Numerical Simulation and Scientific Computing II

Lecture 2: Distributed Parallel Computing II



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Quiz

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

→ <u>tag</u> and <u>dest</u> 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?

 \rightarrow 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

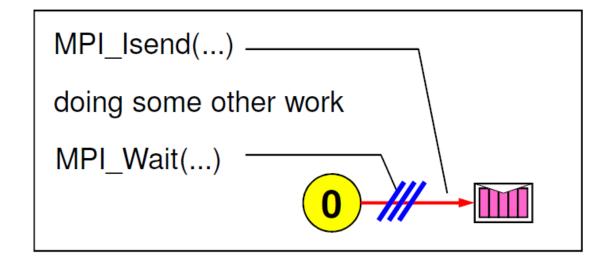
- Distributed Parallel Computing II
 - Non-Blocking Communication
 - Collective Communication
 - Derived Datatypes
 - Virtual Topologies
 - Hybrid MPI+OpenMP
- Quiz

Non-Blocking Communications

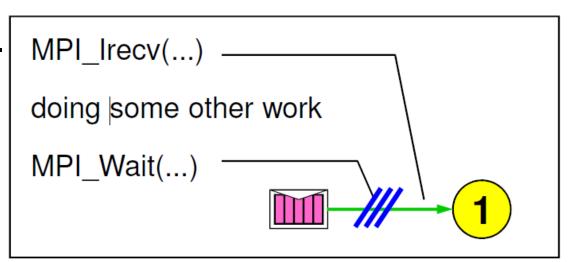
- Separate communication into three phases:
 - Initiate nonblocking communication
 - returns Immediately
 - routine name starting with MPI_I...
 - Do some work (perhaps involving other communications?)
 - If cluster hardware doesn't have dedicated MPI communication logic, don't expect efficient overlapping of communication with computation: Communication requires significant computational resources!
 - Wait for non-blocking communication to complete

Non-Blocking Examples

Non-blocking send

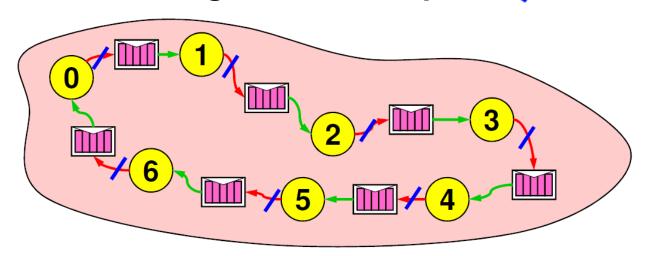


Non-blocking <u>receive</u>



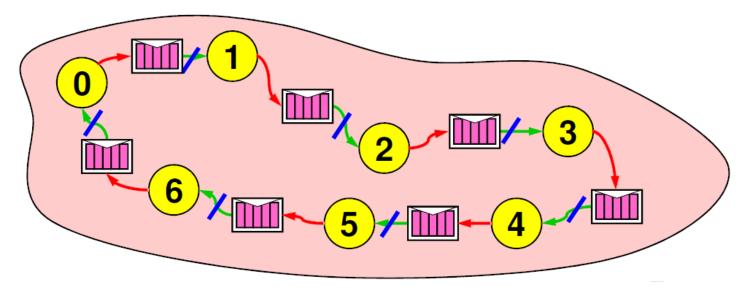
Non-Blocking Send

- 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

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

```
MPI_Issend( buf, count, datatype, dest, tag, comm, [OUT] &request_handle);
MPI Wait( [INOUT] &request handle, &status);
```

Nonblocking Receive

<u>buf</u> must not be used between <u>Irecv</u> and <u>Wait</u>

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

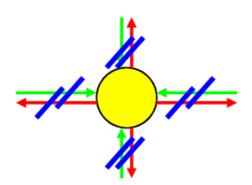
```
MPI_Wait( &request_handle, &status);
MPI_Test( &request_handle, &flag, &status);
```

- 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 (i.e., at least one)
 - 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!

- 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.

