Parallel programming / computation

Sultan ALPAR s.alpar@iitu.edu.kz

IITU

Lecture 5 Collective Communication

Collective Communication

- Communications involving a group of processes.
- Called by all processes in a communicator.
- Examples:
 - Barrier synchronization.
 - Broadcast, scatter, gather.
 - Global sum, global maximum, etc.
 - Neighbor communication in a virtual process grid

New in MPI-3.0

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Should be faster than any programming with point-to-point messages!

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E.g., broadcast

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Sequential algorithm O(# processes)

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 \bigcirc

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Tree based algorithm

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Tree based algorithm O(log₂(# processes))

E.g., broadcast



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Tree based algorithm O(log₂(# processes))

Hardware-broadcast O(1)

E.g., broadcast



And optimized algorithms on clusters of SMP nodes are even more complicated!



- Collective action over a communicator.
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- No tags.
 - For each message, the amount of data sent must exactly match the amount of data specified by the receiver
 - \rightarrow It is forbidden to provide receive buffer count arguments that are too long (and also too short, of course)

Exception with Python (mpi4py): if a buffer argument represents #processes of messages (e.g. snd_buf in comm.Scatter) and the argument count is to be derived from the buffer argument (i.e. is not explicitly defined in the argument list), then this count argument is derived from the inferred number of elements of the buffer divided by the size of the communicator.

e.g., when passing snd buf, or (snd buf, datatype).



very important

C	•	C/C++:	int MPI_Barrier(M	PI_Co	mm comm)	
Fortran	•	Fortran: mpi_f08: mpi & mpif.h:	MPI_BARRIER(co TYPE(MPI_Comm) :: INTEGER comm, ierr	omm, i comm ; or	ierror) INTEGER, OPTIONAL :: ierror	
Python	•	Python:	comm.Barrier()	or	comm.barrier()	

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 - Load imbalance of computation [MPI_Wtime(); MPI_Barrier(); MPI_Wtime()]
 - communication epochs [MPI_Wtime(); MPI_Allreduce(); ...; MPI_Wtime()]

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 - Load imbalance of computation [MPI_Wtime(); MPI_Barrier(); MPI_Wtime()]
 - communication epochs [MPI_Wtime(); MPI_Allreduce(); ...; MPI_Wtime()]
 - if used for synchronizing external communication (e.g. I/O):
 - exchanging tokens may be more efficient and scalable than a barrier on MPI_COMM_WORLD,

see also advanced exercise of this course chapter.

Broadcast



Broadcast









Example: MPI_Scatter(sbuf, 1, MPI_CHAR, *rbuf*, 1, MPI_CHAR, 1, MPI_COMM_WORLD);

Completely ignored at all processes except root











Exercise 1 — Gather

In MPI/tasks/...

- Use C C/Ch6/gather-skel.c or Fortran F_30/Ch6/gather-skel_30.f90
 Or Python PY/Ch6/gather-skel.py (hint: use Gather, i.e. with numPy buffers)
- The skeleton is based on our first example in course Chapter 1.
- Differences:
 - This skeleton first gathers the data into an array at process 0
 - And then, process 0 prints the array.
- In this exercise, you should substitute the point-to-point communication by one call to MPI_Gather
- Hint for Python
 - The result_array (used in MPI_Gather) needs to be declared on all processes. Therefore add "else: result_array = None"

```
if (my_rank == 0):
    result_array = np.empty(num_procs, dtype=np.double)
else:
    result_array = None
```

Advanced Exercise 1b — Barrier / profiling

Based on C/Ch6/solutions/pi.c → pi-mpi.c → pi-mpi-inbalance.c

inbalanced

balanced

- Use C/Ch6/pi-mpi-inbalance-profiling-skel.c
- or Python PY/Ch6/pi-mpi-inbalance-profiling-skel.py
- Or Fortran (my apologies, Fortran does not yet exists, but this shouldn't be a problem)
- This program has several parts:
 - Perfect work-distribution for n=10,000,000 intervals.
 - If 3 or more processes:
 Introducing an inbalance: The last 2 processes get double and zero intervals.
 - Calculation of π with a distributed integral \rightarrow partial sums in p_sum.
 - Global reduction of all p_sum into one global sum.
 - Time measurements for all parts
- Your task, see "// **EXERCISE**" in the skeleton:
 - Add MPI_Barrier wherever useful, and especially to measure idle time due to the bad load balance.
 - Substitute all wt? by wt1 .. wt4 as needed
 - Compile and run it with 2 processes
 - → expected result 99,9% parallel efficiency
 - Run with more than 3 processes
 - \rightarrow about 50% parallel efficiency and 50% in idle time

