Numerical Simulation and Scientific Computing II

Lecture 2:
Distributed Parallel Computing II

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Acknowledgments

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2014 Parallel Programming Workshop Lecture Material on:

Introduction to the Message Passing Interface (MPI)

Thanks to

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Georg Hager (RRZE)

Gabriele Jost (Supersmith)

2013 Supercomputing Tutorial on:

Hybrid MPI and OpenMP Parallel Programming

Sources

- High Performance Computing Center Stuttgart (HLRS) Online Courses https://www.hlrs.de/about-us/media-publications/teaching-training-material/
- YouTube -- search for “Introduction to MPI”, e.g., https://youtu.be/RoQJNx5npF4 -- Part I of III

Additional Courses at TU Wien

ECTS Courses (count as free electives)

- 057.020 (Winter term)
  VSC-School I Courses in High Performance Computing
- 057.021 (Summer term)
  VSC-School II Courses in High Performance Computing

Non-ECTS Trainings (don't count as free electives)

- Node-Level Performance Engineering
- OpenMP
- MPI
- Deep-Learning und GPU programming (OpenACC)
- Hybrid-programming MPI+X

http://typo3.vsc.ac.at/research/vsc-research-center/vsc-school-seminar/

Quiz

Q1: How is it ensured that a specific message is received by a specific process?

→ *tag* and *dest* parameter

Q2: What is the first and last routine to be called in a MPI program?

→ *MPI_Init (…)* and *MPI_Finalize()*

Q3: Is "MPI_Init" executed by one, several or all MPI processes?

→ all

Q4: Name typical reduction operations?

→ sum, min, max, etc.

Q5: How can a point-to-point communication be made non-blocking? What potential advantage is there?

→ MPI_I…, potentially allows to overlap communication with computation

Outline

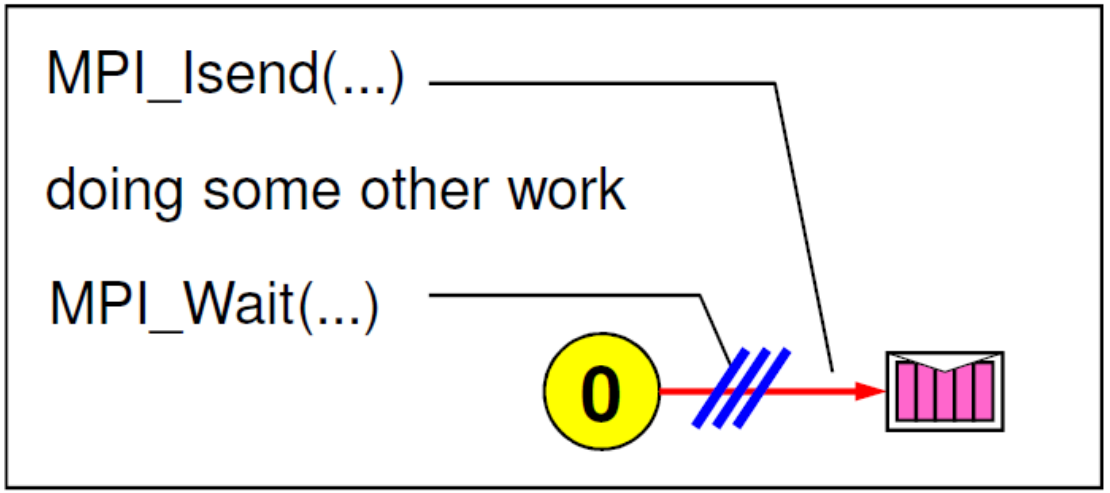
- Distributed Parallel Computing II
  - **Non-Blocking Communication**
  - Collective Communication
  - Derived Datatypes
  - Virtual Topologies
  - Hybrid MPI+OpenMP
- Quiz

Non-Blocking Communications

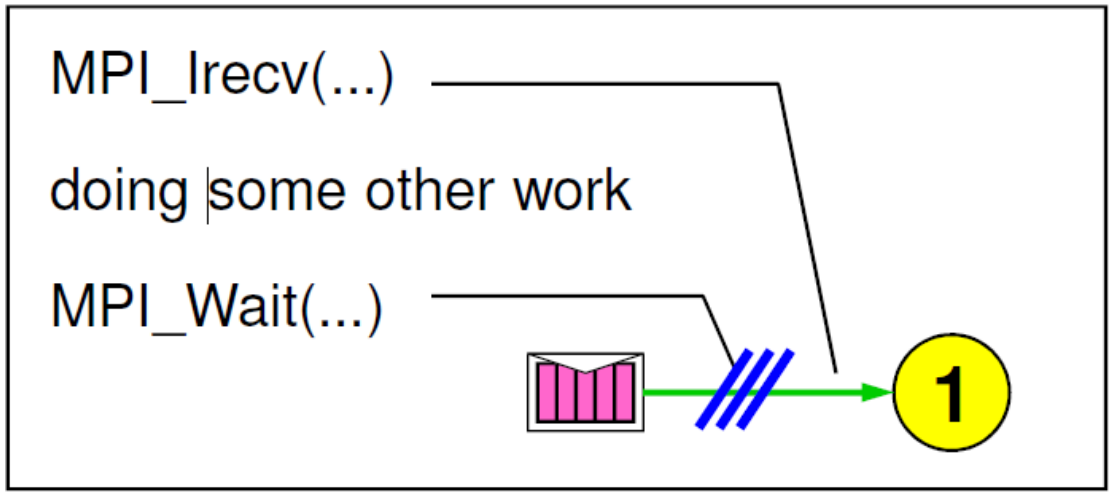
- Separate communication into three phases:
  - Initiate nonblocking communication
    - returns Immediately
    - routine name starting with MPI_I…
  - Do some work (perhaps involving other communications?)
  - Wait for non-blocking communication to complete

Non-Blocking Examples

- **Non-blocking send**

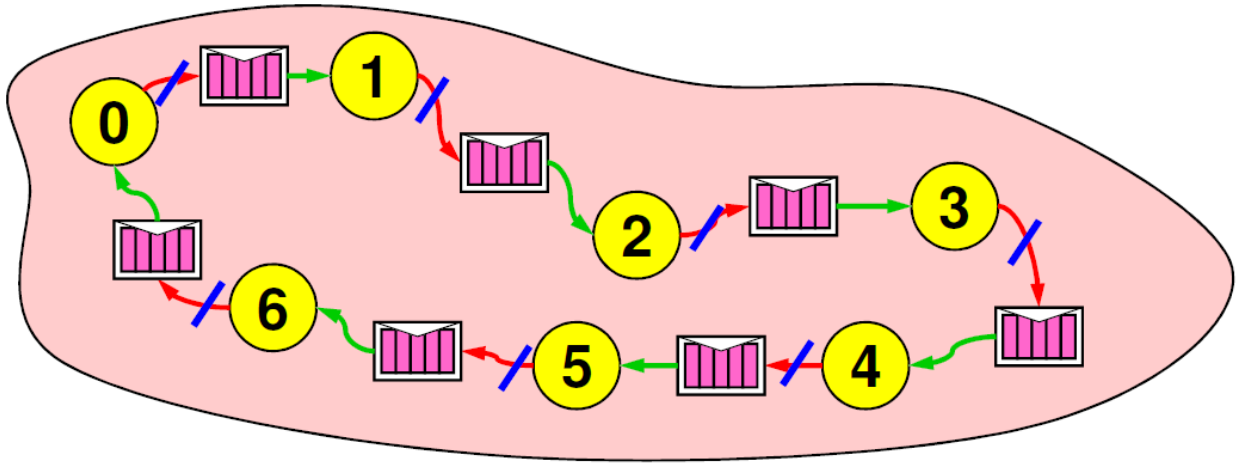


- **Non-blocking receive**



Non-Blocking Send

- Initiate non-blocking send
  - Ring example: Initiate non-blocking send to the right neighbor
- Do some work
  - Ring example: Receiving the message from left neighbor
- Message transfer can be completed
- Wait for non-blocking send to complete

