MPI for Dummies

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General principles in this tutorial

- Everything is practically oriented
- We will use lots of real example code to illustrate concepts
- At the end, you should be able to use what you have learned and write real code, run real programs
- Feel free to interrupt and ask questions
- If our pace is too fast or two slow, let us know

What we will cover in this tutorial

- **What is MPI?**
- How to write a simple program in MPI
- Running your application with MPICH
- Slightly more advanced topics:
  - Non-blocking communication in MPI
  - Group (collective) communication in MPI
  - MPI Datatypes
- Conclusions and Final Q/A

The switch from sequential to parallel computing

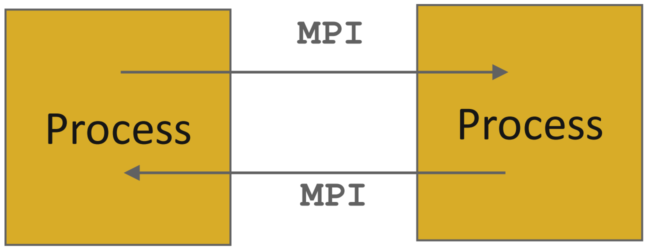
- Moore's law continues to be true, but…
  - Processor speeds no longer double every 18-24 months
  - Number of processing units double, instead
    - Multi-core chips (dual-core, quad-core)
  - No more automatic increase in speed for software
- Parallelism is the norm
  - Lots of processors connected over a network and coordinating to solve large problems
  - Used every where!
    - By USPS for tracking and minimizing fuel routes
    - By automobile companies for car crash simulations
    - By airline industry to build newer models of flights

Sample Parallel Programming Models

- Shared Memory Programming
  - Processes share memory address space (threads model)
  - Application ensures no data corruption (Lock/Unlock)
- Transparent Parallelization
  - Compiler works magic on sequential programs
- Directive-based Parallelization
  - Compiler needs help (e.g., OpenMP)
- Message Passing
  - Explicit communication between processes (like sending and receiving emails)

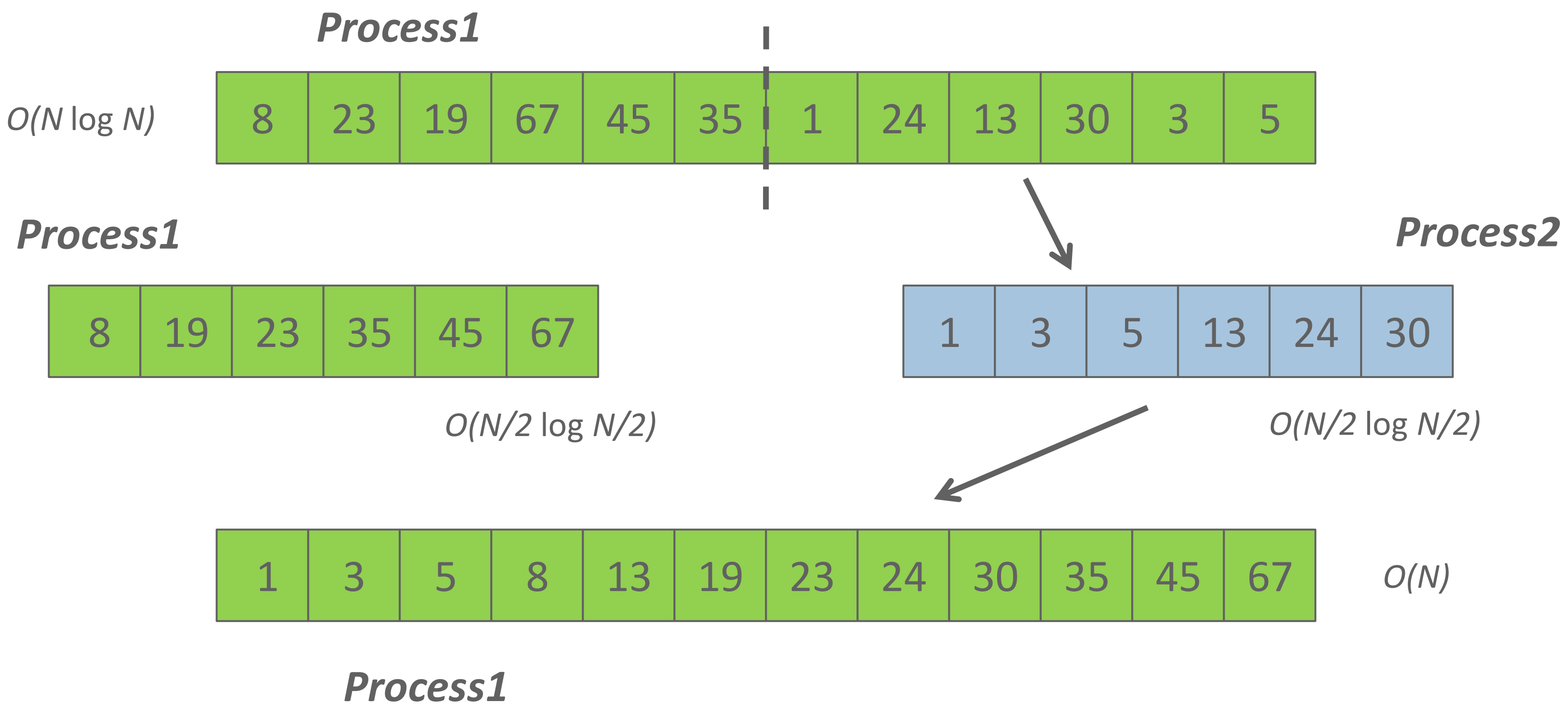
The Message-Passing Model

- A *process* is (traditionally) a program counter and address space.
- Processes may have multiple *threads* (program counters and associated stacks) sharing a single address space. MPI is for communication among processes, which have separate address spaces.
- Inter-process communication consists of
  - synchronization
  - movement of data from one process's address space to another's.



The Message-Passing Model (an example)

- Each process has to send/receive data to/from other processes
- Example: Sorting Integers



Standardizing Message-Passing Models with MPI

- Early vendor systems (Intel’s NX, IBM’s EUI, TMC’s CMMD) were not portable (or very capable)
- Early portable systems (PVM, p4, TCGMSG, Chameleon) were mainly research efforts
  - Did not address the full spectrum of message-passing issues
  - Lacked vendor support
  - Were not implemented at the most efficient level
- The MPI Forum was a collection of vendors, portability writers and users that wanted to standardize all these efforts

What is MPI?

- MPI: Message Passing Interface
  - The MPI Forum organized in 1992 with broad participation by:
    - Vendors: IBM, Intel, TMC, SGI, Convex, Meiko
    - Portability library writers: PVM, p4
    - Users: application scientists and library writers
    - MPI-1 finished in 18 months
  - Incorporates the best ideas in a “standard” way
    - Each function takes fixed arguments
    - Each function has fixed semantics
      - Standardizes what the MPI implementation provides and what the application can and cannot expect
      - Each system can implement it differently as long as the semantics match
- MPI is not…
  - a language or compiler specification
  - a specific implementation or product

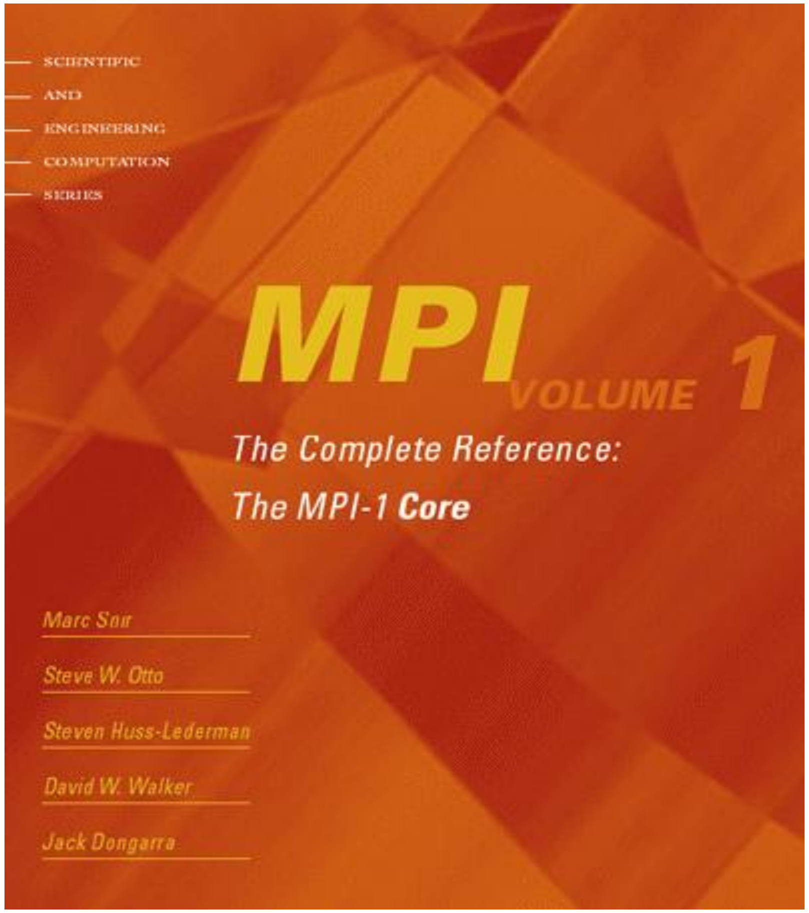
What is in MPI-1

- Basic functions for communication (100+ functions)
- Blocking sends, receives
- Nonblocking sends and receives
- Variants of above
- Rich set of collective communication functions
  - Broadcast, scatter, gather, etc
  - Very important for performance; widely used
- Datatypes to describe data layout
- Process topologies
- C, C++ and Fortran bindings
- Error codes and classes

Following MPI Standards

- MPI-2 was released in 2000
  - Several additional features including MPI + threads, MPI-I/O, remote memory access functionality and many others
- MPI-2.1 (2008) and MPI-2.2 (2009) were recently released with some corrections to the standard and small features
- MPI-3 (2012) added several new features to MPI
- The Standard itself:
  - at http://www.mpi-forum.org
  - All MPI official releases, in both postscript and HTML
- Other information on Web:
  - at http://www.mcs.anl.gov/mpi
  - pointers to lots of material including tutorials, a FAQ, other MPI pages

The MPI Standard (1 & 2)


