# CS420 – Lectures 18, 19 and 20

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## Particle Code – Molecular Dynamics

Simulate movement of bunch of atoms, each with its charge
Highly simplified description: Repeat, for millions of steps

- Compute forces between atoms
  - Coulomb forces, due to atom charge
  - Bond forces
- Update velocity
- Update location

No need to maintain velocity:

$$\vec{x}_{n+1} = 2\vec{x}_n - \vec{x}_{n-1} + \vec{F}_n \cdot mass\, \Delta t^2.$$

Usually compute forces only for nearby atoms, use another method to handle long-range interactions

## Algorithm outline

```
foreach pair of atoms x,y {
$dist = ||x.\vec{loc} - y.\vec{loc}||$;
if $dist < C$ {
    $\vec{direction} = (x.\vec{loc} - y.\vec{loc})/dist$;
    $force = -(x.charge \cdot y.charge)/dist^2$;
    $x.\vec{force} -= force \cdot \vec{direction}$;
    $y.\vec{force} += force \cdot \vec{direction}$;
}
}
foreach atom x {
$\vec{temp} = x.\vec{loc}$;
$x.\vec{loc} = 2 \cdot \vec{temp} - x.\vec{oldloc} + x.\vec{force} \cdot x.mass$;
$x.\vec{oldloc} = \vec{temp}$;
}
```

Will assume world is 2D – to shorten code

C does not have vector operations – need to define them. We do this with C macros

```
#define v_assign(x,y) {y[0]=x[0]; y[1]=x[1];} /* vec=vec */
#define s_times_v(s,x,y) {y[0]=s*x[0]; y[1]=s*x[1];} /* vec=scalar*vec */
#define v_plus_v(x,y,z) {z[0]=x[0]+y[0]; z[1]=x[1]+y[1];} /* vec=vec+vec */
#define v_minus_v(x,y,z) {z[0]=x[0]-y[0]; z[1]=x[1]-y[1];} /* vec=vec-vec */
#define v_norm(x)  sqrt(x[0]*x[0]+x[1]*x[1]) /* vector norm */
```

Can use functions – but then would want the compiler to inline them

```
static inline void
assign (double x[2], double y[2])
{
y[0] = x[0]; y[1] = x[1];
}
```

Inlining: No function call; the code of the function is inserted in place of a function call.

## Data Structure

```
typedef struct Atom {
double loc[2]; /* current location */
double oldloc[2]; /* previous location */
double mass; /* mass */
double charge; /* charge */
double force[2]; /* force operating on atom */
} Atom;
```

## Algorithm outline

```
foreach pair of atoms x,y {
$dist = ||x.\vec{loc} - y.\vec{loc}||$;
if $dist < C$ {
   $\vec{direction} = (x.\vec{loc} - y.\vec{loc})/dist$;
   $force = -(x.charge \cdot y.charge)/dist^2$;
   $x.\vec{force} -= force \cdot \vec{direction}$;
   $y.\vec{force} += force \cdot \vec{direction}$;
}
}
foreach atom x {
$\vec{temp} = x.\vec{loc}$;
$x.\vec{loc} = 2 \cdot \vec{temp} - x.\vec{oldloc} + x.\vec{force} \cdot x.mass$;
$x.\vec{oldloc} = \vec{temp}$;
}
```

```
void interact(Atom *x, Atom *y) {
double force, dist, direction[2];

v_minus_v( x->loc, y->loc, direction)
dist = v_norm(direction);
if (dist < C) {
 s_times_v( (1/dist), direction, direction);
 force = -(x->charge * y->charge)/(dist*dist);
 s_times_v(force, direction, direction);
 v_minus_v(x->force, direction, x->force);
 v_plus_v(y->force, direction, y->force);
 }
}
```

## Move atom

Assume $\Delta t = 1$.

```
void move(Atom *x) {
 double temp[2];
 for (i=0; i<2; i++) {
  temp[i] = x->loc[i];
  x->loc[i] = 2*temp[i] - x->oldloc[i] + x->force[i]*x->mass;
  x->oldloc[i] = temp[i];
  }
 }
```

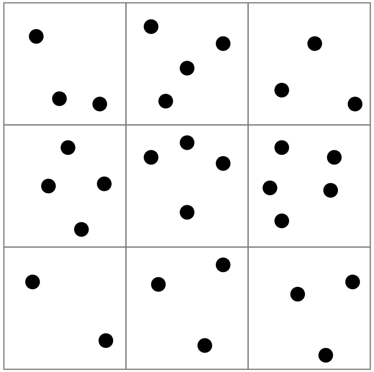
or

```
...
v_assign_v(x->loc, temp);
v_plus_v(temp, temp, x->loc);
v_minus_v(x->loc, x->oldloc, x->loc);
s_times_v(x->mass, x->force, part);
v_plus_v(x->loc, part, x->loc);
V_assign_v(temp,x->oldloc)
```

Functions should be inlined, if possible

## parallel (message-passing) algorithm

- Divide the (2D) domain into cells; assign a cell to each process.
- Results in OK load balancing if atom density is close to constant. (True of molecular simulations, not of cosmology simulations.)
- Usually, cell dimension $\gg$ cutoff radius. Atoms may interact only with atoms in nearby cells.
- Array is periodic

