CPS615 Introduction to Computational Science
The Message Passing Interface MPI

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This presentation contains material from:

Designing and Building Parallel Programs,

by Ian Foster, Gina Goff, Ehtesham Hayder and Charles Koelbel

and

Tutorial on MPI: The Message Passing Interface

by William Gropp

Abstract of MPI Presentation

- This covers MPI from a user's point of view and is meant to be a supplement to other online resources from the MPI Forum, David Walker's Tutorial, Ian Foster's Book "Designing and Building Parallel Programs", Gropp,Lusk and Skjellum "Using MPI"
- An Overview is based on subset of 6 routines that cover send/receive, environment inquiry (for rank and total number of processors) initialize and finalization with simple examples
- Processor Groups, Collective Communication and Computation, Topologies, and Derived Datatypes are also discussed

MPI Overview -- Comparison with HPF -- I

- MPI collected ideas from many previous message passing systems and put them into a "standard" so we could write portable (runs on all current machines) and scalable (runs on future machines we can think of) parallel software
- MPI plays the same role to message passing systems that HPF does to data parallel languages
  - BUT whereas MPI has essentially all one could want -- as message passing is “fully understood”
  - HPF and related technologies will still evolve as there are many unsolved data parallel compiler issues
    - » e.g. HPC++ -- the C++ version of HPF has important differences
    - » and there is no data parallel version of C due to pointers (there is a C* language which has restrictions)
    - » HPJava is our new idea but again not same as HPF or HPC++
  - whereas MPI is fine with Fortran C or C++ and even Java

MPI Overview -- Comparison with HPF -- II

- HPF runs on SIMD and MIMD machines and is high level as it expresses a style of programming or problem architecture
- MPI runs on MIMD machines (in principle it could run on SIMD but unnatural and inefficient) -- it expresses a machine architecture
- Traditional Software Model is
  - Problem --> High Level Language --> Assembly Language --> Machine
    - » Expresses Problem Expresses Machine
- So in this analogy MPI is universal "machine-language" of Parallel processing
- MPI can be built efficiently at low risk whereas HPF compiler is difficult project with many unsolved issues

Some Key Features of MPI

- An MPI program defines a set of processes, each executing the same program (SPMD)
  - (usually one process per parallel computer node)
- … that communicate by calling MPI messaging functions
  - (point-to-point and collective)
- … and can be constructed in a modular fashion
  - (communication contexts are the key to MPI libraries)
- Also
  - Support for Process Groups -- messaging in subsets of processors
  - Support for application dependent (virtual) topologies analogous to distribution types in HPF
  - Inquiry routines to find out properties of the environment such as number of processors

What is MPI?

- A standard message-passing library
  - p4, NX, PVM, Express, PARMACS are precursors
- MPI defines a language-independent interface
  - Not an implementation
- Bindings are defined for different languages
  - So far, C and Fortran 77, C++ and F90
  - Java Grande Forum is defining Java bindings
- Multiple implementations
  - MPICH is a widely-used portable implementation
  - See http://www.mcs.anl.gov/mpi/

History of MPI

- Began at Williamsburg Workshop in April 1992
- Organized at Supercomputing 92 (November 92)
- Followed HPF Forum format and process
  - Met every 6 weeks for two days
  - Extensive, open email discussions
  - Drafts, readings, votes
- Pre-final draft distributed at Supercomputing 93
- Two-month public comment period
- Final version of draft in May 1994
- Widely available now on the Web, ftp sites, netlib
- Public and optimized Vendor implementations available for Unix and Windows NT
- Further MPI Forum meetings through 1995 and 1996 to discuss additions to the standard
- Standard announced at Supercomputing 1996

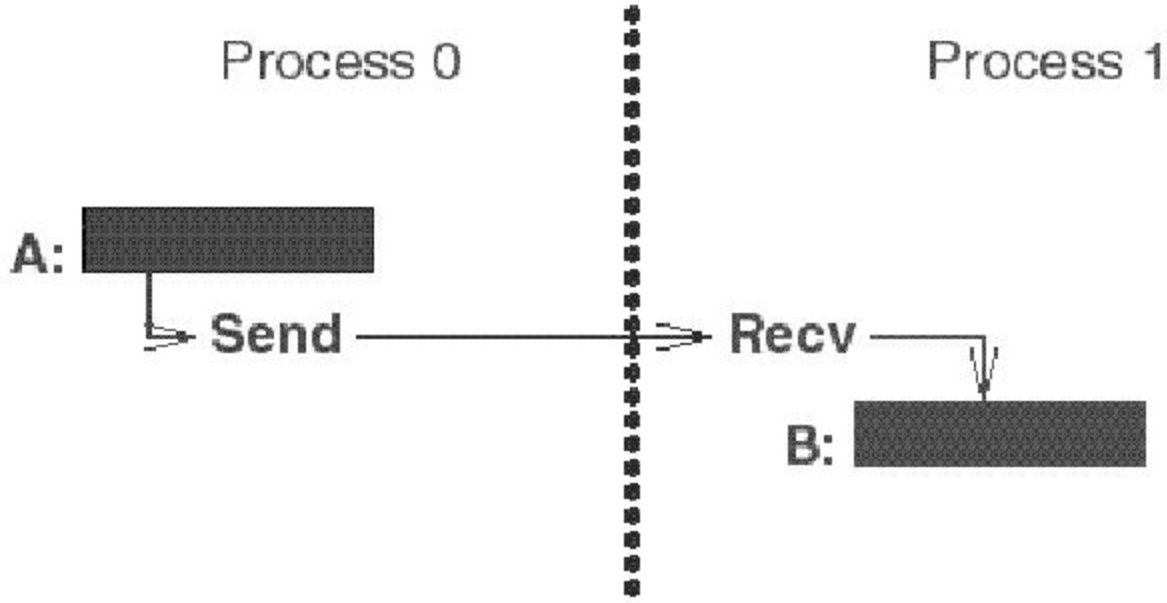
Who Designed MPI?

- Broad Participation
- Vendors
  - IBM, Intel, TMC, Meiko, Cray, Convex, Ncube
- Message Passing Library writers
  - PVM, p4, Zipcode, TCGMSG, Chameleon, Express, Linda
- Application specialists and consultants
- Companies:
  - ARCO, Convex, Cray Research, IBM, Intel, KAI, Meiko, NAG, nCUBE, Parasoft, Shell, TMC
- Laboratories:
  - ANL, GMD, LANL, LLNL, NOAA, NSF, ORNL, PNL, Sandia, SDSC, SRC
- Universities:
  - UC Santa Barbara, Syracuse, Michigan State, Oregon Grad Institute, New Mexico, Miss. State, Southampton, Colorado, Yale, Tennessee, Maryland, Western Michigan, Edinburgh, Cornell, Rice, San Francisco

Some Difficulties with MPI

- MPI was designed by the Kitchen Sink approach and has 129 functions and each has many arguments
  - This completeness is strength and weakness!
  - Hard to implement efficiently and hard to learn all its details
- It is not a complete operating environment and does not have ability to create and spawn processes etc.
- PVM is the previous dominant approach
  - It is very simple with much less functionality than MPI
  - However it runs on essentially all machines including heterogeneous workstation clusters
  - Further it is a complete albeit simple operating environment
- However it seems clear that MPI has been adopted as the standard messaging system by parallel computer vendors

Sending/Receiving Messages: Issues



- **Questions:**
  - **What is sent?**
  - **To whom is the data sent?**
  - **How does the receiver identify it?**

What Gets Sent: The Buffer

- First generation message passing systems only allowed one to transmit information originating in a contiguous array of bytes
  - Hid the real data structure from hardware and programmer
    - » Might make it hard to provide efficient implementations as implied a lot of expensive memory accesses
  - Required pre-packing dispersed data, e.g.:
    - » Rows (in Fortran, columns in C) of a matrix must be transposed before transmission
  - Prevented convenient communication between machines with different data representations

Generalizing the Buffer in MPI

- **MPI specifies the buffer by *starting address*, *datatype*, and *count***
  - **starting address is obvious**
  - **datatypes are constructed recursively from**
    - » **Elementary (all C and Fortran datatypes)**
    - » **Contiguous array of datatypes**
    - » **Strided blocks of datatypes**
    - » **Indexed array of blocks of datatypes**
    - » **General structures**
  - **count is number of datatype elements**

Advantages of Datatypes

- Cominations of elementary datatypes into a derived user defined datatype allows clean communication of collections of disparate types in a single MPI call.
- Elimination of length (in bytes) in favor of count (of items of a given type) is clearer
- Specifying application-oriented layouts allows maximal use of special hardware and optimized memory use
- However this wonderful technology is problematical in Java where layout of data structures in memory is not defined in most cases
  - Java's serialization subsumes user defined datatypes as a general way of packing a class of disparate types into a message that can be sent between heterogeneous computers

To Whom It Gets Sent: Process Identifiers

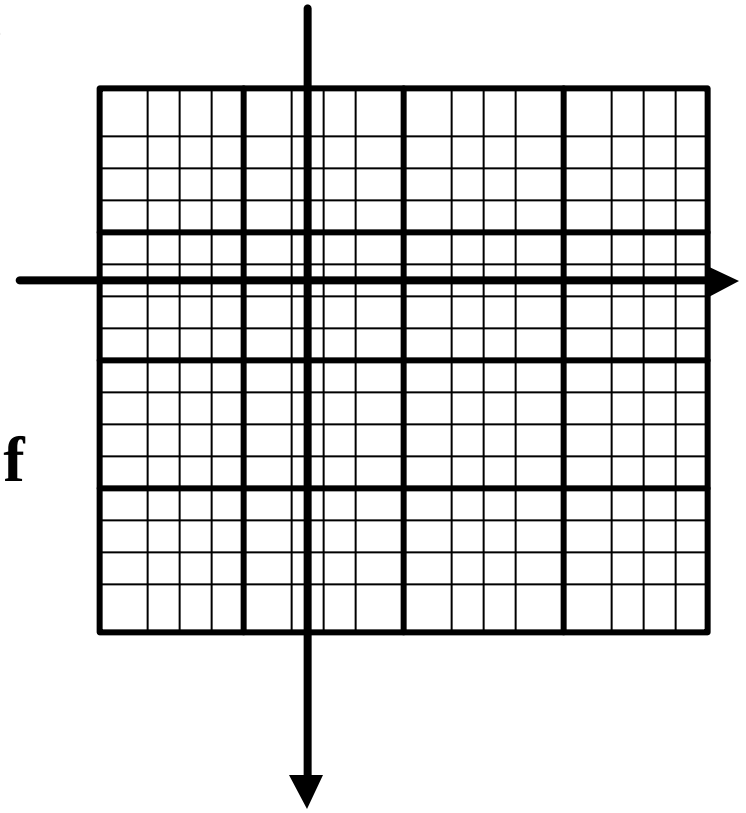
- 1st generation message passing systems used hardware addresses
  - Was inflexible
    - » Had to recode on moving to a new machine
  - Was inconvenient
    - » Required programmer to map problem topology onto explicit machine connections
  - Was insufficient
    - » Didn't support operations over a submachine (e.g., sum across a row of processes)

Generalizing the Process Identifier in MPI

- MPI supports process groups
  - Initial “all” group
  - Group management routines
    - » Split group
    - » Define group from list
- All communication takes place in groups
  - Source/destination identifications refer to rank in group
  - Communicator = group + context

Why use Process Groups?

