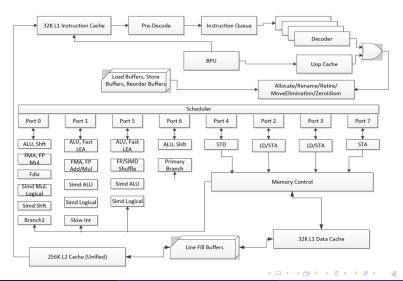
MA6252 Topics in Applied Mathematics II Introduction to MPI

National University of Singapore February 17th 2015

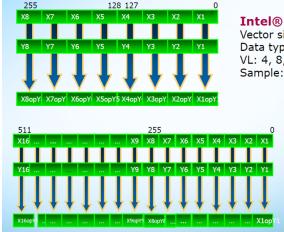
Outline

- Levels of parallelism
- MPI Overview
- Process model and language bindings
- Messages and point-to-point communication
- Non-blocking communication
- Collective communication

CPU Core Pipeline Functionality: Intel Microarchitecture Haswell



Data Parallelism - SIMD



Intel® AVX

Vector size: 256bit

Data types: 32 and 64 bit floats

VL: 4, 8, 16

Sample: Xi, Yi 32 bit int or float

Intel® MIC

Vector size: 512bit

Data types:

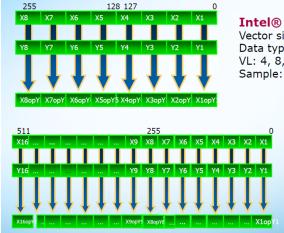
32 and 64 bit integers 32 and 64bit floats (some support for 16 bits floats)

VL: 8,16

Sample: 32 bit float

MA6252 17.12.2015 4 / 90

Data Parallelism - SIMD



Intel® AVX

Vector size: 256bit

Data types: 32 and 64 bit floats

VL: 4, 8, 16

Sample: Xi, Yi 32 bit int or float

Intel® MIC

Vector size: 512bit

Data types:

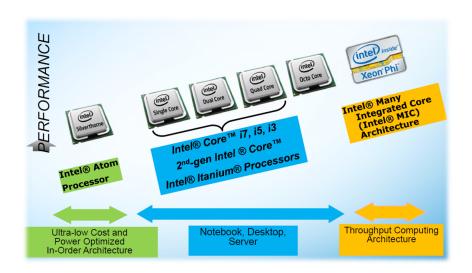
32 and 64 bit integers 32 and 64bit floats (some support for 16 bits floats)

VL: 8,16

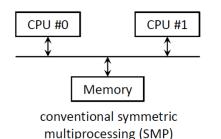
Sample: 32 bit float

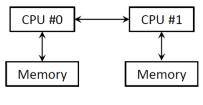
MA6252 17.12.2015 5 / 90

Shared Memory Parallelism



Shared Memory Access





non-uniform memory access (NUMA)

Distributed Memory Machines







	JUGENE	JUQUEEN	SuperMUC
System	IBM Bluegene/P	IBM Bluegene/Q	IBM System x iDataPlex
Processor	PowerPC 450	PowerPC A2	Xeon E5-2680 8C
Clock frequency	o.85 GHz	1.6 GHz	2.8 GHz
#Nodes	73 728	24 576	9 216
#Cores	294 912	393 216	147 456
Network	3D Torus	5D Torus	Tree
GFlop/s per Watt	0.44	2.54	0.94

	Peak	Factor	Paradigm	
Serial	0.5 GFlops			

	Peak	Factor	Paradigm
Serial	0.5 GFlops	_	
Processing units	1 GFlops	×2	balance between adds and mults. CPU

	Peak	Factor	Paradigm
Serial	0.5 GFlops		
Processing units	1 GFlops	x2	balance between adds and mults, CPU
Instruction pipeline	6 GFlops	×6	compiler or CPU

	Peak	Factor	Paradigm
Serial	0.5 GFlops		
Processing units	1 GFlops	x2	balance between adds and mults, CPU
Instruction pipeline	6 GFlops	×6	compiler or CPU
SIMD (AVX)	24 GFlops	x4	compiler, intrinsics, pragmas

	Peak	Factor	Paradigm
Serial	0.5 GFlops		
Processing units	1 GFlops	x2	balance between adds and mults, CPU
Instruction pipeline	6 GFlops	×6	compiler or CPU
SIMD (AVX)	24 GFlops	×4	compiler, intrinsics, pragmas
Shared memory parallel	384 GFLops	×16	OpenMP