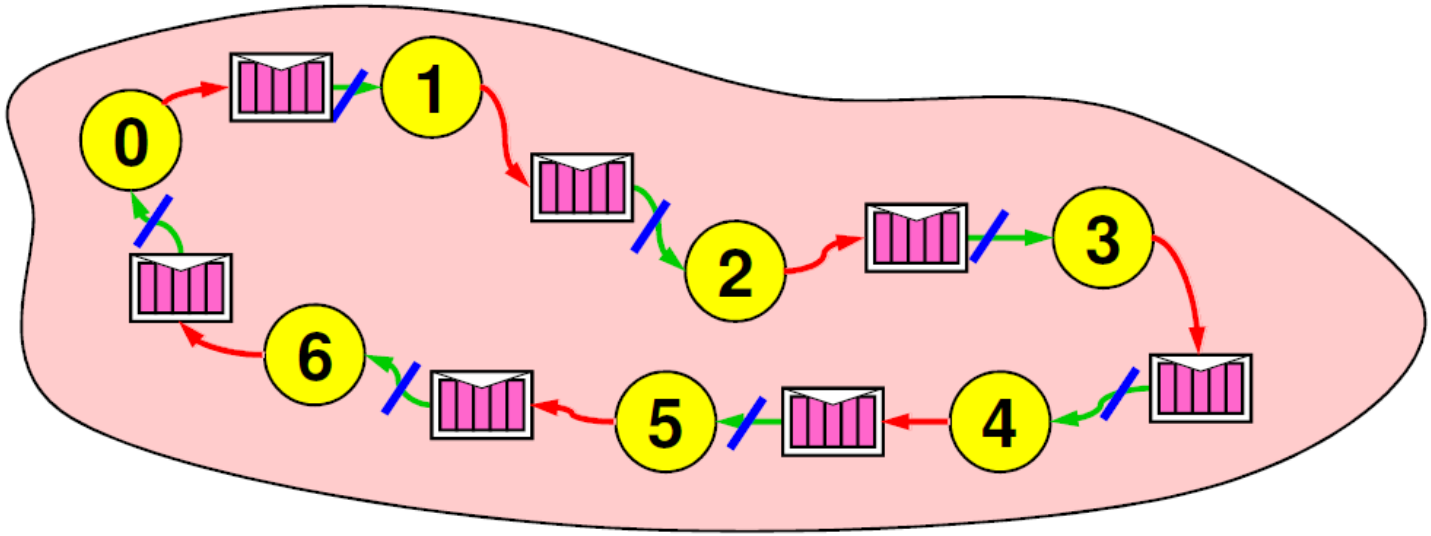


Non-Blocking Receive

- Initiate non-blocking receive
  - Ring example: Initiate non-blocking receive from left neighbor

- Do some work
  - Ring example: Sending the message to the right neighbor

- Message transfer can be completed
- Wait for non-blocking receive to complete



Request Handles

- **Request handles**
  - **Are used for non-blocking communication**
  - **Must be stored in local variables: MPI_Request**
    - **is generated by a non-blocking communication routine**
    - **is used (and freed) in the MPI_WAIT routine**

Non-Blocking Synchronous Send

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

```
MPI_Issend( buf, count, datatype, dest, tag, comm, [OUT] &request_handle);
        ⬇
MPI_Wait( [INOUT] &request_handle, &status);
```

Nonblocking Receive

- **buf must not be used between Irecv and Wait**

MPI_Irecv (buf, count, datatype, source, tag, comm, [OUT] &request_handle);

MPI_Wait([INOUT] &request_handle, &status);

Blocking and Non-Blocking

- Send and receive can be blocking or non-blocking.
- A blocking send can be used with a non-blocking receive, and vice-versa.
- Non-blocking sends can use any mode
  - standard – MPI_ISEND
  - synchronous – MPI_ISSEND
  - buffered – MPI_IBSEND
  - ready – MPI_IRSEND
- Synchronous mode affects completion, i.e. MPI_Wait / MPI_Test, not initiation, i.e., MPI_I...
- The non-blocking operation immediately followed by a matching wait is equivalent to the blocking operation.

Completion

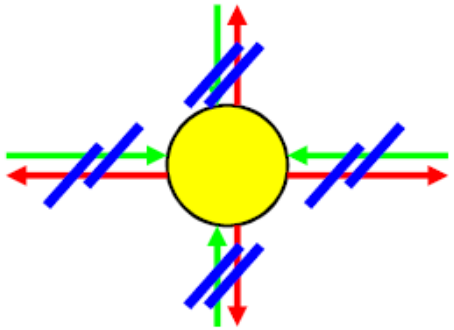
```
MPI_Wait( &request_handle, &status);
MPI_Test( &request_handle, &flag, &status);
```

- **You need to**
  - **WAIT or**
  - **Loop with TEST until request is completed, i.e., flag == 1**

Multiple Non-Blocking Communications

You have several request handles:

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



***) Each status contains an additional error field.**

This field is only used if MPI_ERR_IN_STATUS is returned (also valid for send operations).

Send-Receive in One Routine

- **MPI_Sendrecv & MPI_Sendrecv_replace**
  - **Combines the triple “MPI_Irecv + Send + Wait” into one routine**

Performance Options

Which is the fastest neighbor communication?

- **MPI_Irecv + MPI_Send**
- **MPI_Irecv + MPI_Isend**
- **MPI_Isend + MPI_Recv**
- **MPI_Isend + MPI_Irecv**
- **MPI_Sendrecv**
- **MPI_Neighbor_alltoall**

No answer by the MPI standard, because:

MPI targets portable and efficient message-passing programming but efficiency of MPI application-programming is not portable!

Example Non-Blocking Communication

- **Integration with MPI non-blocking communications**
  - **Example source:** http://www.bu.edu/tech/support/research/training-consulting/online-tutorials/mpi/example1-2/example1_3/
  - **Background on numerical integration:** http://www.bu.edu/tech/support/research/training-consulting/online-tutorials/mpi/example1-2/
- **Until a matching receive has signaled that it is ready to receive, a blocking send will continue to wait.**

```
void other_work(int myid) {
  printf("more work on process %dn", myid);
}
float integral(float ai, float h, int n){
  int j;
  float aij, integ;
  integ = 0.0;                /* initialize */
  for (j=0;j<j++) {          /* sum integrals */
    aij = ai + (j+0.5)*h;      /* mid-point */
    integ += cos(aij)*h;
  }
  return integ;
}
```

Support Functions

Example Non-Blocking Communication

Common Part

```
int n, p, myid, tag, master, proc, ierr;
float h, integral_sum, a, b, ai, pi, my_int;
MPI_Comm comm;
MPI_Request request;
MPI_Status status;
comm = MPI_COMM_WORLD;
ierr = MPI_Init(&argc,&argv);          /* starts MPI */
MPI_Comm_rank(comm, &myid);            /* get current process id */
MPI_Comm_size(comm, &p);               /* get number of processes */
master = 0;
pi = acos(-1.0);  /* = 3.14159... */
a = 0.;           * lower limit of integration */
b = pi*1./2.;     /* upper limit of integration */
n = 500;          /* number of increment within each process */
tag = 123;        /* set the tag to identify this particular job */
h = (b-a)/n/p;    /* length of increment */
ai = a + myid*n*h;  /* lower limit of integration for partition myid */
my_int = integral(ai, h, n);    /* 0<=myid<=p-1 */
printf("Process %d has the partial result of %fn", myid, my_int);
```

Example Non-Blocking Communication

Master Part

```
if(myid == master) {
  integral_sum = my_int;
  for (proc=1;proc<p;proc++) {
    MPI_Recv(
            &my_int, 1, MPI_FLOAT,    /* triplet of buffer, size, data type */
            MPI_ANY_SOURCE,       /* message source */
            MPI_ANY_TAG,          /* message tag */
            comm, &status);       /* status identifies source, tag */
    integral_sum += my_int;
  }
  printf("The Integral =%fn",integral_sum); /* sum of my_int */
}
```

Example Non-Blocking Communication

Worker Part

```
else {
  MPI_Isend(      /* non-blocking send */
            &my_int, 1, MPI_FLOAT,      /* triplet of buffer, size, data type */
            master,
            tag,
            comm, &request);      /* send my_int to master */
  other_work(myid);
  MPI_Wait(&request, &status);    /* block until Isend is done */
 }
 MPI_Finalize();                  /* let MPI finish up ... */
}
```

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- Distributed Parallel Computing II
  - Non-Blocking Communication
  - **Collective Communication**
  - Derived Datatypes
  - Virtual Topologies
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Collective Communication

- Communications involving a group of processes.
- Called by all processes in a communicator.
- Examples:
  - Barrier synchronization.
  - Broadcast, scatter, gather.
  - Global sum, global maximum, etc.
  - Neighbor communication in a virtual grid

Characteristics of Collective Communication

- Collective action over a communicator.
- All processes of the communicator must communicate, i.e., must call the collective routine.
- Synchronization may or may not occur, therefore all processes must be able to start the collective routine.
- On a given communicator, the n-th collective call must match on all processes of the communicator.
- In MPI-1.0 – MPI-2.2, all collective operations are blocking. Non-blocking versions since MPI-3.0.
- No tags.
- Receive buffers must have exactly the same size as send buffers.

