CS420 – Lectures 13 and 14

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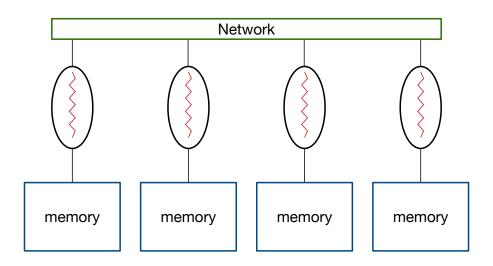
Spring 2023



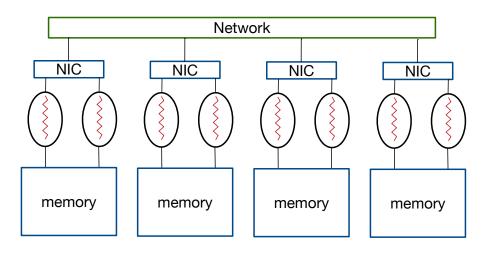
Beyond shared memory

Shared memory becomes expensive and hard to scale beyond a few sockets. Instead we use *distributed memory*

Distributed memory



Hybrid shared memory/distributed memory



Basic communication mechanism

Hardware: • Moves data from the memory of one node to the memory of another node.

Provides indication that transfer is complete

Software: • Calls to move data from one memory to another

Calls to synchronize

Communication is achieved by a matching pair of a send and a receive: $send(to, data) \longrightarrow recv(from, data)$

The communication

- Moves data (from sender to receiver)
- Synchronizes (receive will complete after send started)

MPI

- MPI (Message Passing Interface) is a Standard Message passing library designed by an open forum that is broadly used in HPC.
- Standardization effort started in 1992, MPI-1 was published late 93.
- Has C and Fortran binding



Basic communication mechanism: sending & receiving messages $send(to, data) \longrightarrow recv(from, data)$

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- Who is communicating?
 - In MPI the communication is between *processes*. Typically, processes will be on different nodes, but they could be on the same node.
- Need process ids
 - An MPI computation involves a group of processes. The initial group is MPI_COMM_WORLD. Each process has a rank within MPI_COMM_WORLD; ranks are from 0 to N-1, if there are N processes. (Actually, MPI_COMM_WORLD is a communicator, more about this later.)

Hello world

```
#include <mpi.h>
#include < stdio.h>
int main(int argc, char **argv)) {
int rank, size;
MPI_Init(&argc, &argv);
MPI_comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &size);
printf(''I am %d of %d\n", rank, size);
MPI_Finalize();
return 0;
```

- main is executed by each process.
 Number of processes is fixed
- MPI_comm_rank() returns rank of calling process
- MPI_comm_size() returns number of processes
- Initialization and finalization is required

Simple communication

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char ** argv)
int rank, val[100];
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
if (rank == 0)
MPI_Send(val, 100, MPI_INT, 1, 0, MPI_COMM_WORLD);
else if (rank == 1)
MPI_Recv(val, 100, MPI_INT, 0, 0, MPI_COMM_WORLD,
MPI_STATUS_IGNORE);
MPI Finalize();
return 0;
```

```
MPI_Send(val, 100, MPI_INT, 1, 0, MPI_COMM_WORLD)
```

• I am sending data that is stored in a buffer starting at val (send buffer)