	Peak	Factor	Paradigm
Serial	0.5 GFlops		
Processing units	1 GFlops	x2	balance between adds and mults, CPU
Instruction pipeline	6 GFlops	×6	compiler or CPU
SIMD (AVX)	24 GFlops	×4	compiler, intrinsics, pragmas
Shared memory parallel	384 GFLops	×16	OpenMP
(Accelerators, e.g. GPU)			CUDA, OpenCL

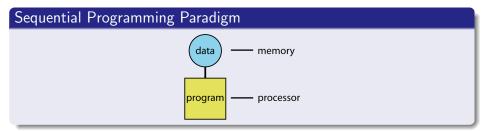
	Peak	Factor	Paradigm
Serial	0.5 GFlops		
Processing units	1 GFlops	×2	balance between adds and mults, CPU
Instruction pipeline	6 GFlops	×6	compiler or CPU
SIMD (AVX)	24 GFlops	×4	compiler, intrinsics, pragmas
Shared memory parallel	384 GFLops	×16	OpenMP
(Accelerators, e.g. GPU)			CUDA, OpenCL
Distributed memory parallel	3.84 PFlops	×10 000	MPI

Outline

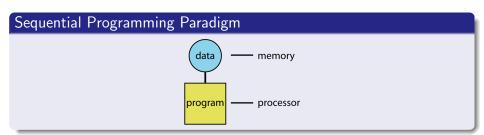
- MPI Overview
 - one program on several processors
 - work and data distribution
 - the communication network
- Process model and language bindings
- Messages and point-to-point communication
- Non-blocking communication
- Virtual topologies
- Collective communication

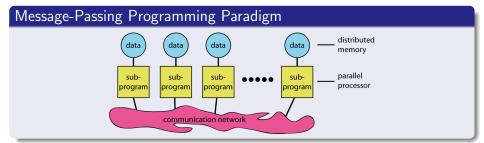


The Message-Passing Programming Paradigm



The Message-Passing Programming Paradigm

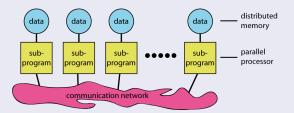




The Message-Passing Programming Paradigm

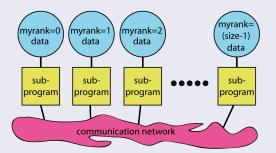
Each processor in a message passing program runs a sub-program

- \bullet written in a conventional sequential language, e.g., C(++) or Fortran
- typically the same on each processor (SPMD)
- the variables of each sub-program have
 - the same name
 - but different locations (distributed memory) and different data!
 - i.e., all variables are private
- communicate via special send & receive routines (message passing)

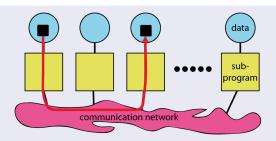


Data and Work Distribution

- the value of myrank is returned by special library function
- the system of size processes is started by special MPI initialization program (mpirun or mpiexec)
- all distribution decisions are based on myrank
- i.e., which process works on which data



Messages



- Messages are packets of data moving between sub-programs
- Necessary information for the message passing system:
 - sending process
 - source location
 - source data type
 - source data size

- receiving process
- destination location
- destination data type
- destination buffer size

Access

- A sub-program needs to be connected to a message passing system
- A message passing system is similar to:
 - mail box
 - phone line
 - fax machine
 - etc.
- MPI:
 - sub-program must be linked with an MPI library
 - the total program (i.e., all sub-programs of the program) must be started with the MPI startup tool

15 / 90

Addressing

- Messages need to have addresses to be sent to
- Addresses are similar to:
 - mail addresses
 - phone number
 - fax number
 - etc.
- MPI: addresses are ranks of the MPI processes (sub-programs)

16 / 90

Point-to-Point communication

- Simplest from of message passing
- One process send a message to another
- Different types of point-to-point communication:
 - non-buffered = synchronous send
 - buffered = asynchronous send

Synchronous/Asynchronous Sends

Synchronous Sends

- The sender gets an information that the message is received
- Analog to the beep or okay-sheet of a fax

Synchronous/Asynchronous Sends

Synchronous Sends

- The sender gets an information that the message is received
- Analog to the beep or okay-sheet of a fax

Buffered = Asynchronous Sends

• We only know when the message has left

Process 0

```
send ( &a, 1, 1 );
receive( &b, 1, 1 );
```

Process 1

```
send ( &a, 1, 0 );
receive( &b, 1, 0 );
```

19 / 90

Process 0

```
send ( &a, 1, 1 );
receive( &b, 1, 1 );
```

Process 1

```
send ( &a, 1, 0 );
receive( &b, 1, 0 );
```

Depending on the implementation of send and receive this might lead to a **deadlock**!

