

MPI Programming

Intel Software College



Course Objectives

After successfully completing this module, you will be able to:

- Compile and run MPI programs using the MPICH implementation
- Write MPI programs using the core library



2

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Agenda

What is MPI? Core MPI Library

Basic Communication

Non-Blocking Communications

Collective Communications

Advanced MPI

- Useful Features
- Factors Affecting MPI Performance



3

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Agenda

What is MPI?

- **Core MPI Library**
- **Basic Communication**
- **Non-Blocking Communications**
- **Collective Communications**
- Advanced MPI
 - Useful Features
 - Factors Affecting MPI Performance



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MPI

A library - not a language

A library for inter-process communication and data exchange

Function categories

- Initialization/finalization
- Point-to-point communication
- Collective communication
- Communicator topologies
- User-defined data types
- Utilities (e.g.- timing and initialization)

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5

Parallel Models Compared

	MPI	Threads	OpenMP*
Portable	✓		✓
Scalable	✓	✓	✓
Performance Oriented	✓		\checkmark
Supports Data Parallel	✓	✓	\checkmark
Incremental Parallelism			\checkmark
High Level			\checkmark
Serial Code Intact			\checkmark
Verifiable Correctness			\checkmark
Distributed Memory	✓		



6

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Common MPI Implementations

MPICH* (Argonne National Laboratory)

- Most common MPI implementation
- Derivatives
 - MPICH GM* Myrinet* support (available from Myricom)
 - MVAPICH* InfiniBand* support (available from Ohio State University)
 - Intel® MPI version tuned to Intel Architecture systems
 - LAM/MPI* (Indiana University)
 - Contains many MPI 2.0 features
 - Daemon-based MPI implementation
 - MPI/Pro* (MPI Software Technology)
 - Scali MPI Connect*
 - Provides native support for most high-end interconnects



7

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Getting Started

OSCAR? NPACI Rocks?

- MPI Implementation(s) pre-configured
- For a manual build see material in backup to these slides

What do you need to run?

- Program supplied or build with mpicc <program.c> or mpif77 <program.f>
- Which machines to use? (machines file)
- A way to launch programs on remote machines (ssh for both OSCAR and Rocks)

Run with:

8

 mpirun -n xx <program name> where xx is the number of processes (ranks) to launch



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Absolute Minimum MPI Program Skeleton

Initialize MPI Lib on my node – required

Do work – optional, but important ©

Wrap it up once we are finished – required



9

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Compiling an MPI Program

Most MPI implementations supply compilation scripts:

mpif77 mpi_prog.f
mpicc mpi_proc.c
mpif90 mpi_prof.f90
mpiCC mpi_prof.C

Manual compilation/linking also possible:

ifc mpi_prog.f -L/usr/local/mpich-1.2.5/lib -lfmpich -lmpich



10

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MPI Machine File

A text file telling MPI where to launch processes

Put separate machine name on each line

Example:

compute-0-0		
compute-0-1		
compute-0-2		
compute-0-3		

Check implementation for multi-processor node formats Default file found in MPI installation



11

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Parallel Program Execution

Launch scenario for MPIRUN

- Find machine file (to know where to launch)
- Use SSH or RSH to execute a copy of program on each node in machine file
- Once launched, each copy establishes communication with local MPI lib (MP_Init)
- Each copy ends MPI interaction with MPI_Finalize



12

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Starting an MPI Program





13

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Activity 1: "Hello, World" in MPI

Demonstrates how to create, compile and run a simple MPI program on the lab cluster using the Intel MPI implementation

```
#include <stdio.h>
#include ``mpi.h"
int main (int argc, char* argv[])
{
    MPI_Init (&argc, &argv); /* Initialize the library */
    printf (``Hello world\n");
    MPI_Finalize (); /* Wrap it up. */
}
```



14

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Agenda

What is MPI?

