MPI - Message Passing Interface

Overview

MPI core routines
  Example: Hello World
Modes for point-to-point communication
Collective communication operations
  Example: 1D Finite Differences
Virtual processor topologies
Group concept
Communicator concept
One-sided communication (MPI-2)
Additional features
Literature

MPI - principles

MPI standard for message passing created in 1993

- API with C, C++ and Fortran bindings
- replaced vendor-specific message passing libraries
- replaced other de-facto standards: PICL, PARMACS, PVM
- abstraction from machine-specific details
- enhanced portability (though at a low level)
- efficient implementations (avoid unnecessary copying)
- implemented on almost all parallel machines

MPI-1.1 1995
Extension MPI-2 1997 (MPI-2.1 2008, MPI-2.2 2009)

Free implementations (e.g. for PCs, NOWs, Linux clusters):
  MPICH (Argonne), OpenMPI (www.open-mpi.org), CHIMP (Edinburgh), ...

Commercial implementations (optimized) e.g. Scali MPI (on Neolith)

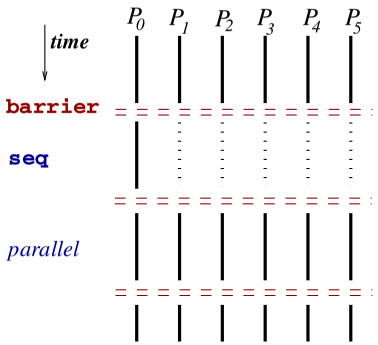
MPI - program execution

Run a MPI executable: with (platform-dependent) shell script

`mpirun` -np 6 `a.out` [args]

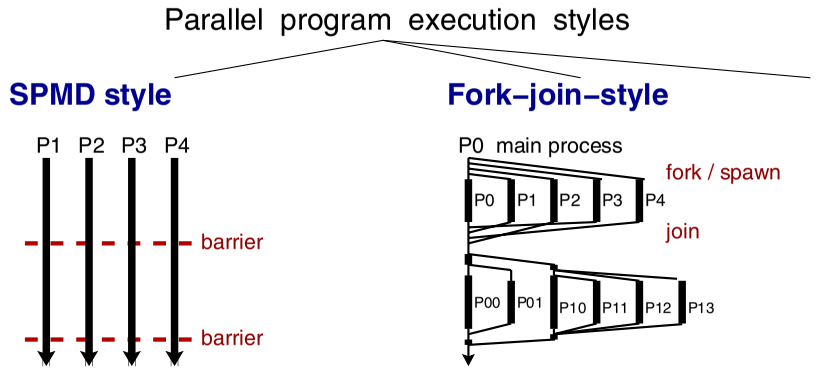
creates fixed set of 6 processes that execute `a.out`

- fixed set of processors
- no spawn() command
- main() executed by all started processors as one group



SPMD execution style

Background: SPMD execution style vs. Fork-join execution style



SPMD style	Fork–join–style
constant number of parallel activities (processors / processes / threads)	dynamic creation and deletion of parallel activities
static mapping to processors	needs dynamic scheduling (overhead)
mostly flat parallelism (nested parallelism by group splitting)	naturally nested parallelism (nested parallelism by nested spawning)
Example: MPI, HPF, UPC, NestStep	Example: pthreads, Java threads, Unix–fork, OpenMP, PVM, MPI–2, Cilk

MPI - determinism

Message passing is generally nondeterministic:
Arrival order of two sent messages is unspecified.

MPI guarantees that two messages sent from processor A to B will arrive in the order sent.

Messages can be distinguished by sender and a tag (integer).

User-defined nondeterminism in receive operations:

wildcard `MPI_ANY_SOURCE`

wildcard `MPI_ANY_TAG`

MPI core routines (C API)

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

MPI_Finalize( void );

MPI_Send( void *sbuf, int count, MPI_Datatype datatype,
                          int dest, int tag, MPI_Comm comm );

int MPI_Recv( void *dbuf, int count, MPI_Datatype datatype,
     int source, int tag, MPI_Comm comm, MPI_Status *status );

MPI_Comm_size( MPI_Comm comm, int *psize);