- We find a good example when we consider typical Matrix Algorithm
  - (matrix multiplication)
  - $A_{i,j} = S_k B_{i,k} C_{k,j}$
  - summed over k'th column of B and k'th row of C
- Consider a block decomposition of 16 by 16 matrices B and C as for Laplace's equation. (Efficient Decomposition as we will see later)
- Each sum operation involves a subset(group) of 4 processors



How It Is Identified: Message Tags

- 1st generation message passing systems used an integer “tag” (a.k.a. “type” or “id”) to match messages when received
  - Most systems allowed wildcard on receive
    - » wildcard means match any tag i.e. any message
    - » Unsafe due to unexpected message arrival
  - Most could match sender id, some with wildcards
    - » Wildcards unsafe; strict checks inconvenient
  - All systems let users pick the tags
    - » Unsafe for libraries due to interference

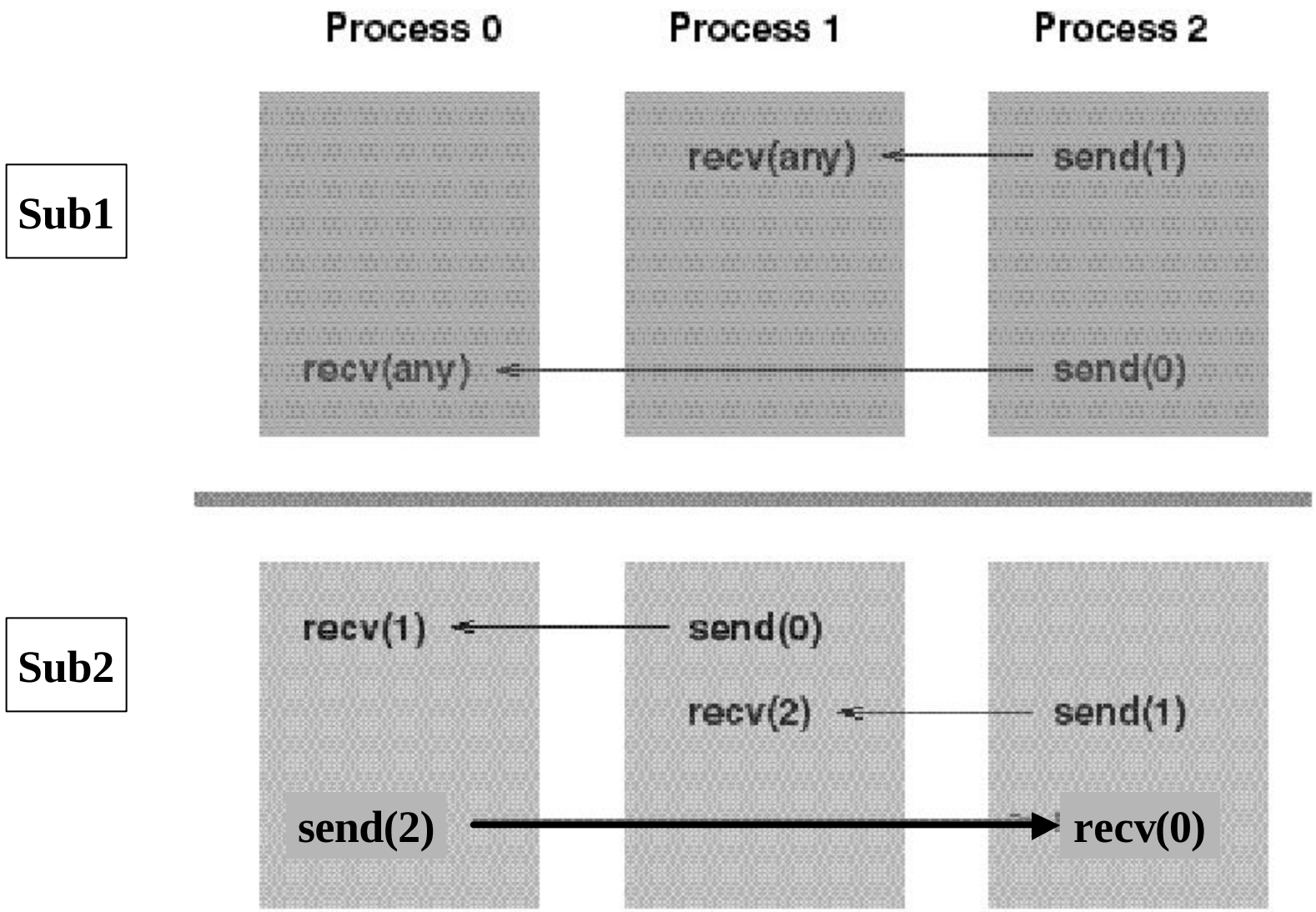
Sample Program using Library

- **Calls Sub1 and Sub2 are from different libraries**
- **Same sequence of calls on all processes, with no global synch**

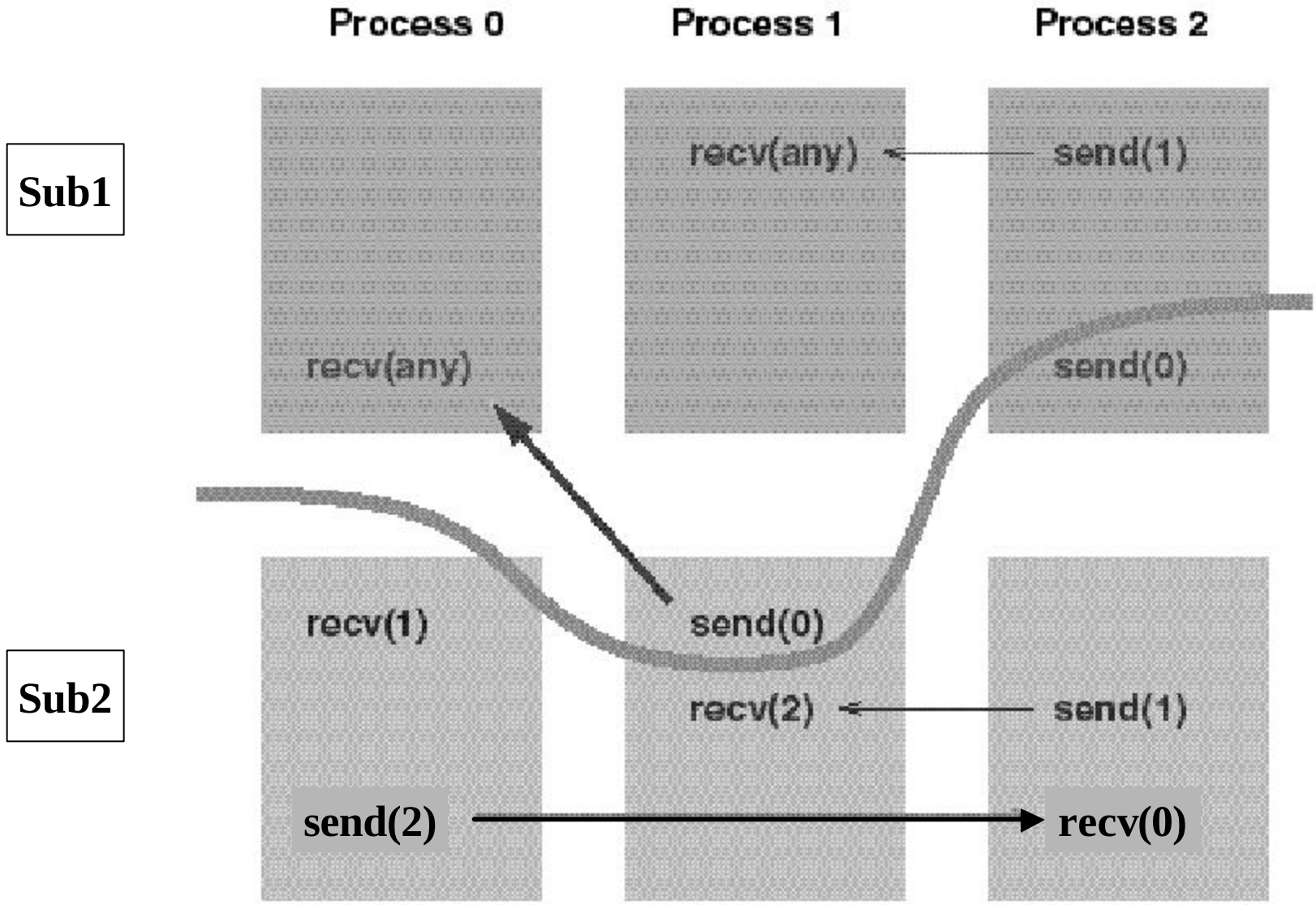
```
Sub1();
Sub2();
```

- We follow with two cases showing possibility of error with messages getting mixed up between subroutine calls

Correct Library Execution



Incorrect Library Execution



What Happened?

- Each library was self-consistent
  - Correctly handled all messages it knew about
- Interaction between the libraries killed them
  - "Intercepting" a message broke both
- The lesson:
  - Don't take messages from strangers
- Other examples teach other lessons:
  - Clean up your own messages
  - Don't use other libraries' tags
  - Etc. …

Solution to the Tag Problem

- Generalize tag to tag and communicator
- A separate communication *context* for each family of messages
  - Used for queuing and matching
  - This is the context for communicators
- No wild cards allowed in communicator, for security
- Communicator allocated by the system, for security
- Tags retained for use within a context
  - wild cards OK for tags

MPI Conventions

- All MPI routines are prefixed by MPI_
  - C is always MPI_Xnnnnn(parameters) : C is case sensitive
  - Fortran is case insensitive but we will write MPI_XNNNNN(parameters)
- MPI constants are in upper case as are MPI datatypes, e.g. MPI_FLOAT for floating point number in C
- Specify overall constants with
  - #include "mpi.h" in C programs
  - include "mpif.h" in Fortran
- C routines are actually integer functions and always return an integer status (error) code
- Fortran routines are really subroutines and have returned status code as last argument
  - Please check on status codes although this is often skipped!