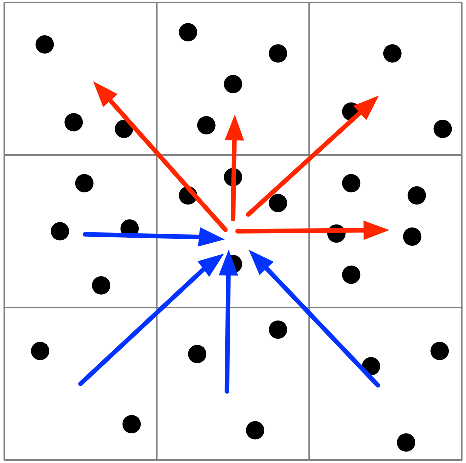


## Algorithm outline

Repeat

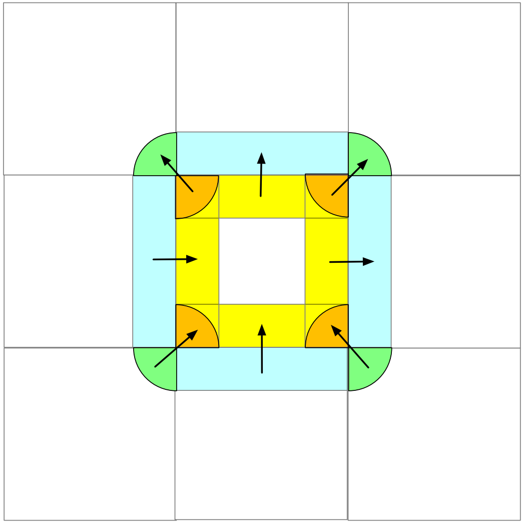
1. Broadcast atoms to neighbor cells
2. Compute atom-atom interactions
3. Collect back computed forces
4. Update locations
5. Move particles that crossed cell boundaries

To compute each force only once, send in 4 directions and receive from 4 directions



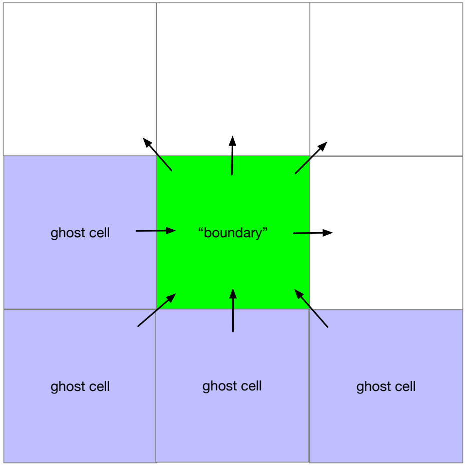
## Interactions

- Atoms at the boundary of a cell interact with atom on the corresponding boundary of the neighboring cell
- Can use “ghost cell” pattern – but need to recompute boundary at each iteration (atom moves!)
- Have a pretty good estimate of number of atoms in each slice ($\sim$ constant density)



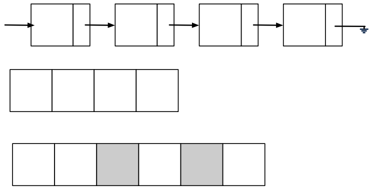
## Simplified algorithm

- Assume all atoms could interact with atoms in neighboring cells (they are all “on the boundary”)
- Superflous work and communication but correct, since check cuttoff before computing atom-atom interaction
- “boundary” communicated to four other processess (NE, N, NW, E)
- Process stores 4 ghost cells, where it receives atoms from W, SE, S, SW



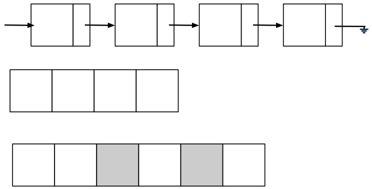
## Implementation choices

- No need to communicate all atom fields: Need to broadcast location and charge and receive back (reduce) forces– might be worthwhile to keep these fields separately
- How do we store atom list?
  - Don't care the order in which they are stored
  - Need to insert and delete atoms in the list (when they move from cell to cell)
  - But few atoms change cell at each iteration (pragmatic knowledge)



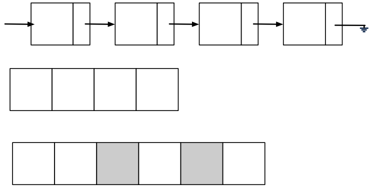
linked list

- Easy to insert or delete
- Data not contiguous and links take space



linked list
- Easy to insert or delete
- Data not contiguous and links take space

contiguous array
- Easy to insert (at array end)
- Expensive to delete, if deletes are at arbitrary locations

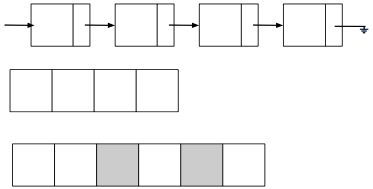


linked list

- Easy to insert or delete
- Data not contiguous and links take space

contiguous array

- Easy to insert (at array end)
- Expensive to delete, if deletes are at arbitrary locations
- Easy to delete (and compress) if deletes done while traversing the array sequentially



linked list

- Easy to insert or delete
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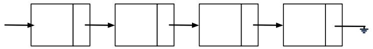
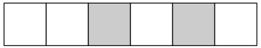
contiguous array

- Easy to insert (at array end)
- Expensive to delete, if deletes are at arbitrary locations
- Easy to delete (and compress) if deletes done while traversing the array sequentially

Array with "holes": Deleted items are marked invalid

- Easy to insert or delete
- OK if deletes are small fraction of accesses: Can compress periodically





- Will use array
- Will split parts to send and to receive
- “struct of arrays” or “array of structs”? so that parts sent and received are contiguous, and vectorization easier.

“struct of arrays” so that parts sent and received are contiguous, and vectorization easier.

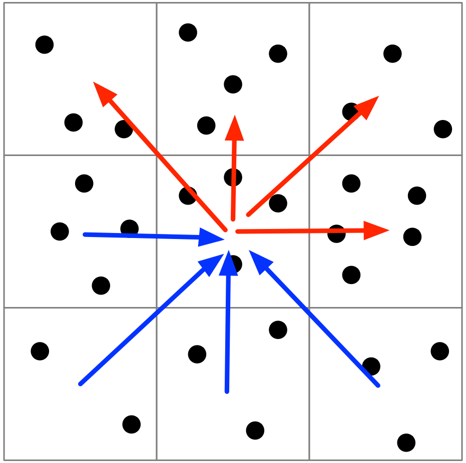
```
/* atom data structures */
double loc[MAXATOMS][2];
double oldloc[MAXATOMS][2];
double mass[MAXATOMS];
double charge[MAXATOMS];
double force[MAXATOMS][2];
```

## Communication

How do we communicate?