SCIENTIFIC AND ENGINEERING COMPUTATION SERIES

MPI VOLUME 1

The Complete Reference: The MPI-1 Core

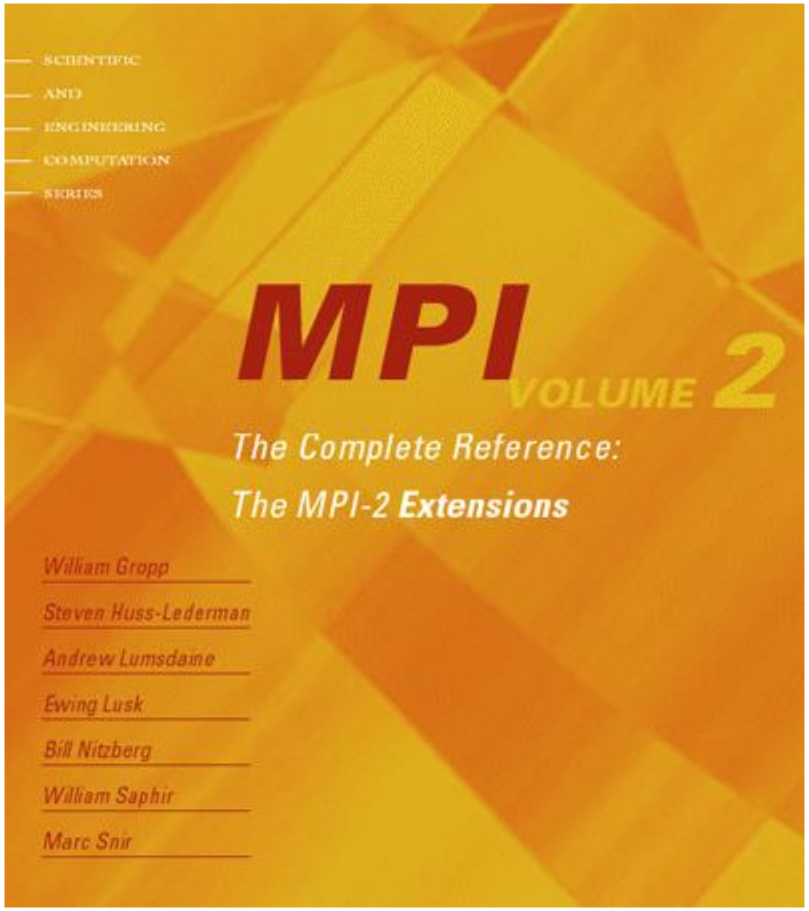
Marc Snir

Steve W. Otto

Steven Huss-Lederman

David W. Walker

Jack Dongarra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MPI VOLUME 2

The Complete Reference: The MPI-2 Extensions

William Gropp

Steven Huss-Lederman

Andrew Lumsdaine

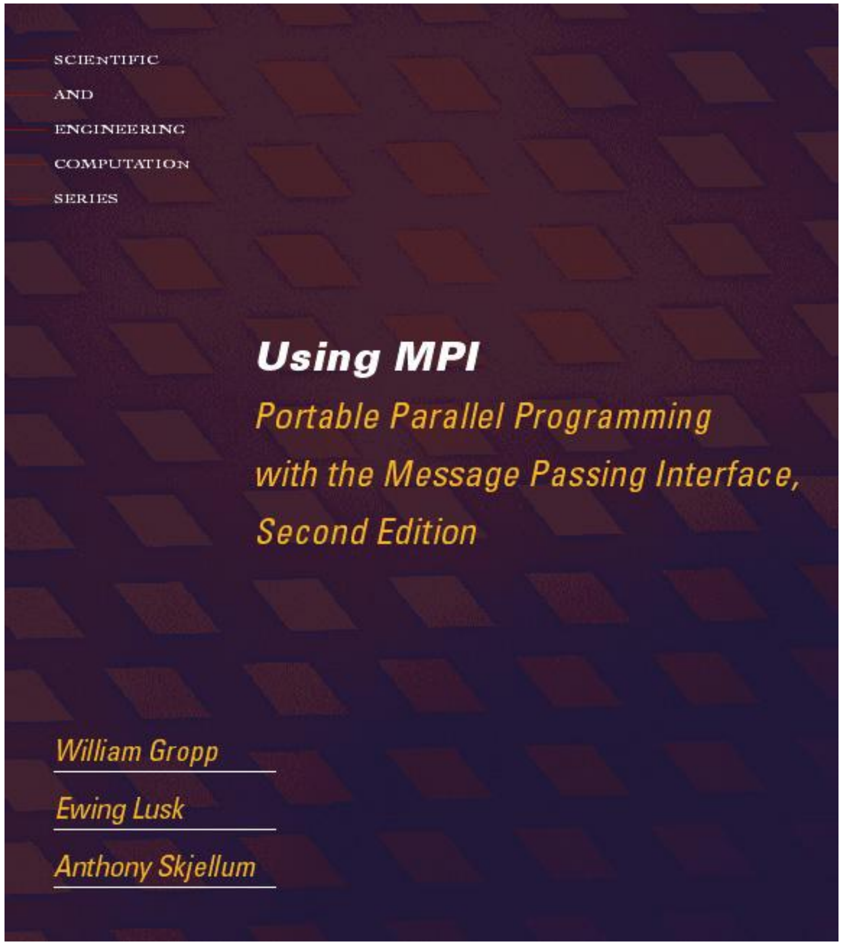
Ewing Lusk

Bill Nitzberg

William Saphir

Marc Snir

Tutorial Material on MPI-1 and MPI-2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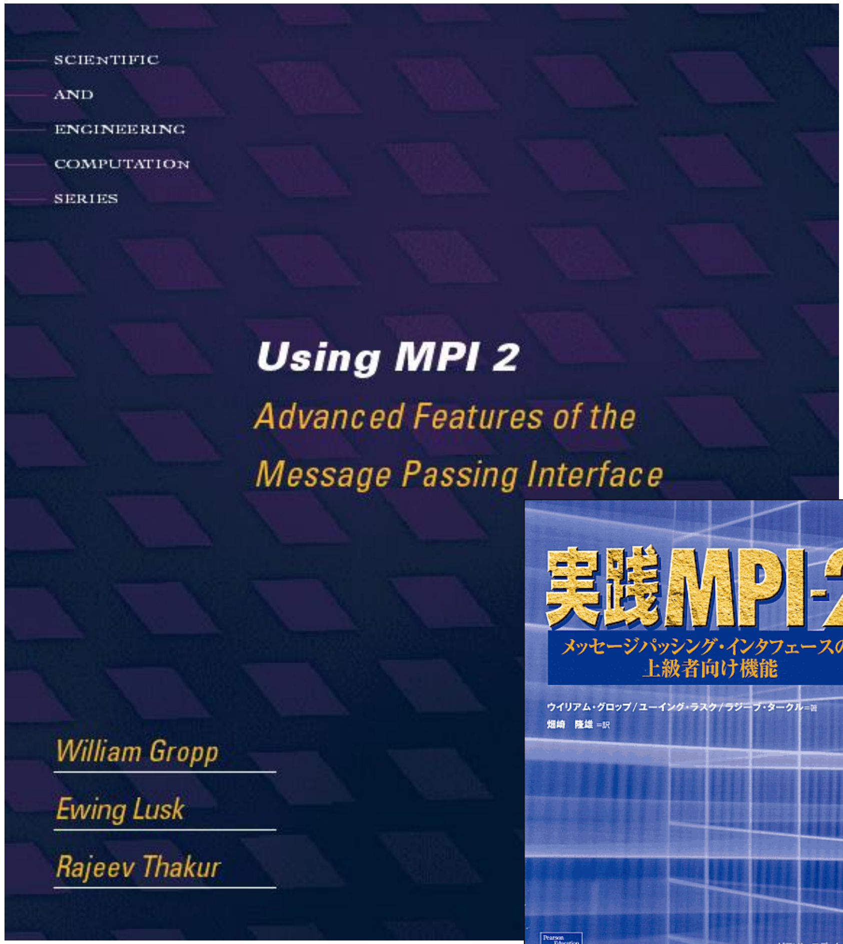
Using MPI
Portable Parallel Programming with the Message Passing Interface, Second Edition

William Gropp
Ewing Lusk
Anthony Skjellum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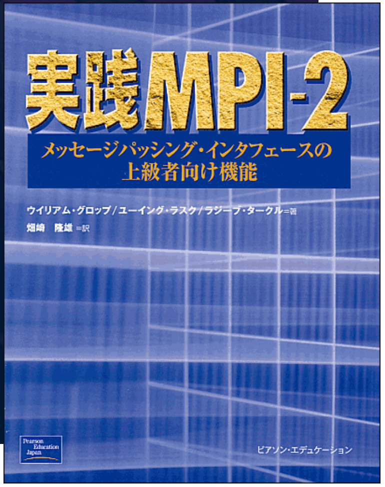
Using MPI 2
Advanced Features of the Message Passing Interface

William Gropp
Ewing Lusk
Rajeev Thakur


実践MPI-2
メッセージパッシング・インタフェースの
上級者向け機能

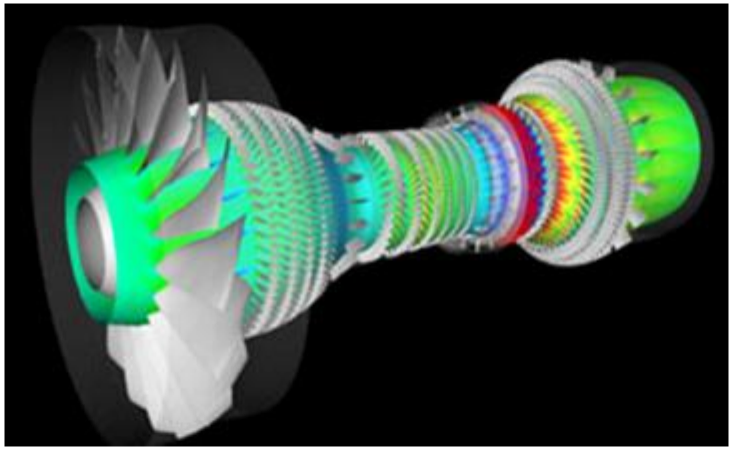
ウイリアム・グロップ/ユーイング・ラスク/ラジーブ・タークル=著
畑崎　隆雄 =訳

Pearson Education Japan
ピアソン・エデュケーション

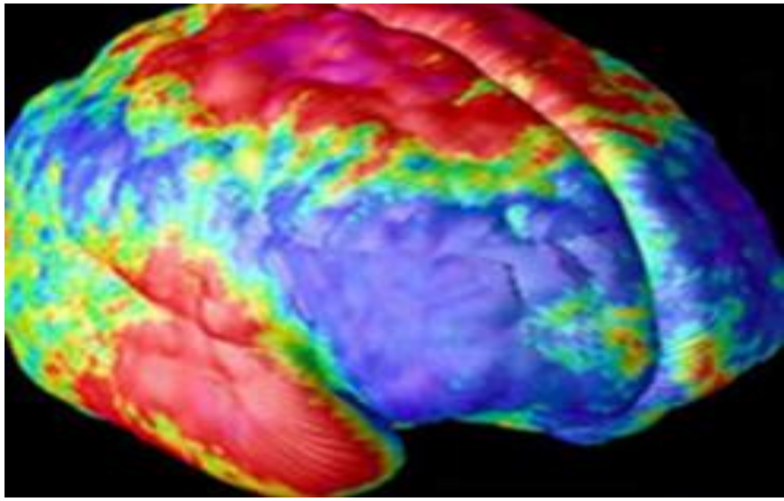
http://www.mcs.anl.gov/mpi/usingmpi
http://www.mcs.anl.gov/mpi/usingmpi2

Applications (Science and Engineering)

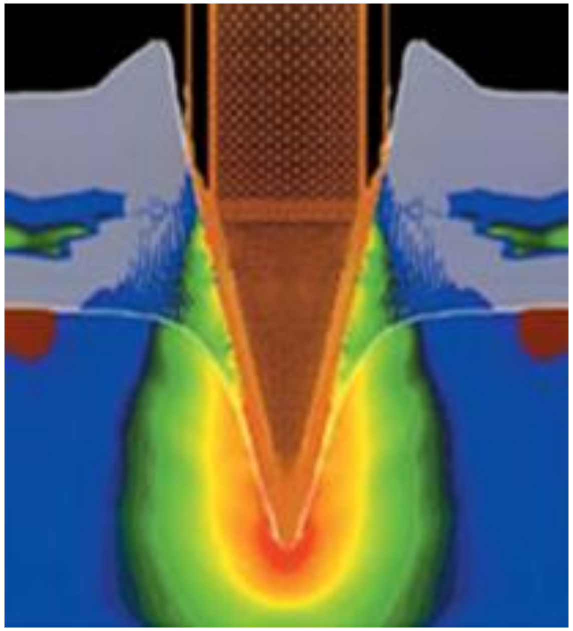
- MPI is widely used in large scale parallel applications in science and engineering
  - Atmosphere, Earth, Environment
  - Physics - applied, nuclear, particle, condensed matter, high pressure, fusion, photonics
  - Bioscience, Biotechnology, Genetics
  - Chemistry, Molecular Sciences
  - Geology, Seismology
  - Mechanical Engineering - from prosthetics to spacecraft
  - Electrical Engineering, Circuit Design, Microelectronics
  - Computer Science, Mathematics



Turbo machinery (Gas turbine/compressor)

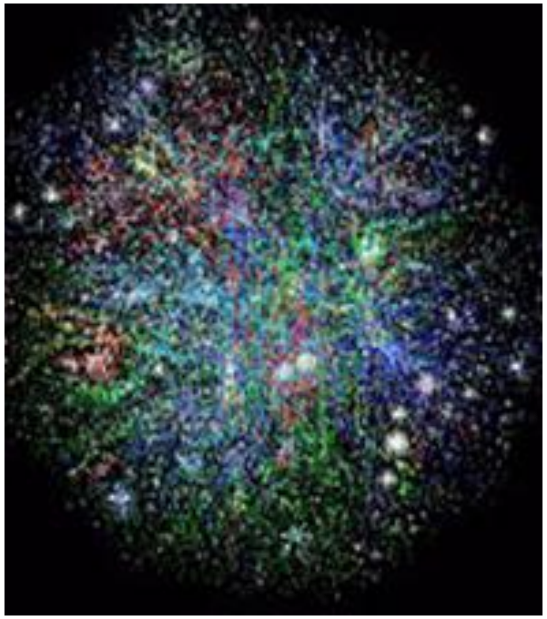


Biology application



Drilling application

Transportation & traffic application



Astrophysics application

Reasons for Using MPI

- **Standardization** - MPI is the only message passing library which can be considered a standard. It is supported on virtually all HPC platforms. Practically, it has replaced all previous message passing libraries
- **Portability** - There is no need to modify your source code when you port your application to a different platform that supports (and is compliant with) the MPI standard
- **Performance Opportunities** - Vendor implementations should be able to exploit native hardware features to optimize performance
- **Functionality** – Rich set of features
- **Availability** - A variety of implementations are available, both vendor and public domain
  - MPICH is a popular open-source and free implementation of MPI
  - Vendors and other collaborators take MPICH and add support for their systems
    - Intel MPI, IBM Blue Gene MPI, Cray MPI, Microsoft MPI, MVAPICH, MPICH-MX

Important considerations while using MPI

- All parallelism is explicit: the programmer is responsible for correctly identifying parallelism and implementing parallel algorithms using MPI constructs

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- **How to write a simple program in MPI**
- Running your application with MPICH
- Slightly more advanced topics:
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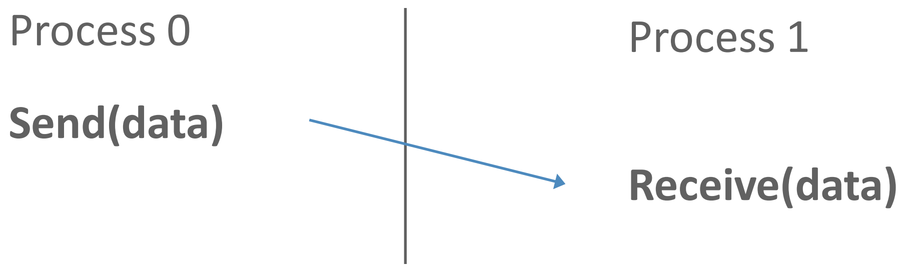
  - Group (collective) communication in MPI
  - MPI Datatypes
- Conclusions and Final Q/A

MPI Basic Send/Receive

- Simple communication model



- Application needs to specify to the MPI implementation:
  1. How do you compile and run an MPI application?
  2. How will processes be identified?
  3. How will "data" be described?

Compiling and Running MPI applications (more details later)

- MPI is a library
  - Applications can be written in C, C++ or Fortran and appropriate calls to MPI can be added where required
- Compilation:
  - Regular applications:
    - `gcc test.c -o test`
  - MPI applications
    - `mpicc test.c -o test`
- Execution:
  - Regular applications
    - `./test`
  - MPI applications (running with 16 processes)
    - `mpiexec –np 16 ./test`

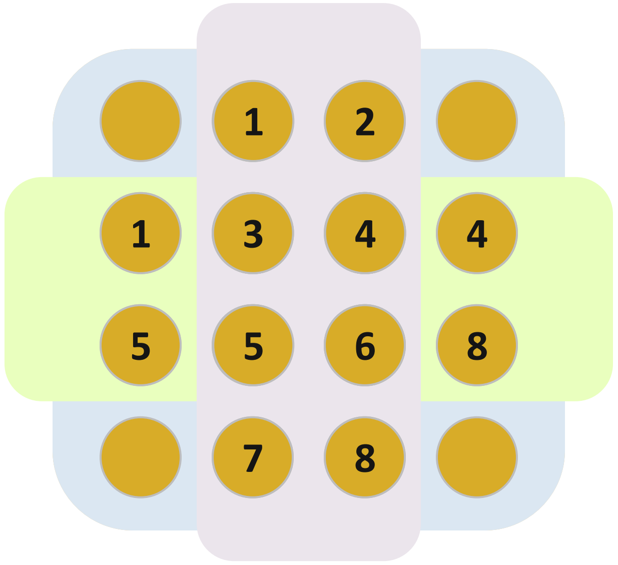
Process Identification

- MPI processes can be collected into groups
  - Each group can have multiple colors (some times called context)
  - *Group + color == communicator (it is like a name for the group)*
  - When an MPI application starts, the group of all processes is initially given a predefined name called **`MPI_COMM_WORLD`**
  - The same group can have many names, but simple programs do not have to worry about multiple names
- A process is identified by a unique number within each communicator, called *rank*
  - For two different communicators, the same process can have two different ranks: so the meaning of a "rank" is only defined when you specify the communicator

Communicators

```
mpiexec -np 16 ./test
```

Communicators do not need to contain all processes in the system



When you start an MPI program, there is one predefined communicator **MPI_COMM_WORLD**

