HPCSE - II

«MPI - part 2 »

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Outline

- Broadcast and MPI data types
- Groups and communications
- Topologies

Credit for these slides: Prof. M. Troyer

Parallelizing Simpson integration

- Only the master rank (0) reads the input data. How do we share it?

```
int main(int argc, char** argv)
{
  MPI_Init(&argc,&argv);

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

  double a;            // lower bound of integration
  double b;            // upper bound of integration
  int nsteps; // number of subintervals for integration

  // read the parameters on the master rank
  if (rank==0)
    std::cin >> a >> b >> nsteps;

  // we need to share the parameters with the other ranks
  ???

  // integrate just one part on each thread
  double delta = (b-a)/size;
  double result = simpson(func,a+rank*delta,a+(rank+1)*delta,nsteps/size);

  //  collect all to the master (rank 0)
  MPI_Reduce(rank == 0 ? MPI_IN_PLACE : &result, &result, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);

   // the master prints
  if (rank==0)
    std::cout << result << std::endl;

  MPI_Finalize();
  return 0;
}
```

Broadcast

- MPI provides a collective broadcast operation

```
int MPI_Bcast( void *buffer, int count, MPI_Datatype datatype, int root,
               MPI_Comm comm )
// broadcast the data from the root rank to all others
```

- We can use this to broadcast the data

```
// and then broadcast the parameters to the other ranks
 MPI_Bcast(&a, 1, MPI_DOUBLE,0, MPI_COMM_WORLD);
 MPI_Bcast(&b, 1, MPI_DOUBLE,0, MPI_COMM_WORLD);
 MPI_Bcast(&nsteps, 1, MPI_INT,0, MPI_COMM_WORLD);
```

- This is inefficient since we use three broadcasts.
- We will later pack all parameters into one buffer and broadcast that buffer.

Sending it bitwise

- The dangerous solution: pack it all into a struct and send it bitwise
- This assumes a homogeneous machine with identical integer and floating point formats.

```
// define a struct for the parameters
struct parms {
  double a;            // lower bound of integration
  double b;            // upper bound of integration
  int nsteps; // number of subintervals for integration
};

parms p;

// read the parameters on the master rank
if (rank==0)
  std::cin >> p.a >> p.b >> p.nsteps;

// broadcast the parms as bytes - warning, not portable on heterogeneous machines
MPI_Bcast(&p, sizeof(parms), MPI_BYTE, 0, MPI_COMM_WORLD);
```

Packing and unpacking

- Allocate a sufficiently large buffer and then pack the data into it
- Send/receive the packed buffer with type **MPI_PACKED**
- Finally unpack it on the receiving side

```
int MPI_Pack(void *inbuf, int incount, MPI_Datatype datatype,
             void *outbuf, int outcount, int *position, MPI_Comm comm)
// packs the data given as input into the outbuf buffer starting at a given position.
// outcount is the size of the buffer and position gets updated to point to the first
// free byte after packing in the data.
// An error is returned if the buffer is too small.

int MPI_Unpack(void *inbuf, int insize, int *position,
               void *outbuf, int outcount, MPI_Datatype datatype, MPI_Comm comm)
// unpack data from the buffer starting at given position into the buffer outbuf.
// position is updated to point to the location after the last byte read

int MPI_Pack_size(int incount, MPI_Datatype datatype, MPI_Comm comm, int *size)
// returns in size an upper bound for the number of bytes needed to pack incount
// values of type datatype. This can be used to determine the required buffer size
```

Packing data into a buffer

- Pack the input data, broadcast it and unpack

```
// create a buffer and pack the values.
// first get the size for the buffer and allocate a buffer
int size_double, size_int;
MPI_Pack_size(1, MPI_DOUBLE, MPI_COMM_WORLD,&size_double);
MPI_Pack_size(1, MPI_INT,    MPI_COMM_WORLD,&size_int);
int buffer_size = 2*size_double+size_int;
char* buffer = new char[buffer_size];

// pack the values into the buffer on the master
if (rank==0) {
  int pos=0;
  MPI_Pack(&a, 1, MPI_DOUBLE, buffer, buffer_size, &pos, MPI_COMM_WORLD);
  MPI_Pack(&b, 1, MPI_DOUBLE, buffer, buffer_size, &pos, MPI_COMM_WORLD);
  MPI_Pack(&nsteps, 1, MPI_INT, buffer, buffer_size, &pos, MPI_COMM_WORLD);
  assert ( pos <= buffer_size );
}

// broadcast the buffer
MPI_Bcast(buffer, buffer_size, MPI_PACKED, 0, MPI_COMM_WORLD);

// and unpack on the receiving side
int pos=0;
MPI_Unpack(buffer, buffer_size, &pos, &a, 1, MPI_DOUBLE, MPI_COMM_WORLD);
MPI_Unpack(buffer, buffer_size, &pos, &b, 1, MPI_DOUBLE, MPI_COMM_WORLD);
MPI_Unpack(buffer, buffer_size, &pos, &nsteps, 1, MPI_INT, MPI_COMM_WORLD);
assert ( pos <= buffer_size );

// and finally delete the buffer
delete[] buffer;
```

Recall sending the parameters

- We had three options, none was ideal
  - three individual broadcasts: wasteful since three communications
  - packing it into a buffer: wasteful since it involves copying
  - sending the struct bitwise: dangerous since it assumes homogeneity
- What we want to do here and for the ghost cells is to send non-contiguous or heterogeneous data without copying.
- The solution are MPI datatypes: describe your data layout to MPI and MPI uses that information in the communication.

```
struct parms {
  double a;
  double b;
  int nsteps;
};
```

type	count	offset
MPI_DOUBLE	2	0
MPI_INT	1	16

Building an MPI data type

- The most general function is MPI_Type_create_struct, taking numbers, offsets and types