Global Reduction Operations

- To perform a global reduce operation across all members of a group.
- $d_0 \circ d_1 \circ d_2 \circ d_3 \circ \dots \circ d_{s-2} \circ d_{s-1}$
 - d_i = data in process rank i
 - single variable, or
 - vector
 - o = associative operation
 - Example:
 - global sum or product
 - global maximum or minimum
 - global user-defined operation

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 - Example:
 - global sum or product
 - global maximum or minimum
 - global user-defined operation
- floating point rounding may depend on usage of associative law:
 - $[(d_0 \circ d_1) \circ (d_2 \circ d_3)] \circ [\dots \circ (d_{s-2} \circ d_{s-1})]$
 - $((((((d_0 \circ d_1) \circ d_2) \circ d_3) \circ \dots) \circ d_{s-2}) \circ d_{s-1})$ modify last 3 or 4 digits!
 - May be even worse through partial sums in each process: $\sum_{i=0}^{n-1} x_i \rightarrow [[[(\sum_{i=0}^{n/s-1} x_i \circ \sum_{i=n/s}^{2n/s-1} x_i) \circ (\dots \circ \dots)] \circ [\dots \circ (\dots \circ \dots)]]]$

E.g., with $n=10^8$ rounding errors may
Example of Global Reduction

• Global integer sum.

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- Sum of all inbuf values should be returned in *resultbuf*.
- C/C++: root=0; MPI_Reduce(&inbuf, &*resultbuf*, 1, MPI_INT, MPI_SUM, root, MPI_COMM_WORLD);
- Fortran: root=0 CALL MPI_REDUCE(inbuf, *resultbuf*, 1, MPI_INTEGER, MPI_SUM, root, MPI_COMM_WORLD, *IERROR*)
- Python: comm_world = MPI.COMM_WORLD snd_buf = np.array(value, dtype=np.intc) resultbuf = np.empty((), dtype=np.intc) comm_world.Reduce(snd_buf, resultbuf, op=MPI.SUM)
 - The result is only placed in *resultbuf* at the root process.

Predefined Reduction Operation Handles

Predefined operation handle	Function
MPI_MAX	Maximum
MPI_MIN	Minimum
MPI_SUM	Sum
MPI_PROD	Product
MPI_LAND	Logical AND
MPI_BAND	Bitwise AND
MPI_LOR	Logical OR
MPI_BOR	Bitwise OR
MPI_LXOR	Logical exclusive OR
MPI_BXOR	Bitwise exclusive OR
MPI_MAXLOC	Maximum and location of the maximum
MPI_MINLOC	Minimum and location of the minimum











User-Defined Reduction Operations

- Operator handles
 - predefined see table above
 - user-defined
- User-defined operation \square :
 - associative
 - user-defined function must perform the operation vector_A
 vector_B
 - syntax of the user-defined function \rightarrow MPI standard
- Registering a user-defined reduction function:
 - C/C++: MPI_Op_create(MPI_User_function *func, int commute, MPI_Op *op)



С

- Fortran: MPI_OP_CREATE(FUNC, COMMUTE, OP, IERROR)
- Python: op = MPI.Op.Create(func, commute=True or False)
- COMMUTE tells the MPI library whether FUNC is commutative.

Variants of Reduction Operations

- MPI_Allreduce
 - no root,
 - returns the result in all processes
- New in MPI-2.2
 - MPI_Reduce_scatter_block and MPI_Reduce_scatter
 - result vector of the reduction operation is scattered to the processes into the real result buffers



- MPI_Scan
 - prefix reduction
 - result at process with rank i := reduction of inbuf-values from rank 0 to rank i
- MPI_Exscan
 - result at process with rank i :=