Every process in a communicator has an ID called as “rank”

Can make copies of this communicator (same group of processes, but different “aliases”)

The same process might have different ranks in different communicators

Communicators can be created “by hand” or using tools provided by MPI (not discussed in this tutorial)

Simple programs typically only use the predefined communicator **MPI_COMM_WORLD**

Simple MPI Program Identifying Processes

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

int main(int argc, char ** argv)
{
    int rank, size;

    MPI_Init(&argc, &argv);

    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    printf("I am %d of %d\n", rank, size);

    MPI_Finalize();
    return 0;
}
```

Basic requirements for an MPI program

Data Communication

- Data communication in MPI is like email exchange
  - One process sends a copy of the data to another process (or a group of processes), and the other process receives it
- Communication requires the following information:
  - Sender has to know:
    - Whom to send the data to (receiver's process rank)
    - What kind of data to send (100 integers or 200 characters, etc)
    - A user-defined "tag" for the message (think of it as an email subject; allows the receiver to understand what type of data is being received)
  - Receiver "might" have to know:
    - Who is sending the data (OK if the receiver does not know; in this case sender rank will be **`MPI_ANY_SOURCE`**, meaning anyone can send)
    - What kind of data is being received (partial information is OK: I might receive *up to* 1000 integers)
    - What the user-defined "tag" of the message is (OK if the receiver does not know; in this case tag will be **`MPI_ANY_TAG`**)

More Details on Using Ranks for Communication

- When sending data, the sender has to specify the destination process’ rank
  - Tells where the message should go
- The receiver has to specify the source process’ rank
  - Tells where the message will come from
- `MPI_ANY_SOURCE` is a special “wild-card” source that can be used by the receiver to match any source

More Details on Describing Data for Communication

- MPI Datatype is very similar to a C or Fortran datatype
  - `int` → `MPI_INT`
  - `double` → `MPI_DOUBLE`
  - `char` → `MPI_CHAR`
- More complex datatypes are also possible:
  - E.g., you can create a structure datatype that comprises of other datatypes → a char, an int and a double.
  - Or, a vector datatype for the columns of a matrix
- The "count" in **`MPI_SEND`** and **`MPI_RECV`** refers to how many datatype elements should be communicated

More Details on User "Tags" for Communication

- Messages are sent with an accompanying user-defined integer *tag*, to assist the receiving process in identifying the message
- For example, if an application is expecting two types of messages from a peer, tags can help distinguish these two types
- Messages can be screened at the receiving end by specifying a specific tag
- **`MPI_ANY_TAG`** is a special "wild-card" tag that can be used by the receiver to match any tag

MPI Basic (Blocking) Send

```
MPI_SEND(buf, count, datatype, dest, tag, comm)
```

- The message buffer is described by (`buf, count, datatype`).
- The target process is specified by `dest` and `comm`.
  - `dest` is the rank of the target process in the communicator specified by `comm`.
- `tag` is a user-defined “type” for the message
- When this function returns, the data has been delivered to the system and the buffer can be reused.
  - The message may not have been received by the target process.

MPI Basic (Blocking) Receive

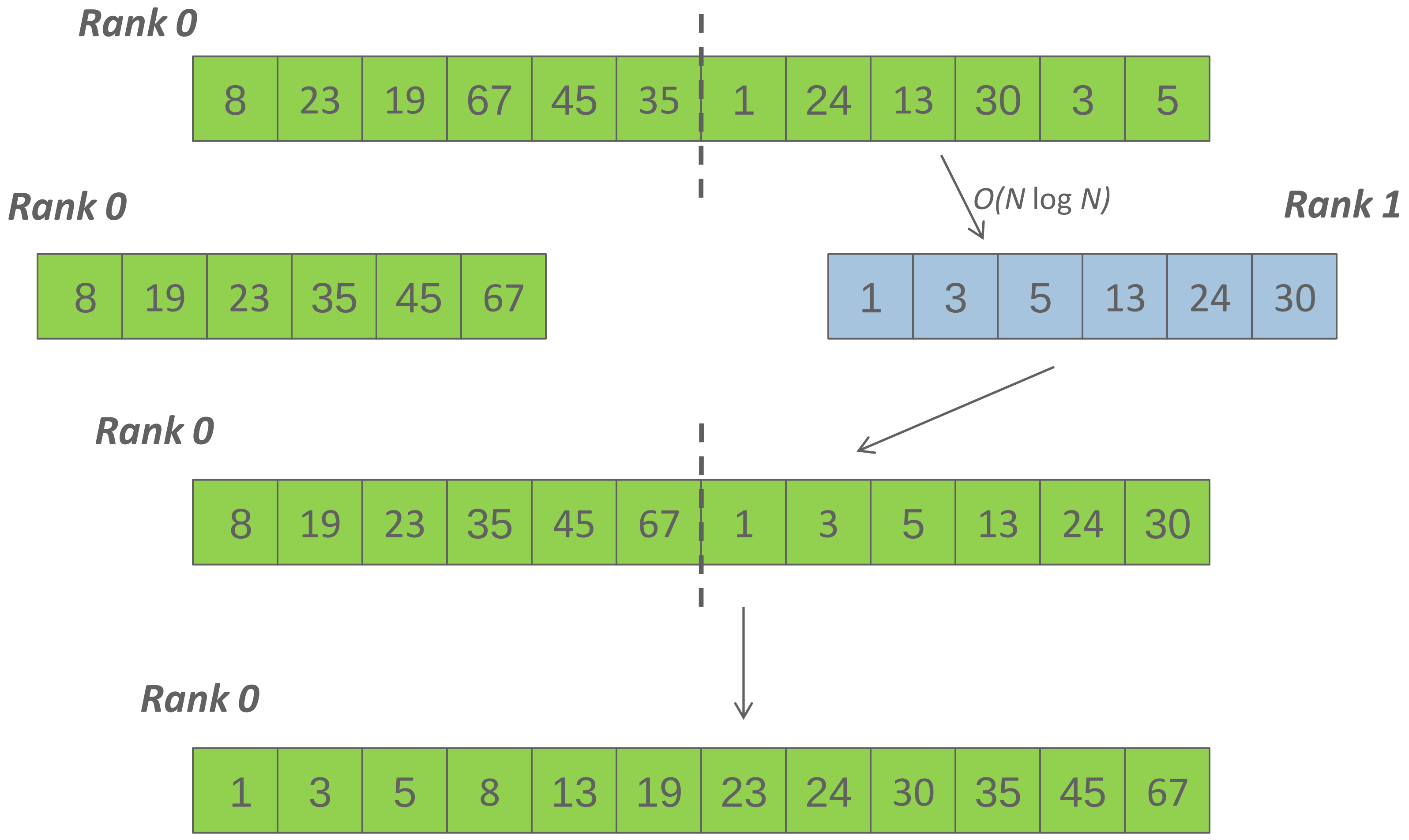
`MPI_RECV(buf, count, datatype, source, tag, comm, status)`

- Waits until a matching (on **`source`**, **`tag`**, **`comm`**) message is received from the system, and the buffer can be used.
- **`source`** is rank in communicator **`comm`**, or **`MPI_ANY_SOURCE`**.
- Receiving fewer than **`count`** occurrences of **`datatype`** is OK, but receiving more is an error.
- **`status`** contains further information:
  - Who sent the message (can be used if you used **`MPI_ANY_SOURCE`**)
  - How much data was actually received
  - What tag was used with the message (can be used if you used **`MPI_ANY_TAG`**)
  - **`MPI_STATUS_IGNORE`** can be used if we don't need any additional information

Simple Communication in MPI

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

int main(int argc, char ** argv)
{
    int rank, data[100];

    MPI_Init(&argc, &argv);

    MPI_Comm_rank(MPI_COMM_WORLD, &rank);

    if (rank == 0)
        MPI_Send(data, 100, MPI_INT, 1, 0, MPI_COMM_WORLD);
    else if (rank == 1)
        MPI_Recv(data, 100, MPI_INT, 0, 0, MPI_COMM_WORLD,
                 MPI_STATUS_IGNORE);

    MPI_Finalize();
    return 0;
}
```

Parallel Sort using MPI Send/Recv



Parallel Sort using MPI Send/Recv (contd.)

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char ** argv)
{
    int rank;
    int a[1000], b[500];

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    if (rank == 0) {
        MPI_Send(&a[500], 500, MPI_INT, 1, 0, MPI_COMM_WORLD);
        sort(a, 500);
        MPI_Recv(b, 500, MPI_INT, 1, 0, MPI_COMM_WORLD, &status);

        /* Serial: Merge array b and sorted part of array a */
    }
    else if (rank == 1) {
        MPI_Recv(b, 500, MPI_INT, 0, 0, MPI_COMM_WORLD, &status);
        sort(b, 500);
        MPI_Send(b, 500, MPI_INT, 0, 0, MPI_COMM_WORLD);
    }

    MPI_Finalize(); return 0;
}
```

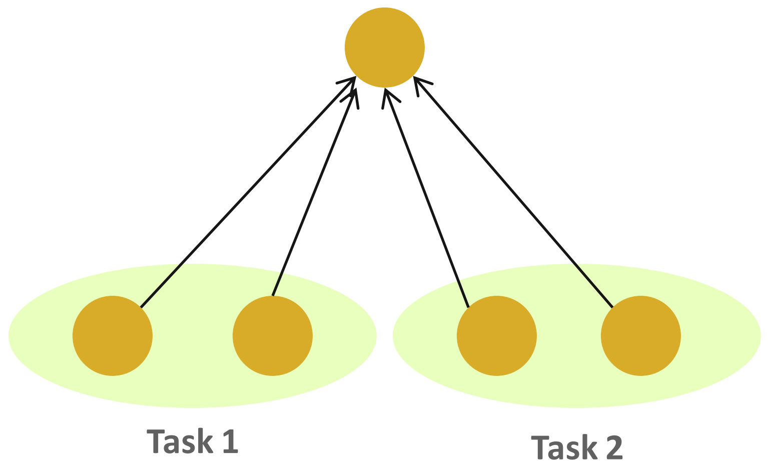
Status Object

- The status object is used after completion of a receive to find the actual length, source, and tag of a message
- Status object is MPI-defined type and provides information about:
  - The source process for the message (`status.MPI_SOURCE`)
  - The message tag (`status.MPI_TAG`)
  - Error status (`status.MPI_ERROR`)
- The number of elements received is given by:

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

`status`	return status of receive operation (status)
`datatype`	datatype of each receive buffer element (handle)
`count`	number of received elements (integer)(OUT)

Using the “status” field



- Each “worker process” computes some task (maximum 100 elements) and sends it to the “master” process together with its group number: the “tag” field can be used to represent the task
  - Data count is not fixed (maximum 100 elements)
  - Order in which workers send output to master is not fixed (different workers = different src ranks, and different tasks = different tags)

Using the “status” field (contd.)

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

int main(int argc, char ** argv)
{
    [...snip...]

    if (rank != 0)
        MPI_Send(data, rand() % 100, MPI_INT, 0, group_id,
                 MPI_COMM_WORLD);
    else {
        for (i = 0; i < size – 1 ; i++) {
            MPI_Recv(data, 100, MPI_INT, MPI_ANY_SOURCE,
                     MPI_ANY_TAG, MPI_COMM_WORLD, &status);
            MPI_Get_count(&status, MPI_INT, &count);
            printf(“worker ID: %d; task ID: %d; count: %d\n”,
                   status.source, status.tag, count);
        }
    }

    [...snip...]
}
```

MPI is Simple

- Many parallel programs can be written using just these six functions, only two of which are non-trivial:
  - `MPI_INIT – initialize the MPI library (must be the first routine called)`
  - `MPI_COMM_SIZE - get the size of a communicator`
  - `MPI_COMM_RANK – get the rank of the calling process in the communicator`
  - `MPI_SEND – send a message to another process`
  - `MPI_RECV – send a message to another process`
  - `MPI_FINALIZE – clean up all MPI state (must be the last MPI function called by a process)`
- For performance, however, you need to use other MPI features

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- **Running your application with MPICH**
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  - Group (collective) communication in MPI
  - MPI Datatypes
- Conclusions and Final Q/A

What is MPICH

- MPICH is a high-performance and widely portable implementation of MPI
- It provides all features of MPI that have been defined so far (including MPI-1, MPI-2.0, MPI-2.1, MPI-2.2, and MPI-3.0)
- Active development lead by Argonne National Laboratory and University of Illinois at Urbana-Champaign
  - Several close collaborators who contribute many features, bug fixes, testing for quality assurance, etc.
    - IBM, Microsoft, Cray, Intel, Ohio State University, Queen’s University, Myricom and many others
- Current release is MPICH-3.0.2

Getting Started with MPICH

- Download MPICH
  - Go to http://www.mpich.org and follow the downloads link
  - The download will be a zipped tarball
- Build MPICH2
  - Unzip/untar the tarball
  - `tar -xzvf mpich-3.0.2.tar.gz`
  - `cd mpich-3.0.2`
  - `./configure --prefix=/where/to/install/mpich`
  - `make`
  - `make install`
  - `Add /where/to/install/mpich/bin to your PATH`

Compiling MPI programs with MPICH

- Compilation Wrappers
  - For C programs: `mpicc test.c –o test`
  - For C++ programs: `mpicxx test.cpp –o test`
  - For Fortran 77 programs: `mpif77 test.f –o test`
  - For Fortran 90 programs: `mpif90 test.f90 –o test`
- You can link other libraries are required too
  - To link to a math library: `mpicc test.c –o test -lm`
- You can just assume that "mpicc" and friends have replaced your regular compilers (gcc, gfortran, etc.)