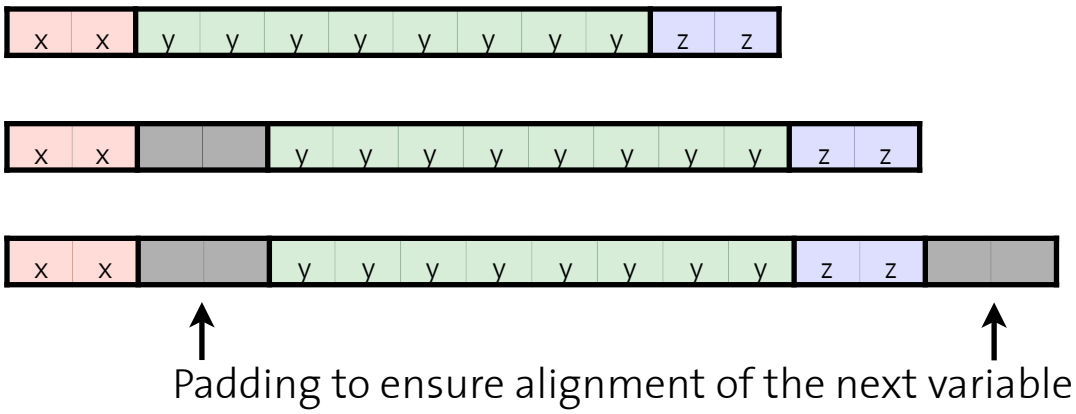
```
// define a struct for the parameters
struct parms {
  double a;            // lower bound of integration
  double b;            // upper bound of integration
  int nsteps; // number of subintervals for integration
};

// describe this struct through sizes, offsets and types
// and create an MPI data type
// still dangerous since it assumes that we know any potential padding
MPI_Datatype parms_t;
int          blocklens[2]  =  {2,1};
MPI_Aint     offsets[2]    =  {0,2*sizeof(double)};
MPI_Datatype types[2]      =  {MPI_DOUBLE, MPI_INT};
MPI_Type_create_struct(2, blocklens, offsets, types,&parms_t);
MPI_Type_commit(&parms_t); // finish building the type

parms p;

// read the parameters on the master rank
if (rank==0);
  std::cin >> p.a >> p.b >> p.nsteps;

// broadcast the parms now using our type
MPI_Bcast(&p, 1, parms_t, 0, MPI_COMM_WORLD);

// and now free the type
MPI_Type_free(&parms_t);
```

Alignment and padding

- This code was dangerous since we assumed that we know how the compiler lays out a struct in memory.

```
struct parms {
  short  x;
  double y;
  short  z;
};
```

- We might be wrong due to padding and alignment. Consider the following three examples of how this could be stored in memory



Safer way of using MPI_Type_create_struct

- To get the right offsets and size we take actual addresses
  - use MPI_Get_address to convert pointers to integers
  - specify lower bound and upper bound of the struct

```
// define a struct for the parameters
struct parms {
  double a;            // lower bound of integration
  double b;            // upper bound of integration
  int nsteps; // number of subintervals for integration
};

parms p;

// describe the struct through sizes, offsets and types
// the safe way getting addresses

MPI_Aint p_lb, p_a, p_nsteps, p_ub;
MPI_Get_address(&p,       &p_lb);      // start of the struct is the lower bound
MPI_Get_address(&p.a,     &p_a);       // address of the first double
MPI_Get_address(&p.nsteps, &p_nsteps); // address of the integer
MPI_Get_address(&p+1,     &p_ub);      // start of the next struct is the upper bound

int          blocklens[] =  {0, 2, 1, 0};
MPI_Datatype types[]     =  {MPI_LB, MPI_DOUBLE, MPI_INT, MPI_UB};
MPI_Aint     offsets[]   =  {0, p_a-p_lb, p_nsteps-p_lb, p_ub-p_lb};

MPI_Datatype parms_t;
MPI_Type_create_struct(4, blocklens, offsets, types,&parms_t);
MPI_Type_commit(&parms_t);
```

MPI_Type_create_struct

- The declaration of the functions used in the previous examples

```
int MPI_Type_create_struct(int count, int blocklengths[], MPI_Aint offsets[],
                           MPI_Datatype types[], MPI_Datatype *newtype)
// builds an MPI data type for a data type for a general data structure given by
// types, counts (blocklengths) and their offsets relative to the start of the data structure

int MPI_Get_address(void *location, MPI_Aint *address)
// converts a pointer to the integer type used internally by MPI to store pointers

int MPI_Type_commit(MPI_Datatype *datatype)
// commits the data type: finished building it. It can now be used.

int MPI_Type_free(MPI_Datatype *datatype)
// frees the data type, releasing any allocated memory
```