Support Functions

```
int n, p, myid, tag, master, proc, ierr;
                                                               Common Part
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 */
                                  /* get current process id */
MPI_Comm_rank(comm, &myid);
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);
```

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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

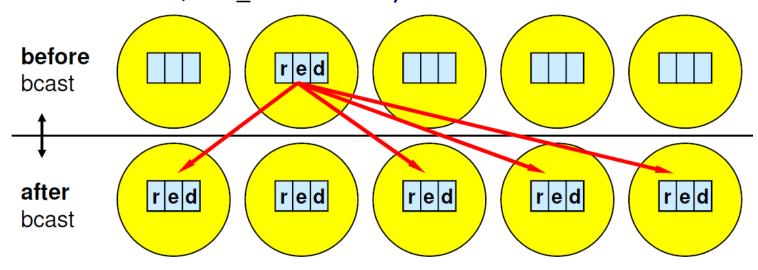
- Collective action over a communicator.
- All processes of the communicator must communicate, i.e., must call the collective routine.
- Synchronization may or may not occur, therefore all processes must be able to start the collective routine.
- On a given communicator, the n-th collective call must 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.
 - Not covered in this lecture
- 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 measurements

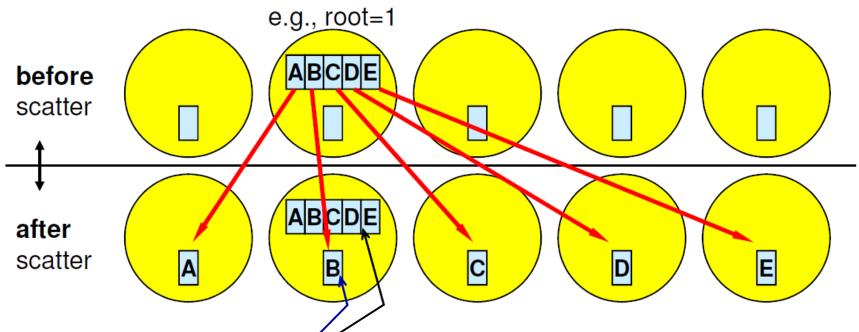
Broadcast



E.g. <u>root</u>=1: all processes must use same "root"

```
Example
std::vector<char> buf(3);
if(myrank == 1) { buf[0]='r'; buf[1]='e'; buf[2]='d'; }
MPI_Bcast(buf.data(), buf.size(), MPI_CHAR, 1, MPI_COMM_WORLD);
```

Scatter



int MPI_Scatter(void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype,

int root, MPI_Comm comm)

Example

If data cannot be equally distributed to all processes, use:

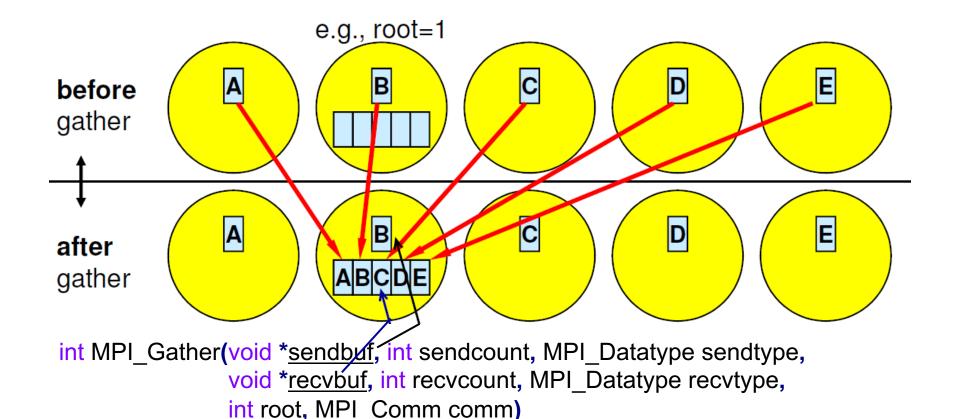
MPI_Scatterv: allows for variable send/recvcounts.

Sum of transmitted data size must match: sendcount x sendtype =

recvcount x recvtype

In principle: allowed to mix data types!
But typically: counts and types the same.

Gather



Example

See notes for Scatter, same here.

Global Reduction Operations

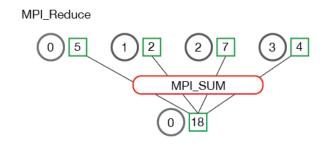
- To perform a global reduce operation across
- d0 o d1 o d2 o d3 o ... o ds-2 o ds-1
 - di = data in process rank i
 - single variable, or
 - vector
 - o = associative operation
 - Example:
 - global sum or product
 - global maximum or minimum
 - global user-defined operation

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

int MPI_Reduce(void *inbuf, void *result, int count, MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm)