Running MPI programs with MPICH

- Launch 16 processes on the local node:
  - `mpiexec -np 16 ./test`
- Launch 16 processes on 4 nodes (each has 4 cores)
  - `mpiexec -hosts h1:4,h2:4,h3:4,h4:4 -np 16 ./test`
    - Runs the first four processes on h1, the next four on h2, etc.
  - `mpiexec -hosts h1,h2,h3,h4 -np 16 ./test`
    - Runs the first process on h1, the second on h2, etc., and wraps around
    - So, h1 will have the 1st, 5th, 9th and 13th processes
- If there are many nodes, it might be easier to create a host file
  - cat hf

    ```
    h1:4
    h2:2
    ```
  - `mpiexec -hostfile hf -np 16 ./test`

Trying some example programs

- MPICH comes packaged with several example programs using almost of MPICH's functionality
- A simple program to try out is the PI example written in C (cpi.c) – calculates the value of PI in parallel (available in the examples directory when you build MPICH)
  - `mpiexec -np 16 ./examples/cpi`
- The output will show how many processes are running, and the error in calculating PI
- Next, try it with multiple hosts
  - `mpiexec -hosts h1:2,h2:4 -np 16 ./examples/cpi`
- If things don't work as expected, send an email to discuss@mpich.org

Interaction with Resource Managers

- Resource managers such as SGE, PBS, SLURM or Loadleveler are common in many managed clusters
  - MPICH automatically detects them and interoperates with them
- For example with PBS, you can create a script such as:

```
#! /bin/bash

cd $PBS_O_WORKDIR
# No need to provide –np or –hostfile options
mpiexec ./test
```

- Job can be submitted as: `qsub –l nodes=2:ppn=2 test.sub`
  - "mpiexec" will automatically know that the system has PBS, and ask PBS for the number of cores allocated (4 in this case), and which nodes have been allocated
- The usage is similar for other resource managers

Debugging MPI programs

- Parallel debugging is trickier than debugging serial programs
  - Many processes computing; getting the state of one failed process is usually hard
  - MPICH provides in-built support for some debugging
  - And it natively interoperates with commercial parallel debuggers such as Totalview and DDT
- Using MPICH with totalview:
  - `totalview -a mpiexec -np 6 ./test`
- Using MPICH with ddd (or gdb) on one process:
  - `mpiexec -np 4 ./test : -np 1 ddd ./test : -np 1 ./test`
  - Launches the 5th process under "ddd" and all other processes normally

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- Conclusions and Final Q/A

Blocking vs. Non-blocking Communication

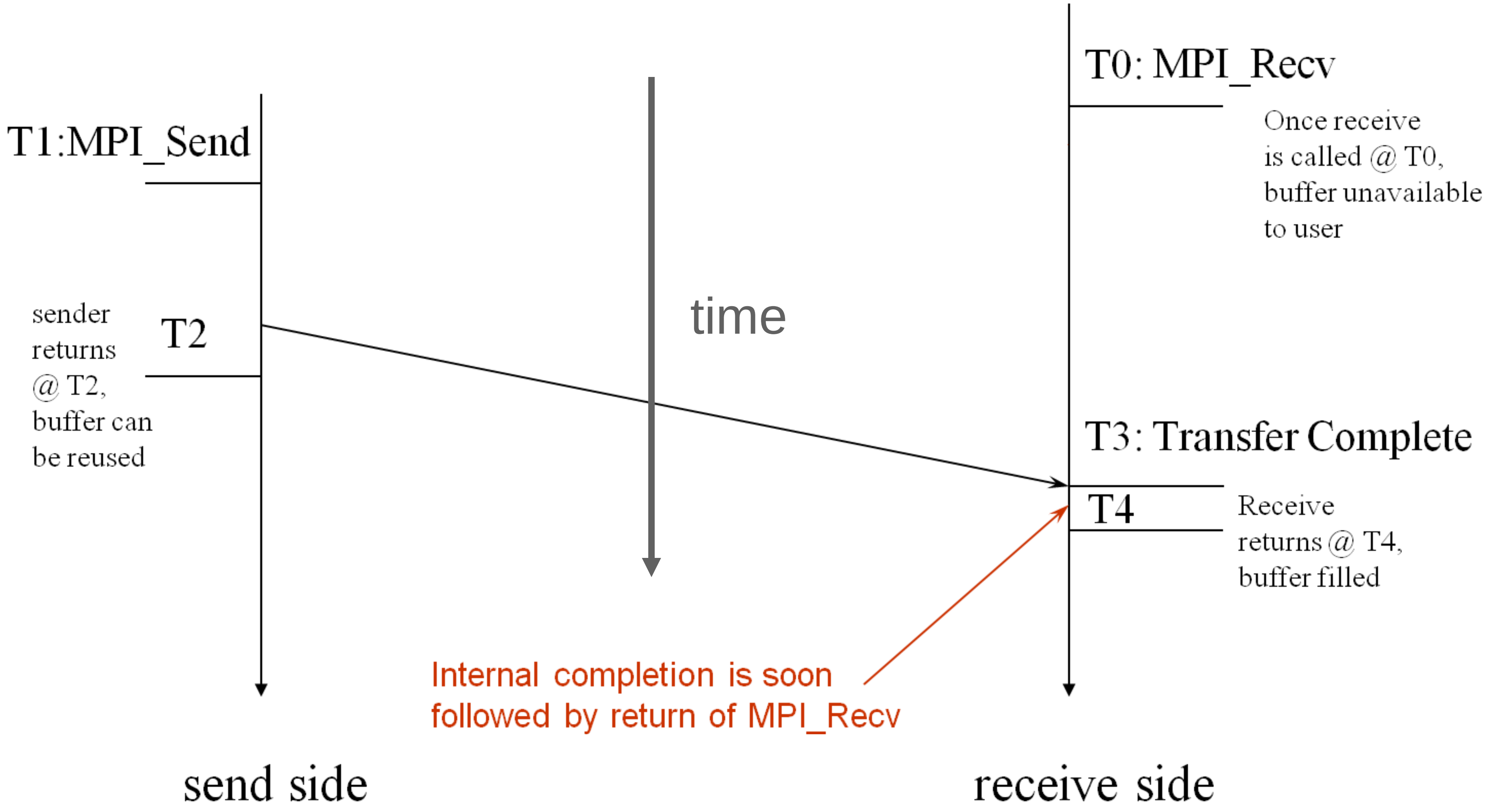
- `MPI_SEND/MPI_RECV` are blocking communication calls
  - Return of the routine implies completion
  - When these calls return the memory locations used in the message transfer can be safely accessed for reuse
  - For "send" completion implies variable sent can be reused/modified
  - Modifications will not affect data intended for the receiver
  - For "receive" variable received can be read
- `MPI_ISEND/MPI_IRECV` are non-blocking variants
  - Routine returns immediately – completion has to be separately tested for
  - These are primarily used to overlap computation and communication to improve performance

Blocking Communication

- In blocking communication.
  - **`MPI_SEND`** does not return until buffer is empty (available for reuse)
  - **`MPI_RECV`** does not return until buffer is full (available for use)
- A process sending data will be blocked until data in the send buffer is emptied
- A process receiving data will be blocked until the receive buffer is filled
- Exact completion semantics of communication generally depends on the message size and the system buffer size
- Blocking communication is simple to use but can be prone to deadlocks

```
                        If (rank == 0) Then
                              Call mpi_send(..)
                              Call mpi_recv(..)
Usually deadlocks →     Else
                              Call mpi_send(..)     ← UNLESS you reverse send/recv
                              Call mpi_recv(..)
                        Endif
```

Blocking Send-Receive Diagram


T0: MPI_Recv
Once receive is called @ T0, buffer unavailable to user
T1:MPI_Send
time
sender returns @ T2, buffer can be reused
T2
T3: Transfer Complete
T4
Receive returns @ T4, buffer filled
Internal completion is soon followed by return of MPI_Recv
send side
receive side

Non-Blocking Communication

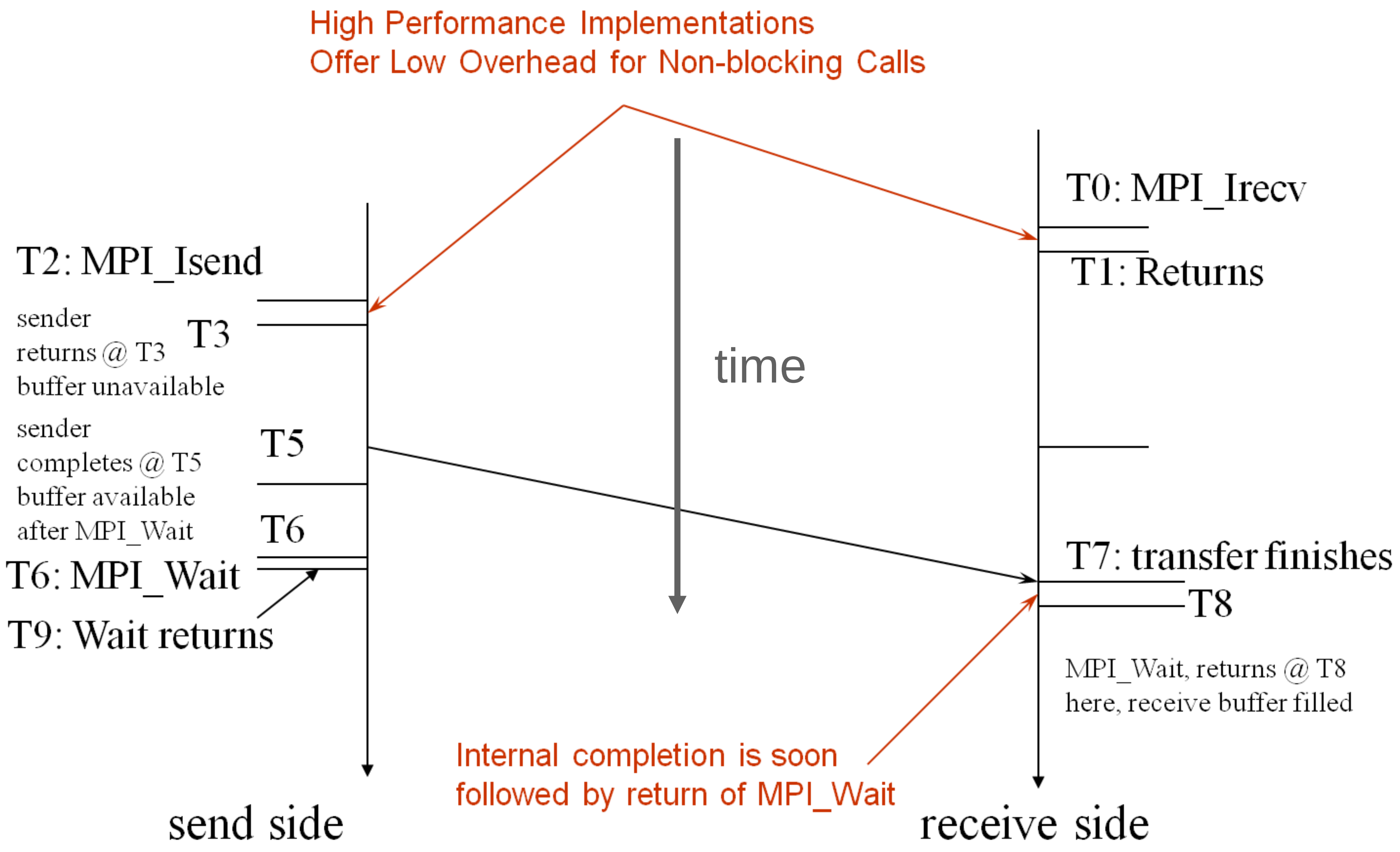
- Non-blocking (asynchronous) operations return (immediately) "request handles" that can be waited on and queried
  - `MPI_ISEND(start, count, datatype, dest, tag, comm, request)`
  - `MPI_IRECV(start, count, datatype, src, tag, comm, request)`
  - `MPI_WAIT(request, status)`
- Non-blocking operations allow overlapping computation and communication
- One can also test without waiting using **MPI_TEST**
  - **MPI_TEST(request, flag, status)**
- Anywhere you use **MPI_SEND** or **MPI_RECV**, you can use the pair of **MPI_ISEND/MPI_WAIT** or **MPI_IRECV/MPI_WAIT**
- Combinations of blocking and non-blocking sends/receives can be used to synchronize execution instead of barriers

Multiple Completions

- It is sometimes desirable to wait on multiple requests:
  - `MPI_Waitall(count, array_of_requests, array_of_statuses)`
  - `MPI_Waitany(count, array_of_requests, &index, &status)`

  -
    ```
    MPI_Waitsome(count, array_of_requests, array_of_indices,
                 array_of_statuses)
    ```
- There are corresponding versions of `test` for each of these

Non-Blocking Send-Receive Diagram



Message Completion and Buffering

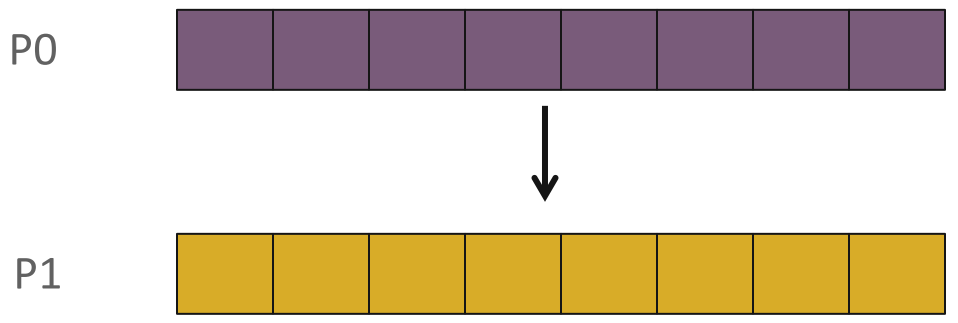
- For a communication to succeed:
  - Sender must specify a valid destination rank
  - Receiver must specify a valid source rank (including MPI_ANY_SOURCE)
  - The communicator must be the same
  - Tags must match
  - Receiver's buffer must be large enough
- A send has completed when the user supplied buffer can be reused