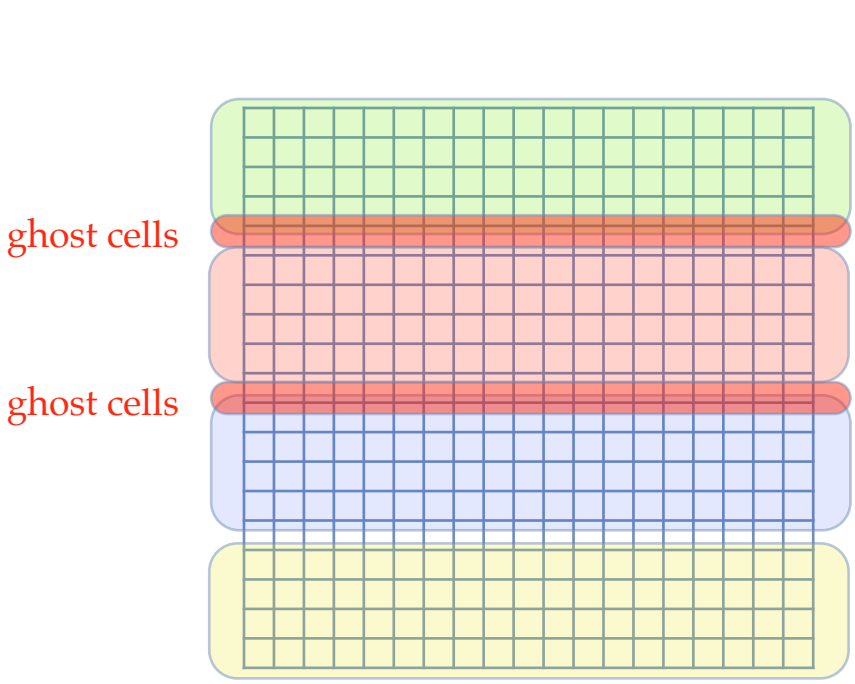
- We can use MPI_Type_create_struct to send the contents of linked lists
  - we view the whole memory as a huge struct from which we send some select data
  - thus give absolute addresses as offsets
  - pass **MPI_BOTTOM** as the buffer pointer in communication to indicate that the type uses absolute addresses

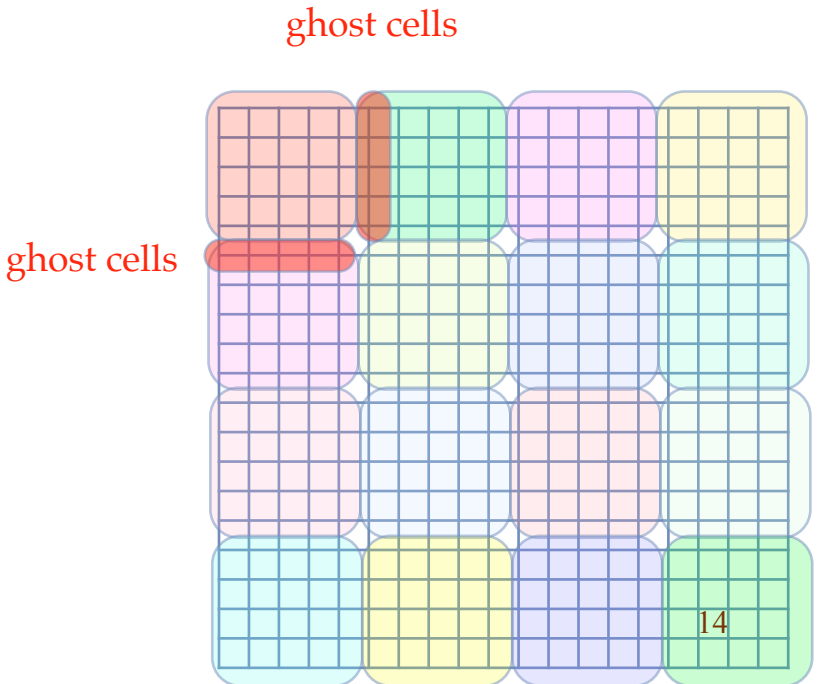
Receiving a list into a vector

```
if(num==0) {
  // receive data into a vector and print it
  std::vector<int> data(10);
  MPI_Status status;
  MPI_Recv(&data[0], 10, MPI_INT, 1, 42, MPI_COMM_WORLD, &status);
  for (int i=0; i < data.size(); ++i)
    std:: cout << data[i] << "\n";
}
else {
  // fill a list with the numbers 0-9 and send it
  std::list<int> data;
  for (int i=0; i<10; ++i)
    data.push_back(i);

  std::vector<MPI_Datatype> types(10,MPI_INT);
  std::vector<int>          blocklens(10,1);
  std::vector<MPI_Aint>     offsets;

  for (int& x : data) {
    MPI_Aint address;
    MPI_Get_address(&x, &address); // use absolute addresses
    offsets.push_back(address);
  }

  MPI_Datatype list_type;
  MPI_Type_create_struct(10, &(blocklens[0]), &offsets[0], &types[0] ,&list_type);
  MPI_Type_commit(&list_type);

  MPI_Send(MPI_BOTTOM, 1, list_type, 0, 42, MPI_COMM_WORLD);

  MPI_Type_free(&list_type);
}
```

Recall domain decomposition and ghost cells

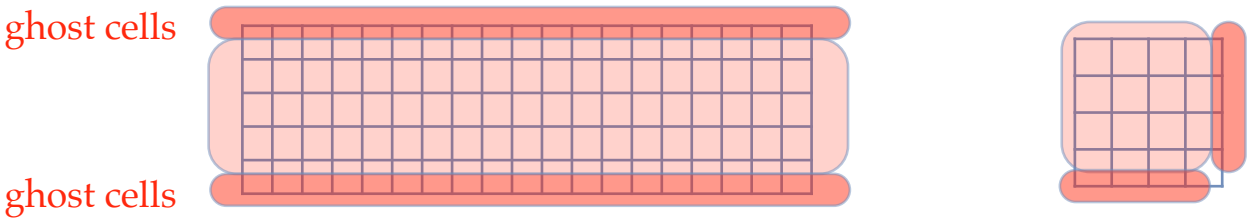
- How do we best exchange boundary values with the neighboring ranks?
  - In 1D it was just a single number and was easy
  - Sometimes we might be lucky and they could be contiguous arrays
- What shall we do in the general case?
  - pack them into buffers?
  - or just describe to MPI where they are in memory?