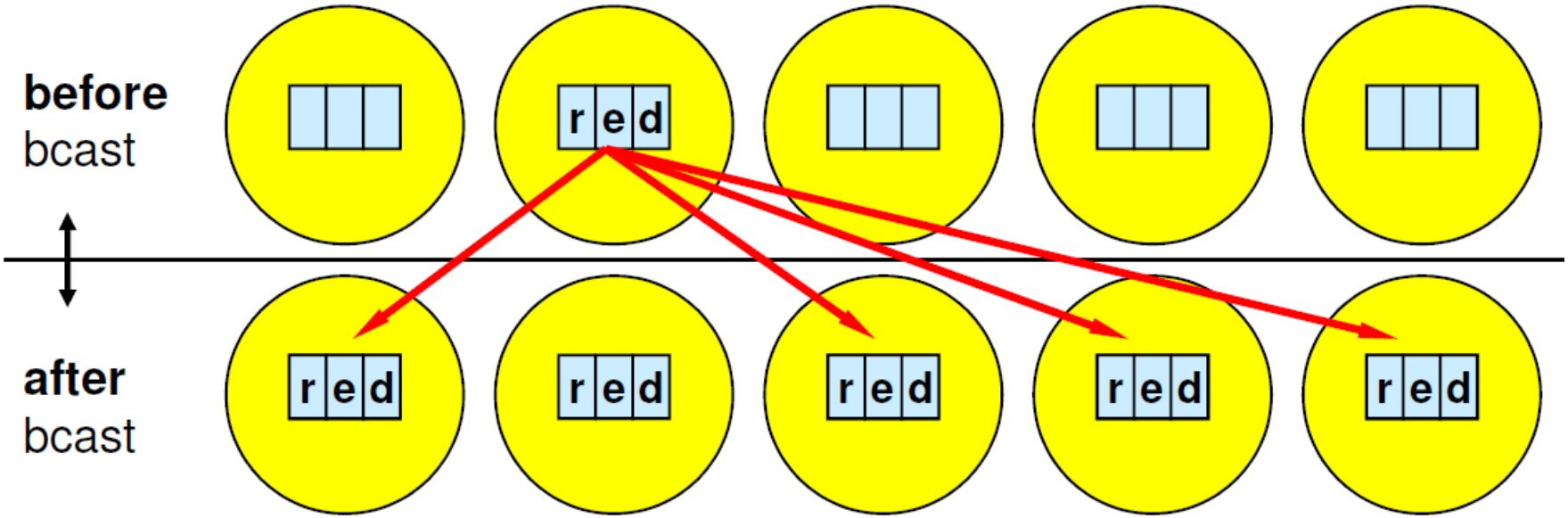
Barrier Synchronization

MPI_Barrier is normally never needed:

- **all synchronization is done automatically by the data communication:**
  a process cannot continue before it has the data that it needs.
- **if used for debugging:**
  please guarantee, that it is removed in production.
- **for profiling: to separate time measurement of**
  - **Load imbalance of computation [MPI_Wtime(); MPI_Barrier(); MPI_Wtime()]**
  - **communication epochs [MPI_Wtime(); MPI_Allreduce(); …; MPI_Wtime()]**

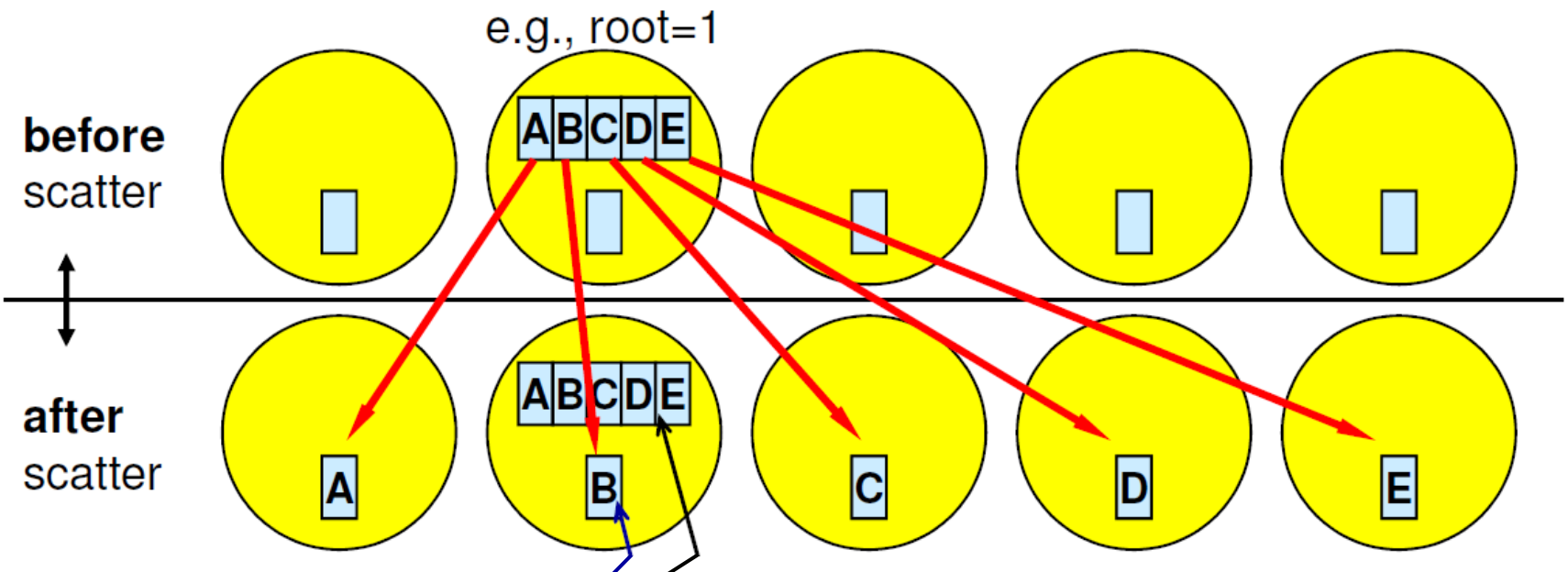
Broadcast

```
int MPI_Bcast(void *buf, int count, MPI_Datatype datatype,
              int root, MPI_Comm comm)
```



- **E.g. root=1**
- **Rank of the sending process (i.e., root process) must be given identically by all processes**

Scatter

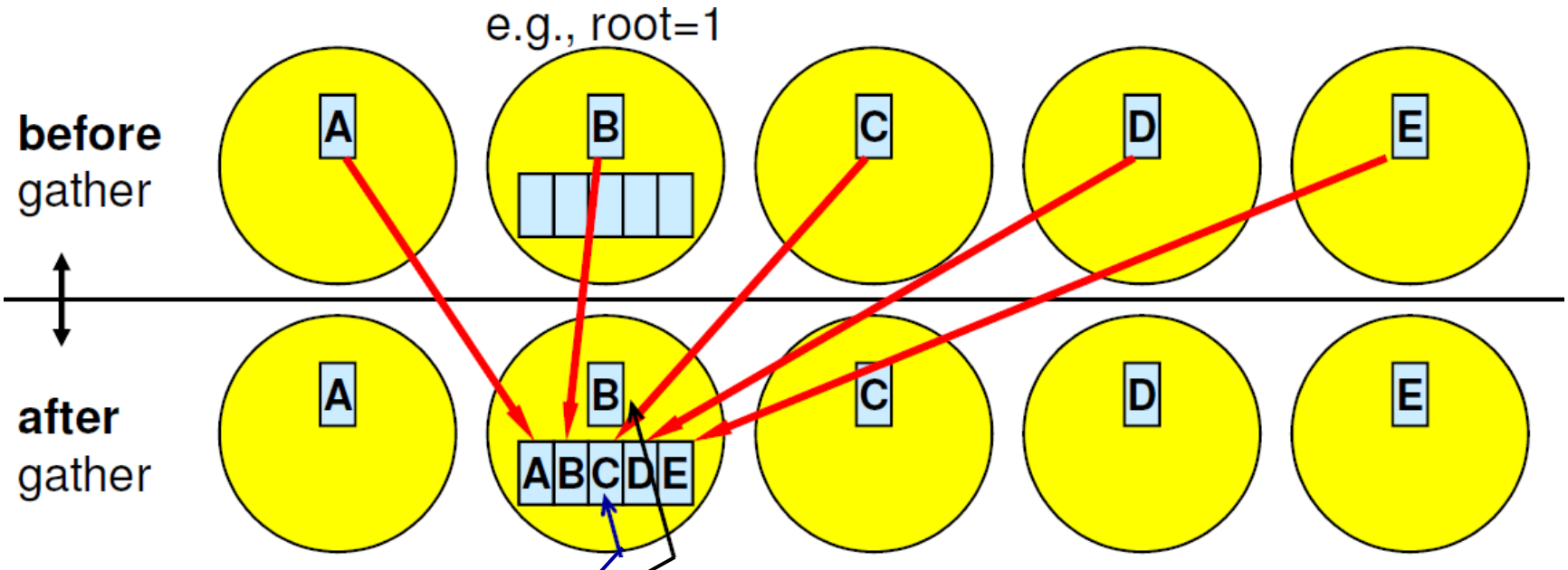



```
int MPI_Scatter(void *sendbuf, int sendcount, MPI_Datatype sendtype,
                void *recvbuf, int recvcount, MPI_Datatype recvtype,
                int root, MPI_Comm comm)
```

- **Example**

```
MPI_Scatter(sbuf, 1, MPI_CHAR,
            rbuf, 1, MPI_CHAR,
            1, MPI_COMM_WORLD)
```

Gather




```
int MPI_Gather(void *sendbuf, int sendcount, MPI_Datatype sendtype,
               void *recvbuf, int recvcount, MPI_Datatype recvtype,
               int root, MPI_Comm comm)
```

- **Example**

```
MPI_Gather(sbuf, 1, MPI_CHAR,
           rbuf, 1, MPI_CHAR,
           1, MPI_COMM_WORLD)
```

Global Reduction Operations

- To perform a global reduce operation across all members of a group.
- d0 o d1 o d2 o d3 o … o ds-2 o ds-1
  - di = data in process rank i
    - single variable, or
    - vector
  - o = associative operation
  - Example:
    - global sum or product
    - global maximum or minimum
    - global user-defined operation
- Floating point rounding may depend on usage of associative law
  - [(d**0** **o** d**1**) **o** (d**2** **o** d**3**)] **o** [… **o** (d**s-2** **o** d**s-1**)]