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

Support Function

Example Collective Communication

```
int n, p, myid, tag, proc, ierr, i;
                                                                 First Part
float h, integral_sum, a, b, ai, pi, my_int(buf[50];
int master = 0; /* processor performing total sum */
MPI Comm comm;
                                                           buf-size >= p
                                                           (see next slide)
comm = MPI COMM WORLD;
ierr = MPI Init(&argc,&argv);
                                    /* starts MPT */
MPI_Comm_rank(comm, &myid);
                                        7* get current process id */
                                       /* get number of processes */
MPI Comm size(comm, &p);
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 */
                                                                  Second Part
   &my int, 1, MPI FLOAT, /* send buffer, size, data type */
   &buf[0], 1, MPI FLOAT, /* receive buffer, size, data type */
   master, comm):
if(myid == master) {
                                         buf must fit all ranks!
 integral sum = 0.0;
 for (i=0; i<p; i++) {
  integral sum += buf[i];
 printf("The Integral =%fn",integral sum);
MPI Finalize();
                                          Is there another collective
                                          operation which could be used
                                          here?
                                          Yes, MPI Reduce with MPI SUM
```

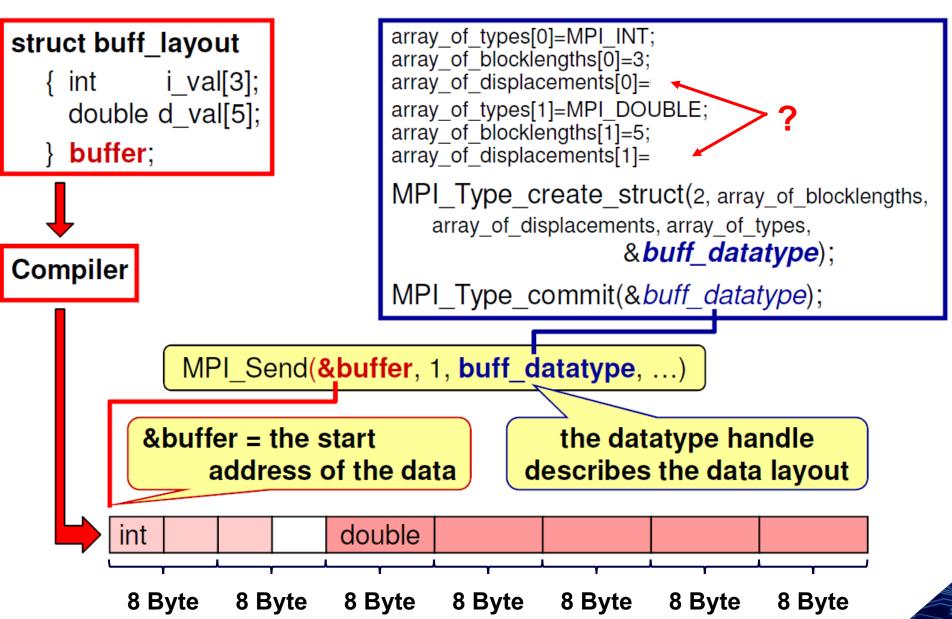
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Derived Datatypes

- 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



Compute Displacement

```
array of types[0]=MPI INT;
           array of blocklengths[0]=3;
           array of displacements[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);
In principle:
array of displacements[i] = address(block i) - address(block 0);
Use:
int MPI Get address(vold* location, MPI Aint *address)
Continuing the example:
int address base, address 0, address 1;
MPI Get address(&buffer, &address base);
                                                           struct buff layout
MPI_Get_address(&buffer.i_val[0], &address_0);
                                                             { int
MPI_Get_address(&buffer.d_val[0], &address_1);
                                                               double d_val[5];
array of displacements[0] = address 0 - address base;
                                                               buffer;
array_of_displacements[1] = address_1 - address_base;
```

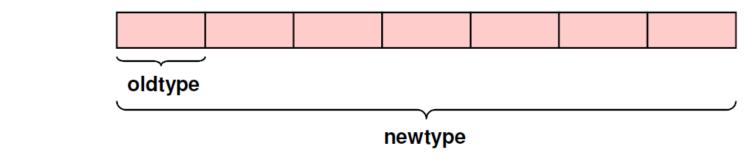
i val[3];

Derived Datatype: Another Example

```
typedef struct {
 char
         a:
 int
         b;
 double c;} mystruct;
mystruct mydata;
int baseaddr, addr0, addr1, addr2;
MPI Get address (&mydata, &baseaddr);
MPI_Get_address ( &mydata.a, &addr0);
MPI_Get_address ( &mydata.b, &addr1);
MPI Get address (&mydata.c, &addr2);
displ[0] = addr0 - baseaddr;
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 );
```

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).
- If type no longer required, one may call MPI_TYPE_FREE() to free a datatype and its internal resources.