MPI data types for ghost cells

- The ghost cells in a 2D array or column and rows in a matrix can be described as strided vectors




```
int MPI_Type_contiguous(int count, MPI_Datatype old_type, MPI_Datatype *new_type_p)
// build an MPI datatype for a contiguous array

int MPI_Type_vector(int count, int blocklength, int stride,
                    MPI_Datatype old_type, MPI_Datatype *newtype_p)
// build an MPI datatype for a vector array of blocklength contiguous entries that are
// spaced at a given stride. stride is like the leading dimension in BLAS and specifies
// the distance between blocks

int MPI_Type_create_hvector(int count, int blocklen,  MPI_Aint stride,
                            MPI_Datatype old_type, MPI_Datatype *newtype_p)
// like MPI_Type_vector but now the stride is given in bytes
```

Row and column data types

- We can use this to create data types for rows and columns of a matrix, and similarly for slices of an array

```
hpc12::matrix<double,hpc12::column_major> a(4,4);

MPI_Datatype row, col;

MPI_Type_contiguous(4,       MPI_DOUBLE, &col);
MPI_Type_vector    (4, 1, 4, MPI_DOUBLE, &row);

MPI_Type_commit(&row);
MPI_Type_commit(&col);

// use them
// ...
// and finally free them

MPI_Type_free(&row);
MPI_Type_free(&col);
```

1	5	9	13
2	6	10	14
3	7	11	15
4	8	12	16

Subarrays

- More general is the creation of subarrays, especially for boundary layers and ghost cells

```
int MPI_Type_create_subarray(int ndims, int sizes[], int subsizes[], int starts[],
                             int order, MPI_Datatype oldtype, MPI_Datatype *newtype)
// build an MPI datatype for a subarray of a larger array:
//   ndims:    number of dimensions
//   sizes:    extent of the full array in each dimension
//   subsizes: extent of the subarray in each dimension
//   starts:   starting index of the subarray
//   order:    array storage order, can be either of MPI_ORDER_C or MPI_ORDER_FORTRAN
```

- Use it for the 2D diffusion equation parallelized using MPI

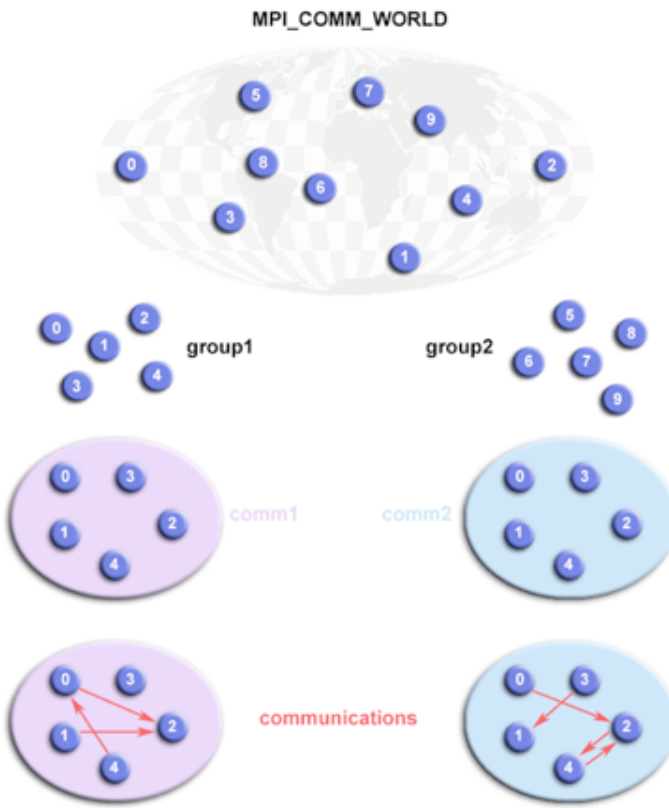
Indexed data types

- Finally, we want to send just some elements of an array. For example, send some particles to a different cell list.

```
int MPI_Type_indexed(int count, int blocklens[], int indices[],
                     MPI_Datatype old_type, MPI_Datatype *newtype)
// build an MPI datatype selecting specific entries from a contiguous array. Starting a
// at each of the given indices a number of elements given in the corresponding entry
// of blocklens is chosen.

int MPI_Type_create_hindexed(int count, int blocklens[], MPI_Aint displacements[],
                             MPI_Datatype oldtype, MPI_Datatype *newtype)
// same as MPI_Type_indexed but now instead of indices the displacement in bytes from the
// start of the array is specified

int MPI_Type_create_indexed_block(int count, int blocklength, int array_of_displacements[],
                                  MPI_Datatype oldtype, MPI_Datatype *newtype)
// same as MPI_Type_indexed but with constant sized blocks
```

Groups and Communicators

- Imagine we want to split a computation into individual tasks that run on subsets of the ranks:
  - do multiple integrations at the same time
  - operate on rows or columns of a matrix
  - operate on slices of a 3D mesh
- We want to split the ranks into groups and build a new communicator for each group
- We can then do collective operations within a group instead of within all ranks