```
*buf =3;
MPI_Send(buf, 1, MPI_INT …)
*buf = 4; /* OK, receiver will always
receive 3 */
```

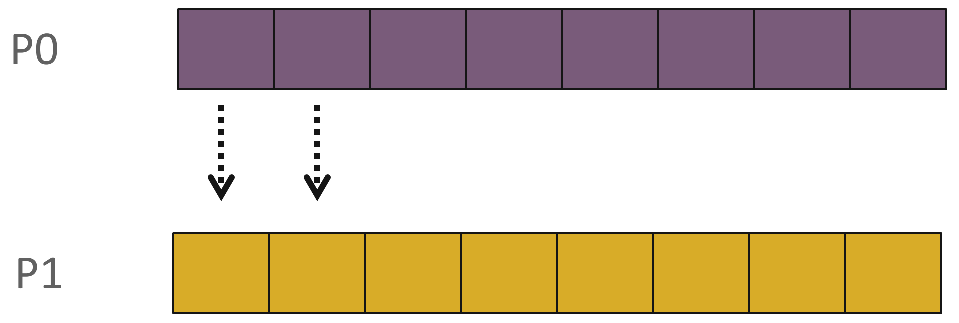
```
*buf =3;
MPI_Isend(buf, 1, MPI_INT …)
*buf = 4; /*Not certain if receiver
gets 3 or 4 or anything else */
MPI_Wait(…);
```

- Just because the send completes does not mean that the receive has completed
  - Message may be buffered by the system
  - Message may still be in transit

A Non-Blocking communication example



Blocking
Communication



Non-blocking
Communication

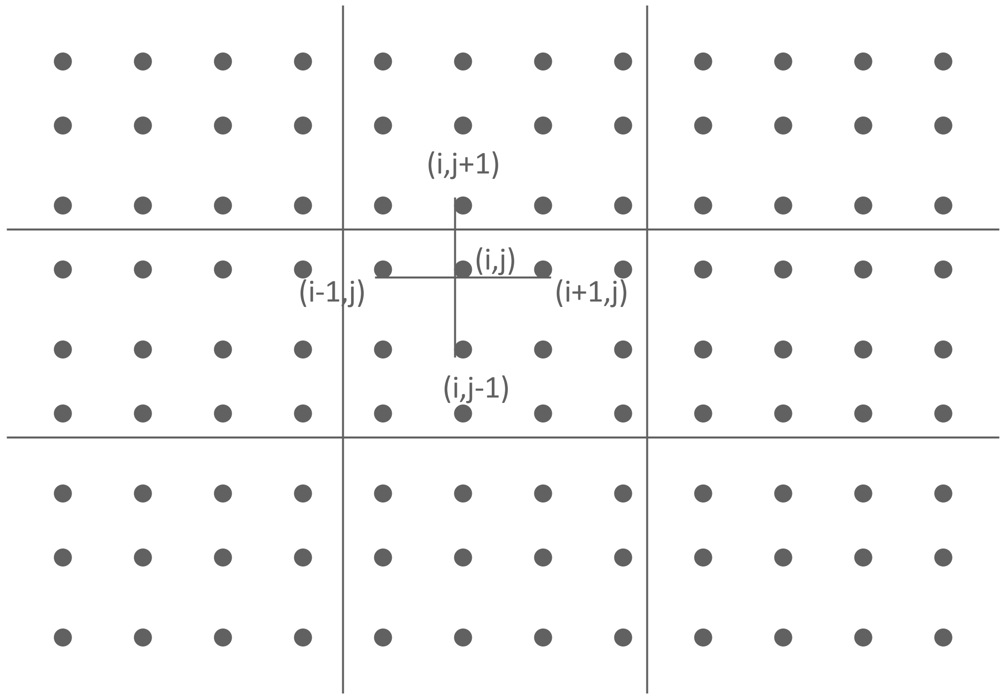
A Non-Blocking communication example

```
int main(int argc, char ** argv)
{
    [...snip...]
    if (rank == 0) {
        for (i=0; i< 100; i++) {
            /* Compute each data element and send it out */
            data[i] = compute(i);
            MPI_ISend(&data[i], 1, MPI_INT, 1, 0, MPI_COMM_WORLD,
                      &request[i]);
        }
        MPI_Waitall(100, request, MPI_STATUSES_IGNORE)
    }
    else {
        for (i = 0; i < 100; i++)
            MPI_Recv(&data[i], 1, MPI_INT, 0, 0, MPI_COMM_WORLD,
                     MPI_STATUS_IGNORE);
    }
    [...snip...]
}
```

Understanding Performance: Unexpected Hot Spots

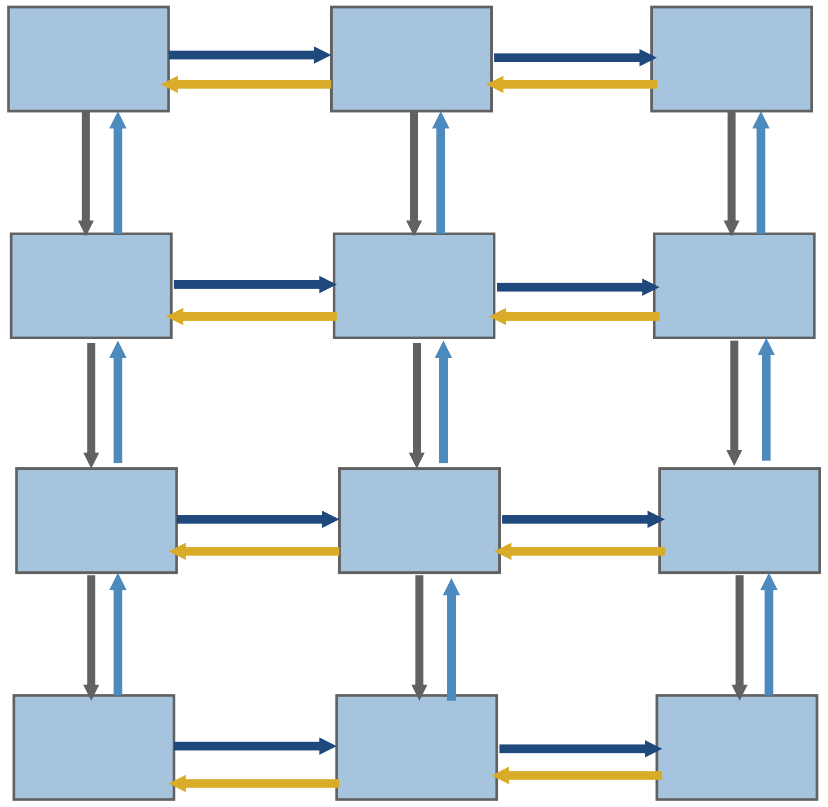
- Basic performance analysis looks at two-party exchanges
- Real applications involve many simultaneous communications
- Performance problems can arise even in common grid exchange patterns
- Message passing illustrates problems present even in shared memory
  - Blocking operations may cause unavoidable memory stalls

2D Poisson Problem



Mesh Exchange

- Exchange data on a mesh



Sample Code

```
Do i=1, n_neighbors
  Call MPI_Send(edge, len, MPI_REAL, nbr(i), tag,
                                 comm, ierr)
Enddo

Do i=1, n_neighbors
  Call MPI_Recv(edge, len, MPI_REAL, nbr(i), tag,
                                comm, status, ierr)
Enddo
```

- What is wrong with this code?

Deadlocks!

- All of the sends may block, waiting for a matching receive (will for large enough messages)
- The variation of

```
if (has down nbr)
    Call MPI_Send( … down … )
if (has up nbr)
    Call MPI_Recv( … up … )
…
```

sequentializes (all except the bottom process blocks)

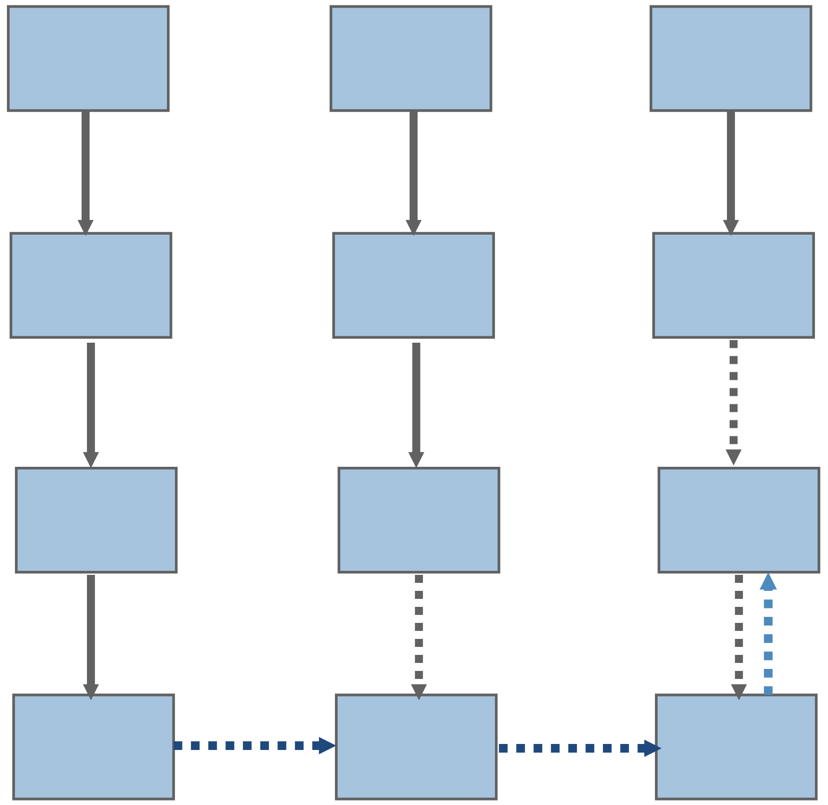
Fix 1: Use Irecv

```
Do i=1, n_neighbors
  Call MPI_Irecv(edge, len, MPI_REAL, nbr(i), tag, comm,
                                requests[i], ierr)
Enddo

Do i=1, n_neighbors
  Call MPI_Send(edge, len, MPI_REAL, nbr(i), tag, comm, ierr)
Enddo