Example of Global Reduction

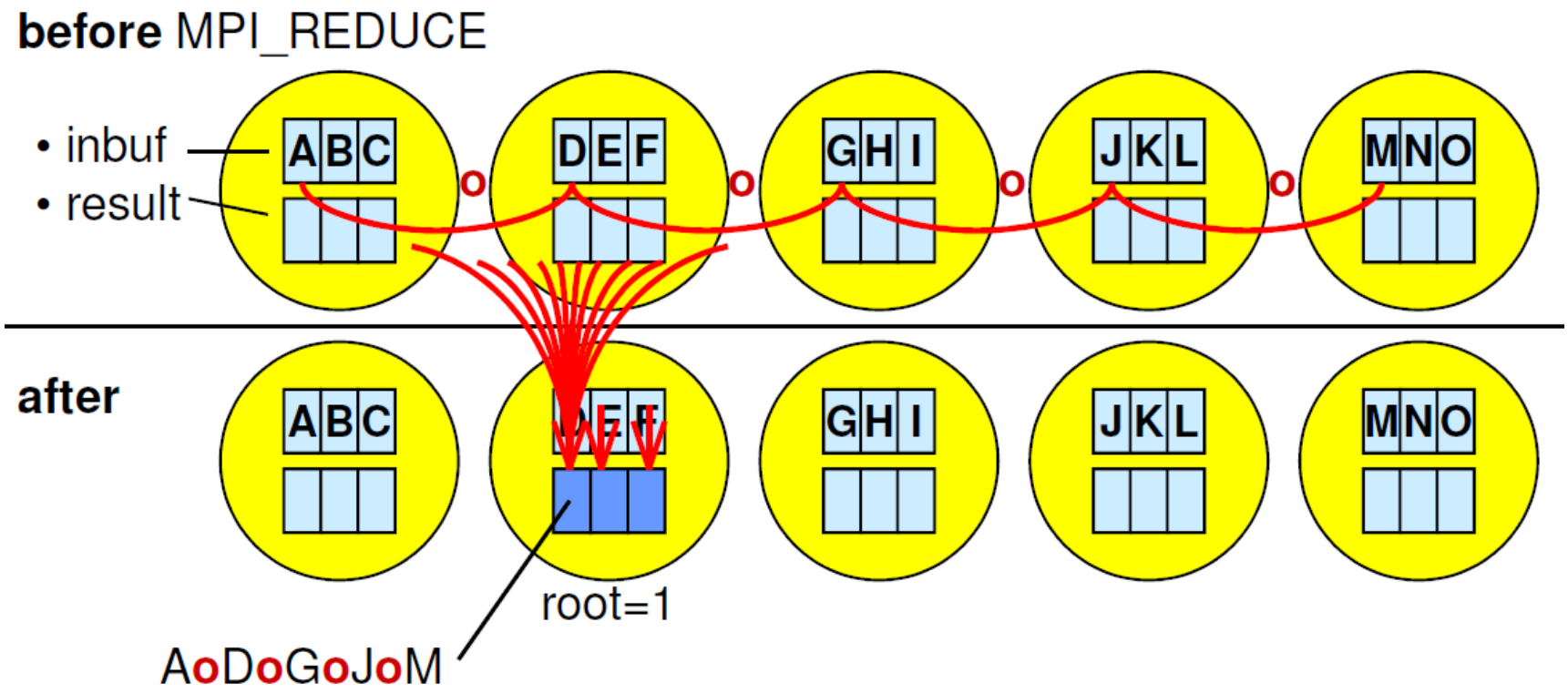
- **Global integer sum.**
- **Sum of all inbuf values should be returned in *resultbuf*.**
- **The result is only placed in *resultbuf* at the root process.**

```
root=0;
MPI_Reduce(&inbuf, &resultbuf, 1, MPI_INT, MPI_SUM,
                   root, MPI_COMM_WORLD);
```

Predefined Reduction Operation Handles

Predefined operation handle	Function
MPI_MAX	Maximum
MPI_MIN	Minimum
MPI_SUM	Sum
MPI_PROD	Product
MPI_LAND	Logical AND
MPI_BAND	Bitwise AND
MPI_LOR	Logical OR
MPI_BOR	Bitwise OR
MPI_LXOR	Logical exclusive OR
MPI_BXOR	Bitwise exclusive OR
MPI_MAXLOC	Maximum and location of the maximum
MPI_MINLOC	Minimum and location of the minimum

Reduce



- **User-defined reduction operations possible**
  - **Not covered here**

Non-Blocking Collective Communication

- MPI_I..... Non-blocking variants of all collective communication:
  - MPI_Ibarrier, MPI_Ibcast, …
- Collective initiation and completion are separated
- May have multiple outstanding collective communications on same communicator
- Ordered initialization on each communicator
- Offers opportunity to overlap
  - several collective communications, e.g., on several overlapping communicators
    - Without deadlocks or serializations!
  - computation and communication

Example Collective Communication

- **Integration with MPI collective communications**
  - **Example source: http://www.bu.edu/tech/support/research/training-consulting/online-tutorials/mpi/example1-2/example1_4/**
  - **Adaption of previous example based on non-blocking communication**

```
float integral(float ai, float h, int n){
  int j;
  float aij, integ;
  integ = 0.0;              /* initialize */
  for (j=0;j<j++) {         /* sum integrals */
    aij = ai + (j+0.5)*h;     /* mid-point */
    integ += cos(aij)*h;
  }
  return integ;
}
```

Support Function

Example Collective Communication

First Part

```
int n, p, myid, tag, proc, ierr, i;
float h, integral_sum, a, b, ai, pi, my_int, buf[50];
int master = 0;  /* processor performing total sum */
MPI_Comm comm;
comm = MPI_COMM_WORLD;
ierr = MPI_Init(&argc,&argv);          /* starts MPI */
MPI_Comm_rank(comm, &myid);          /* get current process id */
MPI_Comm_size(comm, &p);            /* get number of processes */
pi = acos(-1.0);  /* = 3.14159... */
a = 0.;          /* lower limit of integration */
b = pi*1./2.;    /* upper limit of integration */
n = 500;         /* number of increment within each process */
tag = 123;       /* set the tag to identify this particular job */
h = (b-a)/n/p;    /* length of increment */
ai = a + myid*n*h;  /* lower limit of integration for partition myid */
my_int = integral(ai, h, n);   /* 0<=myid<=p-1 */
printf("Process %d has the partial sum of %fn", myid,my_int);
```

Example Collective Communication

```
MPI_Gather(      /* collects my_int from all processes to master */
     &my_int, 1, MPI_FLOAT,      /* send buffer, size, data type */
     buf, 1, MPI_FLOAT,     /* receive buffer, size, data type */
     master, comm);

if(myid == master) {
  integral_sum = 0.0;
  for (i=0; i< i++) {
    integral_sum += buf[i];
  }
  printf("The Integral =%fn",integral_sum);
}

MPI_Finalize();
```

Second Part

Outline

- Distributed Parallel Computing II
  - Non-Blocking Communication
  - Collective Communication
  - **Derived Datatypes**
  - Virtual Topologies
  - Hybrid MPI+OpenMP
- Quiz

- Description of the memory layout of the buffer
  - for sending
  - for receiving
- Basic types
- Derived types
  - vectors
  - structs
  - others

Data Layout and the Describing Datatype Handle

```
struct buff_layout
  { int    i_val[3];
    double d_val[5];
  } buffer;
```

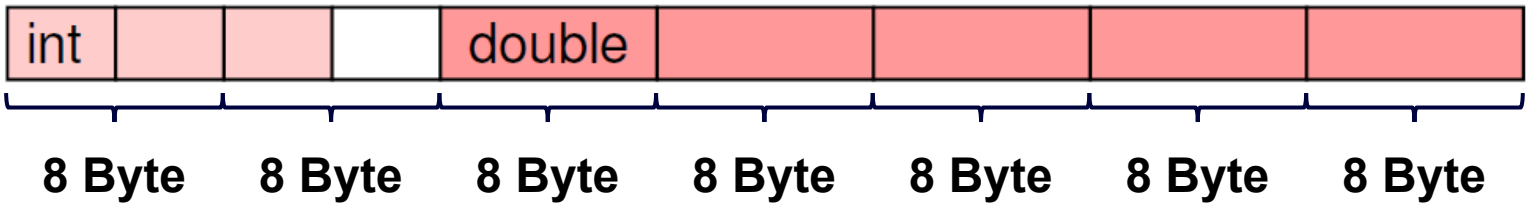
Compiler

```
array_of_types[0]=MPI_INT;
array_of_blocklengths[0]=3;
array_of_displacements[0]=0;
array_of_types[1]=MPI_DOUBLE;
array_of_blocklengths[1]=5;
array_of_displacements[1]=…;
MPI_Type_create_struct(2, array_of_blocklengths,
    array_of_displacements, array_of_types,
                          &buff_datatype);
MPI_Type_commit(&buff_datatype);
```