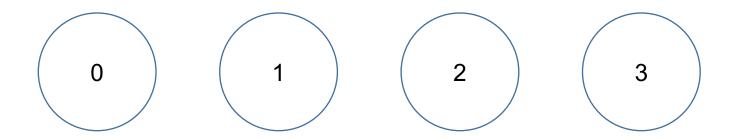
```
int MPI_Type_commit(MPI_Datatype *datatype);
int MPI_Type_free (MPI_Datatype *datatype);
```

Outline

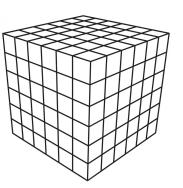
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Virtual Topologies

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



Now consider that you work with this:

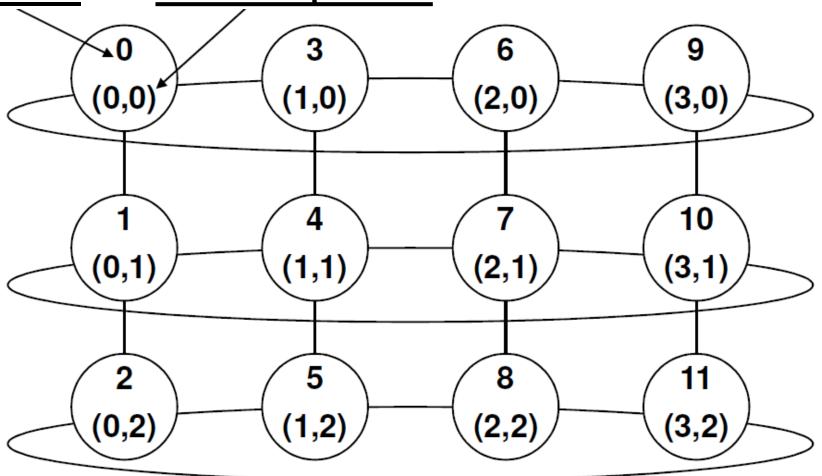


How to Use a Virtual Topology

- 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.

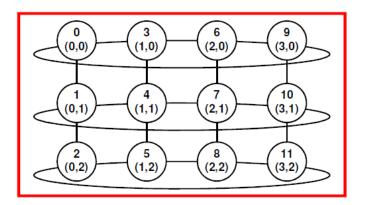
Graph Topologies

- 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
 - → Reorder: 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!

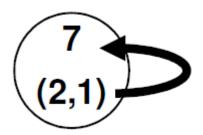


Mapping ranks to process grid coordinates

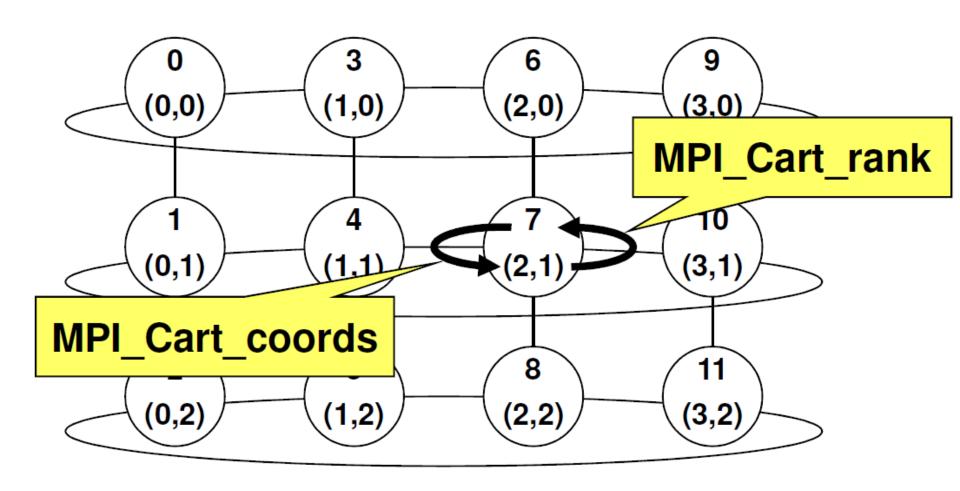


int MPI_Cart_coords(MPI_Comm comm_cart, int rank, int maxdims, int *coords)

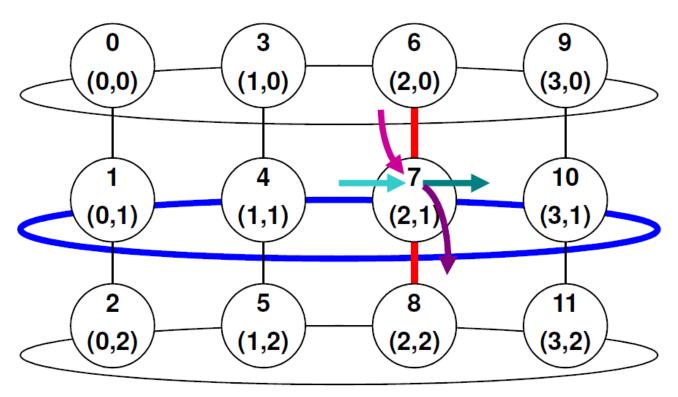
Mapping process grid coordinates to ranks