Standard Constants in MPI

- There a set of predefined constants in include files for each language and these include:
- MPI_SUCCESS -- successful return code
- MPI_COMM_WORLD (everything) and MPI_COMM_SELF(current process) are predefined reserved communicators in C and Fortran
- Fortran elementary datatypes are:
  - MPI_INTEGER, MPI_REAL, MPI_DOUBLE_PRECISION, MPI_COMPLEX, MPI_DOUBLE_COMPLEX, MPI_LOGICAL, MPI_CHARACTER, MPI_BYTE, MPI_PACKED
- C elementary datatypes are:
  - MPI_CHAR, MPI_SHORT, MPI_INT, MPI_LONG, MPI_UNSIGNED_CHAR, MPI_UNSIGNED_SHORT, MPI_UNSIGNED, MPI_UNSIGNED_LONG, MPI_FLOAT, MPI_DOUBLE, MPI_LONG_DOUBLE, MPI_BYTE, MPI_PACKED

The Six Fundamental MPI routines

- MPI_Init (argc, argv) -- initialize
- MPI_Comm_rank (comm, rank) -- find process label (rank) in group
- MPI_Comm_size(comm, size) -- find total number of processes
- MPI_Send (sndbuf,count,datatype,dest,tag,comm) -- send a message
- MPI_Recv (recvbuf,count,datatype,source,tag,comm,status) -- receive a message
- MPI_Finalize( ) -- End Up

MPI_Init -- Environment Management

- This MUST be called to set up MPI before any other MPI routines may be called
- For C: int MPI_Init(int *argc, char **argv[])
  - argc and argv[] are conventional C main routine arguments
  - As usual MPI_Init returns an error
- For Fortran: call MPI_INIT(mpierr)
  - nonzero (more pedantically values not equal to MPI_SUCCESS) values of mpierr represent errors

MPI_Comm_rank -- Environment Inquiry

- This allows you to identify each process by a unique integer called the rank which runs from 0 to N-1 where there are N processes
- If we divide the region 0 to 1 by domain decomposition into N parts, the process with rank r controls
  - subregion covering r/N to (r+1)/N
  - for C:int MPI_Comm_rank(MPI_Comm comm, int *rank)
    - » comm is an MPI communicator of type MPI_Comm
  - for FORTRAN: call MPI_COMM_RANK (comm, rank, mpierr)

MPI_Comm_size -- Environment Inquiry

- **This returns in integer size number of processes in given communicator comm (remember this specifies processor group)**
- **For C: int MPI_Comm_size(MPI_Comm comm,int *size)**
- **For Fortran: call MPI_COMM_SIZE (comm, size, mpierr)**
  - **where comm, size, mpierr are integers**
  - **comm is input; size and mpierr returned**

MPI_Finalize -- Environment Management

- Before exiting an MPI application, it is courteous to clean up the MPI state and MPI_FINALIZE does this. No MPI routine may be called in a given process after that process has called MPI_FINALIZE
- for C: int MPI_Finalize()
- for Fortran:call MPI_FINALIZE(mpierr)
  - mpierr is an integer

Hello World in C plus MPI

- # all processes execute this program
- #include <stdio.h>
- #include <mpi.h>
- void main(int argc,char *argv[])
- { int ierror, rank, size
  - MPI_Init(&argc, &argv); # Initialize
  - # In following Find Process Number
  - MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  - if(rank == 0)
    - » printf ("hello World!\ n");
  - # In following, Find Total number of processes
  - ierror = MPI_Comm_size(MPI_COMM_WORLD, &size);
  - if(ierror != MPI_SUCCESS)
    - » MPI_Abort(MPI_COMM_WORLD,ierror); # Abort
  - printf("I am processor %d out of total of %d\ n", rank, size);
  - MPI_Finalize(); # Finalize }

Comments on Parallel Input/Output - I

- Parallel I/O has technical issues -- how best to optimize access to a file whose contents may be stored on N different disks which can deliver data in parallel and
- Semantic issues -- what does printf in C (and PRINT in Fortran) mean?
- The meaning of printf/PRINT is both undefined and changing
  - In my old Caltech days, printf on a node of a parallel machine was a modification of UNIX which automatically transferred data from nodes to "host e.g. node 0" and produced a single stream
  - In those days, full UNIX did not run on every node of machine
  - We introduced new UNIX I/O modes (singular and multiple) to define meaning of parallel I/O and I thought this was a great idea but it didn't catch on!!

Comments on Parallel Input/Output - II

- Today, memory costs have declined and ALL mainstream MIMD distributed memory machines whether clusters of workstations/PC's or integrated systems such as T3D/ Paragon/ SP-2 have enough memory on each node to run UNIX or Windows NT
- Thus printf today means typically that the node on which it runs will stick it out on "standard output" file for that node
  - However this is implementation dependent
- If on other hand you want a stream of output with information in order
    - » Starting with that from node 0, then node 1, then node 2 etc.
    - » This was default on old Caltech machines but
  - Then in general you need to communicate information from nodes 1 to N-1 to node 0 and let node 0 sort it and output in required order
- MPI-IO standard links I/O to MPI in a standard fashion

Blocking Send: MPI_Send(C) or MPI_SEND(Fortran)

- call MPI_SEND (
  - IN message start address of data to send
  - IN message_len number of items (length in bytes determined by type)
  - IN datatype type of each data element
  - IN dest_rank Process number (rank) of destination
  - IN message_tag tag of message to allow receiver to filter
  - IN communicator Communicator of both sender and receiver group
  - OUT error_message) Error Flag (absent in C)

Example MPI_SEND in Fortran

- integer count, datatype, dest, tag, comm, mpierr
- real sndbuf(50)
- comm = MPI_COMM_WORLD
- tag = 0
- count = 50
- datatype = MPI_REAL
- call MPI_SEND (sndbuf, count, datatype, dest, tag, comm, mpierr)

Blocking Receive: MPI_RECV(Fortran)

- call MPI_RECV(
  - IN start_of_buffer Address of place to store data(address is Input -- values of data are of course output starting at this address!)
  - IN buffer_len Maximum number of items allowed
  - IN datatype Type of each data type
  - IN source_rank Processor number (rank) of source
  - IN tag only accept messages with this tag value
  - IN communicator Communicator of both sender and receiver group
  - OUT return_status Data structure describing what happened!
  - OUT error_message) Error Flag (absent in C)
- Note that return_status is used after completion of receive to find actual received length (buffer_len is a maximum length allowed), actual source processor source_ rank and actual message tag

Blocking Receive: MPI_Recv(C)

- In C syntax is
- int error_message = MPI_Recv(
  - void *start_of_buffer,
  - int buffer_len,
  - MPI_DATATYPE datatype,
  - int source_rank,
  - int tag,
  - MPI_Comm communicator,
  - MPI_Status *return_status)

Fortran example: Receive

- integer status(MPI_STATUS_SIZE) An array to store status of received information
- integer mpierr, count, datatype, source, tag, comm
- integer recvbuf(100)
- count = 100
- datatype = MPI_REAL
- comm = MPI_COMM_WORLD
- source = MPI_ANY_SOURCE accept any source processor
- tag = MPI_ANY_TAG accept any message tag
- call MPI_RECV (recvbuf, count, datatype, source, tag, comm, status, mpierr)
  - Note source and tag can be wild-carded

Hello World:C Example of Send and Receive

- # All processes execute this program
- #include “mpi.h”
- main(int argc, char **argv)
- {
  - char message[20];
  - int i, rank, size, tag=137; # Any value of tag allowed
  - MPI_Status status;
  - MPI_Init (&argc, &argv);
  - MPI_Comm_size(MPI_COMM_WORLD , &size) # Number of Processes
  - MPI_Comm_rank(MPI_COMM_WORLD , &rank); # Who is this process

HelloWorld, continued

- if(rank == 0) { # We are on "root" -- Process 0
  - » strcpy(message,"Hello MPI World"); # Generate message
  - » for(i=1; i<size; i++) # Send message to the size-1 other processes
  - » MPI_Send(message, strlen(message)+1, MPI_CHAR, i, tag, MPI_COMM_WORLD); }
- else { # Any processor except root -- Process 0
  - » MPI_Recv(message,20, MPI_CHAR, 0, tag, MPI_COMM_WORLD , &status); }
- printf('This is a message from node %d saying %s\ n", rank, message);
- MPI_Finalize();

◆ }

Interpretation of Returned Message Status

- In C status is a structure of type MPI_Status
  - status.source gives actual source process
  - status.tag gives the actual message tag
- In Fortran the status is an integer array and different elements give:
  - in status(MPI_SOURCE) the actual source process
  - in status(MPI_TAG) the actual message tag
- In C and Fortran, the number of elements (called count) in the message can be found from call to
- call MPI_GET_COUNT (IN status, IN datatype,
- OUT count, OUT error_message)
  - where as usual in C last argument is missing as returned in function call

Collective Communication

- **Provides standard interfaces to common global operations**
  - **Synchronization**
  - **Communications, i.e. movement of data**
  - **Collective computation**
- **A collective operation uses a process group**
  - **All processes in group call same operation at (roughly) the same time**
  - **Groups are constructed "by hand" with MPI group manipulation routines or by using MPI topology-definition routines**
- **Message tags not needed (generated internally)**
- **All collective operations are blocking.**

Some Collective Communication Operations

- MPI_BARRIER(comm) Global Synchronization within a given communicator
- MPI_BCAST Global Broadcast
- MPI_GATHER Concatenate data from all processors in a communicator into one process
  - MPI_ALLGATHER puts result of concatenation in all processors
- MPI_SCATTER takes data from one processor and scatters over all processors
- MPI_ALLTOALL sends data from all processes to all other processes
- MPI_SENDRECV exchanges data between two processors -- often used to implement "shifts"
  - this viewed as pure point to point by some

Hello World:C Example of Broadcast

- #include "mpi.h"
- main(int argc, char **argv)
- { char message[20];
  - int rank;
  - MPI_Init (&argc, &argv);
  - MPI_Comm_rank(MPI_COMM_WORLD, &rank); # Who is this processor
  - if(rank == 0) # We are on "root" -- Processor 0
    - » strcpy(message,"Hello MPI World"); # Generate message
  - # MPI_Bcast sends from root=0 and receives on all other processor
  - MPI_Bcast(message,20, MPI_CHAR, 0, MPI_COMM_WORLD);
  - printf("This is a message from node %d saying %s\ n", rank, message);
  - MPI_Finalize(); }
- Note that all processes issue the broadcast operation, process 0 sends the message and all processes receive the message.