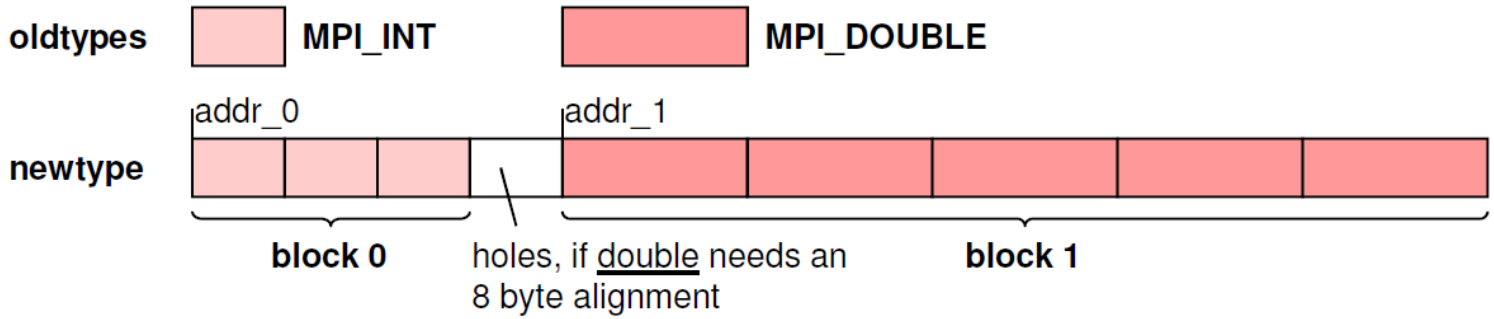
```
MPI_Send(&buffer, 1, buff_datatype, …)
```

&buffer = the start address of the data

the datatype handle describes the data layout



Struct Datatype




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

```
                  count =  2
array_of_blocklengths   = ( 3,          5              )
array_of_displacements  = ( 0,          addr_1 – addr_0 )
          array_of_types = ( MPI_INT,   MPI_DOUBLE     )
```

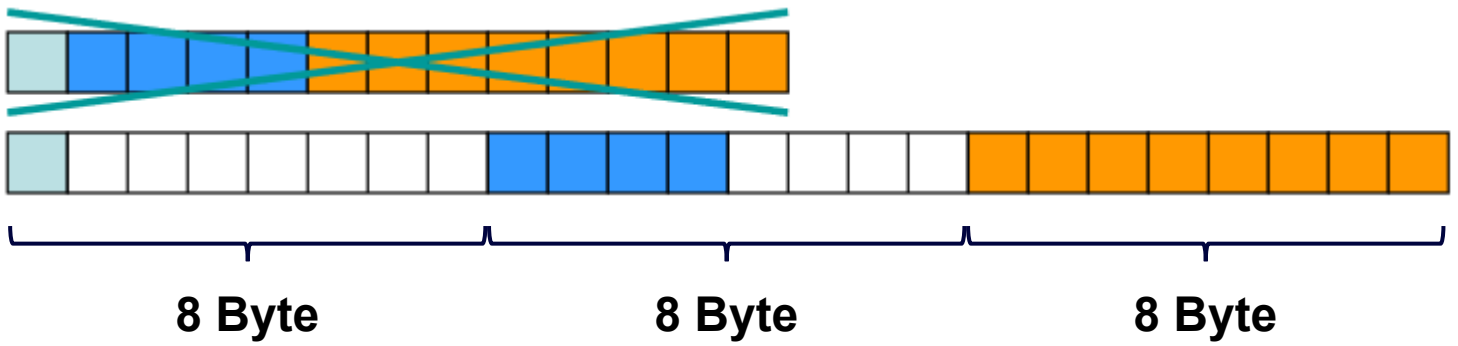
Compute Displacement

- **array_of_displacements[i] := address(block_i) – address(block_0)**

```
int MPI_Get_address(void* location, MPI_Aint *address)
```

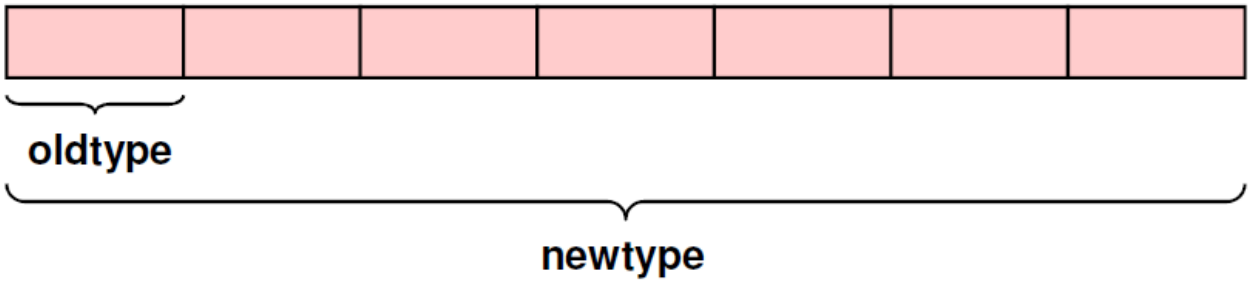
Memory Layout: Another Example

```
typedef struct {
  char      a;
  int       b;
  double    c;
} mystruct;
```



Contiguous Data

- **The simplest derived datatype**
- **Consists of a number of contiguous items of the same datatype**




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

Example

```
int myvec[4];
MPI_Type_contiguous ( 4, MPI_INT, &mybrandnewdatatype);
MPI_Type_commit ( &mybrandnewdatatype );
MPI_Send ( myvec, 1, mybrandnewdatatype, ... );
```

Committing ad Freeing a Datatype

- **Before a dataytype handle is used in message passing communication, it needs to be committed with MPI_TYPE_COMMIT.**
- **This need be done only once (by each MPI process). (More than once use equivalent to additional no-operations.)**
- **If usage is over, one may call MPI_TYPE_FREE() to free a datatype and its internal resources.**

```
int MPI_Type_commit(MPI_Datatype *datatype);
int MPI_Type_free     (MPI_Datatype *datatype);
```

Example Derived Datatype Struct

```
typedef struct {
  char     a;
  int      b;
  double   c;} mystruct;
mystruct mydata;
MPI_Address ( &mydata,   &baseaddr);
MPI_Address ( &mydata.b, &addr1);
MPI_Address ( &mydata.c, &addr2);
displ[0] = 0;
displ[1] = addr1 – baseaddr;
displ[2] = addr2 – baseaddr;
dtype[0] = MPI_CHAR;
blength[0] = 1;
dtype[1] = MPI_INT;
blength[1] = 1;
dtype[2] = MPI_DOUBLE;
blength[2] = 1;
MPI_Type_struct ( 3, blength, displ, dtype, &newtype );
MPI_Type_commit ( &newtype );
```

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  - Derived Datatypes
  - **Virtual Topologies**
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Virtual Topologies

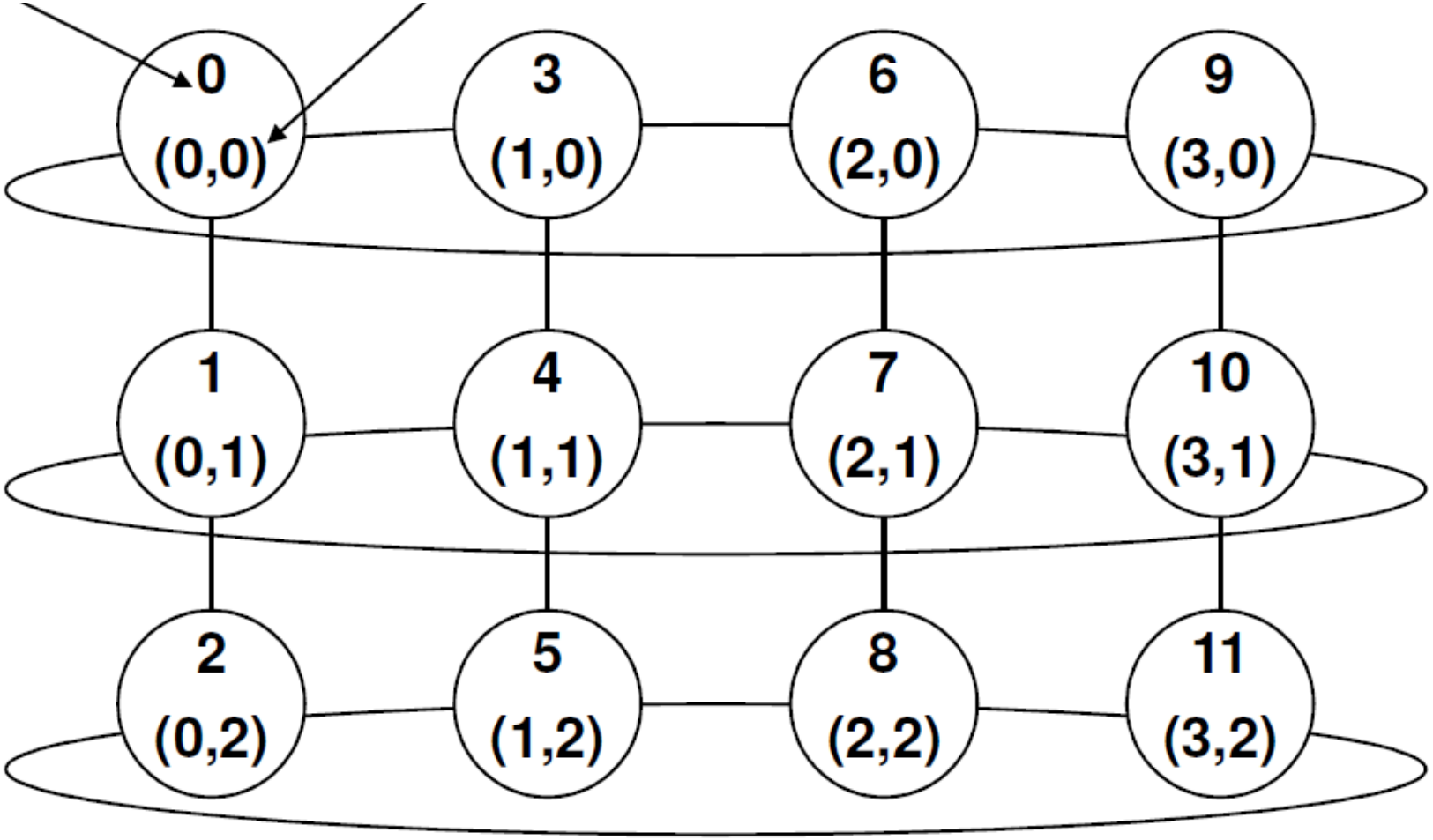
- Convenient process naming.
- Naming scheme to fit the communication pattern.
- Simplifies writing of code.
- Can allow MPI to optimize communications.