19 / 90

Process 0

```
send ( &a, 1, 1 );
receive( &b, 1, 1 );
```

Process 1

```
send ( &a, 1, 0 );
receive( &b, 1, 0 );
```

Depending on the implementation of send and receive this might lead to a **deadlock**!

Process 0

```
receive( &b, 1, 1 );
send ( &a, 1, 1 );
```

Process 1

```
receive( &b, 1, 0 );
send ( &a, 1, 0 );
```

19 / 90

Process 0

```
send ( &a, 1, 1 );
receive( &b, 1, 1 );
```

Process 1

```
send (&a, 1, 0);
receive(&b, 1, 0);
```

Depending on the implementation of send and receive this might lead to a **deadlock**!

Process 0

```
receive( &b, 1, 1 );
send ( &a, 1, 1 );
```

Process 1

```
receive( &b, 1, 0 );
send ( &a, 1, 0 );
```

Even with buffered send this code will lead to a deadlock!

<□▶ <圖▶ <臺▶ <臺▶ 臺 めの

Blocking Operations

- Operations are local activities, e.g.,
 - sending (a message)
 - receiving (a message)
- Some operations may block until another process acts:
 - synchronous send operation blocks until receive is posted
 - receive operation blocks until message is sent
- Relates to the completion of an operation
- Blocking subroutine returns only when the operation has completed

20 / 90

Non-Blocking Operations

- Non-blocking operation: returns immediately and allow the sub-program to perform other work.
- At some later time the sub-program must test or wait for the completion of the non-blocking operation.
- All non-blocking operations must have matching wait (or test) operations. (Some system or application resources can be freed only when the non-blocking operation is completed.)
- A non-blocking operation immediately followed by a matching wait is equivalent to a blocking operation
- Non-blocking operations are not the same as sequential subroutine calls: the operation may continue while the application executes the next statements!

Collective Communications

- Collective communication routines are higher level routines.
- Several processes are involved at a time
- May allow optimized internal implementations, e.g., tree based algorithms
- Can be built out of point-to-point communications

Collective Communications (cont'd)

Broadcast

• A one-to-many communication

Collective Communications (cont'd)

Broadcast

A one-to-many communication

Reduction Operations

• Combine data from several processes to produce a single result

Collective Communications (cont'd)

Broadcast

A one-to-many communication

Reduction Operations

Combine data from several processes to produce a single result

Barriers

Synchronize processes

Outline

- MPI Overview
- Process model and language bindings
 - starting several MPI processes
- Messages and point-to-point communication
- Non-blocking communication
- Derived data types
- Virtual topologies
- Collective communication

24 / 90

MA6252 17.12.2015

Compilation/Header Files/Function Format

Compilation

MA6252 17.12.2015 25 / 90

Compilation/Header Files/Function Format

Compilation

Header files

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

MA6252 17.12.2015 25 / 90

Compilation/Header Files/Function Format

Compilation

Header files

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

MPI Function Format

```
error = MPI_Xxxxx( parameter, ... );
MPI_Xxxxxx( parameter, ... );
```

MA6252 17.12.2015 25 / 90

MPI Function Format Details

- MPI_.... namespace is reserved for MPI constants and routines, i.e., application routines and variable names must not begin with MPI_.
- Output arguments in C(++) are handled via passing-by-pointer:

Function definitions

```
MPI_Comm_rank( ..., int *rank );
MPI_Recv( ..., MPI_Status *status );
```

Usage in your code

```
main( ... ) {
   int myrank;
   MPI_Status recv_status;
   MPI_Comm_rank( ..., &myrank );
   MPI_Recv( ..., &recv_status );
}
```

MA6252 17.12.2015

26 / 90

Initializing MPI

- Should be the very first function call inside the main function
- Must be the very first MPI function call

Function definition

```
MPI_Init( int *argc, char ***argv );
```

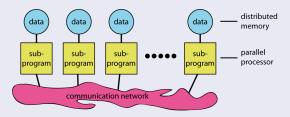
Usage in your code

```
#include <mpi.h>
int main( int argc, char** argv )
{
   MPI_Init( &argc, &argv );
   ...
}
```

MA6252 17.12.2015 27 / 90

Starting the MPI Program

- Start mechanism is implementation dependent
- mpirun -np number_of_processes ./executable (most implementations)
- mpiexec -n number_of_processes ./executable (with MPI-2 standard)

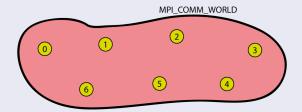


• The parallel MPI processes exist at least after MPI_Init was called.