MPI_Comm_rank( MPI_Comm comm, int *prank);
```

Status object:

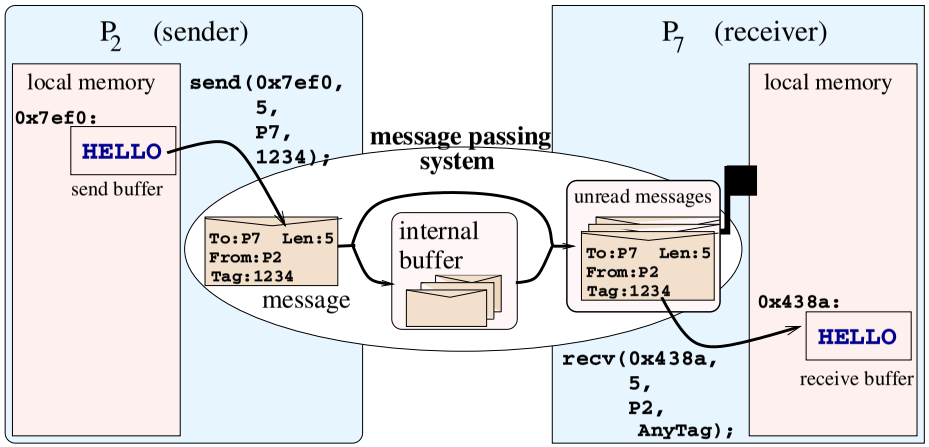
status->MPI_SOURCE indicates the sender of the message received;
status->MPI_TAG indicates the tag of the message received;
status->MPI_ERROR contains an error code.

MPI core routines (C++ API)

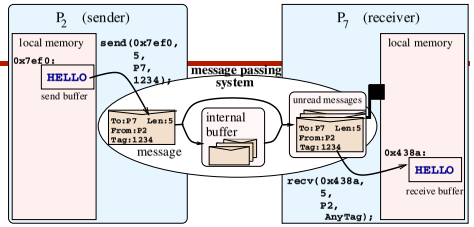
```
void MPI::Init( int &argc, char **&argv );
void MPI::Init( );

void MPI::Finalize( );

void MPI::Comm::Send( void *sbuf, int count,
                                const Datatype& datatype,
                                     int dest, int tag );

void int MPI::Comm::Recv( void *dbuf, int count,
                                const Datatype& datatype,
                          int source, int tag, Status& status );

int MPI::Comm::Get_size( );

int MPI::Comm::Get_rank( );
```

Remark: The C++ API is deprecated in MPI 2.2 (2009), may disappear with MPI 3.0

Hello World (1)



Hello World (2)




```
#include <mpi.h>

void main( void )
{
 MPI_Status status;
 char *string = "xxxxx";  // receive buffer
 int myid;

 MPI_Init( NULL, NULL );
 MPI_Comm_rank( MPI_COMM_WORLD, &myid );
 if (myid==2)
   MPI_Send( "HELLO", 5, MPI_CHAR, 7, 1234, MPI_COMM_WORLD );
 if (myid==7) {
   MPI_Recv( string, 5, MPI_CHAR, 2, MPI_ANY_TAG,
             MPI_COMM_WORLD, &status );
   printf( "Got %s from P%d, tag %d\n",
           string, status.MPI_SOURCE, status.MPI_TAG );
 }
 MPI_Finalize();
}
```


MPI predefined data types

Symbolic constants encode predefined data types in MPI:

MPI_Datatype	Corresponding C type
MPI_CHAR	char
MPI_BYTE	—
MPI_SHORT	short
MPI_INT	int
MPI_LONG	long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double

Recommended for program portability across platforms

MPI communication operations

An MPI communication operation
(i.e., a send or receive routine)
is called