Call MPI_Waitall(n_neighbors, requests, statuses, ierr)
```

- Does not perform well in practice. Why?

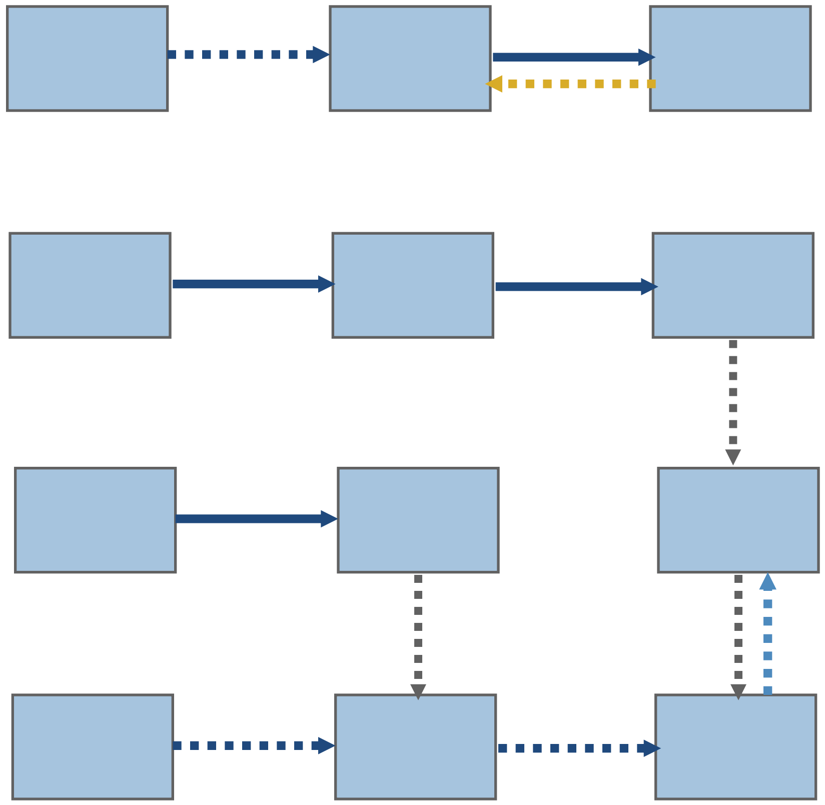
Mesh Exchange - Step 1

- Exchange data on a mesh



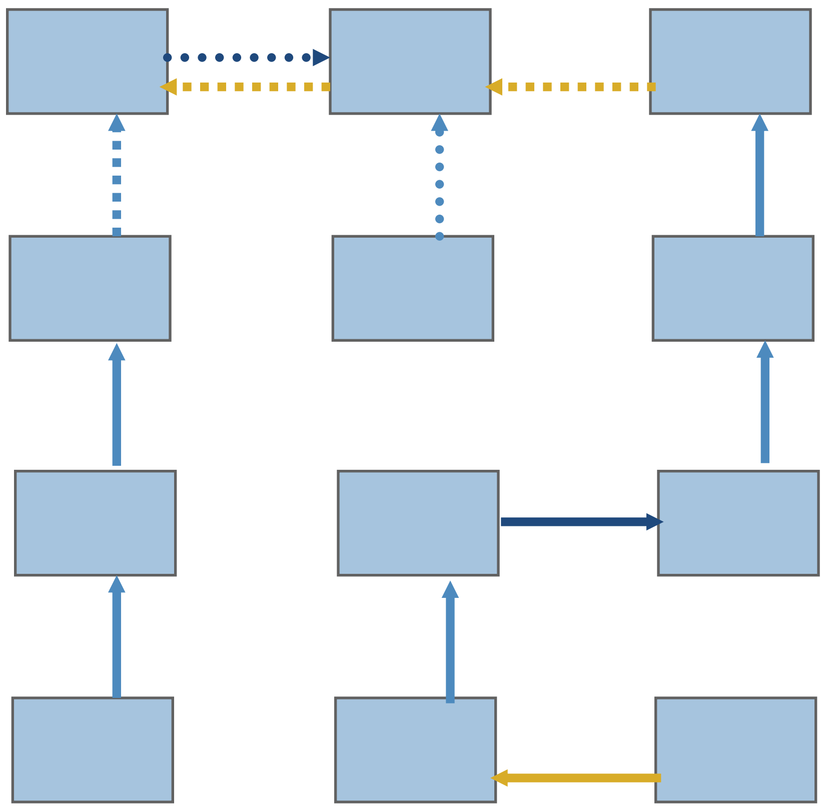
Mesh Exchange - Step 2

- Exchange data on a mesh



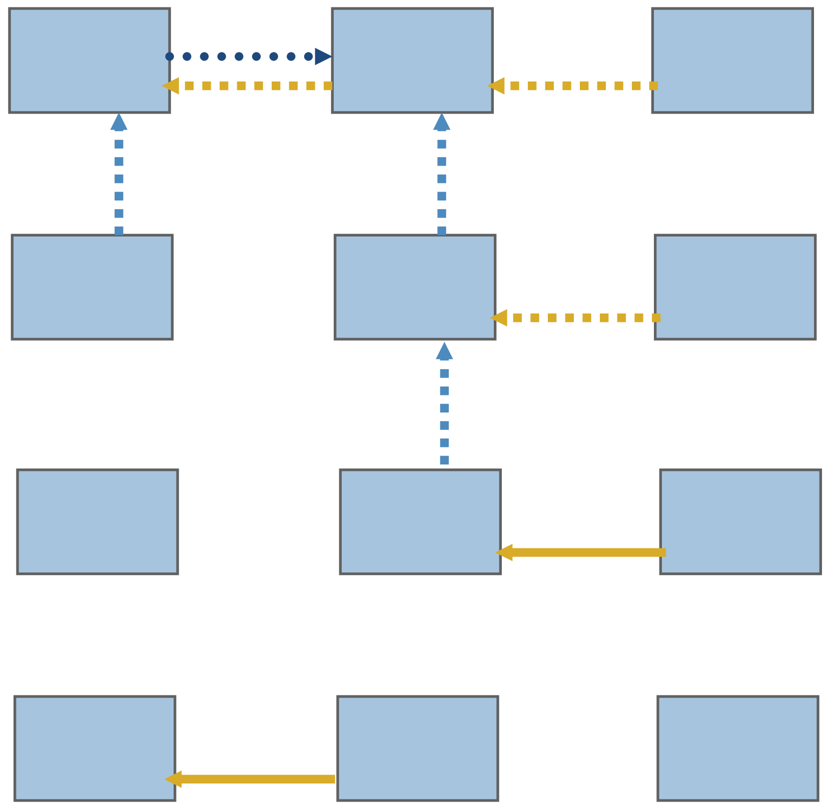
Mesh Exchange - Step 3

- Exchange data on a mesh



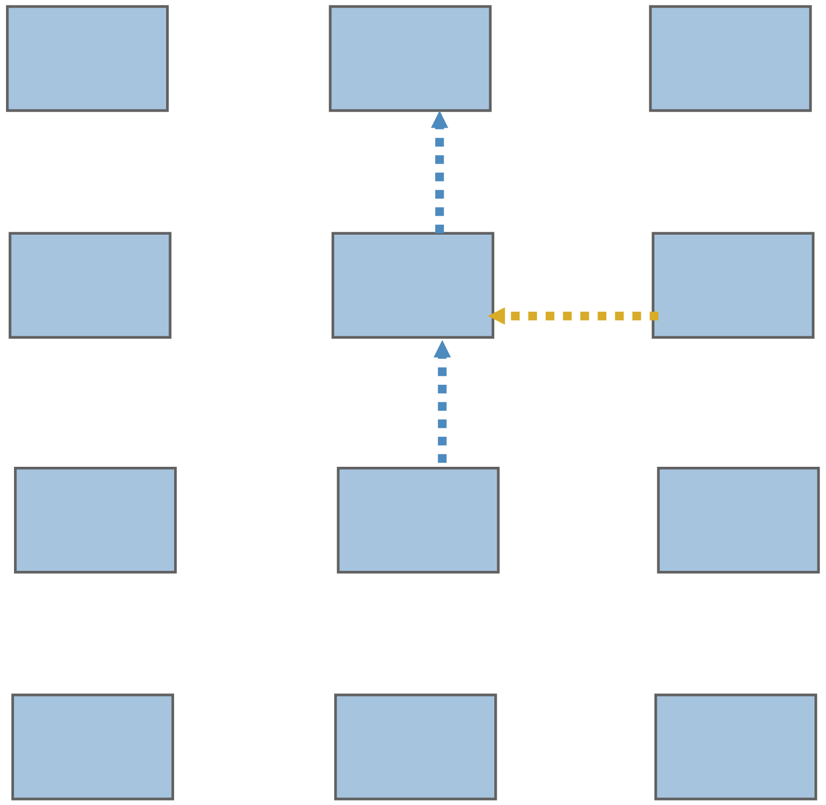
Mesh Exchange - Step 4

- Exchange data on a mesh



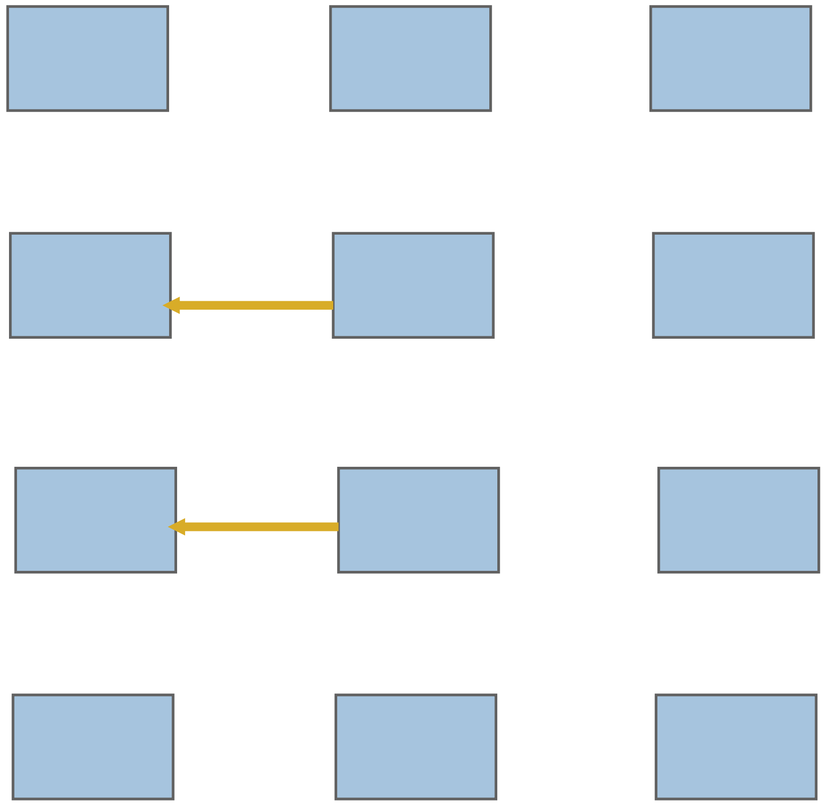
Mesh Exchange - Step 5

- Exchange data on a mesh

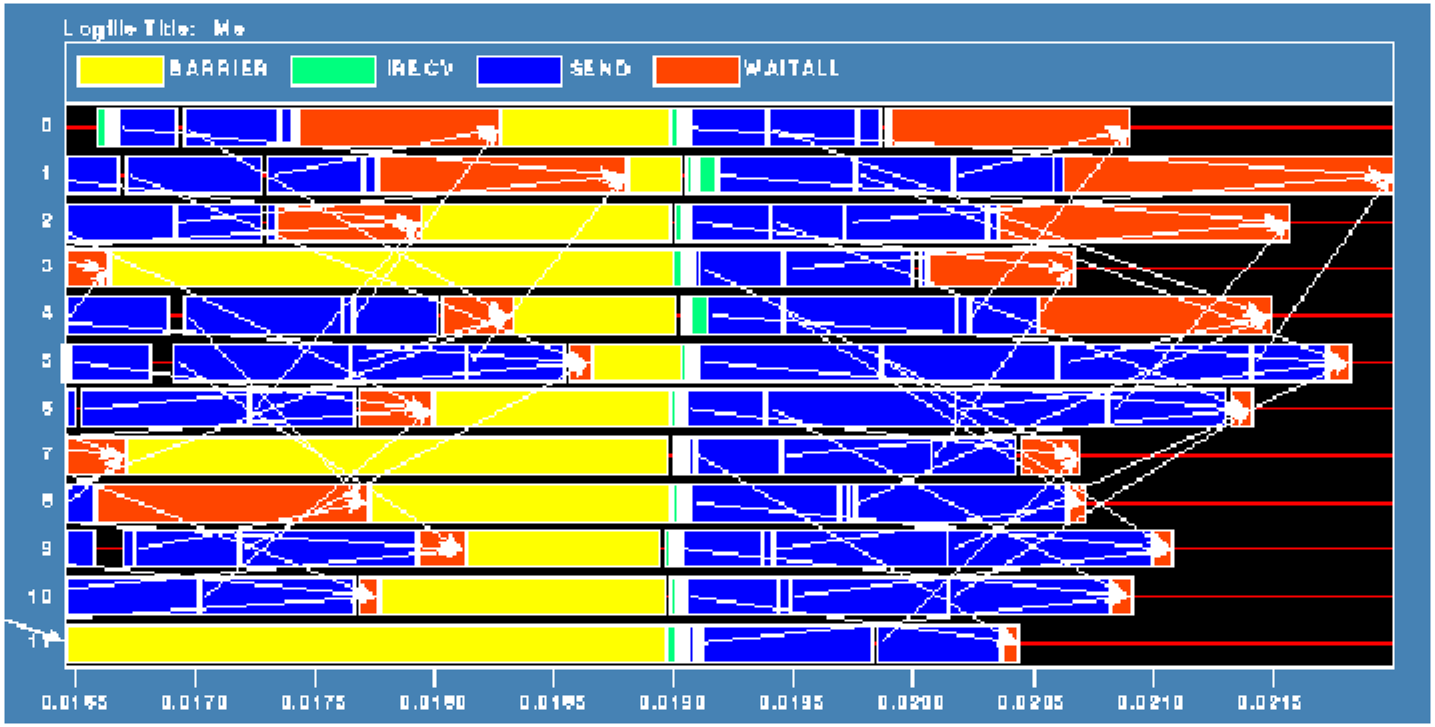


Mesh Exchange - Step 6

- Exchange data on a mesh



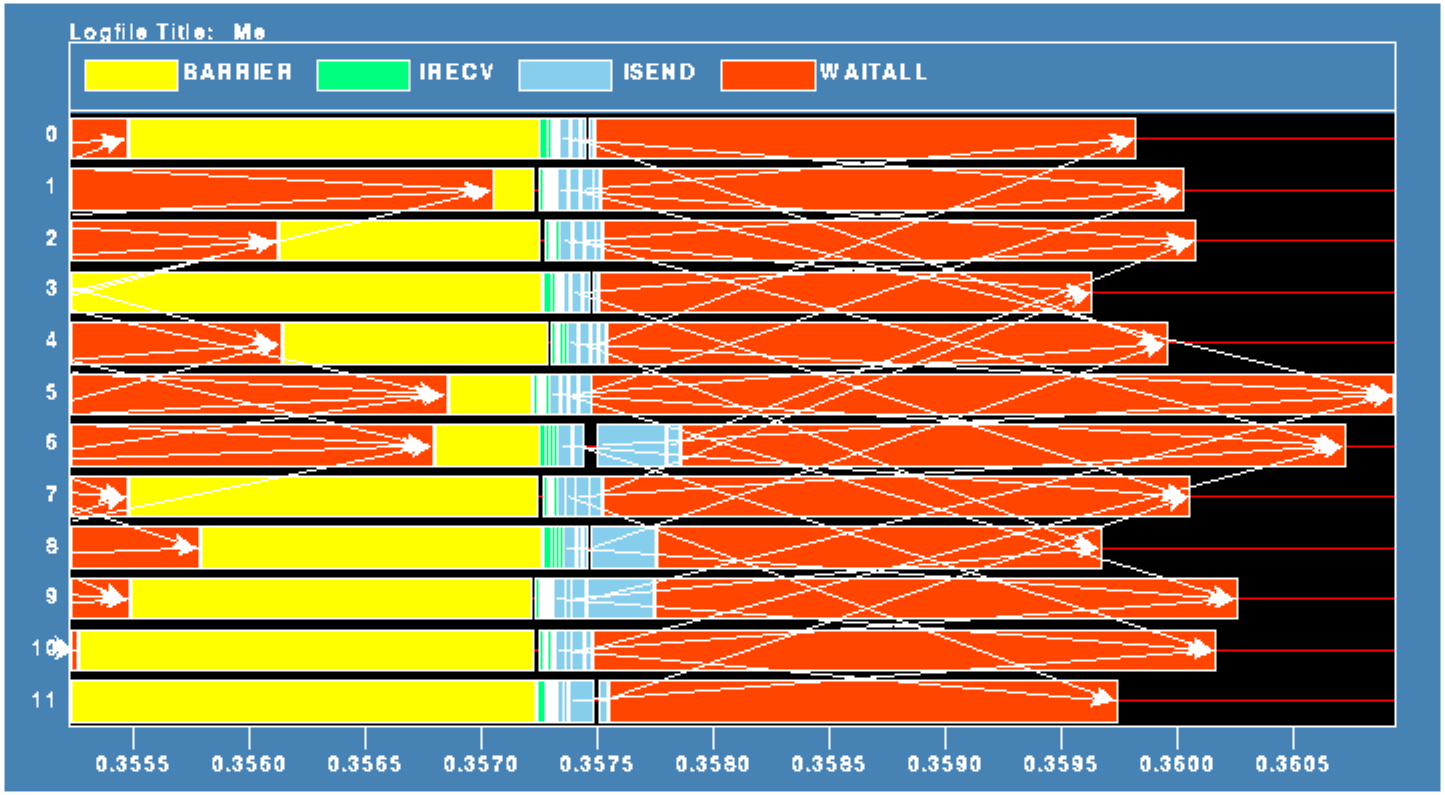
Timeline from IBM SP



Fix 2: Use Isend and Irecv

```
 Do i=1, n_neighbors
  Call MPI_Irecv(edge, len, MPI_REAL, nbr(i), tag, comm,
                           request(i),ierr)
Enddo

Do i=1, n_neighbors
  Call MPI_Isend(edge, len, MPI_REAL, nbr(i), tag, comm,
                           request(n_neighbors+i), ierr)
Enddo