MA6252 17.12.2015 28 / 90

Communicator MPI_COMM_WORLD

- All processes (= sub-programs) of one MPI program are combined in the communicator MPI_COMM_WORLD
- MPI_COMM_WORLD is a predefined handle in mpi.h
- Each process has its own rank in a communicator:
 - starting with 0
 - ending with size-1

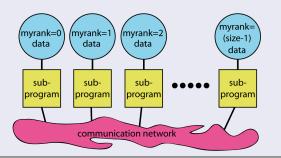


MA6252 17.12.2015 29 / 90

Rank

- The rank identifies different processes
- The rank is the basis for any work and data distribution

int MPI_Comm_rank(MPI_Comm comm, int *rank);



◄□▶◀圖▶◀불▶◀불▶ 불 쒸٩○

MA6252 17.12.2015 30 / 90

Size

• How many processes are contained within a communicator?

```
int MPI_Comm_size( MPI_Comm comm, int *size );
```



MA6252 17.12.2015 31 / 90

Exiting MPI

```
int MPI_Finalize();
```

- MUST be called last by all processes
- After MPI_Finalize:
 - Further MPI-calls are forbidden
 - Especially re-initialization with MPI_Init is forbidden

MA6252 17.12.2015 32 / 90

Example: MPI Hello World (I)

```
#include <mpi.h>
int main( int argc, char **argv )
   // Definition of the variables
   int size; //The total number of processes
   int rank; //The rank/number of this process
   // MPI initialization
   MPI_Init( &argc, &argv );
   // Determining the number of CPUs and the rank for each CPU
   MPI_Comm_size( MPI_COMM_WORLD, &size );
   MPI_Comm_rank( MPI_COMM_WORLD, &rank );
   . . .
```

33 / 90

MA6252 17.12.2015

Example: MPI Hello World (II)

```
// 'Hello World' output for CPU 0
   if(rank == 0)
      cout << " Hello World" << endl;</pre>
   // Output of the own rank and size of each CPU
   cout << " I am CPU " << rank << " of " << size << " CPUs" << endl;
   // MPT finalizations
   MPI_Finalize();
   return 0;
}
```

34 / 90

MA6252 17.12.2015

Example: MPI Hello World (III)

Possible output of the program:

```
I am CPU 2 of 4 CPUs
Hello World
I am CPU 0 of 4 CPUs
I am CPU 3 of 4 CPUs
I am CPU 1 of 4 CPUs
```

Note: The output of the program is non-deterministic!

MA6252 17.12.2015 35 / 90

Outline

- MPI Overview
- Process model and language bindings
- Messages and point-to-point communication
 - the MPI processes can communicate
- Non-blocking communication
- Derived data types
- Virtual topologies
- Collective communication

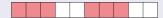


36 / 90

MA6252 17.12.2015

Messages

- A message contains a number of elements of some particular datatype
- MPI datatypes:
 - Basic datatype
 - Derived datatypes



- Derived datatypes can be built up from basic or derived data types
- Data type handles are used to describe the type of the data in the memory.
- Example: message with 5 integers

2345	654	96574	-12	7676
------	-----	-------	-----	------

MA6252 17.12.2015 37 / 90

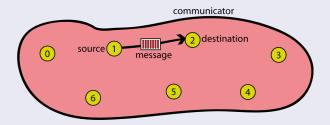
MPI Basic Datatypes

MPI_CHAR	char	Treated as printable character
MPI_SHORT	signed short int	
MPI_INT	signed int	
MPI_LONG	signed long int	
MPI_LONG_LONG	signed long long	
MPI_SIGNED_CHAR	signed char	Treated as integral value
MPI_UNSIGNED_CHAR	unsigned char	Treated as integral value
MPI_UNSIGNED_SHORT	unsigned short int	
MPI_UNSIGNED	unsigned int	
MPI_UNSIGNED_LONG	unsigned long int	
MPI_UNSIGNED_LONG_LONG	unsigned long long	
MPI_FLOAT	float	
MPI_DOUBLE	double	
MPI_LONG_DOUBLE	long double	
MPI_BYTE		
MPI_PACKED		