```
// ... write array A
MPI_Isend(..., A, ...);
// ... no overwriting of the
// ... sent part of A here!
MPI_Wait(...);
// ... can write over A here
```

blocking if the return of program control to the calling process
means that all resources (e.g., buffers) used in the operation
can be reused immediately;

nonblocking or **incomplete** if the operation returns control
to the caller *before* it is completed, such that buffers etc.
may still be accessed afterwards by the started communication activity,
which continues running in the background.

In MPI, nonblocking operations are marked by an `I` prefix.

MPI communication modes

A MPI communication can run in the following modes:

standard mode: the default mode:
synchronicity and buffering depends on the MPI implementation.

synchronous mode:
send and receive operation are forced to work partly simultaneously:
send returns when receive has been started.

buffered mode: (the buffer can be attached by the programmer)
send returns when its send buffer has either been received
or written to a temporary buffer

$\rightarrow$ decouples send and receive

In MPI, the mode is controlled by a prefix (none, `S`, `B`) of the send operation.

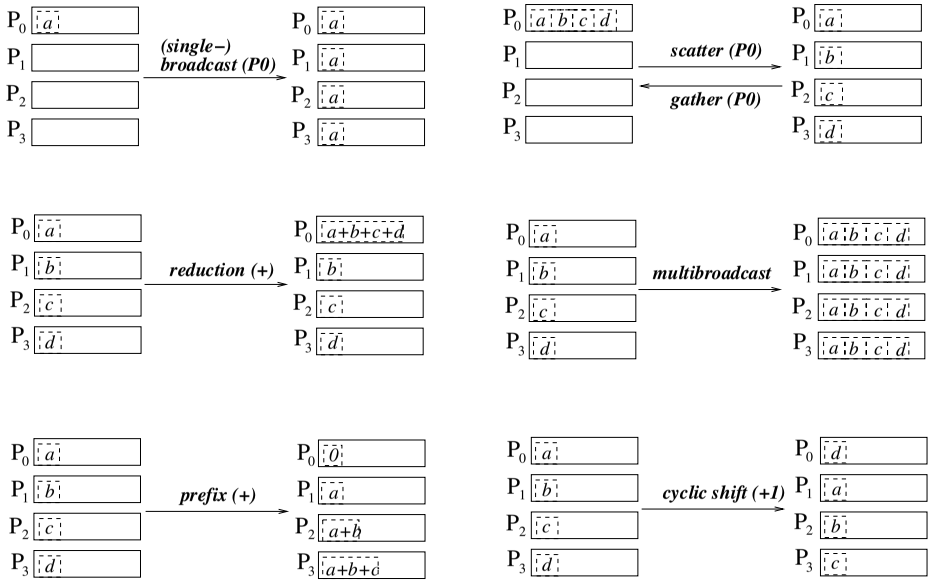
Overview of some important point-to-point communication operations

Operation type	blocking		nonblocking	
Communication mode	send	receive	send	receive
standard	MPI_Send	MPI_Recv	MPI_Isend ... ↓ request MPI_Wait	MPI_Irecv ... ↓ request MPI_Wait
synchronous	MPI_Ssend		MPI_Issend ... ↓ request MPI_Wait	
buffered	MPI_Bsend		MPI_Ibsend ... ↓ request MPI_Wait	
tentative	MPI_*send	MPI_Probe	MPI_I*send ... ↓ request MPI_Wait	MPI_Iprobe ... ↓ request MPI_Wait

Remarks: there are further routines, another mode “ready”,

MPI_TEST as alternative to MPI_WAIT

Collective communication operations



MPI - Collective communication operations: Broadcast, Reduction

Single-Broadcast:

```
MPI_Bcast( void *srbuf, int count, MPI_Datatype datatype,
                                   int rootrank, MPI_Comm comm );
```

Reduction:

```
MPI_Reduce( void *sbuf, void *rbuf, int count,
                MPI_Datatype datatype, MPI_Op op, int rootrank,
                                                  MPI_Comm comm );
```

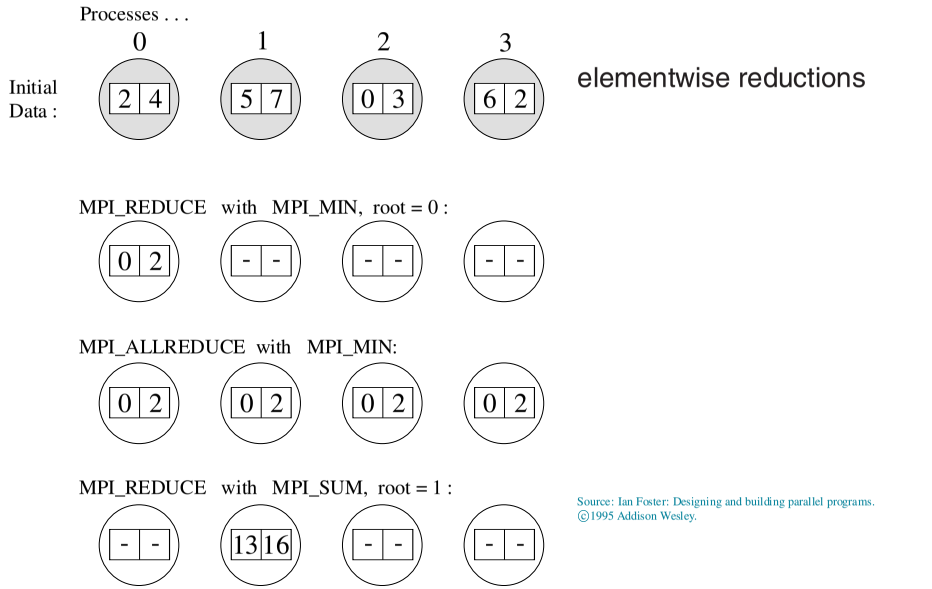
with predefined *op* ∈ { MPI_SUM, MPI_MAX, ... }
or user-defined by MPI_Op_Create.

MPI_Allreduce

Barrier synchronization:

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

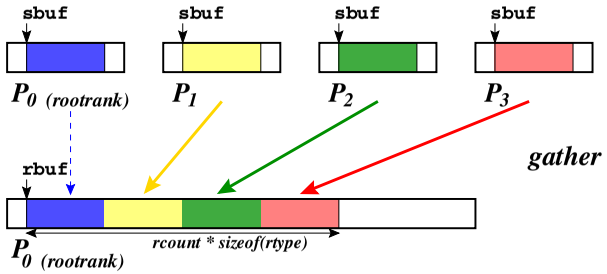

MPI - Collective communication operations (3): Reductions



Source: Ian Foster: Designing and building parallel programs.

MPI - Collective communication operations: Scatter, Gather

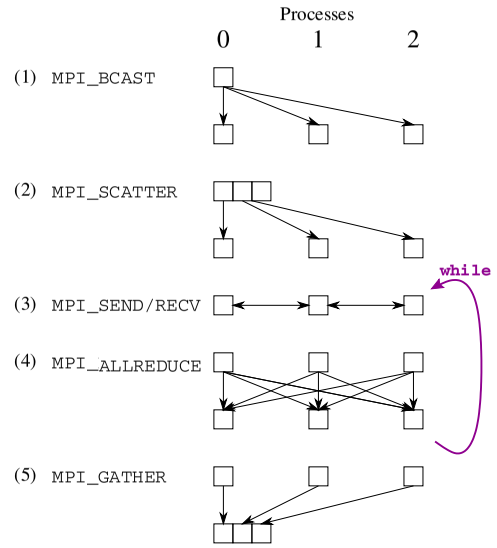
```
int MPI_Scatter( void *sbuf, int scount, MPI_datatype stype,
                 void *rbuf, int rcount, MPI_datatype rtype,
                             int rootrank, MPI_Comm comm );

int MPI_Gather( void *sbuf, int scount, MPI_datatype stype,
                void *rbuf, int rcount, MPI_datatype rtype,
                            int rootrank, MPI_Comm comm );
```



Also, `MPI_Scatterv` and `MPI_Gatherv` for variable-sized local partitions

Example: 1D Finite Differences with collective communication

```
main(int argc, char *argv[]) {
  MPI_Comm com = MPI_COMM_WORLD;
  MPI_Init(&argc, &argv);
  MPI_Comm_size(com, &np);
  MPI_Comm_rank(com, &me);
  if (me == 0) {                    /* Read problem size at process 0 */
    read_problem_size(&size);
    buff[0] = size;
  }
  /* Global broadcast propagates this data to all processes */
  MPI_Bcast(buff, 1, MPI_INT, 0, com);
  /* Extract problem size from buff; allocate space for local data */
  lsize = buff[0]/np;
  local = malloc(lsize+2);
  /* Read input data at process 0; then distribute to processes */
  if (me == 0) { work = malloc(size); read_array(work); }
  MPI_Scatter(work, lsize, MPI_FLOAT, local+1, lsize,
              MPI_FLOAT, 0, com);
  lnbr = (me+np-1)%np;              /* Determine my neighbors in ring */
  rnbr = (me+1)%np;
  globalerr = 99999.0;
  while (globalerr > 0.1) {         /* Repeat until termination */
    /* Exchange boundary values with neighbors */
    ls = local+lsize;
    MPI_Send(local+2, 1, MPI_FLOAT, lnbr, 10, com);
    MPI_Recv(local+1, 1, MPI_FLOAT, rnbr, 10, com, &status);
    MPI_Send(ls-2, 1, MPI_FLOAT, rnbr, 20, com);
    MPI_Recv(ls-1, 1, MPI_FLOAT, lnbr, 20, com, &status);
    compute(local);
    localerr = maxerror(local); /* Determine local error */
    /* Find maximum local error, and replicate in each process */
    MPI_Allreduce(&localerr, &globalerr, 1, MPI_FLOAT,
                  MPI_MAX, com);
  }
  /* Collect results at process 0 */
  MPI_Gather(local, lsize, MPI_FLOAT, work, size,
             MPI_FLOAT, 0, com);
  if (me == 0) { write_array(work); free(work); }
  MPI_Finalize();
}
```



Source: Ian Foster: Designing and building parallel programs.
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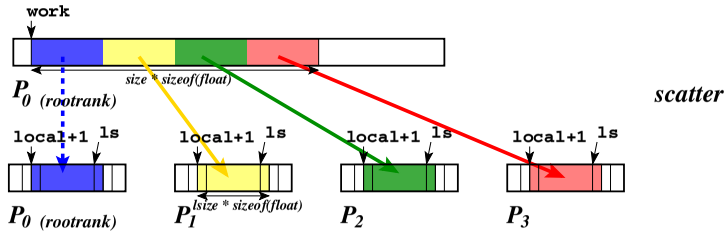
Example, detailed look (1)