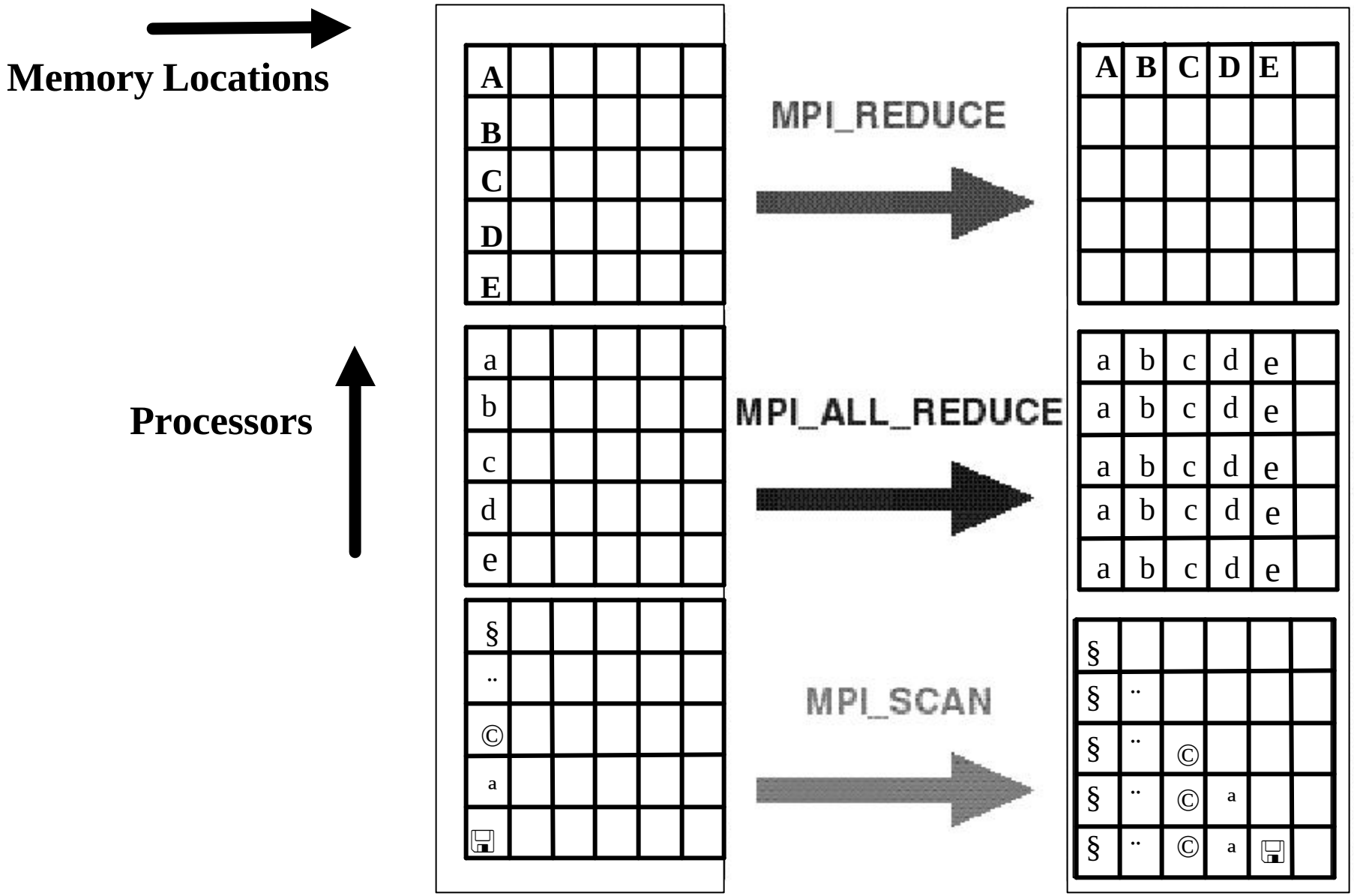
Collective Computation

- One can often perform computing during a collective communication
- MPI_REDUCE performs reduction operation of type chosen from
  - maximum(value or value and location), minimum(value or value and location), sum, product, logical and/or/xor, bit-wise and/or/xor
  - e.g. operation labeled MPI_MAX stores in location result of processor rank the global maximum of original in each processor as in
  - call MPI_REDUCE(original, result, 1, MPI_REAL, MPI_MAX, rank, comm, ierror)
    - » One can also supply one's own reduction function
- MPI_ALLREDUCE is same as MPI_REDUCE but it stores result in all -- not just one -- processors
- MPI_SCAN performs reductions with result for processor r depending on data in processors 0 to r

Examples of Collective Communication/Computation

- Four Processors where each has a send buffer of size 2
  - 0 1 2 3 Processors
  - (2,4) (5,7) (0,3) (6,2) Initial Send Buffers
  - MPI_BCAST with root=2
  - (0,3) (0,3) (0,3) (0,3) Resultant Buffers
  - MPI_REDUCE with action MPI_MIN and root=0
  - (0,2) (_,_) (_,_) (_,_) Resultant Buffers
  - MPI_ALLREDUCE with action MPI_MIN and root=0
  - (0,2) (0,2) (0,2) (0,2) Resultant Buffers
  - MPI_REDUCE with action MPI_SUM and root=1
  - (_,_) (13,16) (_,_) (_,_) Resultant Buffers

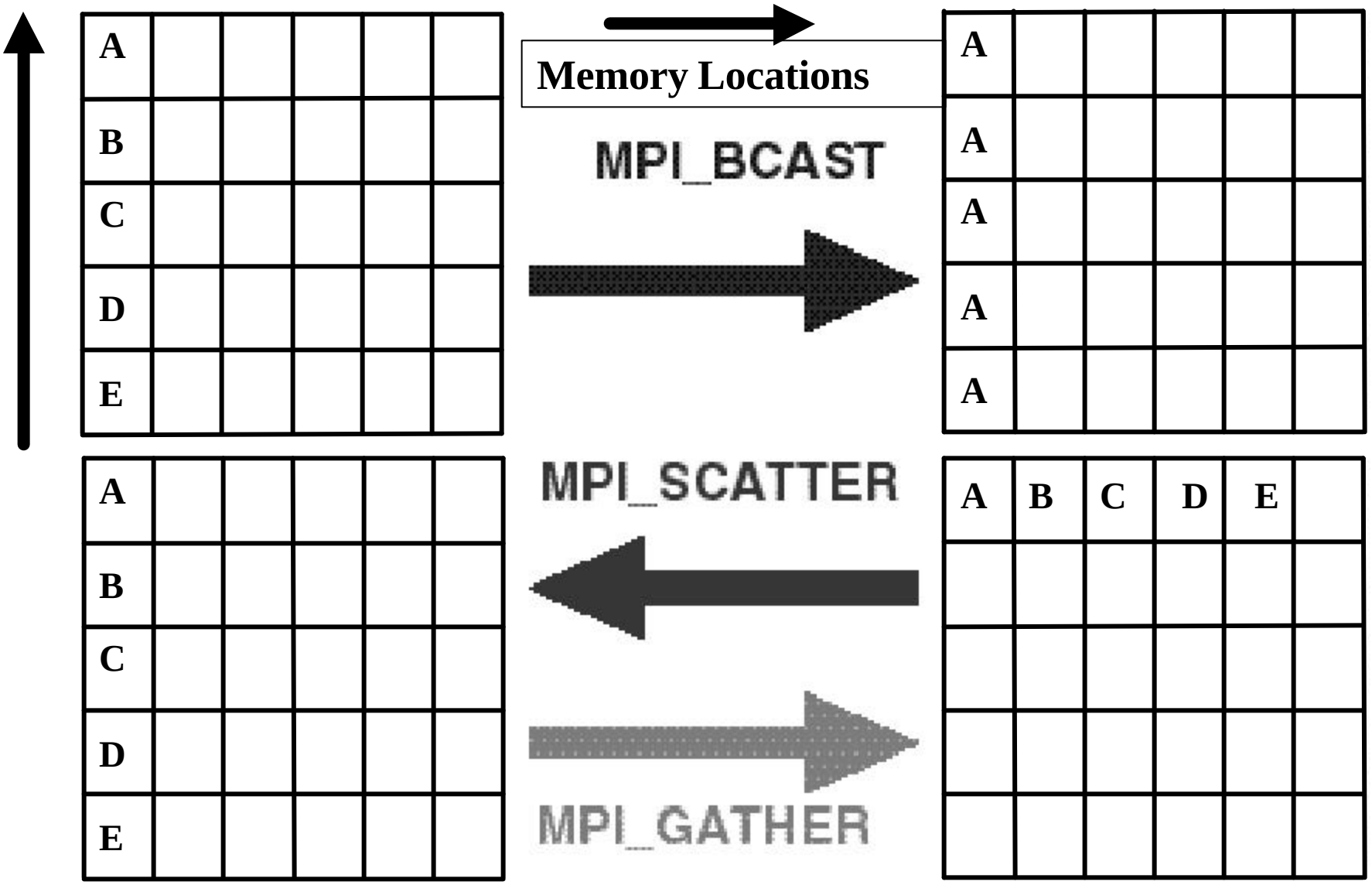
Collective Computation Patterns



More Examples of Collective Communication/Computation

- Four Processors where each has a send buffer of size 2
  - 0 1 2 3 Processors
  - (2,4) (5,7) (0,3) (6,2) Initial Send Buffers
  - MPI_SENDRECV with 0,1 and 2,3 paired
  - (5,7) (2,4) (6,2) (0,3) Resultant Buffers
  - MPI_GATHER with root=0
  - (2,4,5,7,0,3,6,2) (_,_) (_,_) (_,_) Resultant Buffers
  - Now take four Processors where only rank=0 has send buffer
  - (2,4,5,7,0,3,6,2) (_,_) (_,_) (_,_) Initial send Buffers
  - MPI_SCATTER with root=0
  - (2,4) (5,7) (0,3) (6,2) Resultant Buffers

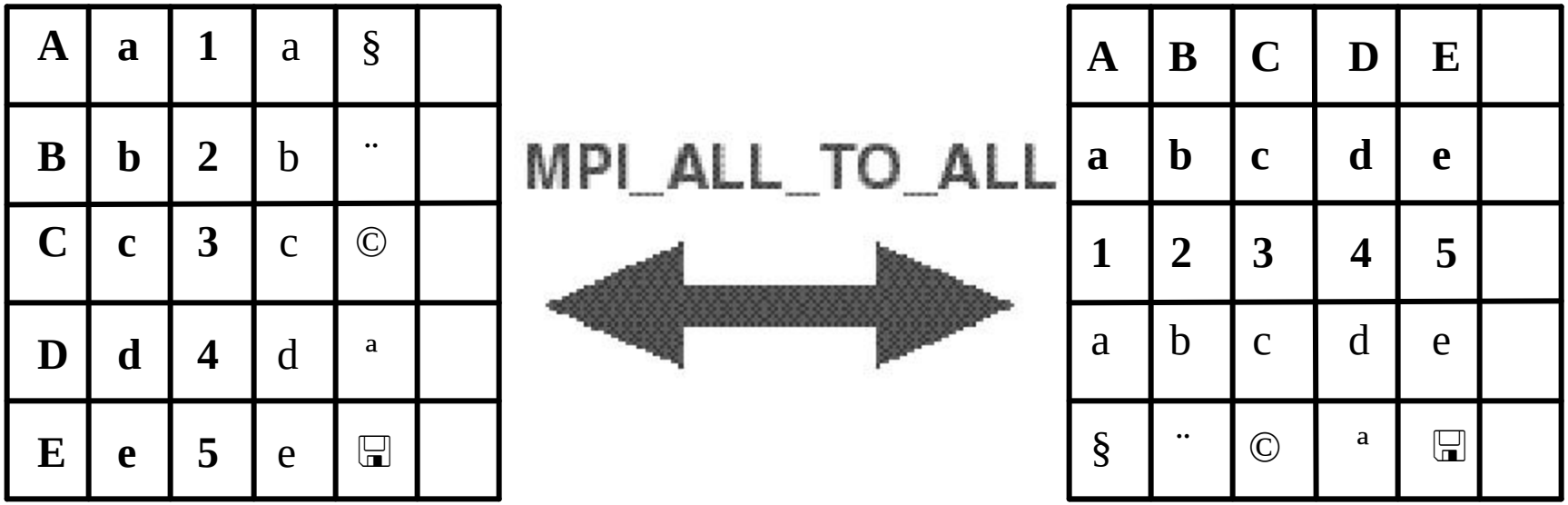
Data Movement (1)