MA6252 17.12.2015 38 / 90

Point-to-Point Communication

- Communication between two processes
- Source process sends message to destination process
- Communication takes place within a communication, e.g., MPI_COMM_WORLD
- Processes are identified by their ranks in the communicator



MA6252 17.12.2015 39 / 90

Sending a Message

- buf is the starting point of the message with count elements
- dest is the rank of the destination process within the communicator comm
- tag is an additional nonnegative integer piggyback information, additionally transferred with the message
- The tag can be used by the program to distinguish different types of messages

MA6252 17.12.2015 40 / 90

Receiving a Message

- buf, count, datatype describe the receive buffer
- Receiving the message sent by process with rank source in comm
- Envelope information is returned in status
- Only messages with matching tag are received

MA6252 17.12.2015 41

Requirements for Point-to-Point Communications

For a communication to succeed:

- Sender must specify a valid destination rank
- Receiver must specify a valid source rank
- The communicator must be the same
- Tags must match
- Message datatypes must match
- Receiver's buffer must be large enough

MA6252 17.12.2015 42 / 90

Wildcarding

- Receiver can wildcard
- To receive from any source ⇒ source = MPI_ANY_SOURCE
- To receive from any tag ⇒ tag = MPI_ANY_TAG
- Actual source and tag are returned in the receiver's status parameter

MA6252 17.12.2015 43 / 90

Communication Envelope

Envelope information is returned from MPI_Recv in status

```
status.MPI_SOURCE
status.MPI_TAG
status.MPI_ERROR
count via MPI_Get_count()
```

```
From: source rank
     tag
To: destination rank
 Item 1
 Item 2
            "count"
 Item 3
           elements
 Item 4
 Item n
```

```
int MPI_Get_count( MPI_Status *status,
                   MPI_Datatype datatype, int *count );
```

17.12.2015 44 / 90

Communication Modes

Send communication modes

- synchronous send \Rightarrow

- buffered [asynchronous] send ⇒ MPI_Bsend

 \Rightarrow

MPI Ssend

- standard send \Rightarrow MPI_Send

- ready send \Rightarrow MPI_Rsend

Receiving all modes \Rightarrow MPI_Recv

MA6252 17.12.2015 45 / 90

Communication Modes – Definitions

Sender mode	Definition	Notes
Synchronous send MPI Ssend	Only completes when the receive has started	
Buffered send MPI_Bsend	Always completes (unless an error occurs), irrespective of receiver	needs application- defined buffer to be declared with MPI_Buffer_attach
Standard send MPI_Send	Either synchronous or buffered	Uses an internal buffer
Ready send MPI_Rsend	May be started only if the matching receive is already posted!	Highly dangerous!
Receive MPI_Recv	Completes when a message has arrived	same routine for all communication modes

MA6252 17.12.2015 46 / 90

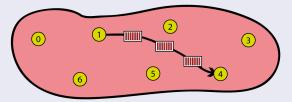
Rules for the Communication Modes

- Standard send (MPI_Send)
 - minimal transfer time
 - may block due to synchronous mode
 - ullet ightarrow risks with synchronous send
- Synchronous send (MPI_Ssend)
 - risk of deadlock
 - risk of serialization
 - ullet risk of waiting o idle time
 - high latency / best bandwidth
- Buffered send (MPI_Bsend)
 - low latency / bad bandwidth
- Ready send (MPI_Rsend)
 - use never, except you have a 200% guarantee that Recv is already called in the current version and all future versions of your code

17.10.001E 17.100

Message Order Preservation

- Rule for messages on the same connection, i.e., same communicator, source, and destination rank:
- Messages do not overtake each other
- This is true even for non-synchronous sends.



• If both receives match both messages, the order is preserved.

MA6252 17.12.2015 48 / 90

Outline

- MPI Overview
- Process model and language bindings
- Messages and point-to-point communication
- Non-blocking communication
 - to avoid idle time and deadlocks
- Derived data types
- Virtual topologies
- Collective communication

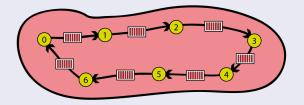


MA6252 17.12.2015 49

Deadlock

Code in each MPI process:

```
// This will block and never return, because MPI_Recv
// cannot be called in the right-hand MPI process
MPI_Ssend( ..., right_rank, ... );
MPI_Recv( ..., left_rank, ... );
```



 Same problem with standard send mode (MPI_Send) if MPI implementation chooses synchronous protocol

MA6252 17.12.2015 50 / 90

Non-Blocking Communications

Separate communication into three phases:

- Initiate non-blocking communication
 - returns immediately
 - routine name starting with MPI_I...
- Do some work (perhaps involving other communications?)
- Wait for non-blocking communication to complete

MA6252 17.12.2015 51 /

Non-Blocking Examples

Non-blocking send

MPI_Isend(...)
doing some other work
MPI_Wait(...)