- 4 sends & 4 receives (of atom lists) followed by 4 receives and 4 sends (of forces) (13 in 3D)
- 1 broadast as root and 4 broadcasts as receiver, followed by one reduce as root and 4 reduces as senders (adding forces) (1 and 13, in 3D)

*Not sure which is better – will use collectives in example*



## Create Cartesian topology

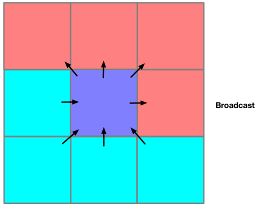
```
/* create 2D torus */
MPI_Comm_size(MPI_COMM_WORLD, &size);
MPI_Dims_create(size, 2, dims);
if (int dim = dims[0] != dims[1]) exit(1); /* should be square */
period[0]=period[1]=true;
MP_Cart_create(MPI_COMM_WORLD,2,dims,periods,true, &torus);
MPI_Comm_rank(torus, &myrank);
MPI_Cart_coords(torus, myrank, 2, mycoords); /* returns x,y coordinates */

...
```

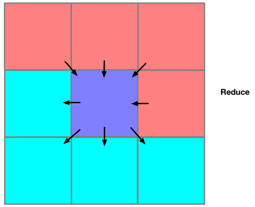
## Basic algorithm

repeat:

1. Send atom list to neighbors in directions NE, N, NW, E
2. Receive atom list from neighbors in directions W, SE, S, SW
3. Compute all interactions between local atoms and other atoms at process (local-local, local-W, local-SE, local-S,local-SW
4. Gather and sum forces acting on local atoms from neighbors in directions NE, N, NW, E and from local-local interactions
5. Compute new positions for local atoms
6. Communicate atoms that crossed boundaries

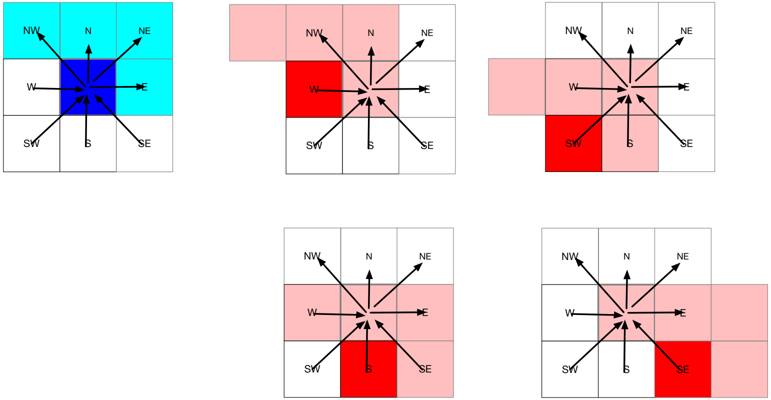
Need four ghost cells





## Communicators for broadcast-reduce

- process is root in the group containing itself, and neighbors in directions NW, N, NE, E.
- It participates in four other groups rooted at neighbors in directions W, SW, S, SE



## Splitting Communicators

```
MPI_Comm_split(comm, color, key, newcomm)
```

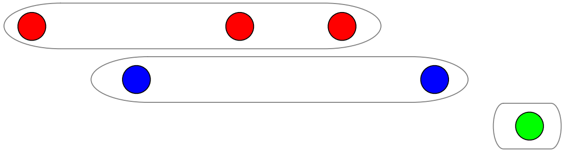
- Called collectively by all processes in `comm`
- One new communicator is created for each distinct value of `color`
- All processes that provides the same 'color' (an integer) end up in the same communicator
- They are ordered in increasing value of key (with ties broken according to the old rank)

| | |
|---|---|
| comm | communicator being split |
| color | integer used to partition the processes |
| key | integer used to specify process order in new communicator |
| newcomm | new communicator |

arguments passed to MPI_Comm_split

| | | | | | | |
|---|---|---|---|---|---|---|
| ranks in comm | 0 | 1 | 2 | 3 | 4 | 5 |
| color | 0 | 1 | 0 | 0 | 1 | 2 |
| key | 2 | 0 | 0 | 0 | 0 | 0 |

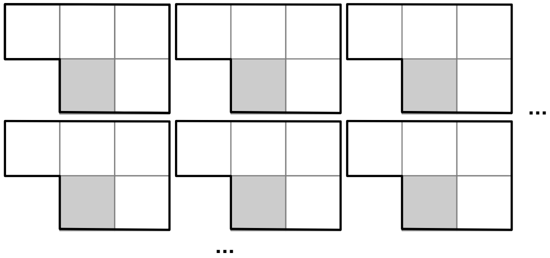
new communicators



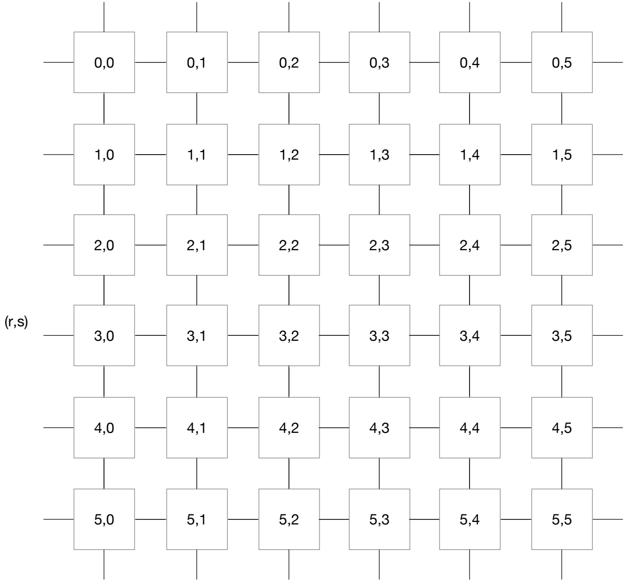
| | | | | | | |
|---|---|---|---|---|---|---|
| new ranks | 2 | 0 | 0 | 1 | 1 | 0 |