```
MPI_Send(sendbuf, count, type, dest, tag, comm)
```

```
MPI_Send(val, 100, MPI_INT, 1, 0, MPI_COMM_WORLD)
```

- I am sending data that is stored in a buffer starting at val (send buffer)
- I am sending 100 items

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MPI_Send(sendbuf, count, type, dest, tag, comm)
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- These items are integers

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- I am sending 100 items
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- The *destination* is the process with rank 1 in MPI_COMM_WORLD
- The message is *tagged* with the value 0.

• I am receiving data into the buffer starting at location val (receive buffer)

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- I am receiving (up to) 100 items

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- I am receiving data into the buffer starting at location val (receive buffer)
- I am receiving (up to) 100 items
- These items are integers
- The source should be the process with rank 0 in MPI_COMM_WORLD
- The message should be *tagged* with the value 0.

- I am receiving data into the buffer starting at location val (receive buffer)
- I am receiving (up to) 100 items
- These items are integers
- The source should be the process with rank 0 in MPI_COMM_WORLD
- The message should be tagged with the value 0.
- I don't need for MPI to return in status information on how the communication completed

Rules

- The receive will match a message sent to the right destination (communicator and rank, with the correct information on the "envelope": sender and tag.
- The programmer must ensure that
 - The datatypes match
 - The sent message does not overflow the receive buffer (OK to send fewer items, the status parameter will tell how many were actually received).
- The send will complete as soon as the message was copied out of the sender memory
 - Possibly before the receive started, if there is buffering
 - Possibly only after the receive is posted, if there is no buffering
- The receive will complete as soon as all the data has been copied into the receive buffer
- Mismatched sends and receives can cause deadlocks!

Communicators

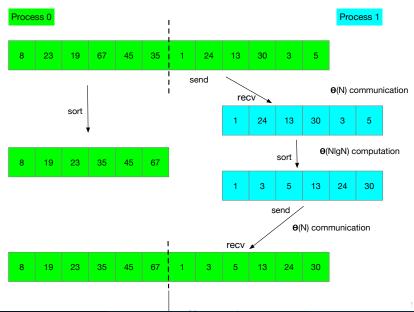
- A communicator is
 - An ordered set of processes
 - A context, a "color"

A process can be in multiple communicators, with a different rank in each

- Communications with different communicators do not interfere with each other
 - Important in the design of parallel libraries
- Simple programs only use MPI_COMM_WORLD

Example

(Naive) parallel sort with 2 processes

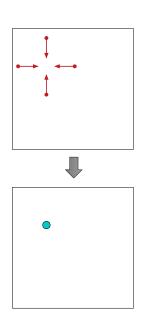