Core MPI Library

Basic Communication

Non-Blocking Communications

Collective Communications

Advanced MPI

- Useful Features
- Factors Affecting MPI Performance



15

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The Whole Library

MPI is large and complex

- MPI 1.0 125 functions
- MPI 2.0 is even larger

But, many MPI features are rarely used

- Inter-communicators
- Topologies
- Persistent communication
- Functions designed for library developers



16

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The Absolute Minimum

Six MPI functions:

- MPI_Init 🖈
- MPI_Comm_size
- MPI_Comm_rank
- MPI_Send
- MPI_Recv
- MPI_Finalize 🖈

Many parallel algorithms can be implemented efficiently with only these functions



17

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Initializing the MPI Library



MPI Init prepares the system for MPI execution

Call to MPI_Init may update arguments in C

• Implementation dependent

No MPI functions may be called before MPI_Init



18

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Shutting Down MPI



MPI_Finalize frees any memory allocated by the MPI library

No MPI functions may be called after calling MPI_Finalize

• Exception: MPI_Init



19

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Sizing the MPI Communicator



MPI_Comm_size returns the number of processes in the specified
communicator

The communicator structure, MPI_Comm, is defined in mpi.h



20

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Determining MPI Process Rank



MPI_Comm_rank returns the rank of calling process within the specified communicator

Processes are numbered from 0 to N-1



21

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Activity 2: "Hello, World" with IDs

Demonstrates how to modify, compile and run a simple MPI program on the lab cluster using the Intel MPI implementation

```
#include <stdio.h>
#include "mpi.h"
int main (int argc, char* argv[])
{
   int numProc, myRank;
  MPI Init (&argc, &argv); /* Initialize the library */
  MPI Comm rank (MPI COMM WORLD, &myRank); /* Who am I?" */
  MPI Comm size (MPI COMM WORLD, &numProc); /*How many? */
  printf ("Hello. Process %d of %d here.\n", myRank, numProc);
  MPI Finalize (); /* Wrap it up. */
}
```



22

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Agenda

What is MPI? Core MPI Library

Basic Communication

Non-Blocking Communications

Collective Communications

Advanced MPI

- Useful Features
- Factors Affecting MPI Performance



23

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Sending Data

MPI_Send performs a blocking send of the specified data to the specified destination



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Receiving Data



MPI_Recv performs a blocking receive of the specified data from the specified source



25

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MPI Data Types for C

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

MPI provides predefined data types that must be specified when passing messages.



26

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MPI Data Types for Fortran

MPI Data Type	Fortran Data Type
MPI_BYTE	
MPI_CHARACTER	CHARACTER
MPI_COMPLEX	COMPLEX
MPI_DOUBLE_PRECISION	DOUBLE PRECISION
MPI_INTEGER	INTEGER
MPI_LOGICAL	LOGICAL
MPI_PACKED	
MPI_REAL	REAL

MPI provides predefined data types that must be specified when passing messages.



27

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MPI Status Details

C

type MPI_Status has three fields

- MPI_SOURCE
- MPI_TAG
- MPI_ERROR

Fortran

Status is an array indexed by

- MPI_SOURCE
- MPI_TAG
- MPI_ERROR

status.MPI_SOURCE status.MPI_TAG status.MPI_ERROR status(MPI_SOURCE)
status(MPI_TAG)
status(MPI_ERROR)



28

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Blocking Communication



Key Points

- Sending and receiving data is a paired operation. Ignoring this principle can result in deadlock.
- Communication and synchronization are coupled.

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29

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Activity 3: "Hello, World" with Message

Modify the "Hello, World" example so that the MPI processes pass an integer variable from left to right, reporting and incrementing its value at each step.





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Activity 4: "Hello, World" with Finish

Modify the "Hello, World" example so that the MPI processes pass an integer variable from left to right, reporting and incrementing its value at each step. The master process should report when all processes are finished.



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Thought Problem

Consider a 2D mesh with nearest-neighbor communication, coded in MPI:



What is wrong with this code?



32

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Definite Deadlock

This program should always deadlock because each MPI process executes a blocking 'receive' before the corresponding 'send'.



33

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Possible Deadlock

This program may deadlock.

In some MPI implementations, MPI_SEND returns when the send buffer is copied to the system buffer. Result:

 Program might work if messages are small, but would deadlock when messages are larger than the system buffer



34

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Worth Repeating



Key Points

• Sending and receiving data is a paired operation.