## Splitting communicators

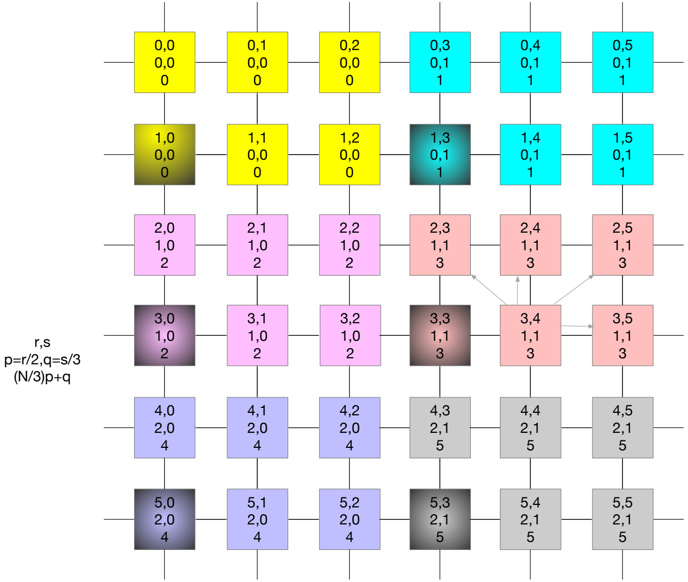
- It is “easy” to split a communicator into sub-communicators with disjoint process groups; not possible to create overlapping communicators.
- Need to create the new communicators in successive phases, where communicators created at the same phase do not overlap
- Can do it in 6 phases, assuming `dimm` divides by 6: Slide basic template across $3 \times 2$ positions.



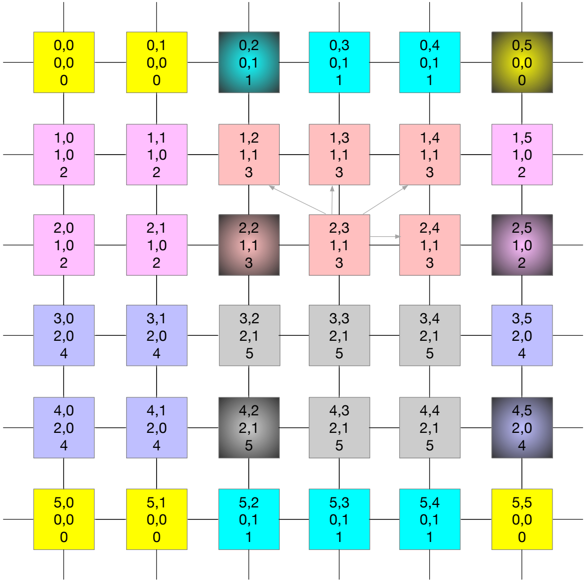
## MD – process mesh (Cartesian topology)



## Splitting communicators

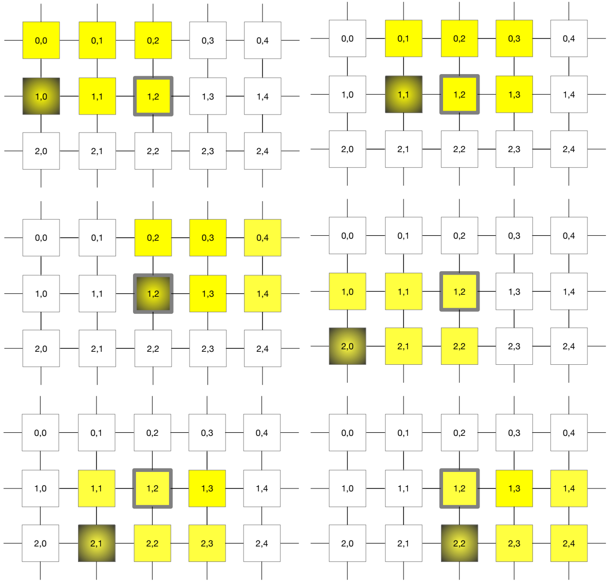


## Splitting communicators shift (1,1)



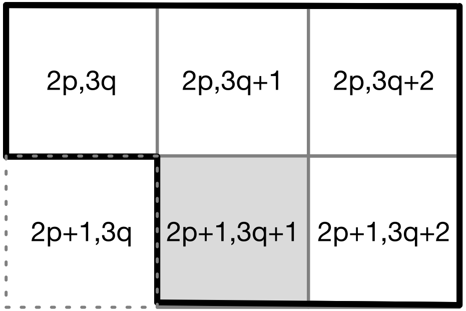
r,s
p=(r+1)/2,q=(s+1)/3
(N/3)p+q

# Communicators defined at process (1,2)

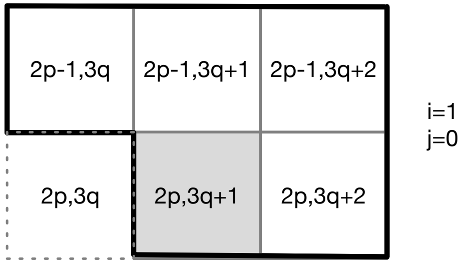


Assume `dimm` is a multiple of 6

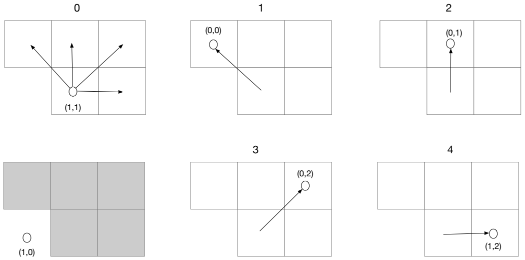
- Let $(r, s)$ be the coordinates of a cell.
- Compute $p = r/2$ and $q = s/3$.
- Six processes, in the $2 \times 3$ rectangle with cell $2p, 3q$ in the upper left corner, will compute the same $(p, q)$ values.
- The plane will be tesselated by $(\texttt{dimm}/2)\times(\texttt{dimm}/3)$ $2\times3$ rectangles



- Compute, for $i = 0, 1$ and $j = 0, 1, 2$
  $p = ((r + i) \mod dimm)/2$ and
  $q = ((s + j) \mod dimm)/3$.
- Six processes, in the $2 \times 3$ rectangle with cell $(2p - i, 3q - j)$ in the upper left corner, will compute the same $(p, q)$ values.
- Each $2 \times 3$ rectangle will obtain once
- Only five of the processes in the rectangle should be in the newly created communicator



- Let $m = (r + i) \mod 2$ and $n = (s + j) \mod 3$
- If $(m, n) = (1, 1)$ then process $(r, s)$ is the root of the broadcast
- If $(m, n) = (0, 0)$ then process $(r, s)$ receives a broadcast from SE process
- If $(m, n) = (0, 1)$ then process $(r, s)$ receives a broadcast from S process
- If $(m, n) = (0, 2)$ then process $(r, s)$ receives a broadcast from SW process
- If $(m, n) = (1, 2)$ then process $(r, s)$ receives a broadcast from W process
- If $(m, n) = (1, 0)$ then process should not be in communicator.