How to Use a Virtual Topology

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

Example – A Two-Dimensional Cylinder

- **Ranks and Cartesian process coordinates**



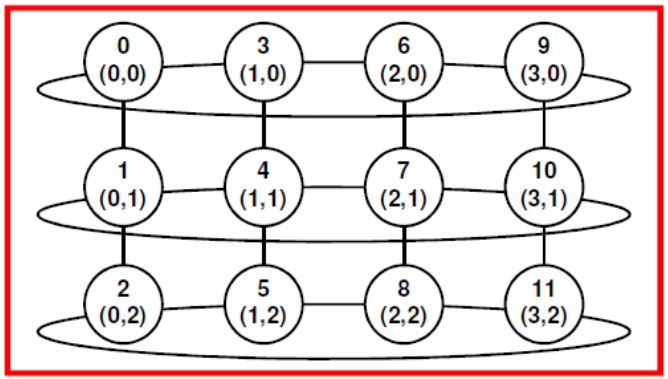
Topology Types

- Cartesian Topologies
  - each process is connected to its neighbor in a virtual grid,
  - boundaries can be cyclic, or not,
  - processes are identified by Cartesian coordinates,
  - of course, communication between any two processes is still allowed.
- Graph Topologies
  - general graphs,
  - two interfaces:
    - MPI_GRAPH_CREATE (since MPI-1)
    - MPI_DIST_GRAPH_CREATE_ADJACENT &
    - MPI_DIST_GRAPH_CREATE (new scalable interface since MPI-2.2)
  - not covered here.

Creating a Cartesian Virtual Topology

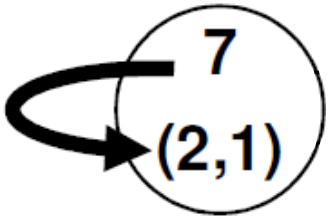
```
int MPI_Cart_create(MPI_Comm comm_old, int ndims,
                    int *dims, int *periods, int reorder,
                    MPI_Comm *comm_cart)
```

- **Comm_old = MPI_COMM_WORLD**
- **ndims = 2**
- **Dims = (4, 3)**
- **Periods = (1, 0)**
- **Reorder = 0 or 1**
  → Task MPI backend to optimally assign MPI ranks to specific Cartesian coordinates considering communication ramifications!
  → But then ranks in comm_cart differ from comm_old!



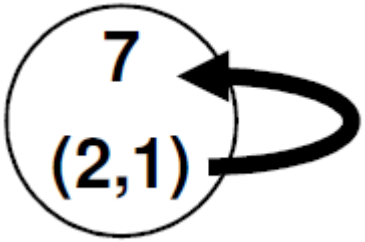
Cartesian Mapping Functions

- **Mapping ranks to process grid coordinates**



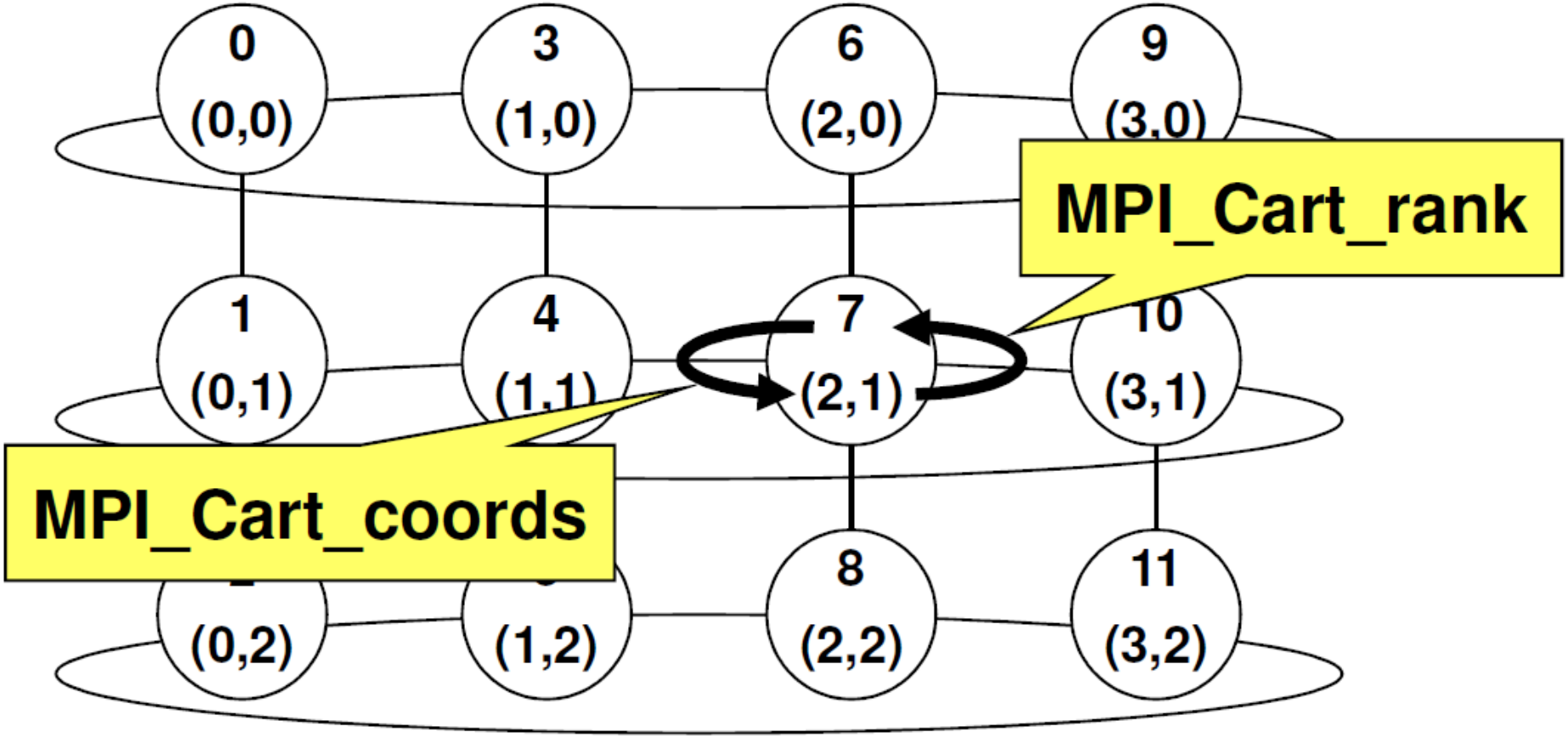

```
int MPI_Cart_coords(MPI_Comm comm_cart, int rank, int maxdims, int *coords)
```

- **Mapping process grid coordinates to ranks**




```
int MPI_Cart_rank(MPI_Comm comm_cart, int *coords, int *rank)
```