reduction of inbuf-values from rank 0 to rank i-1

MPI_Allreduce





Interface of MPI_Allreduce

L ir S (Language independent specification (LIS)	MPI_ALLREDUCE(sendbuf, recvbuf, count, datatype, op, comm)			
		IN	sendbuf	starting address of send buffer (choice)	
		OUT	recvbuf	starting address of receive buffer (choice)	
		IN	count	number of elements in send buffer (non-negative integer)	
		IN	datatype	data type of elements of send buffer (handle)	
		IN	ор	operation (handle) Additional MPI Count	
		IN	comm	communicator (handle) version since MPI-4.0: MPI_Allreduce_c	
C	C/C++ binding	<pre>int MPI_Allreduce(const void* sendbuf, void* recvbuf, int count, MPI_Datatype datatype, MPI_Op op, MPI_Comm comm)</pre>			
Fortran	mpi_f08 Module Fortran binding	<pre>MPI_Allreduce(sendbuf, recvbuf, count, datatype, op, comm, ierror) TYPE(*), DIMENSION(), INTENT(IN) :: sendbuf TYPE(*), DIMENSION() :: recvbuf INTEGER, INTENT(IN) :: count TYPE(MPI_Datatype), INTENT(IN) :: datatype Version si TYPE(MPI_Op), INTENT(IN) :: op TYPE(MPI_Comm), INTENT(IN) :: comm INTEGER, OPTIONAL, INTENT(OUT) :: ierror</pre>			
	mpi module + mpif.h Fortran binding	<pre>MPI_ALLREDUCE(SENDBUF, RECVBUF, COUNT, DATATYPE, OP, COMM, IERROR)</pre>			
Python	Python:	<i>win</i> = con	nm.Allreduce(sendbuf, re	ecvbuf, op) op=MPI.SUM is the default	
			sendbuf, (recvbuf, 1,	MPI.INT)	



MPI_Scan:



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Other Collective Communication Routines

 MPI_Allgather → similar to MPI_Gather, but all processes receive the result vector



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- MPI_Alltoall → each process sends messages to all processes



A1	B1	C1		A1	A2	A3
A2	B2	C2	⇒	B1	B2	B3
A3	B3	C3		C1	C2	C3

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- MPI_.....v (Gatherv, Scatterv, Allgatherv, Alltoallv, Alltoallw)
 - → Each message has a different count and displacement
 - \rightarrow array of counts and array of displs (Alltoallw: also array of types)
 - → interface does **not scale** to thousands of MPI processes!
 - → Recommendation: One should try to use data structures with same communication size on all ranks.

Exercise 2 — Global reduction

- Rewrite the pass-around-the-ring program to use the MPI global reduction to perform the global sum of all ranks of the processes in the ring (and print it from all processes).
- Use C C/Ch6/allreduce-skel.c or Fortran F_30/Ch6/allreduce-skel_30.f90 or Python PY/Ch6/allreduce-skel.py
- I.e., the pass-around-the-ring communication loop must be totally substituted by one call to the MPI collective reduction routine.
- For the argument list, of MPI_Allreduce, please look into the MPI standard:
 - Go to the end of the standard (=<u>end of the MPI function index of MPI-4.0</u>)
 - Go backward in the alphabet to MPI_Allreduce
 - Click on the underlined reference
 - MPI_Allreduce, <u>239</u>, (in MPI-4.0), <u>187</u>, (in MPI-3.1)
 - Python: see also, e.g., mpi4py.MPI.Comm MPI for Python 3.1.1 documentation
 - Specify sum in the same way as the **rcv_buf** in the ring algorithm

Advanced Exercises — Global scan and sub-groups

- 1. Global scan:
 - Rewrite the last program so that each process computes a partial sum, i.e., with MPI_Scan().
 - mpirun -np 5 ./a.out | **sort** -**n** to get the output sorted by the ranks:
 - rank= $0 \rightarrow sum=0$ rank= $1 \rightarrow sum=1$
 - rank= $2 \rightarrow$ sum=3
 - rank= $3 \rightarrow sum=6$
 - rank= 4 \rightarrow sum=10

Quiz on Chapter 6-(1) – Collective communication

- Why should you use MPI collective routines?
- MPI Collective communication: Which are the major rules when using collective communication routines and that do not apply to point to point communication?
 Please try to find at least two or three:



New in MPI-3.0 MPI_I..... Nonblocking variants of all collective communication: MPI_Ibarrier, MPI_Ibcast, ...

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- May have multiple outstanding collective communications on same communicator
- Ordered initialization on each communicator
- Parallel MPI I/O (except with shared file pointer):

New in MPI-3.1

The split collective interface may be deprecated in a future version of MPI

General progress rule of MPI

- MPI is mainly defined in a way that **progress** on communication (and ...) is **required only during MPI procedure calls.**
- But then, progress is required
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- See, e.g., in MPI-4.0
 - Sect. 3.5, page 54, and 3.7.4, page 75; Paragr.s "Progress", esp. progress of repeated MPI_Test, p.75₃₈₋₄₀
 - Sect. 3.8.1 and 3.8.2 about MPI_(I)(M)PROBE
 - Sect. 3.8.4 Cancel, esp. page 94 lines 8-16 & MPI_Finalize Example 11.6, page 496₂₆₋₄₈
 & MPI_Session_finalize, esp. page 503₃₀₋₄₇ and Example 11.8 on page 804
 - Sect. 4.2.2 MPI_Parrived: Same progress rule as for repeated MPI_Test, see page 111₃₁₋₃₄
 - Sect. 5.12: Nonblocking collectives: Same rules as for nonblocking pt-to-pt
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 - By several calls to MPI_Test(), which enables progress