## Create communicators

```
for(i=0; i<2; i++)
 for(j=0; j<3 ; j++) {
  p= ((mycoords[0]+i)%dimm)/2; m = (mycoords[0]+i)%2;
  q= ((mycoords[1]+j)%dimm)/3; n = (myccords[1]+j)%3;
  color = (N/3)*p+q;
  if ((m==1) && (n==0)) color = MPI_UNDEFINED;
  k = 3*m+n+1;
  if(k==4) k=0; /* find communicator index */
  if(k==6) k=4;
  MPI_Comm_split(torus, color, 0, &comm[k]);
  }
```

- Each process belongs to 5 new communicators
- In one of the 6 calls, the color was `MPI_UNDEFINED` and the call returned `MPI_COMM_NULL`
- In each new communicator the processes are ordered in row major order (according to previous rank), so root has rank 3 in each of the new communicators
- Communicators are numbered as indicated in Figure

- Each process calls `MPI_Comm_split` 6 times (i-shift of 0 and 1 and j-shift of 0,1 and 2).
- In one of the calls it is passes argument `color=MPI_UNDEFINRRED`
- Each process constructs 5 communicators each containing 5 processes
- In each of these communicators, the process is in a different position of a 2×3 rectangle that includes it (except the bottom left position)

## communication

```
/* broadcast number of atoms at root process */
numreq=0;
count[0]=numatoms;
for (k=1; k<5; k++)
 MPI_Ibcast(&count[k], 1, MPI_INT, 3, comm[k], req[numreq++]);
MPI_Waitall(5,req, MPI_STATUSES_IGNORE);
```

Assume that locations are stored in an array `loc[5][MAXATOMS][2]`: One MAXATOMS$\times$2 array for local coordinates and 4 for coordinates of atoms in neighbor cells. Charges are stored in array `charge[5][MAXATOMS]`

```
/* broadcast atoms */
numreq=0;
for(k=0;k<5;k++)
  MPI_Ibcast(loc[k][MAXATOMS], 2*count[k], MPI_DOUBLE, 3,
      comm[k], req[numreq++]);
MPI_Waitall(5, req, MPI_STATUSES_IGNORE);
```

## Reduce

Broadcast is followed by force computations, next by the gathering of the computed forces

```
/* collect forces*/
numreq=0;
for(k=0;k<5;k++)
 MPI_Ireduce(force[k][MAXATOMS], 2*count[k], MPI_DOUBLE, 3, comm[k],
 req[numreq++]);
MPI_Waitall(5, req, MPI_STATUSES_IGNORE);
```

## Algorithm steps

1. Broadcast atom list to neighbors in directions NE, N, NW, W
2. Receive atom list from neighbors in directions E, SE, S, SW
3. Compute all interactions between local atoms and other atoms at process (local-local, local-E, local-SE, local-S,local-SW
4. Gather and sum forces acting on local atoms from neighbors in directions NE, N, NW, W and from local-local interactions.
5. Compute new positions for local atoms
6. Communicate atoms that crossed boundaries

## Algorithm steps

Shown how to implement the following:

1. Broadcast atom list to neighbors in directions NE, N, NW, W
2. Receive atom list from neighbors in directions E, SE, S, SW
3. Compute all interactions between local atoms and other atoms at process (local-local, local-E, local-SE, local-S,local-SW
4. Gather and sum forces acting on local atoms from neighbors in directions NE, N, NW, W and from local-local interactions.
5. Compute new positions for local atoms
6. Communicate atoms that crossed boundaries

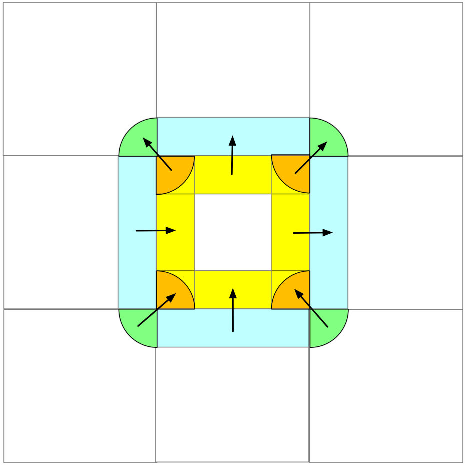
Reference Slides

* Need not be used to prepare for the exam.