Cartesian Mapping Functions

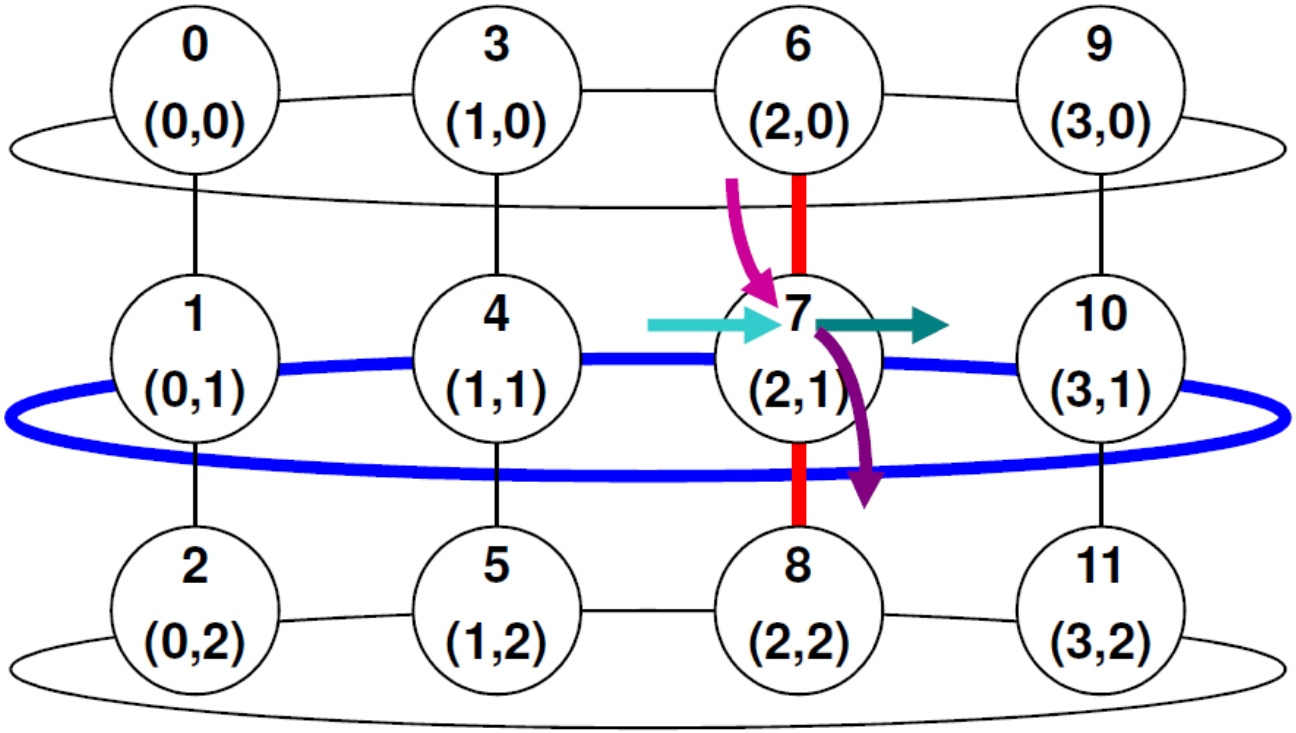


Cartesian Mapping Functions

- **Computing ranks of neighboring processes**
- **Returns MPI_PROC_NULL if there is no neighbor.**
- **MPI_PROC_NULL can be used as source or destination rank in each communication. →**
  Then, this communication will be a no-operation!

```
int MPI_Cart_shift(MPI_Comm comm_cart, int direction, int disp,
                   int *rank_source, int *rank_dest)
```

Cartesian Mapping Functions



invisible input argument: **my_rank** in cart

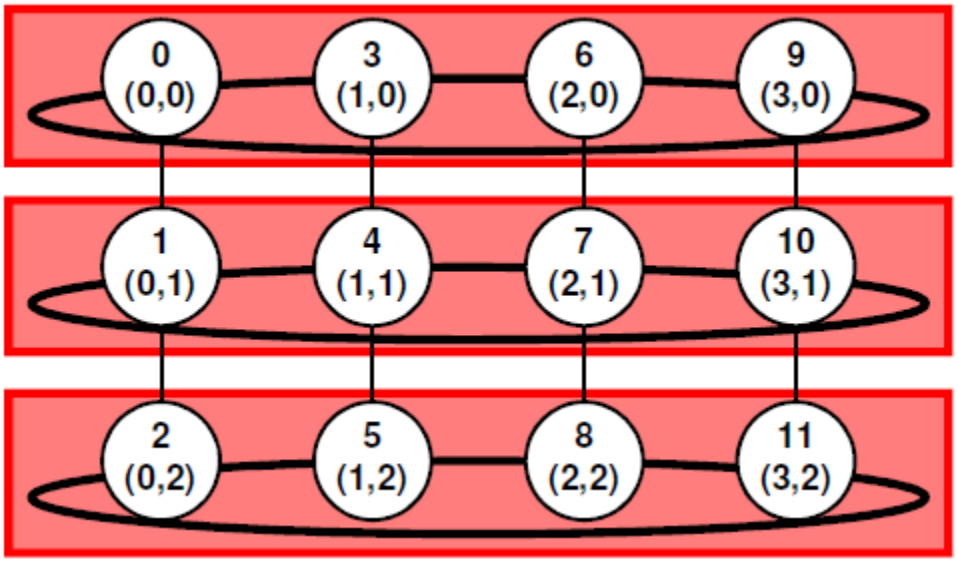
MPI_Cart_shift(cart, direction, displace, *rank_source*, *rank_dest*, *ierror*)

example on	**0** or	**+1**	4	10
process rank=**7**	1	+1	6	8

Cartesian Partitioning

- **Cut a grid up into slices.**
- **A new communicator is produced for each slice.**
- **Each slice can then perform its own collective communications.**

```
int MPI_Cart_sub( MPI_Comm comm_cart, int *remain_dims,
                  MPI_Comm *comm_slice)
```

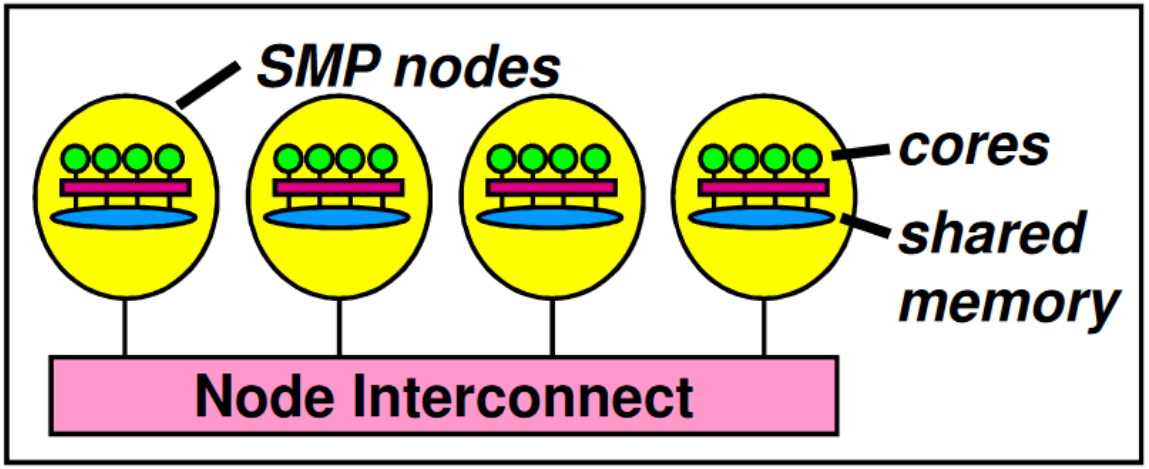


Outline

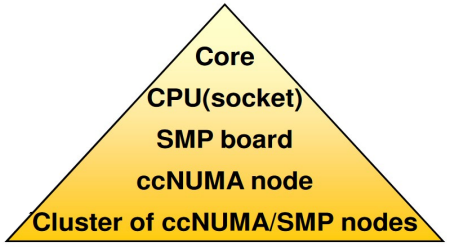
- Distributed Parallel Computing II
  - Non-Blocking Communication
  - Collective Communication
  - Derived Datatypes
  - Virtual Topologies
  - **Hybrid MPI+OpenMP**
- Quiz

Hybrid Parallel Programming

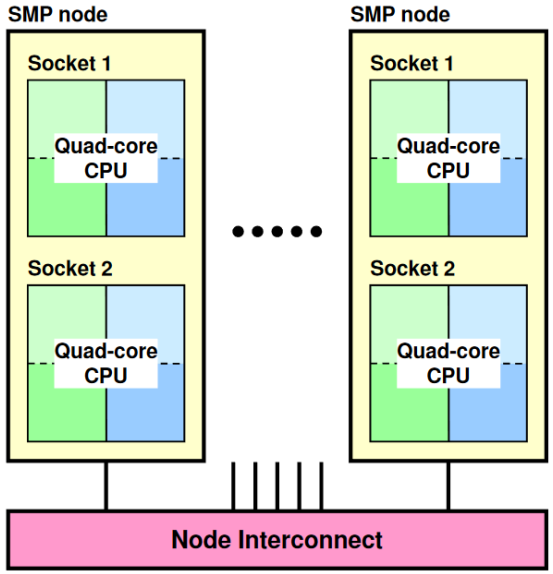
- **Hybrid parallel programming:**
  Mix different parallel programming approaches to efficiently use available computing platforms (heterogeneous computing resources)
- **Typical example:**
  Efficient programming of clusters of shared memory (SMP) nodes



Hybrid Parallel Programming



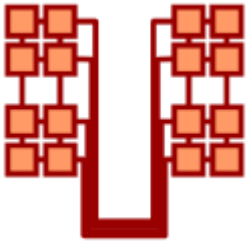
- Hierarchical system layout
- Hybrid programming seems *natural*
  - MPI between the nodes
  - Shared memory programming inside of each SMP node
    - OpenMP
    - MPI-3 shared-memory programming: not covered here
    - Accellerator programming (CUDA, OpenACC, etc): not covered here
    - And others.