Examples of MPI_ALLTOALL

- All to All Communication with i'th location in j'th processor being sent to j'th location in i'th processor
- Processor 0 1 2 3
- Start (a0,a1,a2,a3) (b0,b1,b2,b3) (c0,c1,c2,c3) (d0,d1,d2,d3)
- After (a0,b0,c0,d0) (a1,b1,c1,d1) (a2,b2,c2,d2) (a3,b3,c3,d3)
- There are extensions MPI_ALLTOALLV to handle case where data stored in noncontiguous fashion in each processor and when each processor sends different amounts of data to other processors
- Many MPI routines have such "vector" extensions

Data Movement (2)



List of Collective Routines

Allgather	Allgatherv	Allreduce
Alltoall	Alltoallv	Barrier
Bcast	Gather	Gatherv
Reduce	ReduceScatter	Scan
Scatter	Scatterv	

- "ALL" routines deliver results to all participating processes
- Routines ending in "V" allow different sized inputs on different processors

Example Fortran: Performing a Sum

```
call MPI_COMM_RANK( comm, rank, ierr )
 if (rank .eq. 0) then
   read *, n
 end if
 call MPI_BCAST(n, 1, MPI_INTEGER, 0, comm, ierr )
# Each process computes its range of numbers to sum
 lo = rank*n+1
 hi = lo+n-1
 sum = 0.0d0
 do i = lo, hi
    sum = sum + 1.0d0 / i
 end do
 call MPI_REDUCEALL( sum, sumout, 1, MPI_DOUBLE,
&                    MPI_ADD_DOUBLE, comm, ierr)
```

Example C: Computing Pi

- #include “mpi.h”
- #include <math.h>
- int main (argc, argv)
- int argc; char *argv[];
- {
- int n, myid, numprocs, i, rc;
- double PI25DT = 3.14159265358979323842643;
- double mypi, pi, h, sum, x, a;

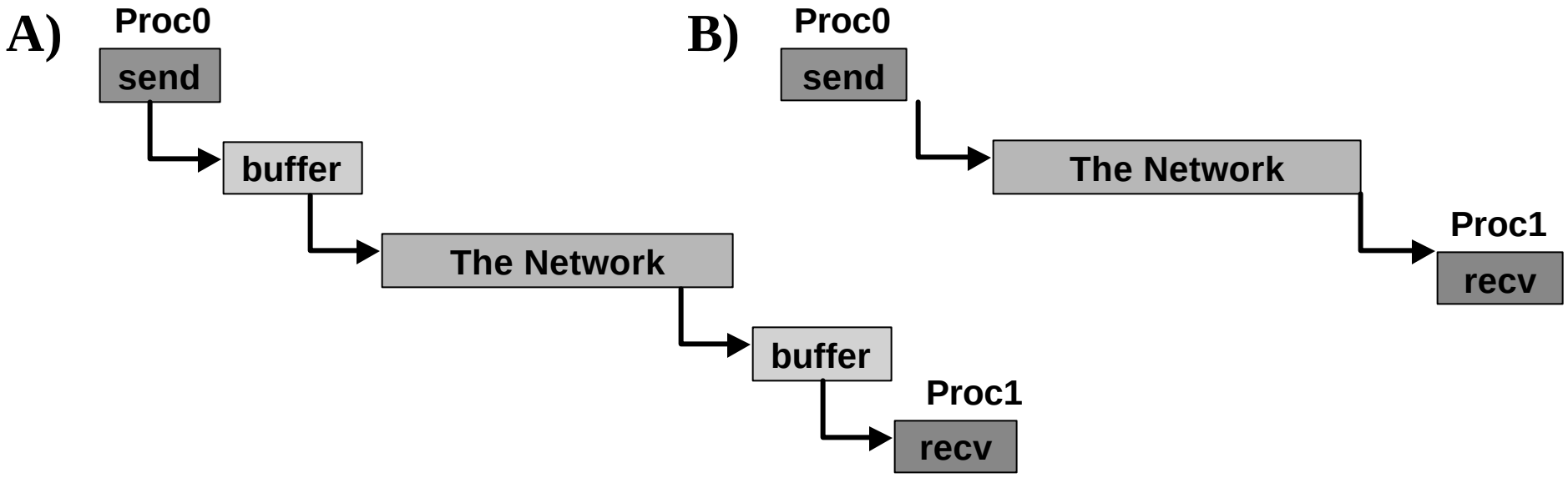
- MPI_Init(&argc, &argv);
- MPI_Comm_size (MPI_COMM_WORLD, &numprocs);
- MPI_Comm_rank (MPI_COMM_WORLD, &myid);

Pi Example continued

- { if (myid == 0)
- { printf ("Enter the number of intervals: (0 quits) ");
- scanf ("%d", &n); }
- MPI_Bcast (&n, 1, MPI_INT, 0, MPI_COMMWORLD);
- if (n == 0) break;
- h = 1.0 / (double) n;
- sum = 0.0;
- for (i = myid+1; i <= n; i += numprocs)
- { x = h * ((double) i - 0.5); sum += 4.0 / 1.0 + x*x): }
- mypi = h * sum;
- MPI_Reduce (&mypi, &pi,1, MPI_DOUBLE,MPI_SUM, 0,MPI_COMMWORLD);
- if (myid == 0)
- printf("pi is approximately %.16f, Error is %.16f\ n",pi, fabs(pi-PI35DT); }
- MPI_Finalize; }

Buffering Issues

- **Where does data go when you send it?**
  - **Multiple buffer copies, as in A)?**
  - **Straight to the network, as in B)?**
- **B) is more efficient than A), but not always correct**



Avoiding Buffering Costs

- **Copies are not needed if**
  - **Send does not return until the data is delivered,**

  or
  - **The data is not touched after the send**
- **MPI provides modes to arrange this**
  - **Synchronous: Do not return until recv is posted**
  - **Ready: Matching recv is posted before send**
  - **Buffered: If you really want buffering**
- **When using asynchronous communication send functions, use MPI_Wait or MPI_WaitAll before reusing the buffer to ensure that all data has been safely transferred on its way.**

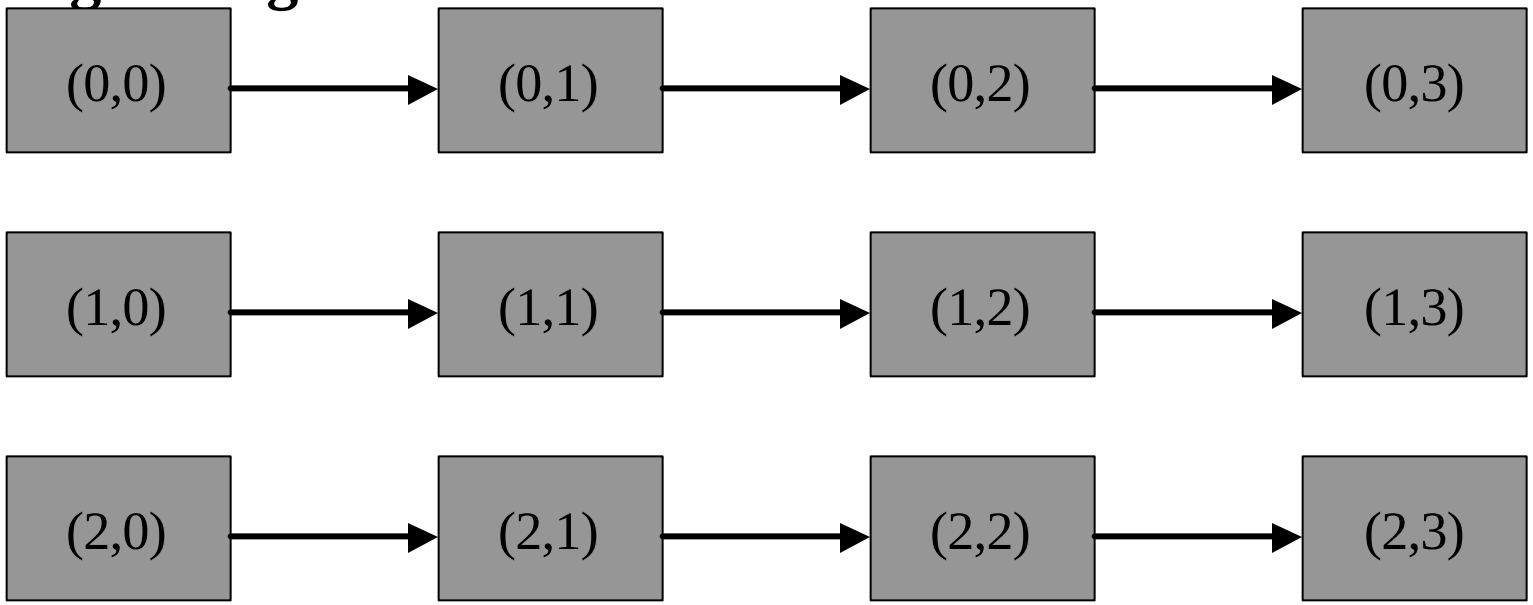
Combining Blocking and Send Modes

- **All combinations are legal**
  - **Red** are fastest, **Blue** are slow

	Blocking	Nonblocking
Normal	`MPI_SEND`	`MPI_ISEND`
Buffering	`MPI_BSEND`	`MPI_IBSEND`
Ready	`MPI_RSEND`	`MPI_IRSEND`
Synchronous	`MPI_SSEND`	`MPI_ISSEND`

Cartesian Topologies

- MPI provides routines to provide structure to collections of processes. Although it also has graph topologies, here we concentrate on cartesian.
- A Cartesian topology is a mesh
- Example of a 3 x 4 mesh with arrows pointing at the right neighbors:



Defining a Cartesian Topology

- The routine MPI_Cart_create creates a Cartesian decomposition of the processes, with the number of dimensions given by the ndim argument. It returns a new communicator (in comm2d in example below) with the same processes as in the input communicator, but different topology.
- ndim = 2;
- dims[0] = 3; dims[1] = 4;
- periods[0] = 0; periods[1] = 0; // periodic is false
- reorder = 1; // reordering is true
- ierr = MPI_Cart_create (MPI_COMM_WORLD, ndim,
- dims, periods, reorder, &comm2d);
  - where reorder specifies that it's o.k. to reorder the default process rank in order to achieve a good embedding (with good communication times between neighbors).