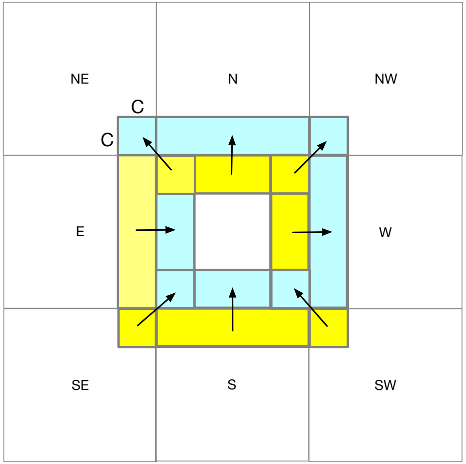
## Possible Improvements (outline)

If cutoff radius is $\ll$ cell size, will want to communicate only cells close to boundary

Boundary regions



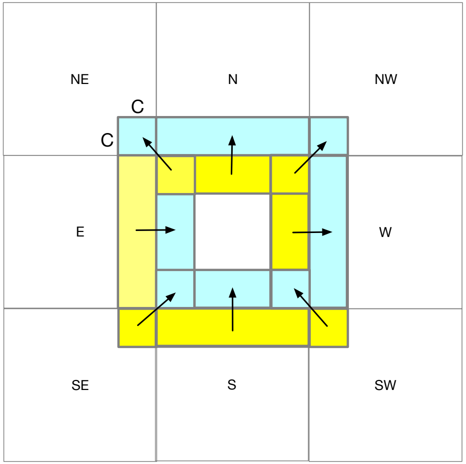
Simplified view (cutting corners)



## Possible implementation

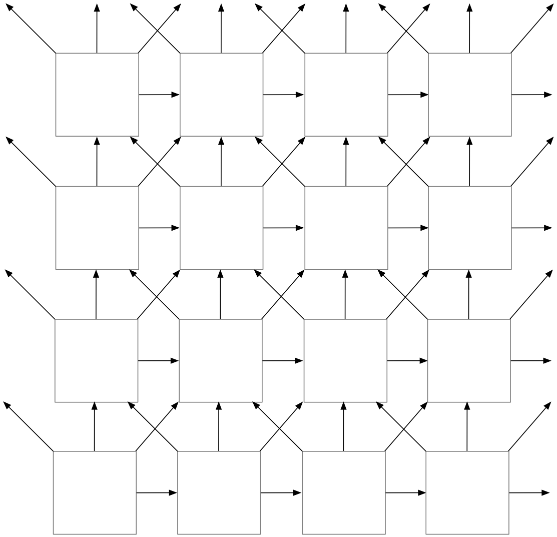
Keep 9 lists for atoms in each of the boundary regions and in center

1. Start send or receive of atoms in boundary regions
2. Compute interactions of atoms in center region
3. complete send/receives
4. Compute interactions of atom in adjacent boundary regions
5. Send/receive back forces
6. Sum forces
7. Update local atom locations
8. Move atoms crossing boundaries



## Alternative Approach – Use Sparse Collectives

- Can create a communicator that has a directed graph topology
- Can execute a *Neighborhood Gather* collective call that sends data on each outgoing edge and receives data on each incoming edge
- Need a graph to send atoms and a reverse graph to receive forces (no reduce)



## Create communicator with graph topology

`MPI_Dist_graph_create_adjacent(comm, indegree, sources, outdegree, destinations, weights, info, reorder, newcomm)`

| | |
|---|---|
| comm | old communicator |
| indegree | number of incoming edges |
| sources | ranks of source nodes |
| outdegree | number of outgoing edges |
| destinations | ranks of destination nodes |
| weights | weights of outgoing edges |
| info | hints |
| reorder | `true` if can reorder processes, `false` otherwise |
| newcomm | new communicator with graph topology. |

## Find neighbors

```
/* assume comm has a Cartesian topology */
...
enum directions {NW, N, NE, E, SE, S, SW, W};
int neighbors[8]; /* ranks of neighbors */
int coords[2], ncoords[2], dims[2], periods[2], neighbor[8];
MPI_Cart_get(comm, 2, dims, periods, coords)
               /* returns info on Cartesian topology */
ncoords[0]=(coords[0]-1)%dims[1];
ncoords[1]=(coords[1]-1)%dims[1];
MPI_Cart_rank(comm, ncoords, &neighbors[NW]);
               /* translates Cartesian coordinates into ranks */
ncoords[0]= (ncoords[0]+1)%dims[0];
MPI_Cart_rank(comm, ncoords, &neighbors[N]);
ncoords[0]= (ncoords[0]+1)%dims[0];
MPI_Cart_rank(comm, ncoords, &neighbors[NE]);
ncoords[1]= (ncoords[1]+1)%dims[1];
MPI_Cart_rank(comm, ncoords, &neighbors[E]);
...
```

```
MPI_Cart_get(comm, maxdims, dims, periods, coords)
```

| | |
|---|---|
| comm | communicator with Cartesian structure |
| maxdims | number of dimensions |
| dims | extent of each dimension |
| periods | periodicity in each dimension |
| coords | Cartesian coordinates of calling process |

`MPI_Cart_rank(comm, coords, rank)`

| | |
|---|---|
| comm | communicator with Cartesian topology |
| coords | Cartesian coordinates of process |
| rank | rank of process |

## Create new communicators

```
...
MPI_Dist_graph_create_adjacent(comm, 4, neighbors[NW], 4,
    &neighbors[SE], MPI_UNWEIGHTED, NULL, false, &outcomm);

MPI_Dist_graph_create_adjacent(comm, 4, neighbors[SE], 4,
&neighbors[NW], MPI_UNWEIGHTED, NULL, false, &outcomm);]
...
```

## Neighborhood collectives

```
MPI_Neighbor_allgather( sendbuf, sendcount, sendtype, recvbuf, recvcount,
recvtype, comm )
```

| | |
|---|---|
| sendbuf | send buffer |
| sendcount | number of elements sent to each destination |
| sendtype | data type of sent elements |
| recvbuf | receive buffer |
| recvcount | number of elements received from each source |
| recvtype | data type of received elements |
| comm | communicator with topology structure |

Same data sent to all destination processes; different data received from source processes

```
MPI_Neighbor_allgatherv(sendbuf, sendcount, sendtype, recvbuf, recvcounts,
displs, recvtype, comm)
```

## Neighborhood collectives

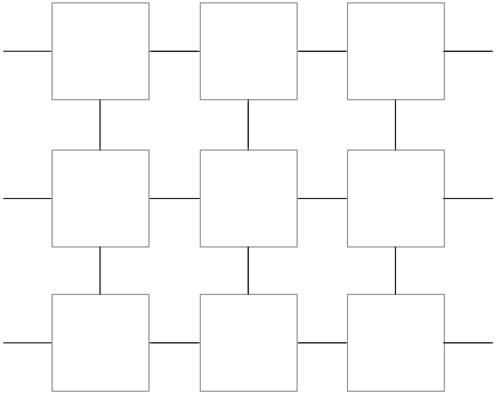
Different data sent to different destinations