Simpson using a communicator

- Simpson integration by MPI using a communicator that might be other than MPI_COMM_WORLD

```
double parallel_simpson(MPI_Comm comm, parms p)
{
  // get the rank and size for the current communicator
  int size;
  int rank;
  MPI_Comm_size(comm,&size);
  MPI_Comm_rank(comm,&rank);

  // integrate just one part on each rank
  double delta = (p.b-p.a)/size;
  double result = simpson(func,p.a+rank*delta,p.a+(rank+1)*delta,p.nsteps/size);

  //  collect the results to all ranks
  MPI_Allreduce(MPI_IN_PLACE, &result, 1, MPI_DOUBLE, MPI_SUM, comm);
  return result;
}
```

Three Simpson integrations at once

```
int main(int argc, char** argv)
{
  MPI_Init(&argc,&argv);
  int rank;
  MPI_Comm_rank(MPI_COMM_WORLD,&rank);

  // we want to do three integrals at once
  parms p[3];
  ...

  // split the ranks into three groups
  int which = rank % 3;
  MPI_Comm comm;
  MPI_Comm_split(MPI_COMM_WORLD, which, rank, &comm);

  // do the integration in each group
  double result = parallel_simpson(comm,p[which]);

  // only the master for each group prints
  int grouprank;
  MPI_Comm_rank(comm, &grouprank);
  if (grouprank==0)
    std::cout << "Integration " << which << " results in " << result << std::endl;

  //  free the type and the new communicator
  MPI_Comm_free(&comm);

  MPI_Finalize();
  return 0;
}
```

Creating and destroying communicators

- The most important functions for communicators

```
int MPI_Comm_rank( MPI_Comm comm, int *rank )

int MPI_Comm_size( MPI_Comm comm, int *size )

int MPI_Comm_compare(MPI_Comm comm1, MPI_Comm comm2, int *result)
// compares two communicators to test is they are the same, i.e. they have the same ranks
// in the same order

int MPI_Comm_dup(MPI_Comm comm, MPI_Comm *newcomm)
// duplicates a communicator.
// this is a collective communication that needs to be called by all ranks.

int MPI_Comm_free(MPI_Comm *comm)
// frees a communicator

int MPI_Comm_split(MPI_Comm comm, int color, int key, MPI_Comm *newcomm)
// splits a communicator into subcommunicators.
// ranks with the same color are grouped together and sorted within each group by key.
// this is a collective communication that needs to be called by all ranks.

int MPI_Comm_create(MPI_Comm comm, MPI_Group group, MPI_Comm *newcomm)
// creates a new communicator based on group that is a subgroup of the ranks in comm.
// this function allows more flexible creation of subcommunicators than MPI_Comm_split.
// this is a collective communication that needs to be called by all ranks.
```

Working with groups (1)

- There are **many** useful functions for group creation

```
int MPI_Group_rank(MPI_Group group, int *rank)
int MPI_Group_size(MPI_Group group, int *size)
// are similar to the corresponding communicator functions

int MPI_Group_translate_ranks(MPI_Group group1, int n, int *ranks1, MPI_Group group2, int *ranks2)
// translates ranks between group: given a set of ranks1 in group1 it sets their ranks in group2
// in the array ranks2, or sets them to MPI_UNDEFINED if no correspondence exists

int MPI_Group_compare(MPI_Group group1, MPI_Group group2, int *result)

int MPI_Comm_group(MPI_Comm comm, MPI_Group *group)
// extracts the group from a communicator

int MPI_Group_free(MPI_Group *group)

int MPI_Group_union(MPI_Group group1, MPI_Group group2, MPI_Group *newgroup)
int MPI_Group_intersection(MPI_Group group1, MPI_Group group2, MPI_Group *newgroup)
int MPI_Group_difference(MPI_Group group1, MPI_Group group2, MPI_Group *newgroup)
// newgroup is the union, intersection, or difference of the given groups
```

Working with groups (2)

- selectively choosing ranks

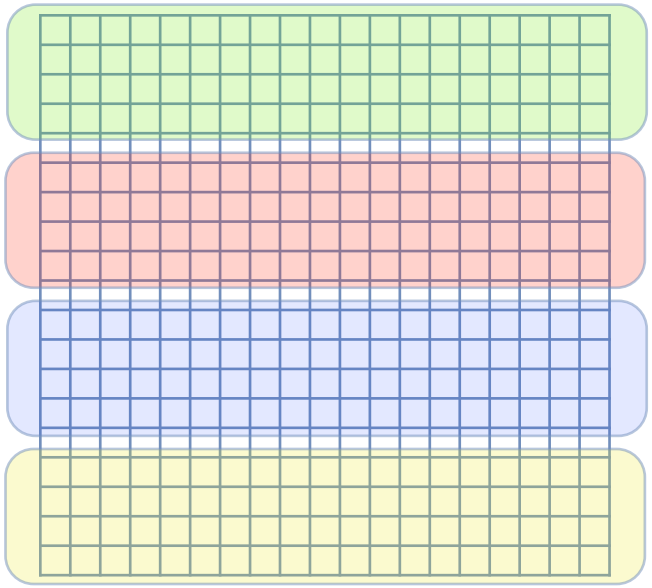
```
int MPI_Group_incl(MPI_Group group, int n, int *ranks, MPI_Group *newgroup)
// create a newgroup containing only the given ranks of a group

int MPI_Group_excl(MPI_Group group, int n, int *ranks, MPI_Group *newgroup)
// create a newgroup containing all except the given ranks of a group

int MPI_Group_range_incl(MPI_Group group, int n, int ranges[][3], MPI_Group *newgroup)
// create a newgroup containing only the given ranges of ranks of a group

int MPI_Group_range_excl(MPI_Group group, int n, int ranges[][3], MPI_Group *newgroup)
// create a newgroup containing all except the given ranges of ranks of a group
```