MA6252 17.12.2015 52 / 90

Non-Blocking Examples

Non-blocking send

MPI_Isend(...)
doing some other work
MPI_Wait(...)



Non-blocking receive

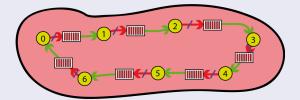
MPI_Irecv(...)
doing some other work
MPI_Wait(...)



MA6252 17.12.2015 52 /

Non-Blocking Send

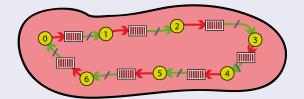
- Initiate non-blocking send
 - ightarrow In the ring example: initiate non-blocking send to the right neighbor
- Do some work:
 - ightarrow In the ring example: Receive the message from left neighbor
- Now, the message transfer can be completed
- Wait for non-blocking send to complete



MA6252 17.12.2015 53 / 90

Non-Blocking Receive

- Initiate non-blocking receive
 In the ring example: Initiate non-blocking receive from left neighbor
- Do some work:
 in the ring example: Sending the message to the right neighbor
- Now, the message transfer can be completed
- Wait for non-blocking receive to complete



MA6252 17.12.2015

Request Handles

Request handles

- are used for non-blocking communication
- must be stored in local variables (MPI_Request)
- the value
 - is generated by a non-blocking communication routine
 - is used (and freed) in the MPI_Wait routine

MA6252 17.12.2015 55 / 90

Non-Blocking Synchronous Send

- buf must not be accessed between Issend and Wait (In MPI-2.2, this restriction is relaxed to "must not be modified")
- "Issend + Wait directly after Issend" is equivalent to blocking call (Ssend)
- status is not used in Issend, but in Wait (with send: nothing returned)

MA6252 17.12.2015 56 / 90

Non-Blocking Receive

```
int MPI_Irecv( void* buf, int count,
                 MPI_Datatype datatype, int source,
                 int tag, MPI_Comm comm,
                 MPI_Request *request);
 int MPI_Wait( MPI_Request *request, MPI_Status *status );

    buf must not be used between Irecv and Wait
```

◆ロト ◆団ト ◆豆ト ◆豆ト ・豆 ・ からぐ ・

MA6252 17.12.2015 57 / 90

Blocking and Non-Blocking

- Send and receive can be blocking or non-blocking
- A blocking send can be used with a non-blocking receive, and vice-versa.
- Non-blocking sends can use any mode standard – MPI Isend

synchronous – MPI_Issend

buffered – MPLIbsend

ready – MPI_Irsend

- Synchronous mode affects completion, i.e., MPI_Wait/MPI_Test, not initiation, i.e., MPI_I...
- The non-blocking operation immediately followed by a matching wait is equivalent to the blocking operation

MA6252 17.12.2015 58 / 90

Completion

One must

- Wait or
- ullet loop with Test until request is completed, i.e., flag ==1

MA6252 17.12.2015 59 / 90

Multiple Non-Blocking Communications

You have several request handles:

- Wait or test for completion of one message MPI_Waitany / MPI_Testany
- Wait or test for completion of all messages MPI_Waitall / MPI_Testall *)
- Wait or test for completion of as many messages as possible MPI_Waitsome / MPI_Testsome *)



*) Each status contains an additional error field. This field is only used if MPI_ERR_IN_STATUS is returned (also valid for send operations)

> MA6252 17.12.2015 60 / 90

Outline

- MPI Overview
- Process model and language bindings
- Messages and point-to-point communication
- Non-blocking communication
- Derived data types
- Virtual topologies
- Collective communication
 - - e.g., broadcast



MA6252 17.12.2015 61 / 90

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.