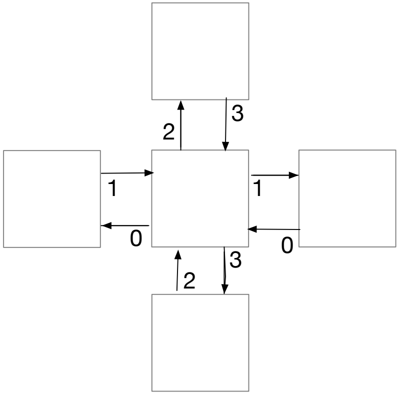
```
MPI_Neighbor_alltoall(sendbuf, sendcount,sendtype, recvbuf, recvcount,
recvtype, comm)
MPI_neighbor_alltoallv(sendbuf, sendcounts, sdispls, sendtype, recvbuf,
recvcounts, rdispls, recvtype, comm)
```

| | |
|---|---|
| sendbuf | send buffer |
| sendcounts | number of elements sent to each destination |
| sdispls | displacement to 1st element sent to each destination |
| sendtype | type of sent elements |
| recvbuf | receive buffer |
| recvcounts | number of elements received from each destination |
| rdispls | displacement to 1st element received form each source |
| recvtype | tyoe of received elements |
| comm | communicator |

## Sparse collectives

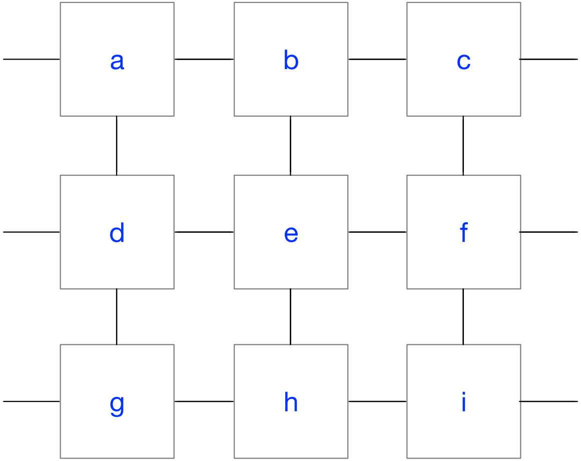
Cartesian topology is also a graph topology: Each node has 2D incoming and 2D outgoing edges (with possible exception of boundaries).





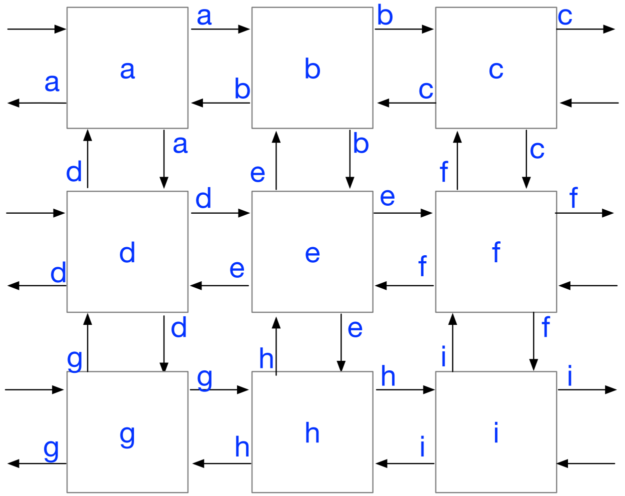
## MPI_Neighbor_allgather

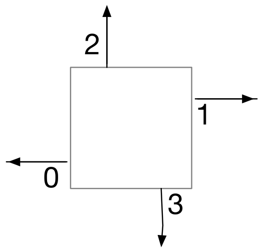
```
MPI_Neighbor_allgather(sendbuf, 1, MPI_CHAR, recvbuf, 1, MPI_CHAR, comm)
```



# MPI_Neighbor_allgather – communication

```
MPI_Neighbor_allgather(sendbuf, 1, MPI_CHAR, recvbuf, 1, MPI_CHAR, comm)
```

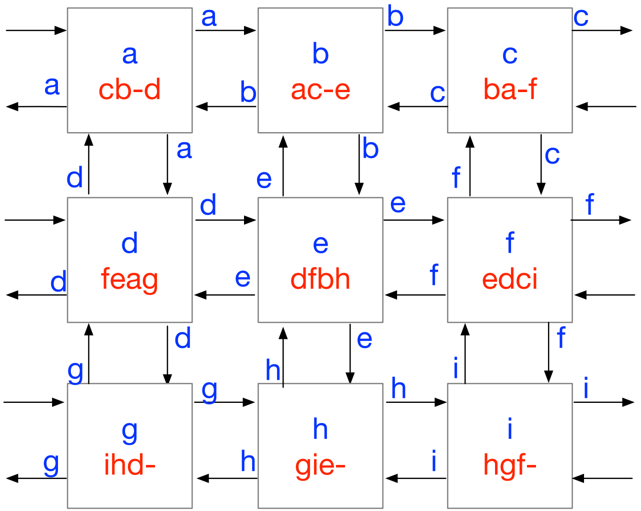


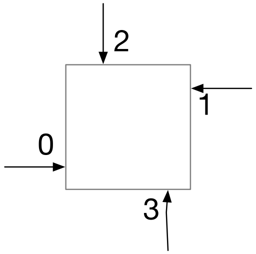


## MPI_Neighbor_allgather – result

```
MPI_Neighbor_allgather(sendbuf, 1, MPI_CHAR, recvbuf, 1, MPI_CHAR, comm)
```

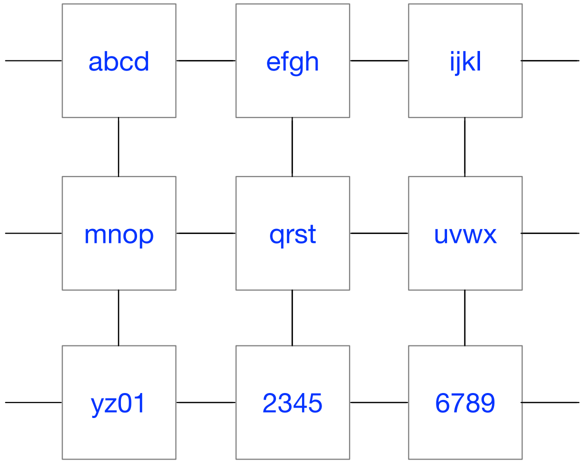
Dash (-) indicates locations that is not updated by call