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 - E.g., with MPICH: export MPICH_ASYNC_PROGRESS=1

Implies a helper thread and MPI_THREAD_MULTIPLE

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Implies a helper thread and MPI_THREAD_MULTIPLE

• Offers opportunity to overlap

- Offers opportunity to overlap
 - several collective communications,
 - e.g., on several overlapping communicators
 - Without deadlocks or serializations!



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 - For this, progress is needed
 - See previous slide



- The receiver
 - needs information and
 - does not know the sending processes nor the <u>n</u>umber of <u>sending processes</u> (<u>nsp</u>)
 - and this number is small compared to the total number.
 - The sender knows all its neighbors, which need some data.
- Non-scalable solution to exchange number of neighbors:
 - MPI_Alltoall, MPI_Reduce_scatter (array with one logical entry per process)
 - Each sender tells all processes whether they will get a message or not.



- For the example with MPI_Ibarrier on next slide, we also need the following *local inquiry procedure*:
 - MPI_lprobe(int source, int tag, MPI_Comm comm, int *flag, MPI_Status *status);
 Python: flag = comm.lprobe(source, tag, status)
 - Result: flag == non-zero or .TRUE. → a message arrived and can be received with a local MPI_Recv,
 - i.e., a subsequent corresponding MPI_Recv will **not** block



























Collective Operations for Intercommunicators

- In MPI-1, collective operations are restricted to ordinary (intra) communicators.
- In MPI-2, most collective operations are extended by an additional functionality for intercommunicators
 - e.g., Bcast on a parents-children intercommunicator: sends data from one parent process to all children.
- Intercommunicators do not apply in
 - MPI_Scan, MPI_Iscan, MPI_Exscan, MPI_Iexscan,
 - MPI_(I)Neighbor_allgather(v)
 - MPI_(I)Neighbor_alltoall(v,w)

New in MPI-3.0

Sparse Collective Operations on Process Topology

- MPI process topologies (Cartesian and (distributed) graph) usable for communication
 - MPI_(I)NEIGHBOR_ALLGATHER(V)
 - MPI_(I)NEIGHBOR_ALLTOALL(V,W)
- If the topology is the full graph, then neighbor routine is identical to full collective communication routine
 - Exception: s/rdispls in MPI_NEIGHBOR_ALLTOALLW are MPI_Aint
- Allows for optimized communication scheduling and scalable resource binding
- Cartesian topology:
 - Sequence of buffer segments is communicated with:
 - direction=0 source, direction=0 dest, direction=1 source, direction=1 dest, ...
 - Defined only for disp=1
 - If a source or dest rank is MPI_PROC_NULL then the buffer location is still there but the content is not touched.

Extended Collective Operations — "In place" Buffer Specification



- (I)REDUCE at root
- (I)ALLREDUCE, (I)REDUCE_SCATTER(_BLOCK), (I)SCAN, (I)EXSCAN, (I)ALLTOALL(V,W) at all processes
- Not available for
 - (I)BARRIER, (I)BCAST, (I)NEIGHBOR_ALLGATHER/ALLTOALL(V,W)
- Python: the constant is MPI.IN_PLACE

- Use C C/Ch6/ibarrier-skel.c or Fortran F_30/Ch6/ibarrier-skel_30.f90
 or Python PY/Ch6/ibarrier-skel.py
- Each process sends 0-4 messages to some other processes (see number_of_dests).
- The skeletons include already the Issends of these messages.

- Use C C/Ch6/ibarrier-skel.c or Fortran F_30/Ch6/ibarrier-skel_30.f90 or Python PY/Ch6/ibarrier-skel.py
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- The receiving processes do not know
 - how many messages must be received, and
 - from which processes they will come.