MPI_Cart_coords and MPI_Cart_rank

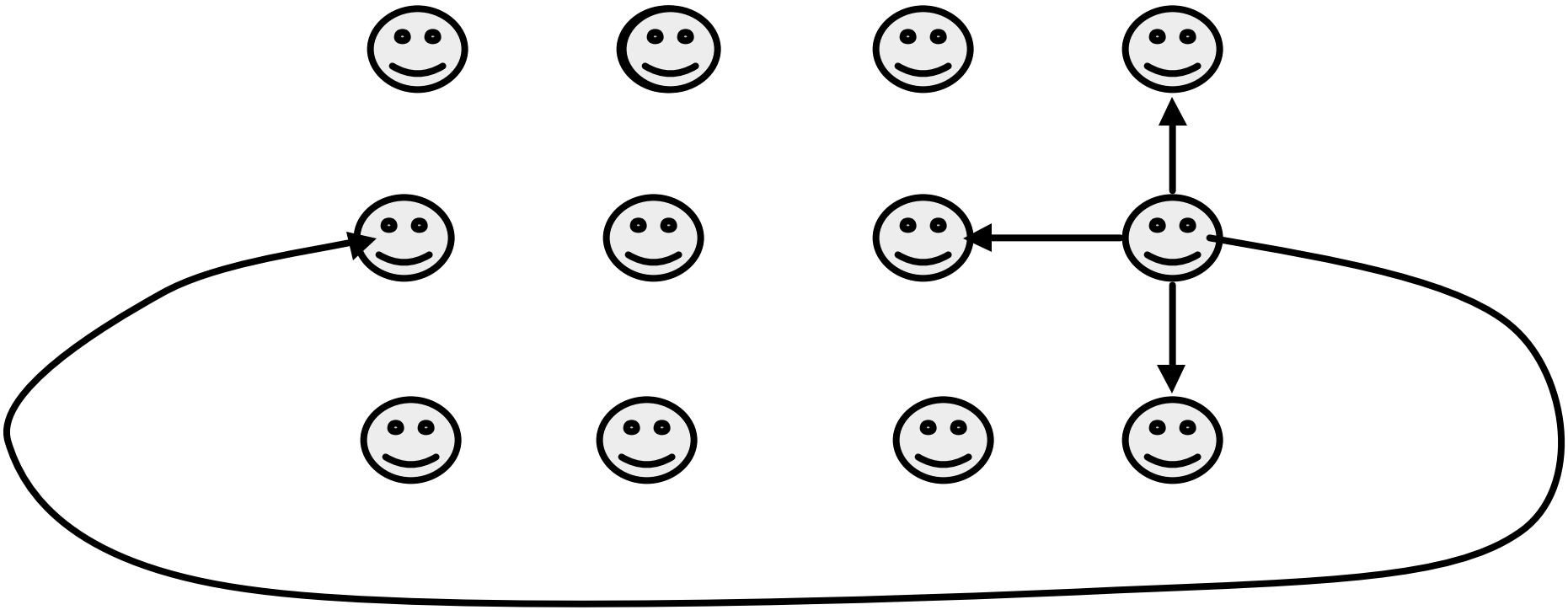
- Given the rank of the process in MPI_COMM_WORLD, this routine gives a two element (for two dimensional topology) array (coords in example below) with the (i, j) coordinates of this process in the new cartesian communicator.
  - ierr MPI_Cart_coords (comm2d, rank, ndim, coords);
  - coords[0] and coords[1] will be the i and j coordinates.
- Given the coords of a process, this routine gives the rank number in the communicator.
  - ierr MPI_Cart_coords (comm2d, coords, &rank);

Who are my neighbors?

- The routine MPI_Cart_shift finds the neighbors in each direction of the new communicator.
- dir = 0; // in C 0 for columns, 1 for rows
- // in Fortran, it's 1 and 2
- disp = 1; // specifies first neighbor to the right and left
- ierr = MPI_Cart_shift (comm2d, dir, disp, &nbrbottom,
- &nbrtop):
- This returns the process numbers (ranks) for a communication of the bottom and top neighbors.
- Typically, the neighbors are used with send/recv to exchange data.
- If a process in a non-periodic mesh is on the border and has no neighbor, then the value MPI_PROCNULL is returned. This process value can be used in a send/recv, but it will have no effect.

Periodic meshes

- In a periodic mesh, as shown below the processes at the edge of the mesh wrap around in their dimension to find their neighbors. The right neighbor is wrapped



Communication in Sub-Grids

- Suppose that you have an algorithm, such as matrix multiply, that requires you to communicate within one row or column of a 2D grid.
  - For example, broadcast a value to all processes in one row.
- MPI_Comm rowcomm;
  freecoords[0] = 0; freecoords[1] = 1;
  ierr = MPI_Cart_sub(comm2d, freecoords, &rowcomm)
- Defines nrow new communicators, each with the processes of that row. The array freecoords has boolean values specifying whether the elements of that dimension "belong" to the communicator.
  - if bcastroot is defined as the root processor in each row, broadcast a value along rows:
    MPI_Bcast(value, 1, MPI_FLOAT, bcastroot, rowcomm);

Motivation for Derived Datatypes in MPI

- These are an elegant solution to a problem we struggled with a lot in the early days -- all message passing is naturally built on buffers holding contiguous data
- However often (usually) the data is not stored contiguously. One can address this with a set of small MPI_SEND commands but we want messages to be as big as possible as latency is so high
- One can copy all the data elements into a single buffer and transmit this but this is tedious for the user and not very efficient
  - It has extra memory to memory copies which are often quite slow
- So derived datatypes can be used to set up arbitary memory templates with variable offsets and primitive datatypes. Derived datatypes can then be used in "ordinary" MPI calls in place of primitive datatypes MPI_REAL MPI_FLOAT etc.

Derived Datatype Basics

- Derived Datatypes should be declared integer in Fortran and MPI_Datatype in C
- Generally have form { (type0,disp0), (type1,disp1) ... (type(n-1),disp(n-1)) } with list of primitive data types typei and displacements (from start of buffer) dispi
- call MPI_TYPE_CONTIGUOUS (count, oldtype, newtype, ierr)
  - creates a new datatype newtype made up of count repetitions of old datatype oldtype
- one must use call MPI_TYPE_COMMIT(derivedtype, ierr) before one can use the type derivedtype in a communication call
- call MPI_TYPE_FREE(derivedtype, ierr) frees up space used by this derived type

Simple Example of Derived Datatype

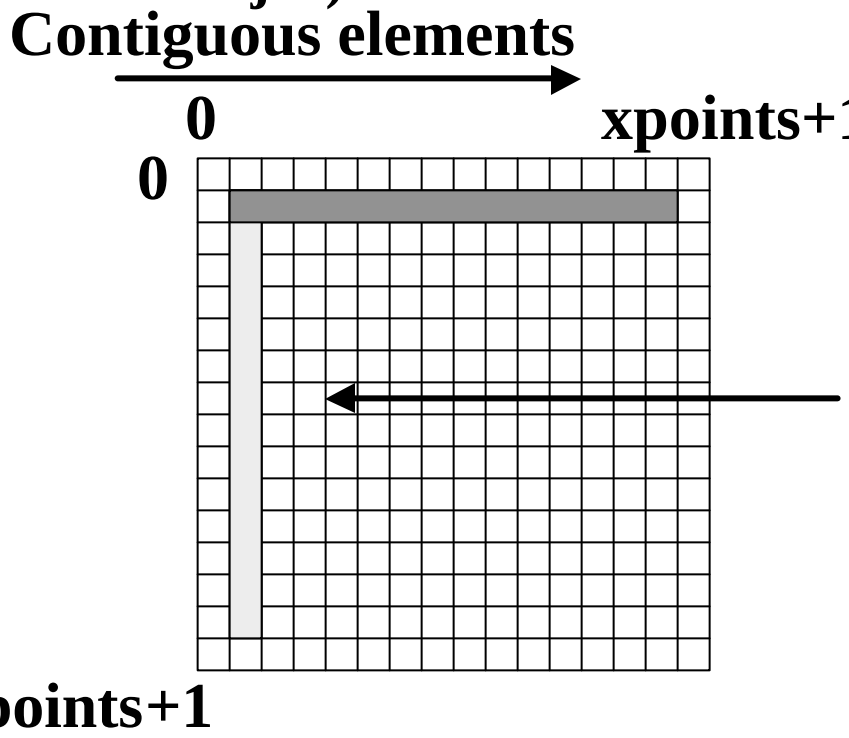
- integer derivedtype, ...
- call MPI_TYPE_CONTIGUOUS(10, MPI_REAL, derivedtype, ierr)
- call MPI_TYPE_COMMIT(derivedtype, ierr)
- call MPI_SEND(data, 1, derivedtype, dest, tag, MPI_COMM_WORLD , ierr)
- call MPI_TYPE_FREE(derivedtype, ierr)
- is equivalent to simpler single call
- call MPI_SEND(data, 10, MPI_REAL, dest, tag, MPI_COMM_WORLD , ierr)
- and each sends 10 contiguous real values at location data to process dest

Derived Datatypes: Vectors

- MPI_TYPE_VECTOR (count, blocklen, stride, oldtype, newtype, ierr)
  - IN count Number of blocks to be added
  - IN blocklen Number of elements in block
  - IN stride Number of elements (NOT bytes) between start of each block
  - IN oldtype Datatype of each element
  - OUT newtype Handle(pointer) for new derived type

Example of Vector type

- **Suppose in C, we have an array**
  - **phi [ypoints+2] [xpoints+2]**
  - **where we want to send rows and columns of elements from 1 : nxblock and 1 : nyblock**
  - **in C, arrays are stored row major order (Fortran is column major)**

