= {'blue ': 0, 'green ': 1, 'red ': 2, 'yellow': 3} and
integer to color= {0: 'blue ', 1: 'green ', 2: 'red ', 3: 'yellow'}
hello from
              of
                  6
hello from 1 of
hello from 2 of 6
hello from 3 of
hello from 4 of
              of
hello from 5
myid=0 color integer = 0
                               color name = blue
myid= 1 color integer = 1
                               color name = green
myid= 2 color integer = 0
                               color name = blue
myid= 3    color integer = 1
                            color name = green
myid= 4 color integer = 0 color name = blue
myid= 5 color integer = 1
                            color name = green
new id is 0 in the blue communicator or 0.blue original id is 0
                                                                id bcast from root 0
new id is 0 in the green communicator or 0.green original id is 1
                                                                id bcast from root 1
new id is 1 in the blue communicator or 1.blue original id is 2
                                                                id bcast from root 0
new id is 1 in the green communicator or 1. green original id is 3
                                                                id bcast from root 1
new id is 2 in the blue communicator or 2.blue original id is 4
                                                                id bcast from root 0
new id is 2 in the green communicator or 2. green original id is 5
                                                                id bcast from root 1
osage:mpi4py tkaiser$
```