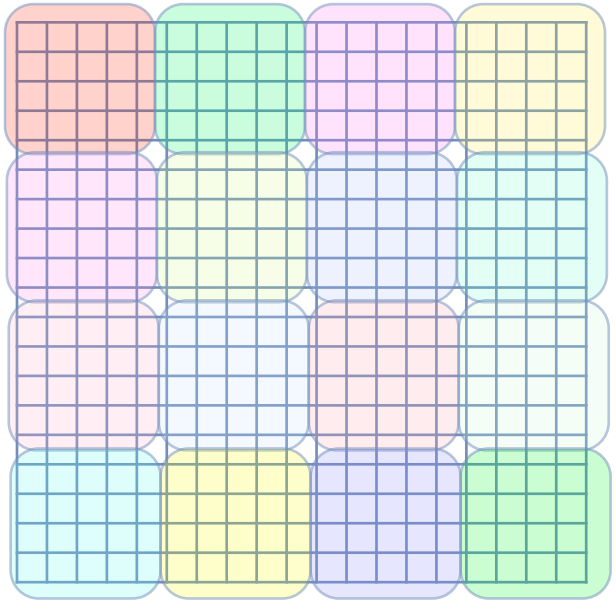
- ranges are given as triples (first, last, stride), and a range includes the ranks

$$\text{first}, \text{first}+\text{stride}, \text{first}+2\,\text{stride}, \ldots, \text{first}+\left\lfloor \frac{\text{last}-\text{first}}{\text{stride}} \right\rfloor \text{stride}$$

Finding the rank of the neighbor

- Easy in a one-dimensional layout
- Harder in two and more dimensions
- Even harder on irregular meshes





- MPI topologies are the solution to easily finding neighbors

MPI topologies

- A (virtual) topology describes the "connectivity" of MPI processes in a communicator. There may be no relation between the physical network and the process topology.
- Two main types
  - **Cartesian topology**: each process is "connected" to its neighbors in a virtual grid. Nodes are labeled by cartesian indices, boundaries can be cyclic (periodic).
  - **Graph topology:** an arbitrary connection graph
- Topologies are essentially a simple graph library built into MPI

Cartesian topologies: MPI_Cart_create

- To work with a regular mesh with row-major ordering we create a cartesian communicator

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

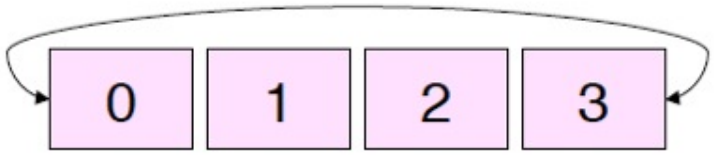
  - **comm_old**: the original communicator
  - **ndims**: number of dimensions
  - **dims**: integer array specifying the number of processes in each dimension
  - **periods**: integer array of boolean values whether the grid is periodic in that dimension
  - **reorder**: boolean flag whether the processes may be reordered
  - **comm_cart**: a new cartesian grid communicator

- To get an automatic splitting into approximately equal counts in each dimension use

```
int MPI_Dims_create(int nnodes, int ndims, int *dims)
// fills in the dims array to be the best fit of arranging nnodes ranks to
// form an ndims dimensional array
```

Periodic boundary conditions

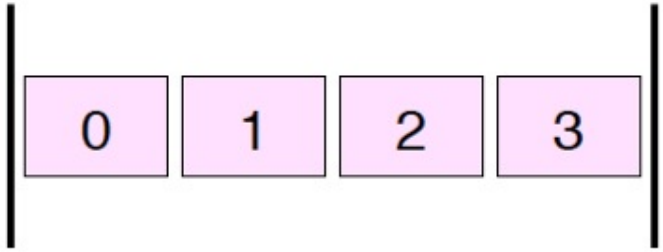
int periods[] = {true}



$left_0 = 3$

$right_3 = 0$

int periods[] = {false}



$left_0$ = MPI_PROC_NULL

$right_3$ = MPI_PROC_NULL

Creating a cartesian communicator

```
int main(int argc, char** argv)
{
  // now initialize MPI and get information about the number of processes

  MPI_Init(&argc,&argv);

  int size;
  int rank;
  MPI_Status status;
  MPI_Comm_size(MPI_COMM_WORLD,&size);
  MPI_Comm_rank(MPI_COMM_WORLD,&rank);

  int nums[3] = {0,0,0};
  int periodic[3] = {false, false, false};

  // split the nodes automatically
  MPI_Dims_create(size, 3, nums);

  if (rank==0)
    std::cout << "We create a " << nums[0] << "x" << nums[1] << "x" << nums[2] << " arrangement.\n";

  // now everyone creates a a cartesian topology
  MPI_Comm cart_comm;
  MPI_Cart_create(MPI_COMM_WORLD, 3, nums, periodic, true, &cart_comm);

  MPI_Comm_free(&cart_comm);
  MPI_Finalize();
 }
```

The most important one: MPI_Cart_shift

- The neighbors are obtained by

```
int MPI_Cart_shift(MPI_Comm comm, int direction, int displacement, int *source, int *dest)
// gives the ranks shifted in the dimension given by direction by a certain displacement, where the
// sign of displacement indicates the direction.
// It returns both the source rank from which the current rank can be reached by that shift
// and the dest rank that is reached from the current rank by that shift.
```