Ignoring this principle can result in deadlock.

• Communication and synchronization are coupled.



35

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Activity 5: Parallelize Pi Integration

```
f(x) = 4 / (1 + x^2)
```



```
#include <stdio.h>
#define INTERVALS 100000
int main (int argc, char* argv[])
   int i;
   double h, x, pi = 0.0;
   h = 1.0 / (double) INTERVALS
   for (i = 0; i < INTERVALS; i++)
      x = h * ((double)i - 0.5);
      pi += 4.0 / (1.0 + x * x);
   pi *= h;
   printf ("Pi = f n'', pi);
```

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36

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No Deadlock

```
Process 0 code
do
<Prepare data>
   call MPI SEND (data, len, MPI REAL, 1,
                   tag, comm, ierr)
   Call MPI REVC (buff, len, MPI REAL, 1,
               taq, comm, ierr)
enddo
Process 1 code
do
   call MPI RECV (buff, len, MPI REAL, 0,
                  taq, comm, ierr)
<Prepare data>
   call MPI SEND (buff, len, MPI REAL, 0,
               tag, comm, ierr)
enddo
```

Though this program will not deadlock, there is another issue . . .



37

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Communication Bottlenecks



Intel® Trace Analyzer MPI timeline showing severe communications bottleneck

Examination of the code revealed that the application was performing data preparation in serial:



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What is MPI? **Core MPI Library Basic Communication Non-Blocking Communications Collective Communications Advanced MPI**

Factors Affecting MPI Performance



39

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Non-Blocking Send



Key Points

- 1. The sender does not wait for message buffering to complete.
- 2. The programmer must guarantee that the send buffer is not modified before the message is delivered.
- 3. It is difficult to debug MPI programs that ignore the previous point.



40

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Non-Blocking Receive



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Key Points
1. The receiver does
not wait for

message to be

received.

2. The program may continue with other processing until message is needed.

3. Call *wait* function to block until message arrives. Cannot guarantee buffer contents until *wait* function returns.





41

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Immediate Send

MPI_Isend performs a non-blocking send of the specified data to the specified destination



42

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Immediate Receive

MPI_Irecv performs a non-blocking receive of the specified data
from the specified source



43

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Confirming Delivery



MPI_Wait returns when the operation that started the specified request gets completed

MPI Send or MPI Recv can also be used to confirm delivery

MPI_Waitall and MPI_Waitany can be used to wait on groups of messages without imposing order



44

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Thought Problem

Consider a two-dimensional mesh with nearest-neighbor communication, coded in MPI



Why does this code perform poorly?

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45





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Increased Parallelism

```
Process 0 code
do
<Prepare data>
   call MPI ISEND (data, len, MPI REAL, 1,
                   tag, comm, request, ierr)
   call MPI REVC (buff, len, MPI REAL, 1,
               tag, comm, ierr)
enddo
Process 1 code
Do
<Prepare data>
   call MPI ISEND (data, len, MPI REAL, 0,
                 tag, comm, request, ierr)
   call MPI RECV (buff, len, MPI REAL, 0,
                 taq, comm, ierr)
```

enddo

46

How does this run?



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Optimizing Communication

Parallel data preparation alleviates the bottleneck





Intel® Trace Analyzer MPI timeline showing improved computation to communication ratio





47

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Agenda

What is MPI? Core MPI Library Basic Communication Non-Blocking Communications Collective Communications Advanced MPI

- Useful Features
- Factors Affecting MPI Performance



48

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Collective Communication

Functions to facilitate communication among all MPI processes in a communicator

Categories:

- Barrier and broadcast
- Gather and scatter
- Reduction

Collective communication functions can be optimized for the underlying network topology



49

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Broadcasting Data

MPI_Bcast sends the specified data to all processes in the communicator



50

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MPI_BCAST Example

```
program BroadcastData
include `mpif.h'
integer, dimension(4) :: msg
call MPI INIT (ierr)
call MPI COMM SIZE (MPI COMM WORLD, nprocs, ierr)
call MPI COMM RANK (MPI COMM WORLD, myrank, ierr)
if (myrank == 0) then
  msg = 1
else
  msq = 0
endif
call MPI BCAST
                 2
   (msg, 4, MPI INTEGER, 0, MPI COMM WORLD, ierr)
call MPI FINALIZE (ierr)
end program BroadcastData
```