```
main ( int argc, char *argv[] )
{
  int np, me, size, lsize, buff[1];
  float *local, *work, localerr, globalerr;

  MPI_Comm com = MPI_COMM_WORLD;
  MPI_Init( &argc, &argv );
  MPI_Comm_size( com, &np );
  MPI_Comm_rank( com, &me );

  if (me == 0) { // read problem size at process 0:
     read_problem_size( &size );
     buff[0] = size;
  }
  // Single-Broadcast of size from P0 to P1...P(np-1):
  MPI_Bcast( buff, 1, MPI_INT, 0, com );
  // Extract problem size from buff; allocate space:
  lsize = buff[0] / np;  // local problem size
  local = (float *) malloc ( (lsize+2) * sizeof(float) );
  ...
```

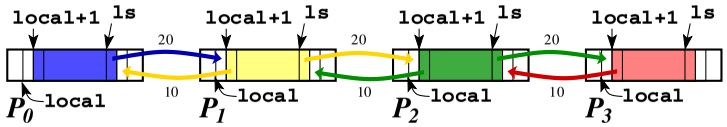

Example, detailed look (2)

```
  ...
  if (me == 0) { // read input data:
     work = (float *) malloc( size * sizeof(float) );
     read_array( work, size );
  }
  // Distribute work's contents from P0 across all processes:
  MPI_Scatter( work, lsize, MPI_FLOAT,
               local+1, lsize, MPI_FLOAT, 0, com );
  lnbr = (me + np - 1) % np;  // left neighbor rank
  rnbr = (me + 1) % np;       // right neighbor rank
  ls = local + lsize;    // points to my last local element
```



Example, detailed look (3)

```
...
globalerr = 99999.0;  // large value
while (globalerr > 0.1) {
   // Exchange boundary values with neighbors:
   MPI_Send( local+1, 1, MPI_FLOAT, lnbr, 10, com );
   MPI_Recv( ls+1, 1, MPI_FLOAT, rnbr, 10, com, &status );
   MPI_Send( ls, 1, MPI_FLOAT, rnbr, 20, com );
   MPI_Recv( local, 1, MPI_FLOAT, lnbr, 20, com, &status );
   compute( local, lsize );   // update my inner elements
   localerr = maxerror( local );
   MPI_Allreduce( &localerr, &globalerr, 1, MPI_FLOAT,
                  MPI_MAX, com );
}
...
```



Questions on the example (for self-evaluation)

Draw a figure that shows in detail which elements are exchanged between neighbor processors in the `send` and `recv` operations.

Question 1:

Is it necessary (for correct execution) to use *different* tags (10, 20) in the exchange phase?

Question 2:

How could this program be improved in efficiency?

(*Hint:* try to overlap communication phases with local computation where possible.)

Question 3:

Try to construct a deadlock situation by reordering the `send` / `recv` operations.

Virtual topologies in MPI

Example: arrange 12 processors in 3×4 grid

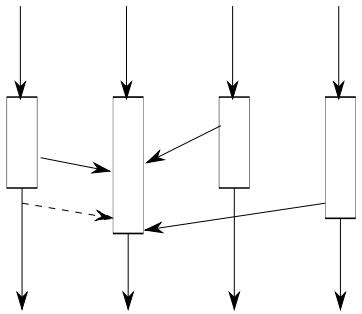
```
int dims[2], coo[2], period[2], src, dest;
period[0]=period[1]=0;  // 0=grid, !0=torus
reorder=0; // 0=use ranks in communicator,
           // !0=MPI uses hardware topology
dims[0] = 3; // extents of a virtual
dims[1] = 4; // 3X4 processor grid