- Example in 3D:

```
int left, right, bottom, top, front, back, newrank;

MPI_Comm_rank(cart_comm,&newrank);

MPI_Cart_shift(cart_comm, 0, 1, &left, &right);
MPI_Cart_shift(cart_comm, 1, 1, &bottom, &top);
MPI_Cart_shift(cart_comm, 2, 1, &front, &back);

std::cout << "Rank " << rank << " has new rank " << newrank << " and neighbors "
          << left << ", " << right << ", "
          << top << ", " << bottom << ", "
          << front << ", " << back << std::endl;
```

Functions for cartesian topologies

- Get number of dimensions

```
int MPI_Cartdim_get(MPI_Comm comm, int *ndims)
```

- Get the cartesian topology information

```
int MPI_Cart_get(MPI_Comm comm, int maxdims, int *dims, int *periods, int *coords)
// retrieves information about the cartesian topology associated with a communicator.
// The arrays are allocated with maxdims dimensions. dims and periods are the numbers used
// when creating the topology. coords are the dimensions of the current rank.
```

- Get the rank of a given coordinate

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

- Get the coordinates of a given rank

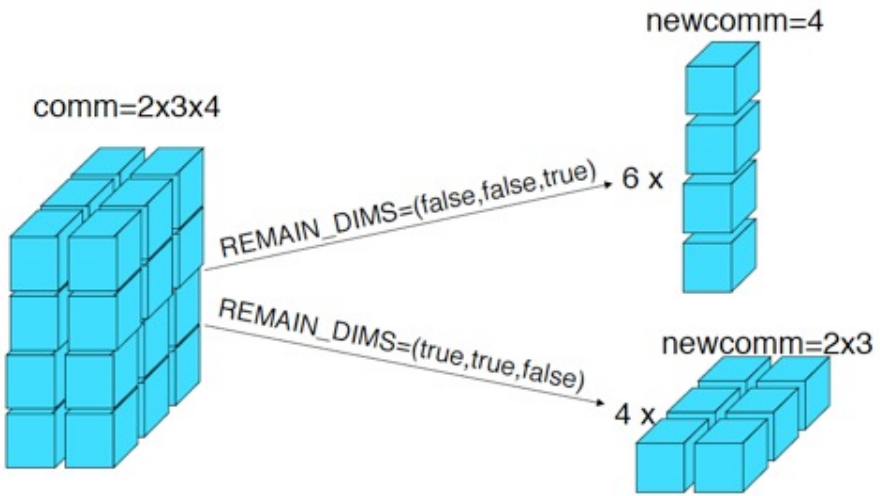
```
int MPI_Cart_coords(MPI_Comm comm, int rank, int maxdims, int *coords)
```

Subgrids of cartesian topologies

- One can split the cartesian communicator into sub grid communicators for columns, rows, planes, ...

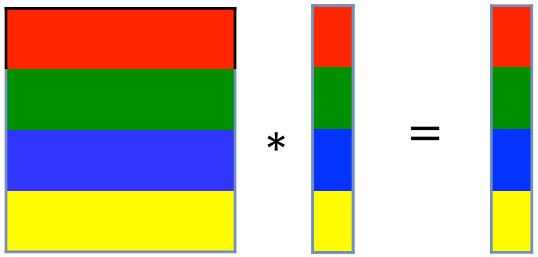
```
int MPI_Cart_sub(MPI_Comm comm, int *remain_dims, MPI_Comm *comm_new)
```

- The remain_dims array specifies whether to keep the processes along a direction joined in a group (true) or split them (false)



Parallel gemv version 1

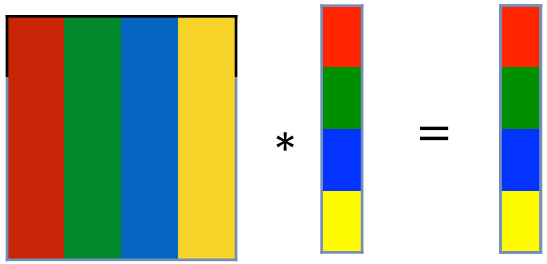
- Block-row distribution
  - Gather all parts of *x* locally
  - and then perform the local multiplications



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

// we want a simple size that can be divided evenly by the number
// of ranks to keep the code simple
int block_size = N/size;
assert(N % size ==0);

// block distribution of the vectors
std::vector<double> x(block_size), y(block_size);

// block row distribution for the matrix: keep only N/size rows
matrix_type A(block_size,N);

...

//Gather all pieces into a big vector and then do a multiplication
std::vector<double> fullx(N);
MPI_Allgather(&x[0], x.size(), MPI_DOUBLE, &fullx[0], x.size(), MPI_DOUBLE, MPI_COMM_WORLD);
dgemv(A,fullx,y);
```

Parallel gemv version 2

- Block-column distribution
  - Perform local multiplications
  - Add all parts (reduction)
  - Finally scatter the results

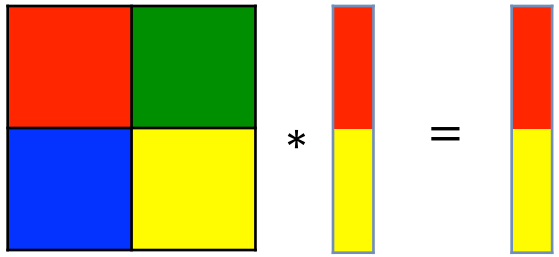



```
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &size);

// we want a simple size that can be divided evenly by the number
// of ranks to keep the code simple
int block_size = N/size;
assert(N % size ==0);

// block distribution of the vectors
std::vector<double> x(block_size), y(block_size);

// block column distribution for the matrix: keep only N/size columns
matrix_type A(N,block_size);

...