- Use C C/Ch6/ibarrier-skel.c or Fortran F_30/Ch6/ibarrier-skel_30.f90 or Python PY/Ch6/ibarrier-skel.py
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 - how many messages must be received, and
 - from which processes they will come.
- The skeleton also includes the lprobe(...) [please add the arguments] and the Recv()

- Use C C/Ch6/ibarrier-skel.c or Fortran F_30/Ch6/ibarrier-skel_30.f90 or Python PY/Ch6/ibarrier-skel.py
- Each process sends 0-4 messages to some other processes (see number_of_dests).
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- The receiving processes do not know
 - how many messages must be received, and
 - from which processes they will come.
- The skeleton also includes the lprobe(...) [please add the arguments] and the Recv()
- You should add the sender-side part of the nonblocking barrier algorithm presented within this course chapter. <u>Hints:</u>
 - With which one call can you check for the completeness of all nonblocking send requests? <a>[]
 - MPI_lbarrier(comm, &ib_rq) should be called only once!
 - The MPI_Test(&ib_rq, ...) can be done only when MPI_Ibarrier is already called (arguments \rightarrow])

- Use C C/Ch6/ibarrier-skel.c or Fortran F_30/Ch6/ibarrier-skel_30.f90
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- The skeleton also includes the lprobe(...) [please add the arguments] and the Recv()
- You should add the sender-side part of the nonblocking barrier algorithm presented within this course chapter. <u>Hints:</u>
 - With which one call can you check for the completeness of all nonblocking send requests?
 - MPI_lbarrier(*comm*, &ib_rq) should be called only once!
 - The MPI_Test(&ib_rq, ...) can be done only when MPI_Ibarrier is already called (arguments \rightarrow])
- Please only fill in the _____ parts. Please do not modify the already given source code.

In MPI/tasks/...

- Use C C/Ch6/ibarrier-skel.c or Fortran F_30/Ch6/ibarrier-skel_30.f90
 or Python PY/Ch6/ibarrier-skel.py
- Each process sends 0-4 messages to some other processes (see number_of_dests).
- The skeletons include already the Issends of these messages.
- The receiving processes do not know

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Exercise

- how many messages must be received, and
- from which processes they will come.
- The skeleton also includes the lprobe(...) [please add the arguments] and the Recv()
- You should add the sender-side part of the nonblocking barrier algorithm presented within this course chapter. <u>Hints:</u>
 - With which one call can you check for the completeness of all nonblocking send requests?
 - MPI_Ibarrier(comm, &ib_rq) should be called only once!
 - The MPI_Test(&ib_rq, ...) can be done only when MPI_Ibarrier is already called (arguments \rightarrow)
- Please only fill in the _____ parts. Please do not modify the already given source code.
- mpirun -np 4 ./a.out | sort +0 -1 +6 -7 +4r -5 (to check whether all messages are received)
- mpirun -np 4 ./a.out | sort +0 -1 +2 -3 +4r -5 +6 -7 (to sort by processes / snd/rcv / partners)

- Use C C/Ch6/ibarrier-skel.c or Fortran F_30/Ch6/ibarrier-skel_30.f90 or Python PY/Ch6/ibarrier-skel.py
- Each process sends 0-4 messages to some other processes (see number_of_dests).
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 - how many messages must be received, and
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Exercise — nonblocking barrier — solutions

In the Ch6/solutions directory, you find

- ibarrier.c / _30.f90 / .py
 - the solution for the ../ibarrier-skel.c / _30.f90 / .py
- ibarrier-optimized.c / _30.f90 / .py
 - an optimized solution that additionally loops over the iprobe & recv
- ibarrier-optimized-test.c / _30.f90 / .py
 - same, but executes only each 10th iprobe & recv
- ibarrier-wrong.c, ibarrier-optimized-wrong.c, ibarrier-optimized-test-wrong.c / _30.f90 / .py
 - All synchronous MPI_Ssend calls are substituted by standard MPI_Send.
 - Therefore, the algorithm will start the ibarrier to early.
 - And therefore may stop before all messages are received.
 - Especially the test version shows always wrong results, whereas the optimized version may sometimes receive all message by luck.
 - − Incorrect programs may produce correct results ⊗
 - \rightarrow therefore correct results never prove that the program is correct \otimes

Advanced Exercise 4 — MPI_IN_PLACE

- C C/Ch6/in-place-skel.c or Fortran F_30/Ch6/in-place-skel_30.f90
- Your tasks:

Use (

- Substitute the several 0 by a root variable initialized with root=0, compile and run
- Substitute root=0 by root=num_procs-1, compile and run
- Modify your program that the MPI_IN_PLACE option is used for MPI_Gather (read the appropriate paragraph in the MPI description of MPI_Gather), compile and run

Any significant difference to your solution?