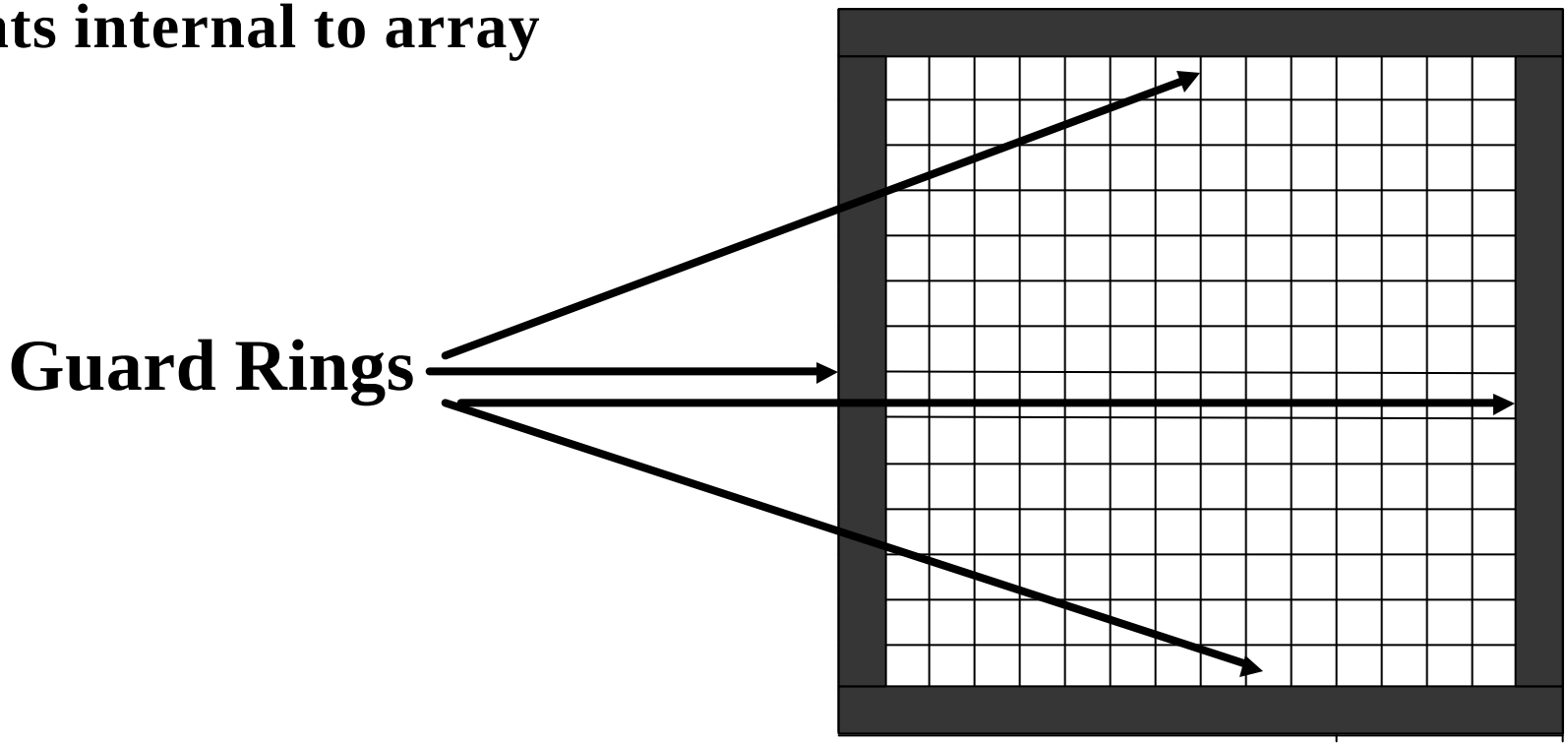



```
MPI_Type_vector
   (xpoints, 1, ypoints+2,
     MPI_DOUBLE, &strided);
```

defines a type called strided which refers to the column of elements

Why is this interesting?

- **In Jacobi like algoritms, each processor stores its own xpoints by ypoints array of variables as well as guard rings containing the rows and columns from neighbours. One loads these guard rings at start of computation iteration and only updates points internal to array**

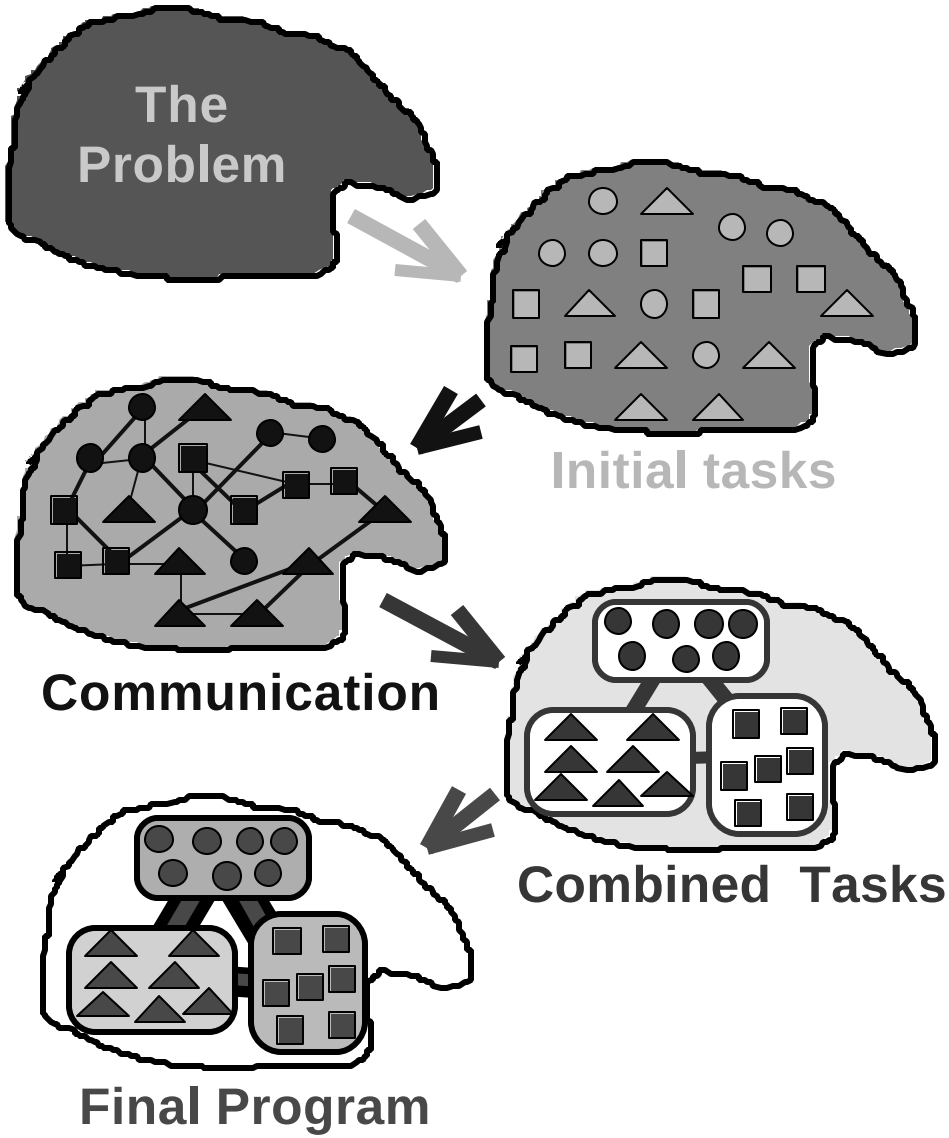


Derived Datatypes: Indexed

- Array of indices, useful for gather/scatter
- MPI_TYPE_INDEXED (count, blocklens, indices, oldtype, newtype, ierr)
  - IN count Number of blocks to be added
  - IN blocklens Number of elements in each block -- an array of length count
  - IN indices Displacements (an array of length count) for each block
  - IN oldtype Datatype of each element
  - OUT newtype Handle(pointer) for new derived type

Designing MPI Programs

- **Partitioning**
  - **Before tackling MPI**
- **Communication**
  - **Many point to collective operations**
- **Agglomeration**
  - **Needed to produce MPI processes**
- **Mapping**
  - **Handled by MPI**



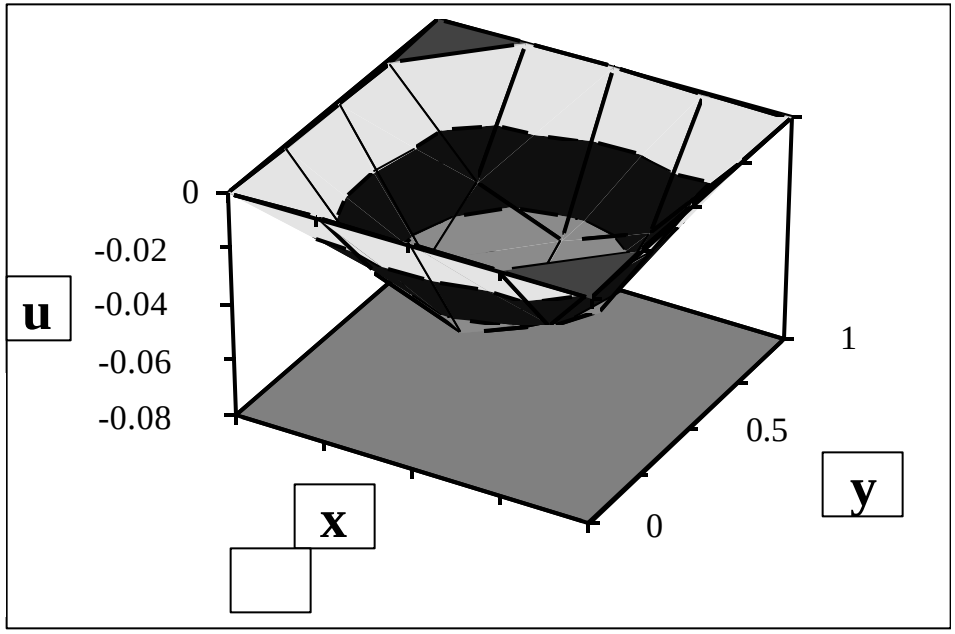
Jacobi Iteration: The Problem

- **Used to numerically solve a Partial Differential Equation (PDE) on a square mesh -- below is Poisson's Equation**
- **Method:**
  - **Update each mesh point by the average of its neighbors**
  - **Repeat until converged**

This is right hand side f(x,y)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -2x^2 + 2x - 2y^2 + 2y$$