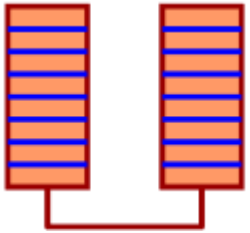
Hybrid Parallel Programming

- **Which programming model is best?**

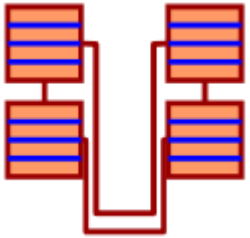
- **"Pure" MPI?**
  (a.k.a. 1 MPI process per CPU core, no shared-memory at all)



- **"Fully hybrid"?**
  (a.k.a. 1 MPI process per node, shared-memory within nodes)

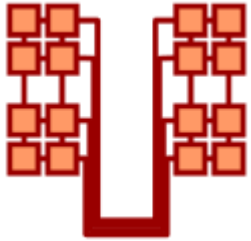


- **"Mixed hybrid"?**
  (a.k.a. 1 MPI process per, e.g., CPU, shared-memory within the CPUs; other combinations possible, e.g., (cc)NUMA specific)

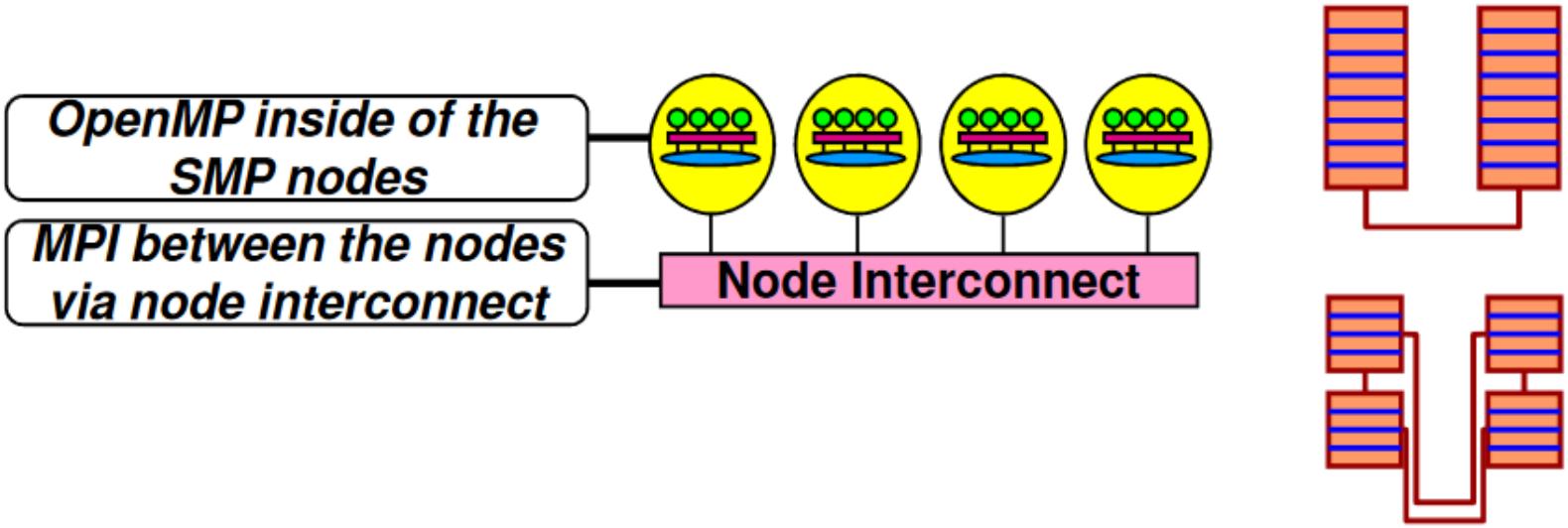


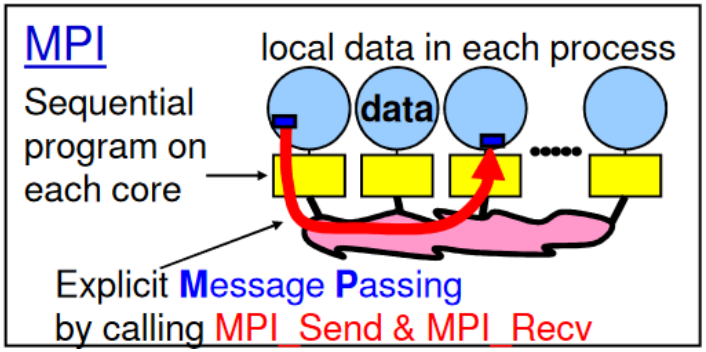
So Far: Pure MPI

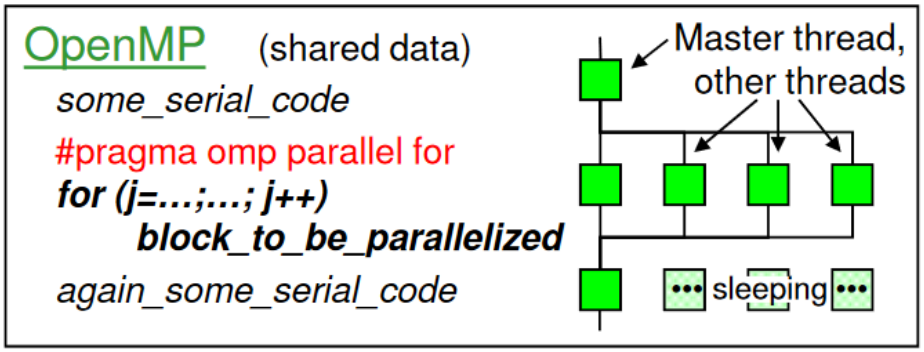
- One MPI process per core
- Major Advantages
  - No modifications on existing MPI codes
  - MPI library need not to support multiple threads
- Major Disadvantages
  - Does MPI library use internally different protocols?
    - Shared memory inside of the SMP nodes
    - Network communication between the nodes
  - Does application topology fit on hardware topology?
  - Unnecessary MPI-communication inside of SMP nodes



Typical Case: MPI+OpenMP







Hybrid MPI+OpenMP *Masteronly*

- **Masteronly:**
  MPI only outside parallel OpenMP regions →
  only the master thread issues MPI calls

```
#pragma omp parallel
  numerical code
/*end omp parallel */

/* on master thread only */
MPI_Send (original data to halo areas in other SMP nodes)
MPI_Recv (halo data from the neighbors)
```

Hybrid MPI+OpenMP *Masteronly*

- **Major Advantages**
  - **No message passing inside of the SMP nodes**
  - **No topology problem**
- **Major Disadvantages**
  - **All other threads are sleeping while master thread communicates**
  - **All communicated data passes through the cache where the master thread is executing**
  - **Strictly speaking: MPI-library must have been compiled with threading support (configure OpenMPI library build with: `--enable-mpi-threads`)**
    and must have been initialized with threading support
    → But masteronly approach will likely work without as well.

MPI Threading Support Handles

- **MPI_THREAD_SINGLE: Only one thread will execute (→ similar to calling MPI_Init ())**
- **MPI_THREAD_FUNNELED: Only master thread will make MPI-calls**
- **MPI_THREAD_SERIALIZED: Multiple threads may make MPI-calls, but only one at a time (not covered here)**
- **MPI_THREAD_MULTIPLE: Multiple threads may call MPI, with no restrictions (not covered here)**

```
int MPI_Init_thread( int * argc, char ** argv[],
                     int thread_level_required,
                     int * thead_level_provided);
```

MPI Library Threading Support

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>
int main(int argc, char* argv[]) {
    // Initilialise MPI and ask for thread support
    int provided;
    MPI_Init_thread(&argc, &argv, MPI_THREAD_SERIALIZED, &provided);
    if(provided < MPI_THREAD_SERIALIZED) {
        printf("The threading support level is lesser than that demanded.\n");
        MPI_Abort(MPI_COMM_WORLD, EXIT_FAILURE);
    }
    else
        printf("The threading support level corresponds to that demanded.\n");
    MPI_Finalize();
}
```

Calling MPI inside of OMP Master

- **Inside of a parallel region with OMP master**
- **Technically requires MPI_THREAD_FUNNELED support, i.e., only master thread will make MPI-calls**
- **Caution: There isn't an implicit synchronization with the OMP master statement → You must guard OMP master+MPI statements with OMP Barriers before and after**

```
#pragma omp barrier
#pragma omp master
MPI_Xxx(...);
#pragma omp barrier
```

- **But this implies that all other threads are sleeping!**
- **The additional barrier implies also the necessary cache flush!**

Calling MPI inside of OMP Master

```
#pragma omp parallel
{
#pragma omp for nowait
  for (i=0; i<1000; i++)
  a[i] = buf[i];

#pragma omp barrier
#pragma omp master
  MPI_Recv(buf,...);
#pragma omp barrier

#pragma omp for nowait
  for (i=0; i<1000; i++)
  c[i] = buf[i];
}
/* omp end parallel */
```

No implicit barrier!

Barriers needed to prevent data races!

Outline

- Distributed Parallel Computing II
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  - Collective Communication
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- **Quiz**

Quiz

- **Q1: How many Bytes would be required to store a derived datatype based on a struct of two characters and one double?**
- **Q2: Can a non-blocking receive be combined with a blocking send?**
- **Q3: Give an example setup for defining a Cartesian MPI communication topology for a three-dimensional setup if you could use up to 1000 MPI processes (make assumptions for all other properties).**
- **Q4: What is the order of the forward/backward Euler method?**
- **Q5: Are Runge-Kutta methods single-step or multi-step methods?**