51

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Data Reduction

MPI_Reduce performs the specified reduction operation on the specified data from all processes in the communicator



52

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MPI Reduction Operations

Operation	Function
MPI_SUM	Summation
MPI_PROD	Product
MPI_MIN	Minimum value
MPI_MINLOC	Minimum value and location
MPI_MAX	Maximum value
MPI_MAXLOC	Maximum value and location
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
User-defined	It is possible to define new reduction operations



53

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MPI_REDUCE Example







54

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Activity 6: Pi Revisited

Simplify your parallel Pi integration using collective communication routines

 $f(x) = 4 / (1 + x^2)$



```
#include <stdio.h>
#define INTERVALS 100000
int main (int argc, char* argv[])
{
   int i;
  double h, x, pi = 0.0;
  h = 1.0 / (double) INTERVALS
   for (i = 0; i < INTERVALS; i++)
   Ł
      x = h * ((double)i - 0.5);
     pi += 4.0 / (1.0 + x * x);
  pi *= h;
  printf ("Pi = f^n, pi);
}
```

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Activity 7: Master-worker



56

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Review

MPI is best for distributed-memory parallel systems

- There are several MPI implementations
- The MPI library is large but the core is small

MPI communication:

- Point-to-point, blocking
- Point-to-point, non-blocking
- Collective



57

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Core MPI

11 Out of 125 Total Functions

Program startup and shutdown

- MPI Init, MPI Finalize
- MPI_Comm_size, MPI_Comm_rank

Point-to-point communication

• MPI Send, MPI Recv

Non-blocking communication

• MPI Isend, MPI Irecv, MPI Wait

Collective communication

• MPI_Bcast, MPI_Reduce



58

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Agenda

What is MPI? Core MPI Library Basic Communication Non-Blocking Communications Collective Communications Advanced MPI

- Useful Features
- Factors Affecting MPI Performance



59

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Useful Features

- Communicators
- Timing routines
- User-defined data types
- Inter-communicators
- Topologies
- Persistent communication
- New features in MPI 2.0



60

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Communicators

MPI uses communicators to direct message traffic. MPI_COMM_WORLD is default communicator of all processes. Program may define other communicators.





61

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Communicators: Example

Each model conveniently maps to its own communicator.





62

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Timing Routines

Performance is a major design goal of MPI

Therefore, MPI provides functions to measure runtime:

- MPI_Wtime returns the number of seconds from some arbitrary starting point
- MPI_Wtick used to determine timer resolution

```
int start = MPI_Wtime ();
// Do some work
int end = MPI_Wtime ();
```





63

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Handling Non-Contiguous Data

How to send only the red elements of V?



One possibility, copy these elements to a temporary array before sending.



64

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Derived Data Types

How to send only the red elements of V, while avoiding copying non-contiguous data to a temporary array?

Define a new data type, in this case a vector with stride of two from original.



MPI_Type_vector (3, 1, 2, MPI_REAL, &vType);
MPI_Send (V[2], 1, vType, dest, tag, MPI_COMM_WORLD);

MPI provides several functions to define new data types. MPICH contains optimizations for user-defined type.



65

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Inter-communicators

Useful for library development to hide library messages from calling program

Can be used to divide the MPI processes among different parallel computations (for example, multi-block CFD)

Functions:

• MPI_Comm_create, MPI_Comm_dup, MPI_Comm_split





66

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Topologies

MPI provides functions to map application topology to processor topology



For example, consider an application that maps naturally onto a 4×3 Cartesian grid. Nearest neighbors are not obvious from process rank

Use MPI_Cart_create function to create a new communicator with the specified topology

Use MPI_Cart_shift to identify nearest neighbors, even for periodic grids

MPI topologies can be user-defined graphs



67

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MPI 2.0 – More Features

One-sided communication

- MPI_Put, MPI_Get
- Uses Remote Memory Access (RMA)
- Separates communication from synchronization