MA6252 17.12.2015 62 / 90

Characteristics of Collective communication

- Collective action over a communicator
- All processes of the communicator must communicate, i.e., must call the collective routine
- Synchronization may or may not occur, therefore all processes must be able to start the collective routine
- All collective operations are blocking
- No tags
- Receive buffers must have exactly the same size as send buffers

MA6252 17.12.2015 63 /

Barrier Synchronization

```
MPI_Barrier( MPI_Comm comm );
```

MPI_Barrier is normally never needed:

- all synchronization is done automatically by the data communication
 - a process cannot continue before it has the data that it needs
- if used for debugging
 - please guarantee, that it is removed in production
- for profiling: to separate time measurement of
 - 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

MA6252 17.12.2015 64 / 90

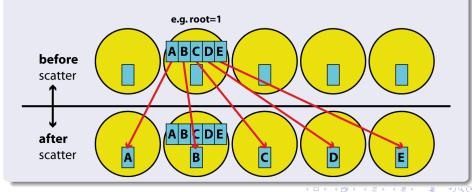
Broadcast

```
int MPI_Bcast( void* buffer, int count,
                MPI_Datatype datatype,
                int root, MPI_Comm comm );
                                e.g.root=2
   before
   bcast
   after
   bcast
```

65 / 90

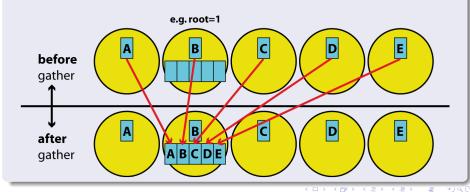
MA6252 17.12.2015

Scatter



MA6252 17.12.2015 66 / 90

Gather



MA6252 17.12.2015 67 / 90

Global Reduction Operations

- To perform a global reduce operation across all members of a group
- $d_0 \circ d_1 \circ d_2 \circ \dots \circ d_{s-2} \circ d_{s-1}$
 - $d_i = \text{data in process rank i}$
 - single variable, or
 - vector
 - o = associative operation
 - Example:
 - global sum or product
 - global maximum or minimum
 - global user-defined operation
 - floating point rounding may depend on usage of associative law
 - $[(d_0 \circ d_1) \circ (d_2 \circ d_3)] \circ [... \circ (d_{s-2} \circ d_{s-1})]$
 - $((((((d_0 \circ d_1) \circ d_2) \circ d_3) \circ ...) \circ d_{s-2}) \circ d_{s-1})$

4□ > 4□ > 4□ > 4□ > 4□ > 9

MA6252 17.12.2015 68 / 90

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

MA6252 17.12.2015 69 / 90

MPI_Reduce

AoDoGoJoM

```
int MPI_Reduce( void* sendbuf, void* recvbuf,
                 int count, MPI_Datatype datatype,
                 MPI_Op op, int root, MPI_Comm comm );
                      e.g.root=1
   before
   reduce
   after
   reduce
```

MA6252 17.12.2015 70 / 90

Example of Global Reduction

- Global integer sum
- Sum of all inbuf values should be returned in resultbuf
- The result is only placed in resultbuf at the root process

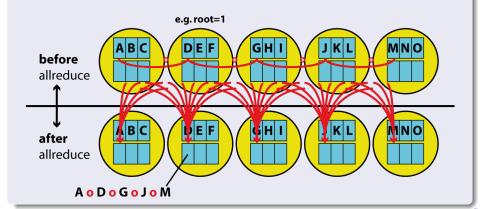
MA6252 17.12.2015 71 / 90

Variants of Reduction Operations

- MPI_Allreduce
 - no root
 - returns the result in all processes
- 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

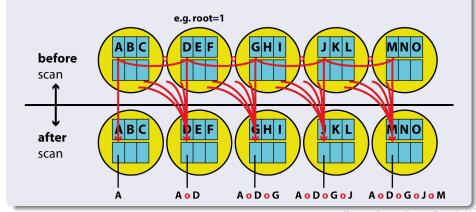
MA6252 17.12.2015 72 / 90

MPI_Allreduce



MA6252 17.12.2015 73 / 90

MPI_Scan



MA6252 17.12.2015 74 / 90

Outline

- MPI Overview
- Process model and language bindings
- Messages and point-to-point communication
- Non-blocking communication
- Derived data types
- Virtual topologies
- Collective communication
- Serialization
 - how to order the execution of MPI processes



MA6252 17.12.2015 75 / 90

Motivation

Question

How can MPI processes be serialized?