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



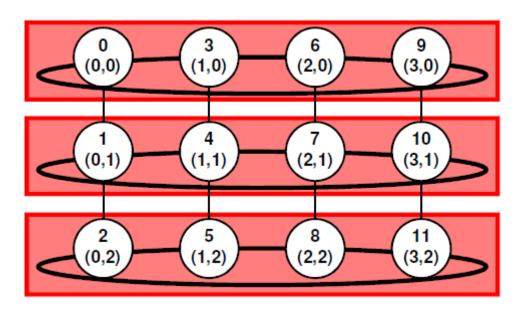
- Compute ranks of neighboring processes
- Returns MPI_PROC_NULL if there is no neighbor.
- In general: MPI_PROC_NULL can be used as source or destination rank in each communication. → This communication will be a no-operation!



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)

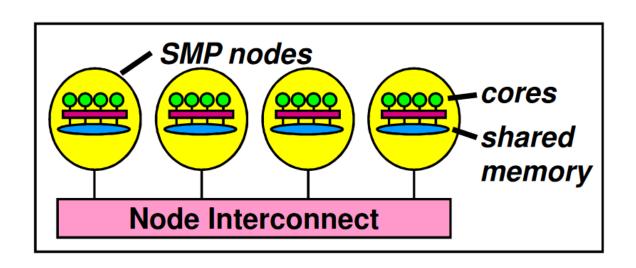


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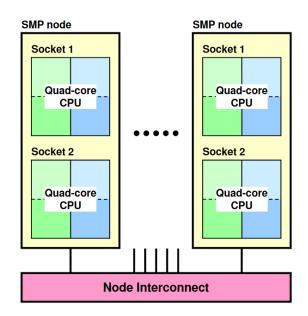
Hybrid Parallel Programming

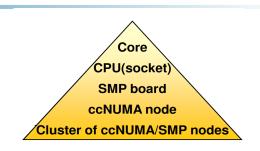
- Hybrid parallel programming:
 Mix different parallel programming approaches to efficiently use available computing platforms (heterogeneous computing resources)
- Typical example: Programming of clusters of shared memory nodes



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
 - Accelerator programming (CUDA, OpenACC, etc): not covered here
 - And others.



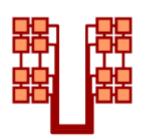


Hybrid Parallel Programming

Which programming model is best?

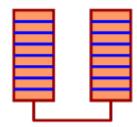
"Pure" MPI?

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



"Fully hybrid"?

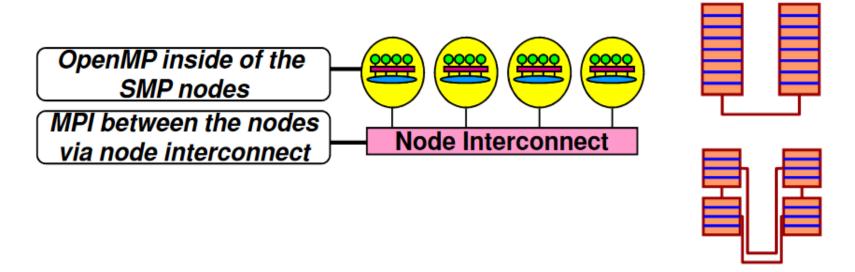
 (a.k.a. 1 MPI process per node, shared-memory within nodes)

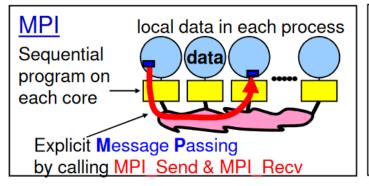


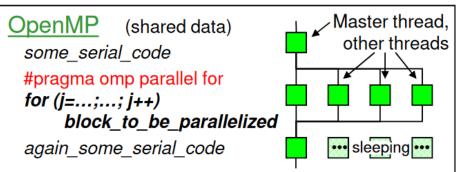
"Mixed hybrid"?

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

Typical Case: MPI+OpenMP







Hybrid MPI+OpenMP *Masteronly*

<u>Master</u>only:
 MPI only outside parallel OpenMP regions →
 only the <u>master</u> 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)

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Quiz

- Q1: How many Bytes would be required to store an MPI 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?