// do a local multiplication, obtaining a full vector
// and then reduce-scatter the result
std::vector<double> fully(N);
dgemv(A,x,fully);
std::vector<int> recvcounts(size, block_size);
MPI_Reduce_scatter(&fully[0],&y[0], &recvcounts[0], MPI_DOUBLE, MPI_SUM, MPI_COMM_WORLD);
```

Parallel gemv version 3

- Block-cyclic distribution on q x q array
  - store vector on diagonal blocks
  - broadcast x_j along column j
  - multiply
  - reduce y_i along row i

$$y_i = \sum_{j=0}^{q-1} A_{i,j} x_j$$



```
// do the multiplication:
// 1. broadcast along columns
MPI_Bcast(&x[0], x.size(), MPI_DOUBLE, col, col_comm);

// 2. do local multiplication
dgemv(A,x,y);

// 3. reduce along row
MPI_Reduce(row==col ? MPI_IN_PLACE : &y[0], &y[0], y.size(), MPI_DOUBLE, MPI_SUM, row, row_comm);
```

Now with communicator construction

```
int N=1024;
int num_blocks = std::sqrt(size);;
int block_size = N/std::sqrt(size);
assert(size = num_blocks * num_blocks);
assert(N % block_size == 0);

// build a cartesian topology
int periodic[2] = {true, true};
int extents[2] = {num_blocks, num_blocks};
MPI_Comm comm;
MPI_Cart_create(MPI_COMM_WORLD, 2, extents, periodic, true, &comm);

// get my row and column number
int coords[2];
MPI_Cart_coords(comm, rank, 2, coords);
int row = coords[0];
int col = coords[1];

// build communicators for rows and columns
MPI_Comm row_comm, col_comm, diag_comm;
MPI_Comm_split(comm,row,col,&row_comm);
MPI_Comm_split(comm,col,row,&col_comm);

// block distribution of the vectors on the diagonal
vector_type x(block_size), y(block_size);
...

// allocate a block of the matrix everywhere and fill it in
matrix_type A(block_size,block_size);
  ...

// do the multiplication:
MPI_Bcast(&x[0], x.size(), MPI_DOUBLE, col, col_comm);
dgemv(A,x,y);
MPI_Reduce(row==col ? MPI_IN_PLACE : &y[0], &y[0], y.size(), MPI_DOUBLE, MPI_SUM, row, row_comm);
```

Exam Question I

In the following MPI code, we want to send some elements of a square matrix from rank 0 to rank 1.

```
1  if (rank == 0)
2  {
3     double A[N][N];
4     // initialization of A
5
6     // TODO: send the anti-diagonal elements of matrix A to rank 1
7  }
8  if (rank == 1)
9  {
10    double buffer[N];
11
12    // TODO: receive elements from rank 0
13
14    // buffer can be used here
15 }
```

a) Build and use an appropriate MPI datatype to send the anti-diagonal elements of matrix A.

b) What modifications to your solution code are required in order to send the diagonal elements of matrix A?

Exam Question II (1)

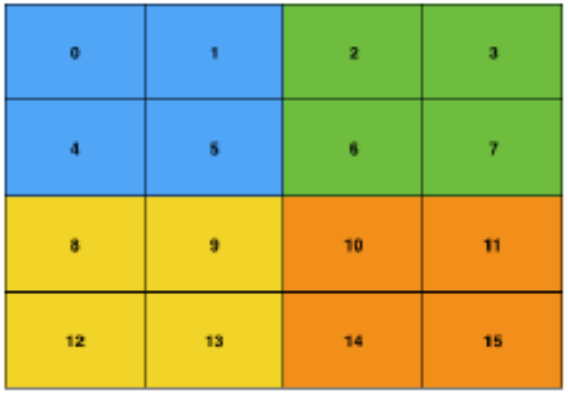
Consider the function `void diffusion_mpi(MPI_Comm comm, int N, int id)`, which solves the diffusion equation in two dimensions on a NxN grid using MPI. The communicator `comm` might be other than `MPI_COMM_WORLD`. The last argument enables users to perform multiple calls to `diffusion_mpi()`, as in the following example:

```
1 // MPI initialization
2
3 // TODO: perform the four calls in parallel, using np=P^2 ranks in total
4 diffusion_mpi(MPI_COMM_WORLD, 1024, 0);
5 diffusion_mpi(MPI_COMM_WORLD, 1024, 1);
6 diffusion_mpi(MPI_COMM_WORLD, 1024, 2);
7 diffusion_mpi(MPI_COMM_WORLD, 1024, 3);
8
9 // MPI shutdown
```

Exam Question II (2)

```
1 // MPI initialization
2
3 // TODO: perform the four calls in parallel, using np=P^2 ranks in total
4 diffusion_mpi(MPI_COMM_WORLD, 1024, 0);
5 diffusion_mpi(MPI_COMM_WORLD, 1024, 1);
6 diffusion_mpi(MPI_COMM_WORLD, 1024, 2);
7 diffusion_mpi(MPI_COMM_WORLD, 1024, 3);
8
9 // MPI shutdown
```

Use MPI groups and communicators to perform the 4 calls to `diffusion_mpi()` at once and within a single MPI application. Assume that the application uses $n_p = P^2$ processes and each call must be performed by a subgroup of processes. There are 4 subgroups of equal size and each subgroup corresponds to a square sub-grid of MPI processes. An example for $n_p = 16$ is depicted in the following figure:



Extend the above MPI code so as to perform the 4 calls in parallel as described above.

Note: Assume that P is even and $P >= 2$.