Call MPI_Waitall(2*n_neighbors, request, statuses, ierr)
```

Timeline from IBM SP



Note processes 5 and 6 are the only interior processors; these perform more communication than the other processors

Lesson: Defer Synchronization

- Send-receive accomplishes two things:
  - Data transfer
  - Synchronization
- In many cases, there is more synchronization than required
- Use non-blocking operations and **`MPI_Waitall`** to defer synchronization
- Tools can help out with identifying performance issues
  - MPE is a profiling library that comes with the MPICH2 implementation of MPI for understanding performance data
  - Jumpshot tool uses MPE datasets to show performance problems graphically

What we will cover in this tutorial

- What is MPI?
- How to write a simple program in MPI
- Running your application with MPICH
- **Slightly more advanced topics:**
  - Non-blocking communication in MPI
  - **Group (collective) communication in MPI**
  - MPI Datatypes
- Conclusions and Final Q/A

Introduction to Collective Operations in MPI

- Collective operations are called by all processes in a communicator.
- **`MPI_BCAST`** distributes data from one process (the root) to all others in a communicator.
- **`MPI_REDUCE`** combines data from all processes in the communicator and returns it to one process.
- In many numerical algorithms, **`SEND/RECV`** can be replaced by **`BCAST/REDUCE`**, improving both simplicity and efficiency.

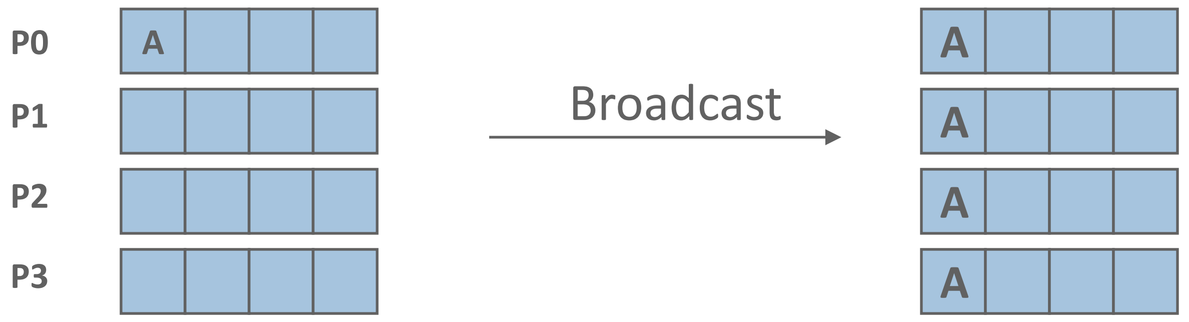
MPI Collective Communication

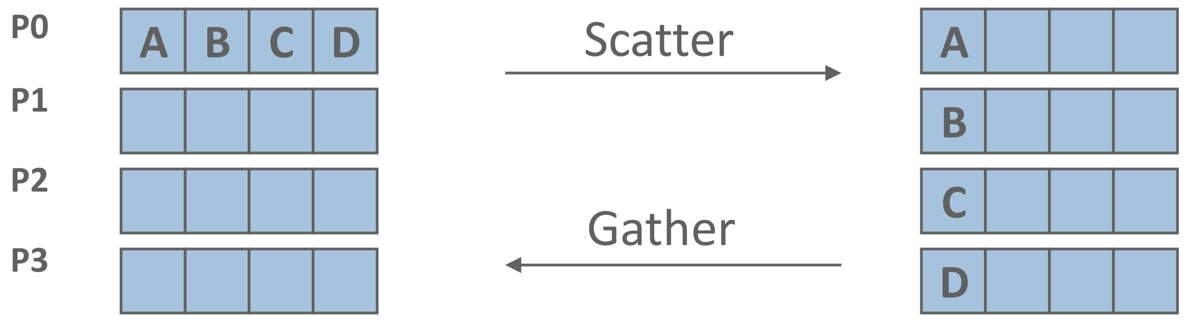
- Communication and computation is coordinated among a group of processes in a communicator
- Tags are not used; different communicators deliver similar functionality
- Non-blocking collective operations in MPI-3
  - Covered in the advanced tutorial (but conceptually simple)
- Three classes of operations: synchronization, data movement, collective computation

Synchronization

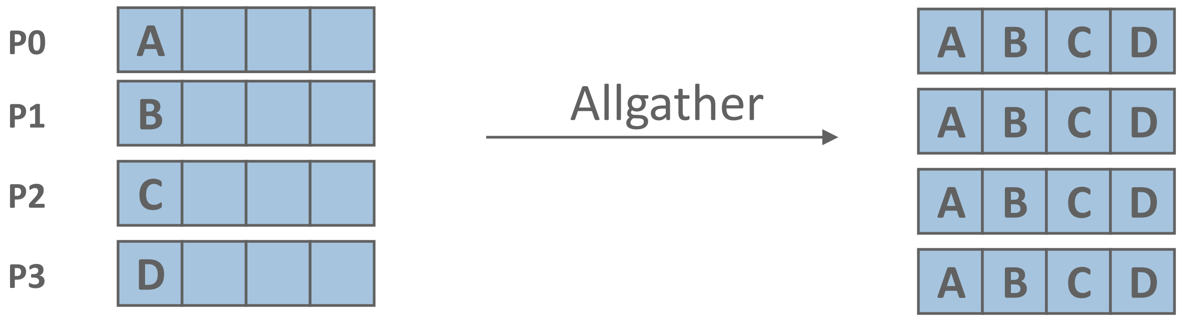
- `MPI_BARRIER(comm)`
  - Blocks until all processes in the group of the communicator `comm` call it
  - A process cannot get out of the barrier until all other processes have reached barrier

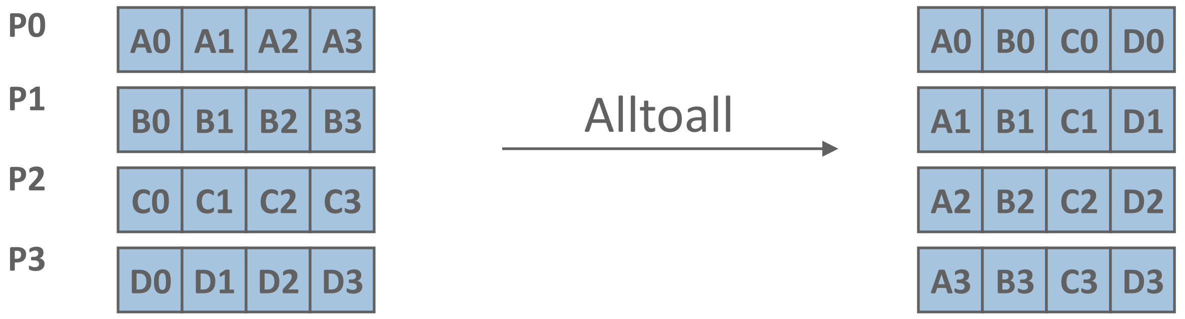
Collective Data Movement



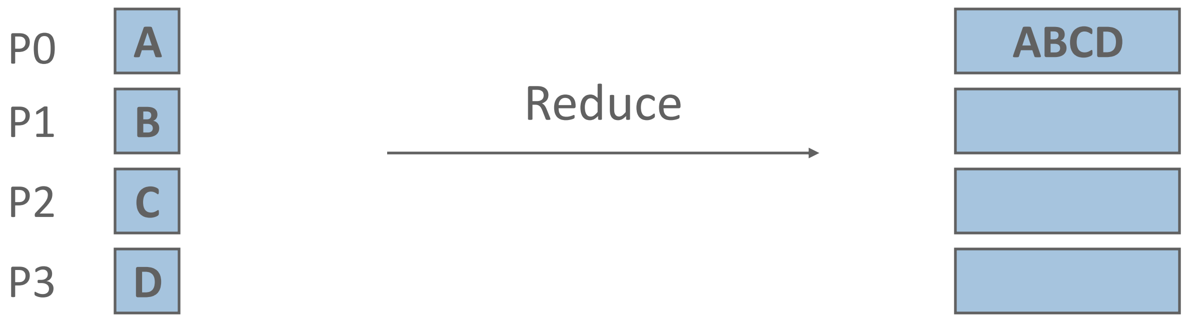


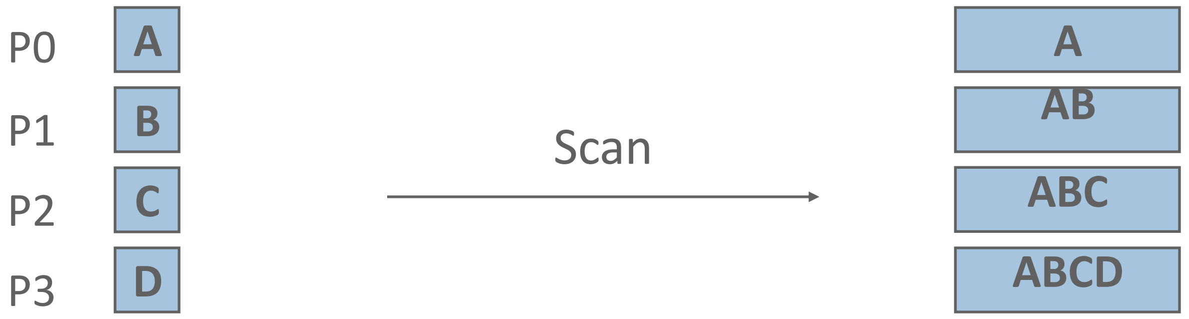
More Collective Data Movement





Collective Computation





MPI Collective Routines

- Many Routines: **`MPI_ALLGATHER`**, **`MPI_ALLGATHERV`**, **`MPI_ALLREDUCE`**, **`MPI_ALLTOALL`**, **`MPI_ALLTOALLV`**, **`MPI_BCAST`**, **`MPI_GATHER`**, **`MPI_GATHERV`**, **`MPI_REDUCE`**, **`MPI_REDUCESCATTER`**, **`MPI_SCAN`**, **`MPI_SCATTER`**, **`MPI_SCATTERV`**
- "**`All`**" versions deliver results to all participating processes
- "**`V`**" versions (stands for vector) allow the hunks to have different sizes
- **`MPI_ALLREDUCE`**, **`MPI_REDUCE`**, **`MPI_REDUCESCATTER`**, and **`MPI_SCAN`** take both built-in and user-defined combiner functions

MPI Built-in Collective Computation Operations

`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 and location
`MPI_MINLOC`	Minimum and location

Defining your own Collective Operations

- Create your own collective computations with:

  ```
  MPI_OP_CREATE(user_fn, commutes, &op);
  MPI_OP_FREE(&op);

  user_fn(invec, inoutvec, len, datatype);
  ```

- The user function should perform:

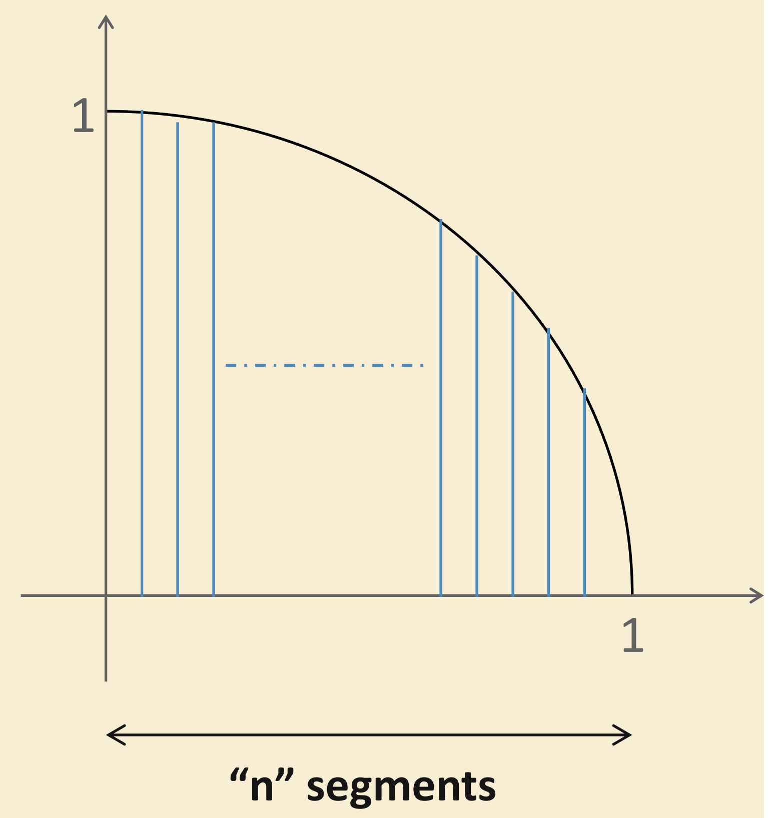
  ```
  inoutvec[i] = invec[i] op inoutvec[i];
  ```

  for i from 0 to len-1

- The user function can be non-commutative, but must be associative

Example: Calculating Pi

- Calculating pi via numerical integration
  - Divide interval up into subintervals
  - Assign subintervals to processes
  - Each process calculates partial sum
  - Add all the partial sums together to get pi



1. Width of each segment (w) will be 1/n
2. Distance (d(i)) of segment "i" from the origin will be "i * w"
3. Height of segment "i" will be sqrt(1 – [d(i)]^2)

Example: PI in C (let us try writing this)