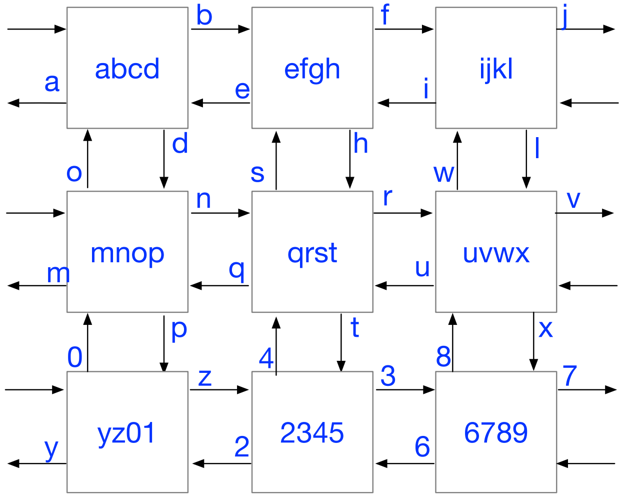
## MPI_Neighbor_alltoall

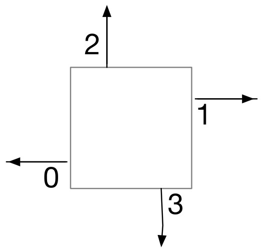
```
MPI_Neighbor_alltoall(sendbuf, 1, MPI_CHAR, recvbuf, 1, MPI_CHAR, comm)
```



## MPI_Neighbor_alltoall – communication

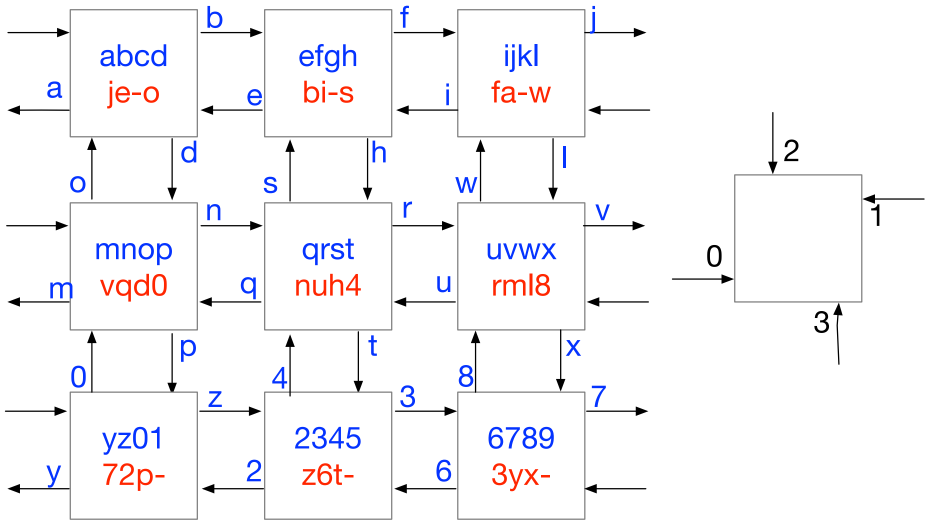
```
MPI_Neighbor_alltoall(sendbuf, 1, MPI_CHAR, recvbuf, 1, MPI_CHAR, comm)
```





# MPI_Neighbor_alltoall – result

```
MPI_Neighbor_alltoall(sendbuf, 1, MPI_CHAR, recvbuf, 1, MPI_CHAR, comm)
```



## Variants

The two calls have a "v" variant where communicated messages can have diffferent lengths:

```
MPI_Neighbor_allgatherv(sendbuf, sendcount, sendtype, recvbuf, recvcounts,
displs, recvtype, comm)
MPI_Neighbor_alltoallv(sendbuf, sendcounts, sdispls, sendtype, recvbuf,
recvcounts, rdispls, recvtype, comm)
```

Each of the four calls have a nonblocking variant.

## Communication

```
\* numatoms -- number of atoms *\
\* loc[k][i] -- coordinates of local atom i *\
\*  (k=0) or i-th atom received from k-th neighbor (k>0) *\
\* mass, charge, force -- ibid *\

int atomcounts[4]; \* number of atoms coords received *\
int displs[4]; \* displacements *\
for(i=0; i<4;i++)
 displs[i] = 2*i*MAXATOMS
\* communicate atom counts *\
MPI_Neighbor_allgather(&numatoms, 1, MPI_INT,
    atomcounts, 1, MPI_INT, incomm);

\* communicate atom locations *\
for(i=0;i<4;i++)
 atomcounts[i]*=2;
MPI_Neighbor_allgatherv(loc, 2*numatoms, MPI_DOUBLE,
    loc[MAXATOMS], atomcounts, MPI_DOUBLE, incomm);
... \* communicate masses and charges *\\
```

## Communication

```
... \* compute forces *\
\* communicate back forces *\
double outforces[5][MAXATOMS][2] \* arrray of locally computed forces *\
double inforces[5][MAXATOMS][2] \* array for received forces *\
MPI_Neighbors_alltoallv(outforces[1], atomcounts, displs, MPI_DOUBLE,
    inforces[1], 2*numatoms, displs, MPI_DOUBLE, outcomm);
\* sum forces *\
for(i=0; i<numatoms, i++) {
 v_assign_v(outforce[0][i],inforce[0][i]);
 for(j=1,j<5;j++)
   v_plus_v(inforce[j][i],inforce[0][i],inforce[0][i]);
```