$u = 0$ if $x = 0, x = 1, y = 0,$ or $y = 1$



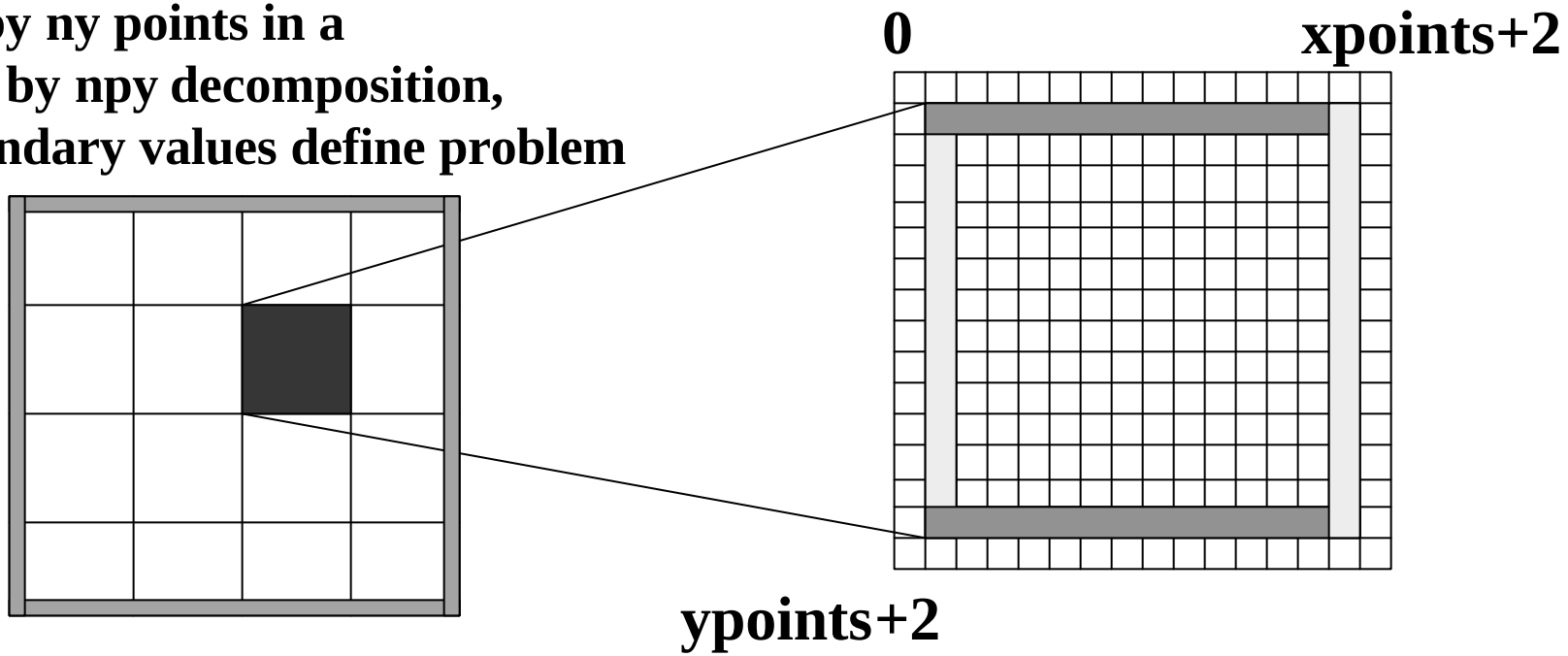
Jacobi Iteration: MPI Program Design

- **Partitioning is simple**
  - **Every point is a micro-task**
- **Communication is simple**
  - **4 nearest neighbors in Cartesian mesh**
  - **Reduction for convergence test**
- **Agglomeration works along dimensions**
  - **1-D packing for high-latency machines (as minimizes number of messages)**
  - **2-D packing for others (most general as minimizes information sent)**
  - **One process per processor practically required**

Jacobi Iteration: MPI Program Design

- Mapping: Cartesian grid supported by MPI virtual topologies
- For generality, write as the 2-D version
  - Create a 1´P (or P´1) grid for 1-D version
- Adjust array bounds, iterate over local array
  - For convenience, include shadow region to hold communicated values (not iterated over)

nx by ny points in a
npx by npy decomposition,
boundary values define problem



Jacobi Iteration: C MPI Program Sketch

```
/ * sizes of data and data files   */
int NDIM = 2;
int xpoints = nx/ npx;  int ypoints = ny/ npy;
double phi[ypoints+2][xpoints+2],
 oldphi[ypoints+2][xpoints+2];

/ *  communication variables */
int rank; int rankx, ranky;
int coords[NDIM];
int reorder = 0;
int dims[NDIM], periods[NDIM];
MPI_Comm comm2d;
MPI_Datatype  contig, strided;
```

Jacobi Iteration: create topology

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

periods[0] = 0;   periods[1] = 0;
dims[0] = npy;   dims[1] = npx;

MPI_Cart_create(MPI_COMM_WORLD, 2, dims, periods,
                reorder, &comm2d);
MPI_Cart_coords(comm2d, rank, 2, coords);
ranky = coords[0];
rankx = coords[1];

MPI_Cart_shift(comm2d, 0, 1, &bottomneighbor, &topneighbor);
MPI_Cart_shift(comm2d, 1, 1, &leftneighbor, &rightneighbor);
```

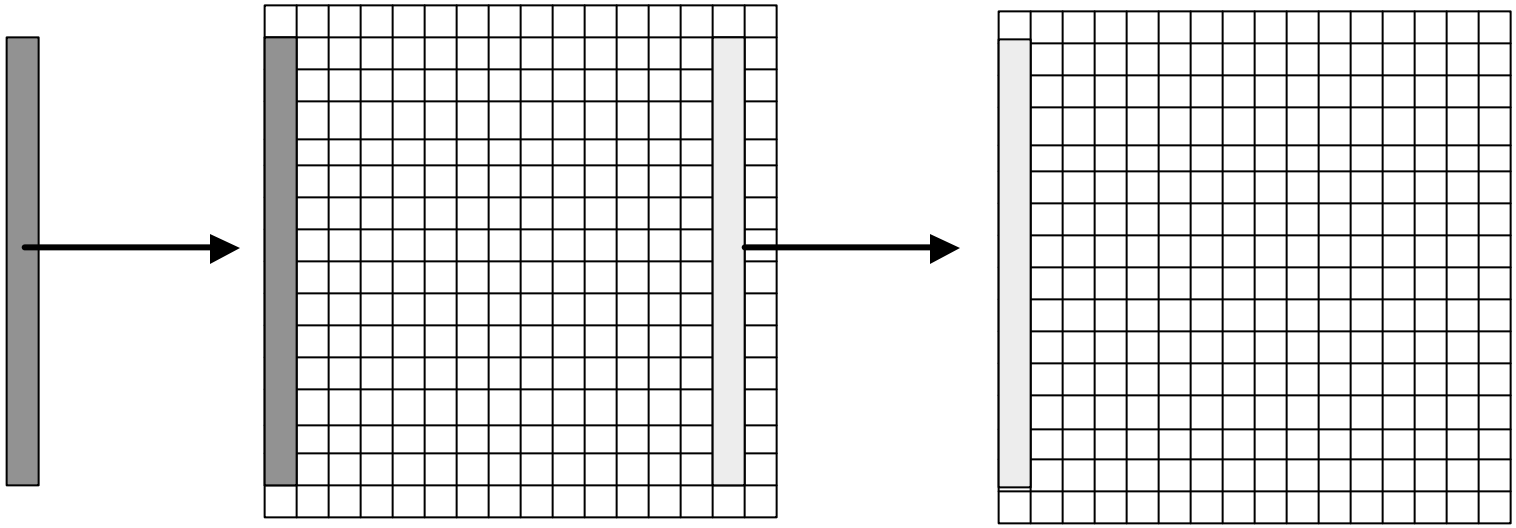
Jacobi iteration: data structures

```
/*  message types  */
MPI_Type_contiguous (ypoints, MPI_DOUBLE, &contig);
MPI_Type_vector (xpoints, 1, ypoints+2, MPI_DOUBLE, &strided);
MPI_Type_commit (&contig);
MPI_Type_commit (&strided);

/* define mask array to be true on boundary and false elsewhere in
   each processor.
   Define boundary values in phi array in each processor.
 */
```

Jacobi Iteration: send guard values

```
while (err > tol) {  /* copy phi array to oldphi */
/ * communicate edge rows and columns to neighboring
    processor  to put in their guard rings          */
    / * Send right boundary to right neighbor
      and receive left ghost vector in return from left neighbor*/
    MPI_Sendrecv (&(oldphi[1][xpoints]), 1, strided,
            rightneighbor, 31, &(oldphi[1][0]), 1, strided,
            leftneighbor, 31, comm2d, &status);
```



Remaining communication

```
/ * Send left boundary in each processor to left neighbor */
 MPI_Sendrecv (&(oldphi[1][1]), 1, strided, leftneighbor, 30,
        &(oldphi[1][xpoints+1]), 1, strided, rightneighbor, 30,
           comm2d, &status);
 / * Send top boundary to top neighbor */
 MPI_Sendrecv (&(oldphi[1][1]), 1, contig, topneighbor, 40,
        &(oldphi[ypoints+1][1]), 1, contig, bottomneighbor, 40,
        comm2d, &status);
 / * Send bottom boundary to bottom neighbor */
 MPI_Sendrecv (&(oldphi[ypoints][1]), 1, contig,
        bottomneighbor, 41, &(oldphi[0][1]), 1, contig,
        topneighbor, 41, comm2d, &status);
```

Jacobi Iteration: update and error

```
for (j = 1; j <= xpoints; j++)
        {
          for (i = 1; i <= ypoints; i++)
            {
              if (mask[i][j]) {
                phi[i][j] = 0.25 * (oldphi[i-1][j] +
                                    oldphi[i+1][j]
                                    + oldphi[i][j-1] +
                                    oldphi[i][j+1]);
                diff = max(diff, abs(phi[i][j] - oldphi[i][j]));
              } }}
 /* maximum difference over all processors */
 MPI_Allreduce(&diff, &err, 1, MPI_DOUBLE, MPI_MAX,
comm2d);
 if (err < ((double)TOLERANCE))    done = 1;
}
```

The MPI Timer

- The elapsed (wall-clock) time between two points in an MPI program can be computed using MPI_Wtime:
  - double t1, t2;
  - t1 = MPI_Wtime ( );
  - . . .
  - t2 = MPI_Wtime ( );
  - printf ("Elapsed time is %f \ n", t2-t1);
- The times are local; the attribute MPI_WTIME_IS_GLOBAL may be used to determine if the times are also synchronized with each other for all processes in MPI_COMM_WORLD .

MPI-2

- The MPI Forum produced a new standard which include MPI 1.2 clarifications and corrections to MPI 1.1
- MPI-2 new topics are:
  - process creation and management, including client/server routines
  - one-sided communications (put/get, active messages)
  - extended collective operations
  - external interfaces
  - I/O
- additional language bindings for C++ and Fortran-90

I/O included in MPI-2

- Goal is to provide model for portable file system allowing for optimization of parallel I/O
  - portable I/O interface POSIX judged not possible to allow enough optimization
- Parallel I/O system provides high-level interface supporting transfers of global data structures between process memories and files.
- Significant optimizations required include:
  - grouping, collective buffering, and disk-directed I/O
- Other optimizations also achieved by
  - asynchronous I/O, strided accesses and control over physical file layout on disks.
- I/O access modes defined by data partitioning expressed with derived datatypes