```
#include <mpi.h>
#include <math.h>
int main(int argc, char *argv[])
{
    [...snip...]
    /* Tell all processes, the number of segments you want */
    MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
    w   = 1.0 / (double) n;
    mypi = 0.0;
    for (i = myid + 1; i <= n; i += numprocs)
        mypi += w * sqrt(1 - (((double) i / n) * ((double) i / n));
    MPI_Reduce(&mypi, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
    if (myid == 0)
        printf("pi is approximately %.16f, Error is %.16f\n", 4 * pi,
               fabs(pi - PI25DT));
    [...snip...]
}
```

What we will cover in this tutorial

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- **Slightly more advanced topics:**
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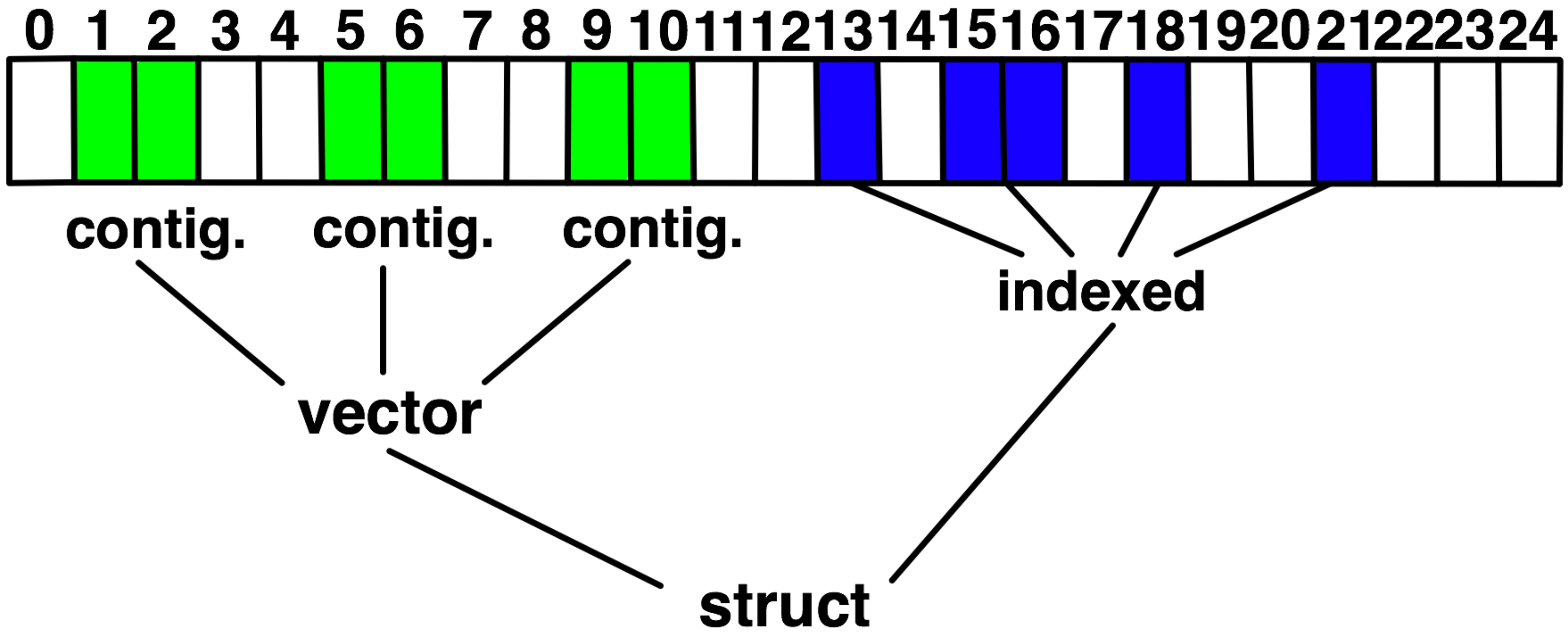
  - Group (collective) communication in MPI
  - **MPI Datatypes**
- Conclusions and Final Q/A

Introduction to Datatypes in MPI

- Datatypes allow to (de)serialize **arbitrary** data layouts into a message stream
  - Networks provide serial channels
  - Same for block devices and I/O
- Several constructors allow arbitrary layouts
  - Recursive specification possible
  - *Declarative* specification of data-layout
    - "what" and not "how", leaves optimization to implementation (*many unexplored* possibilities!)
  - Choosing the right constructors is not always simple

Derived Datatype Example



- Explain Lower Bound, Size, Extent

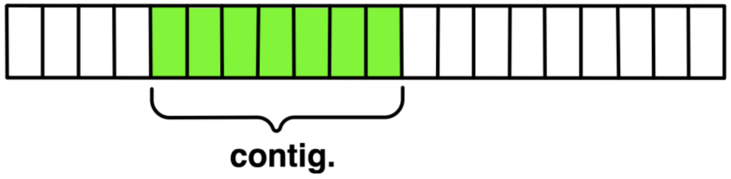
MPI’s Intrinsic Datatypes

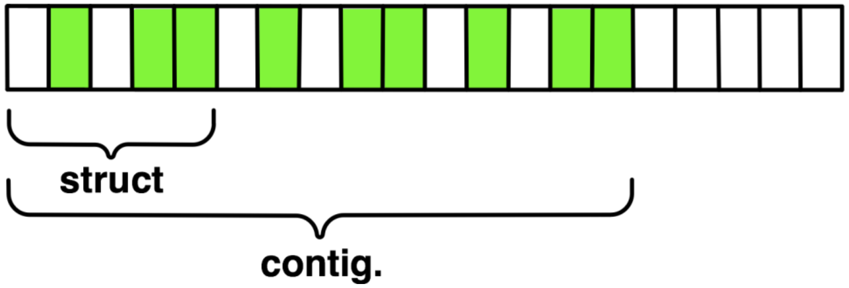
- Why intrinsic types?
  - Heterogeneity, nice to send a Boolean from C to Fortran
  - Conversion rules are complex, not discussed here
  - Length matches to language types
    - No sizeof(int) mess
- Users should generally use intrinsic types as basic types for communication and type construction!
  - MPI_BYTE should be avoided at all cost
- MPI-2.2 added some missing C types
  - E.g., unsigned long long

MPI_Type_contiguous

MPI_Type_contiguous(int count, MPI_Datatype oldtype, MPI_Datatype *newtype)

- Contiguous array of oldtype
- Should not be used as last type (can be replaced by count)

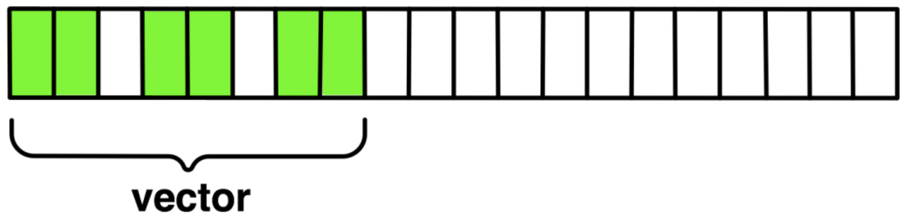


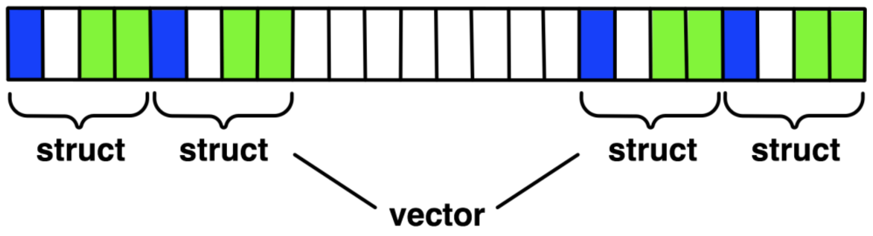


MPI_Type_vector

MPI_Type_vector(int count, int blocklength, int stride, MPI_Datatype oldtype, MPI_Datatype *newtype)

- Specify strided blocks of data of oldtype
- Very useful for Cartesian arrays

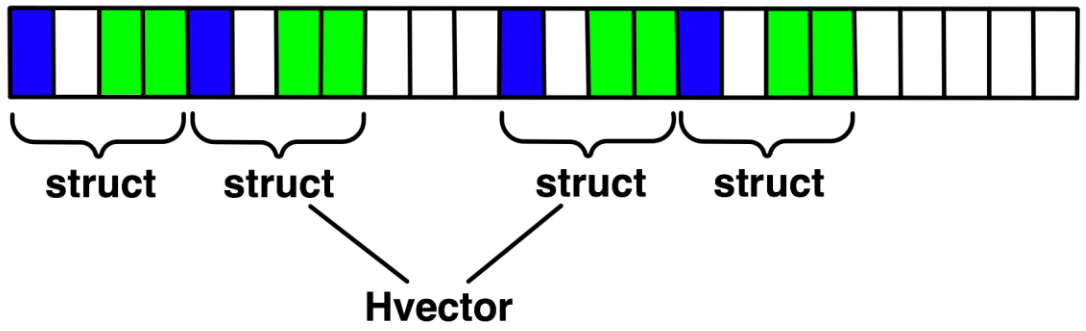




MPI_Type_create_hvector

```
MPI_Type_create_hvector(int count, int blocklength, MPI_Aint
stride, MPI_Datatype oldtype, MPI_Datatype *newtype)
```

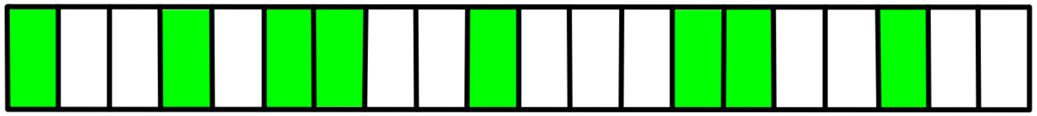
- Create non-unit strided vectors
- Useful for composition, e.g., vector of structs



MPI_Type_indexed

```
MPI_Type_indexed(int count, int *array_of_blocklengths,
int *array_of_displacements, MPI_Datatype oldtype,
MPI_Datatype *newtype)
```

- Pulling irregular subsets of data from a single array (cf. vector collectives)
  - dynamic codes with index lists, expensive though!

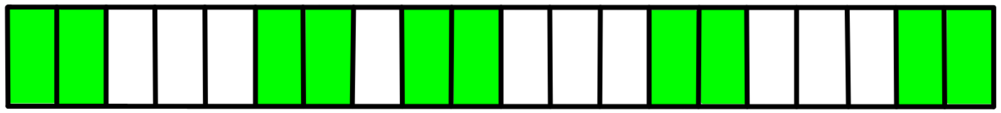


  - blen={1,1,2,1,2,1}
  - displs={0,3,5,9,13,17}

MPI_Type_create_indexed_block

```
MPI_Type_create_indexed_block(int count, int blocklength,
int *array_of_displacements, MPI_Datatype oldtype,
MPI_Datatype *newtype)
```

- Like Create_indexed but blocklength is the same

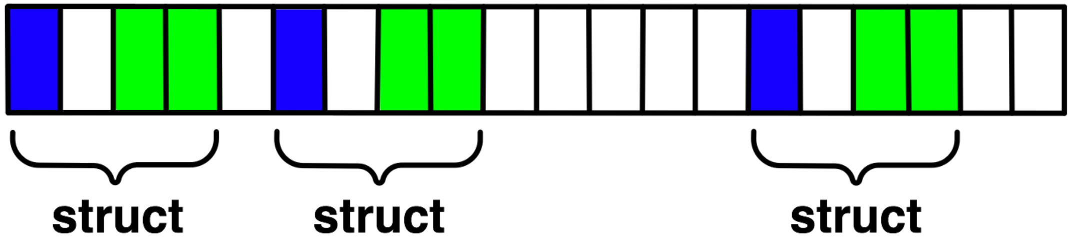


  - blen=2
  - displs={0,5,9,13,18}

MPI_Type_create_hindexed

MPI_Type_create_hindexed(int count, int *arr_of_blocklengths, MPI_Aint *arr_of_displacements, MPI_Datatype oldtype, MPI_Datatype *newtype)

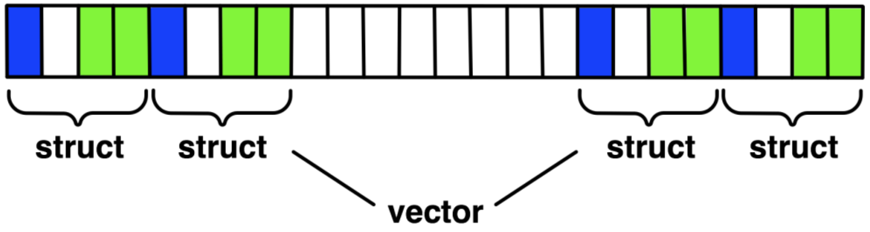
- Indexed with non-unit displacements, e.g., pulling types out of different arrays

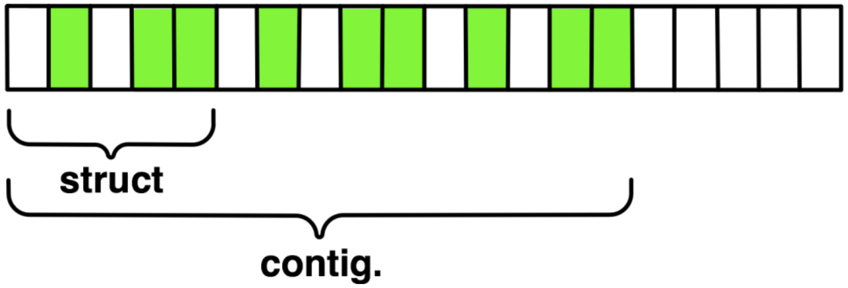


MPI_Type_create_struct

```
MPI_Type_create_struct(int count, int array_of_blocklengths[],
MPI_Aint array_of_displacements[], MPI_Datatype
array_of_types[], MPI_Datatype *newtype)
```

- Most general constructor, allows different types and arbitrary arrays (also most costly)

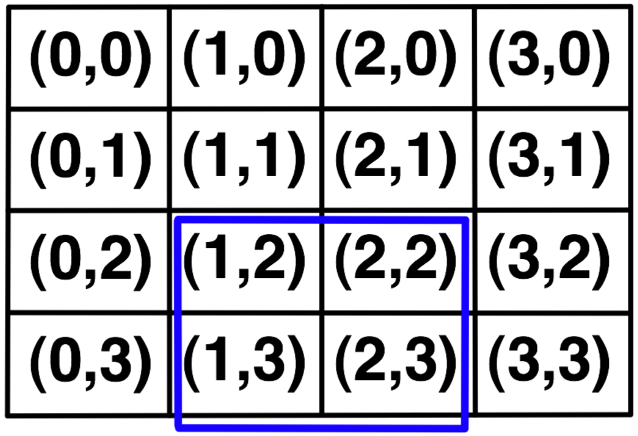




MPI_Type_create_subarray

```
MPI_Type_create_subarray(int ndims, int array_of_sizes[],
int array_of_subsizes[], int array_of_starts[], int order,
MPI_Datatype oldtype, MPI_Datatype *newtype)
```

- Specify subarray of n-dimensional array (sizes) by start (starts) and size (subsize)



MPI_Type_create_darray

```
MPI_Type_create_darray(int size, int rank, int ndims,
int array_of_gsizes[], int array_of_distribs[], int
array_of_dargs[], int array_of_psizes[], int order,
MPI_Datatype oldtype, MPI_Datatype *newtype)
```

- Create distributed array, supports block, cyclic and no distribution for each dimension
  - Very useful for I/O

MPI_BOTTOM and MPI_Get_address

- MPI_BOTTOM is the absolute zero address
  - Portability (e.g., may be non-zero in globally shared memory)
- MPI_Get_address
  - Returns address relative to MPI_BOTTOM
  - Portability (do not use “&” operator in C!)
- Very important to
  - build struct datatypes
  - If data spans multiple arrays

Commit, Free, and Dup

- Types must be committed before use
  - Only the ones that are used!
  - MPI_Type_commit may perform heavy optimizations (and will hopefully)
- MPI_Type_free
  - Free MPI resources of datatypes
  - Does not affect types built from it
- MPI_Type_dup
  - Duplicates a type
  - Library abstraction (composability)

Other DDT Functions

- Pack/Unpack
  - Mainly for compatibility to legacy libraries
  - You should not be doing this yourself
- Get_envelope/contents
  - Only for expert library developers
  - Libraries like MPITypes[1] make this easier
- MPI_Create_resized
  - Change extent and size (dangerous but useful)

1: http://www.mcs.anl.gov/mpitypes/

Datatype Selection Order

- Simple and effective performance model:
  - More parameters == slower
- **contig < vector < index_block < index < struct**
- Some (most) MPIs are inconsistent
  - But this rule is portable
- Advice to users:
  - Try datatype “compression” bottom-up

W. Gropp et al.:Performance Expectations and Guidelines for MPI Derived Datatypes

What we will cover in this tutorial

- What is MPI?
- How to write a simple program in MPI
- Running your application with MPICH
- Slightly more advanced topics:
  - Non-blocking communication in MPI
  - Group (collective) communication in MPI
  - MPI Datatypes
- **Conclusions and Final Q/A**

Conclusions

- Parallelism is critical today, given that that is the only way to achieve performance improvement with the modern hardware
- MPI is an industry standard model for parallel programming
  - A large number of implementations of MPI exist (both commercial and public domain)
  - Virtually every system in the world supports MPI
- Gives user explicit control on data management
- Widely used by many scientific applications with great success
- Your application can be next!

Web Pointers

- MPI standard : http://www.mpi-forum.org/docs/docs.html
- MPICH : http://www.mpich.org
- MPICH mailing list: discuss@mpich.org
- MPI Forum : http://www.mpi-forum.org/
- Other MPI implementations:
  - MVAPICH (MPICH on InfiniBand) : http://mvapich.cse.ohio-state.edu/
  - Intel MPI (MPICH derivative): http://software.intel.com/en-us/intel-mpi-library/
  - Microsoft MPI (MPICH derivative)
  - Open MPI : http://www.open-mpi.org/
- Several MPI tutorials can be found on the web