Dynamic process spawning

- MPI_Spawn function
- Creates a new inter-communicator

Collective communication can be used across disjoint intracommunicators

Parallel I/O

68



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MPI 2.0 – Better Language Support

Fortran 90/95

- Array sections
- Modules

C++

- MPI class library
- MPI functions are methods within MPI classes



69

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Profiling MPI Communications

MPICH* contains profiling tools that are not installed by default

Jumpshot-2

- Installation
 - Install Java Development Kit
 - Additional MPICH configuration option:
 - -mpe-opts=--with-java=/usr/local/jdk
- Usage

70

- Add -mpilog option to MPICH compilation, e.g.:
- mpicc -mpilog -o prog.exe prog.c



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Communications Timeline





71

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What is MPI? Core MPI Library Basic Communication

Non-Blocking Communications

Collective Communications

Advanced MPI

• Useful Features

• Factors Affecting MPI Performance



72

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Network Interconnect

• Timeline shows a repeating pattern of computation and communication but does not indicate a communications bottleneck



• The only way to improve the performance of this application is to use a faster network interconnect

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73

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Network Interconnect

Fast Ethernet

Gigabit Ethernet

Myrinet*

InfiniBand*

Quadrics*

74



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Message Size

In general, given the same amount of data, it is better to send fewer large messages than many small messages

- Fewer MPI function calls, less system overhead
- Fewer messages, less TCP/IP overhead

User-defined data types in MPI can help pack several messages into one



75

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Computation: Communication

Which of these applications is likely to show better parallel speedup and scalability?

Application 1



Application 2



Obviously, Application 1 has a better ratio of computation to communication!



76

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Overlapping Communication & Computation

```
do i = 1, neighbors
   call MPI IRECV (edge(1,i), len, MPI REAL, nbr(i),
                   tag, comm, requests(i), ierr)
enddo
do i = 1, neighbors
   call MPI ISEND (edge(1,i), len, MPI REAL, nbr(i),
                  tag, comm, requests(i), ierr)
enddo
! Perform computation not requiring message data
call MPI WAITALL ((2 * neighbors), requests, status, ierr)
```



77

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MPICH Communication Devices

ch_p4

- General communication device
- Support for SMP nodes
- Supports heterogeneous nodes
- MPICH default communication device

ch_p4mpd

- Only supports homogeneous, uni-processor clusters
- Provides faster, more scalable job startup

ch_shmem - Best for machines supporting shmem

ch_globus2 – Grid-enabled MPICH for Globus

ch_nt – MPICH* for Microsoft Windows*



78

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MPICH SMP Support

Intra-node communication through TCP/IP

Intra-node communication through memcpy



Dual-CPU node



Dual-CPU node

Configure MPICH with the -comm=shared option Set the MPI_MAX_CLUSTER_SIZE environment variable



79

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Backup



80

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Getting Started with MPICH

Step 1: Download most recent package

• <u>ftp://ftp.mcs.anl.gov/pub/mpi/mpich.tar.gz</u>

Step 2: Unpack the archive in /usr/local

Step 3: Patch MPICH

- Download the latest cumulative patch
 - <u>ftp://ftp.mcs.anl.gov/pub/mpi/patch/1.2.5/patch.all</u>
- Copy patch file(s) to /usr/local/mpich-1.2.5

• Execute:

patch -p0 < patch.all</pre>



81

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Configuring MPICH

Step 4: Configure

- Important configuration options
 - Communication device
 - Compilers
 - SMP support

• Execute: configure -with-device=ch_p4 \
 -cc=icc -fc=ifc -f90=ifc -c++=icc \
 -prefix=/usr/local/mpich-1.2.5

Check the configuration log for errors



82

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Installing MPICH

Step 5: Build

- Execute: make >& make.log
- Check the make log for errors

Step 6: Install

• Execute: make install

At this point, anyone logging into the system should have access to the MPI compiler scripts, libraries, mpirun, and machine files.



83

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MPI_GET_COUNT and Wild Card





84

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