76 / 90

MA6252 17.12.2015

Solution 1

```
if( rank == 0 ) /* ... */
MPI_Barrier( MPI_COMM_WORLD );
if( rank == 1 ) /* ... */
MPI_Barrier( MPI_COMM_WORLD );
// ...
```

MA6252 17.12.2015 77 / 90

Solution 1

```
if( rank == 0 ) /* ... */
MPI_Barrier( MPI_COMM_WORLD );
if( rank == 1 ) /* ... */
MPI_Barrier( MPI_COMM_WORLD );
// ...
```

```
MPI_Comm_size( MPI_COMM_WORLD, &size );
MPI_Comm_rank( MPI_COMM_WORLD, &rank );

for( int i=0; i<size; ++i ) {
   if( i == rank ) /* ... */
   MPI_Barrier( MPI_COMM_WORLD );
}</pre>
```

MA6252 17.12.2015 77 / 90

Solution 2

- Each process waits for a message from the processes with rank-1 (blocking receive)
- Do some work
- Send a message to the process with rank rank+1



MA6252 17.12.2015 78 / 90

Outline

- MPI Overview
- Process model and language bindings
- Messages and point-to-point communication
- Non-blocking communication
- Derived data types
- Virtual topologies
 - - a multi-dimensional process naming scheme
- Collective communication



MA6252 17.12.2015 79 / 90

Virtual Topologies

- Convenient process naming
- Naming scheme to fit the communication pattern
- Simplifies writing of code
- Can allow MPI to optimize communications

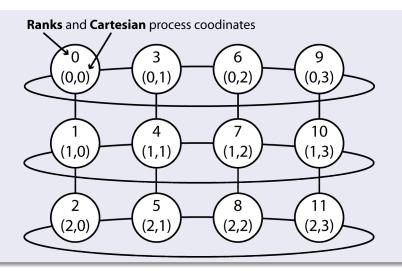
MA6252 17.12.2015 80 / 90

How to use a Virtual Topology

- Creating a topology produces a new communicator
- MPI provides mapping functions
 - to compute process ranks, based on the topology naming scheme
 - and vice versa.

MA6252 17.12.2015 81 / 90

Example – A 2-dimensional Cylinder



◆ロト ◆個ト ◆差ト ◆差ト 差 めらぐ

MA6252 17.12.2015 82 / 90

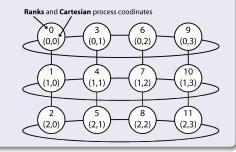
Topology Types

- Cartesian Topologies
 - each process is connected to its neighbor in a virtual grid
 - boundaries can be cyclic, or not
 - processes are identified by Cartesian coordinates
 - of course, communication between any two processes is still allowed
- Graph Topologies
 - general graphs
 - not covered here

MA6252

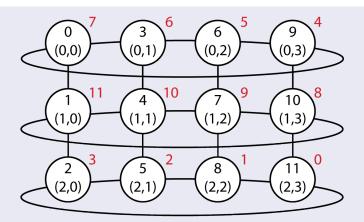
Creating a Cartesian Virtual Topology

```
comm_old = MPI_COMM_WORLD
  ndims = 2
    dim = { 3, 4 }
periods = { 0, 1 }
reorder = see next slide
```



MA6252 17.12.2015 84 / 90

Example – A 2-dimensional Cylinder

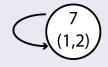


- Ranks in comm and comm_cart may differ, if reorder == 1
- This reordering can allow MPI to optimize communications

MA6252 17.12.2015 85 / 90

Cartesian Mapping Functions

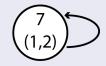
Mapping ranks to process grid coordinates



MA6252 17.12.2015 86 / 90

Cartesian Mapping Functions

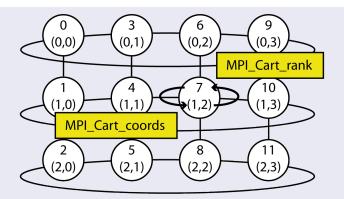
Mapping process grid coordinates to ranks



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

MA6252 17.12.2015 87 / 90

Own Coordinates



Each process gets its own coordinates with

```
MPI_Comm_rank ( comm_cart, &my_rank );
MPI_Cart_coords( comm_cart, my_rank, maxdims, my_coords );
```

MA6252 17.12.2015 88 / 90

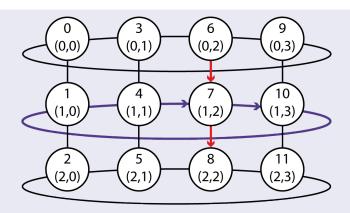
Cartesian Mapping Functions

• Computing ranks of neighboring processes

- Returns MPI_PROC_NULL if there is no neighbor
- \bullet MPI_PROC_NULL can be used as source or destination rank in each communication \to Then, this communication will be a noop!

MA6252 17.12.2015 89 / 90

MPI_Cart_shift - Example



process rank=7 10 +1

90 / 90

MA6252 17.12.2015