// create virtual 2D grid topology:
MPI_Cart_create( comm, 2, dims, period,
                 reorder, &comm2 );

// get my coordinates in 2D grid:
MPI_Cart_coords( comm2, myrank, 2, coo );

// get rank of my grid neighbor in dim. 0
MPI_Cart_shift( comm2, 0, +1, // to south,
                &src, &dest); // from south
...
```

0 (0,0)	**1** (0,1)	**2** (0,2)	**3** (0,3)
4 (1,0)	**5** (1,1)	**6** (1,2)	**7** (1,3)
8 (2,0)	**9** (2,1)	**10** (2,2)	**11** (2,3)

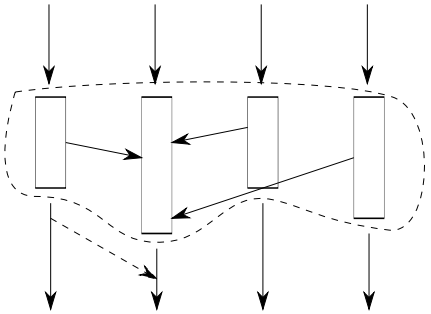
```
...
coo[0]=i; coo[1]=j;

// convert cartesian coordin.
// (i,j) to rank r:
MPI_Cart_rank(comm, coo, &r);

// and vice versa:
MPI_Cart_coords(comm,r,2,coo);
```


Communicator concept – Motivation

Communication error in a sequential composition
where a message is intercepted
by a library routine:



Source: Ian Foster: Designing and building parallel programs.



Avoid error by using a separate context
(separate tag space for messages)

Communicator concept

Communicators provide information hiding when building modular programs.

- identify a process group and the context in which a communication occurs.
- encapsulate internal communication operations within a process group (e.g. through local process identifiers)

→ MPI supports sequential and parallel module composition
(concurrent composition only for MPI-2)

Default communicator: `MPI_COMM_WORLD`

- includes all MPI processes
- defines default context

Communicator functions

`MPI_COMM_DUP` (*comm*, *newcomm*)
creates a new communicator with same processes as *comm*
but with a different context with different message tags.

→ supports sequential composition

Furthermore:

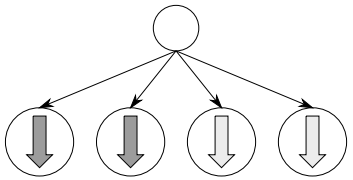
`MPI_COMM_SPLIT` (*comm*, *color*, *key*, *newcomm*)
create a new communicator for a *subset of a group* of processes

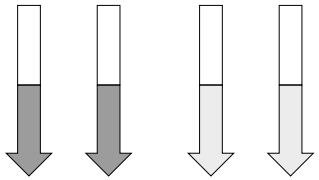
`MPI_INTERCOMM_CREATE` (*comm*, *local_leader*, ... *remote_leader*, ...*intercomm*)
create an intercommunicator, linking processes in different groups

`MPI_COMM_FREE` (*comm*)
release previously created communicator *comm*

Communicators for splitting process sets

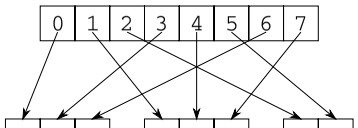
`MPI_COMM_SPLIT` (*comm*, *color*, *key*, *newcomm*)
used for parallel composition of process groups.
A fixed set of processes changes character.





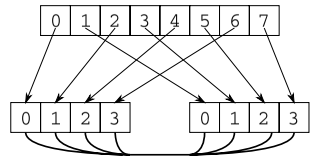
Example:

```
color = myid % 3
   // make color 0, 1, or 2
MPI_COMM_SPLIT( comm, color,
                key, newcomm)
```



Source: Ian Foster: Designing and building parallel programs.

Communicators for communicating between process groups



An *intercommunicator* connects two process groups

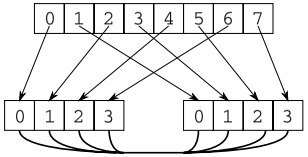
- needs a common parent process (*peercomm*)
- needs a leader process for each process group (*local_leader*, *remote_leader*)
- The local communicator *comm* denotes one of the process groups
- The created intercommunicator is placed in *intercomm*
- The *tag* is used for "safe" communication between the two leaders

`MPI_INTERCOMM_CREATE` (*comm*, *local_leader*,
peercomm, *remote_leader*, *tag*, *intercomm*)

Communicators for communicating between process groups (cont.)

Example:
(program fragment executing on each processor)

split into 2 groups: odd / even numbered




```
call MPI_COMM_SPLIT( MPI_COMM_WORLD, mod(myid,2), myid, comm, ierr)
...
if (mod(myid,2) .eq. 0) then
```

Group 0: create intercommunicator and send message

local leader: 0, remote leader: 1, tag = 99

```
  call MPI_INTERCOMM_CREATE( comm, 0, MPI_COMM_WORLD, 1, 99, intercomm,ierr
  ...
else
```

Group 1: create intercommunicator and send message

note that remote leader has ID 0 in `MPI_COMM_WORLD`:

```
  call MPI_INTERCOMM_CREATE( comm, 0, MPI_COMM_WORLD, 0, 99, intercomm,ierr
  ...
```


One-sided communication (MPI-2)

One-sided communication / Remote memory access (RMA)

- Each MPI process sets up a separate ”thread” for servicing RMA requests
- Limited to a fixed memory block (RMA Window)

RMA Windows

```
int MPI_Win_create ( void *base, MPI_Aint size, int d,
                     MPI_Info info, MPI_Comm comm, MPI_Win *Win )
```

open memory block *base* with *size* bytes for RMA by other processors
displacement unit *d* bytes (distance between neighbored elements)
additional info (typ. MPI_INFO_NULL) to runtime system
$\rightarrow$ window descriptor *Win*

```
MPI_Win_free ( MPI_Win *win )
```


One-sided communication in MPI-2 (2)

3 non-blocking RMA operations:

`MPI_Put`
remote write

`MPI_Get`
remote read

`MPI_Accumulate`
remote reduction

Concurrent read and write leads to unpredictable results.

Multiple Accumulate operations on same location are possible.

One-sided communication in MPI-2 (3)

```
MPI_Win_fence ( int assert, MPI_Win *win )
```

global synchronization of all processors
that belong to the group that declared *win*
flushes all pending writes to *win* ($\rightarrow$ consistency)
assert typ. 0 (tuning parameter for runtime system)

```
while (! converged( A )) {
  update ( A );
  update_buffer( A, from_buf );
  MPI_Win_fence ( 0, win );
  for (i=0; i<num_neighbors; i++)
    MPI_Put ( &from_buf[i], size[i], MPI_INT,
              neighbor[i],
              to_disp[i], size[i], MPI_INT,  win );
  MPI_Win_fence ( 0, win );
}
```

One-sided communication in MPI-2 (4)

Advanced issues

partial synchronization for a subgroup
synchronizing only the accessing and the accessed processor

lock synchronization of two processors
using a window on a third, not involved process as lock holder

Additional MPI / MPI-2 features

- Derived data types
  user can construct and register new data types in MPI type system,
  e.g. row/column vectors of certain length/stride,
  indexed vectors, aggregates of heterogeneous types
  $\rightarrow$ allows for extended type checking for incoming messages
- Dynamic process creation and management in MPI-2
- Additional global communication operations
- Environment inquiry functions

MPI Summary

SPMD style parallelism, p processes with fixed processor ID $0..p-1$
- dynamic process creation / concurrent composition possible in MPI-2

Processes interact by exchanging messages
- messages are typed (but not statically type-safe!)
- point-to-point communication in different modes
- collective communication
- probing for pending messages
- determinism / liveness not guaranteed,
  but can be achieved by careful programming

Modularity through communicators
- combine subprograms by sequential or parallel composition

One-sided communication in MPI-2

Literature on MPI

MPI-Forum: http://www.mpi-forum.org/
Official MPI standard documents
MPI 3.0 expected in the near future

Book series:
Gropp, Lusk, Skjellum: *Using MPI*. Second edition, MIT press, 1999
Gropp, Lusk, Thakur: *Using MPI-2*. MIT press, 1999

Chapter 8 of
Foster: Designing and Building Parallel Programs, Addison-Wesley 1995