```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char ** argv)
int rank:
int a[1000];
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
if (rank == 0) {
MPI Send(&a[500], 500, MPI INT, 1, 0, MPI COMM WORLD);
sort(a, 500);
MPI_Recv(&a[500], 500, MPI_INT, 1, 0, MPI_COMM_WORLD, &status);
merge(a);
else if (rank == 1) {
MPI_Recv(a, 500, MPI_INT, 0, 0, MPI_COMM_WORLD, &status);
sort(a, 500);
MPI_Send(a, 500, MPI_INT, 0, 0, MPI_COMM_WORLD);
MPI_Finalize(); return 0;
```

Is the parallel algorithm faster than sequential?

- Sequential time: $a + bn + cn \lg n$: fixed overhead (e.g., start program), linear overhead (e.g., read/write array) and $n \lg n$, for sorting.
- Parallel time: $al + bn + c(n/2) \lg(n/2) + dn$: fixed, larger overhead to start computation on two nodes; same I/O overhead; sorting work roughly reduced by half; linear communication time added.
- Parallel algorithm is faster if $a + bn + cn \lg n > a' + bn + c(n/2) \lg(n/2) + dn$ or $a + \frac{cn}{2} (\lg n + 1) > a' + dn$
- Parallel algorithm is faster for large n, and sequential algorithm is better for small n (since $al \gg a$); crossing point will depend on exact values of the various coefficients.

Jacobi



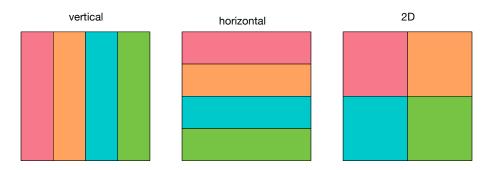
```
do {
 err=0; l=1-1;
  for (i=1; i<N-1; i++)
  for (j=1; j<N-1; j++) {
    a[1-1][i][j]=0.25*(a[1][i-1][j]
    +a[1][i+1][j]+a[1][i][j-1]
    +a[l][i][j+1]);
    err = fmax(err,fabs(a[1][i][j]
    -a[0][i][j]));
} while(err>maxerr);
```

Parallel Jacobi

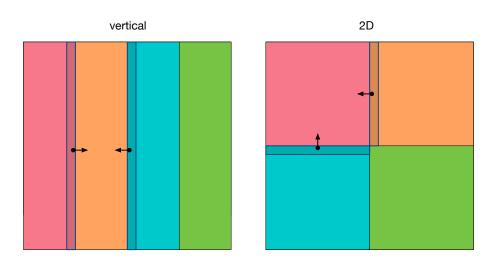
- Need to distribute the two arrays
- Need to distribute the computation
- Data parallelism: distribution of computation follows the distribution of the data
- Simplemost approach is to follow the *owner compute* rule: The process that "owns" an entry (has it in its local memory) is responsible for updating it.

Possible distributions

Need to split the two matrices across the processes



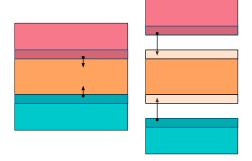
Communication among processes



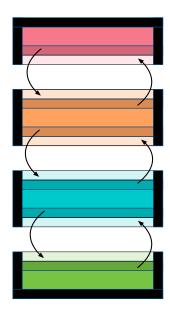
Communication will occur at the boundaries between partitions: Need to send boundary row/column to neighbor

Ghost cells (aka hallo cells)

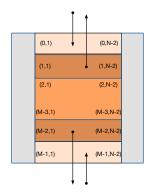
- Need place to receive copy of neighor rows.
- Will add two ghost rows above and beyond the rows owned by the process. These become the boundary for the local Jacobi iteration



Algorithm outline

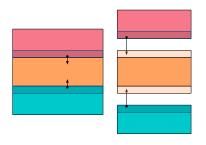


```
repeat {
update ghost rows;
compute new iteration;
}
until(converged)
```



Jacobi

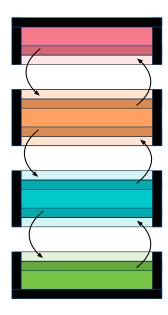
Data distribution



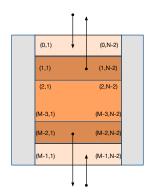
Sequential algorithm

```
do {
  err=0; l=1-1;
  for (i=1;i<N-1; i++)
   for(j=1;j<N-1;j++) {
    a[1-1][i][j]=0.25*(a[1][i-1][j]
      +a[1][i+1][j]+a[1][i][j-1]+a[1][i][j+1]);
    err = fmax(err,fabs(a[1][i][j]-a[0][i][j]));
  }
}
while(err>maxerr);
```

Algorithm outline



```
repeat {
update ghost rows;
compute new iteration;
}
until(converged)
```

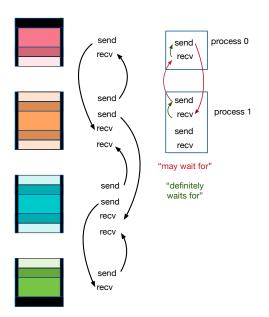


Code – first attempt (ignore convergence test)

```
double a[2][M][N]:
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Comm_size(MPI_COMM_WORLD,&size);
/* assume (M-2)*size=N */
for(iter=0;iter<MAX;iter++) {</pre>
 if(rank>0) {
  /* send up */
  MPI_Send(&a[1][1][1], N-2, MPI_DOUBLE, rank-1,0, MPI_COMM, WORLD);
  /* receive from up */
  MPI_Recv(&a[1][0][1], N-2, MPI_DOUBLE, rank-1,0, MPI_COMM_WORLD,
          MPI STATUS IGNORE):
 if(rank < size-1) {
  /* send down */
  MPI_Send(&a[1][M-2][1], N-2, MPI_DOUBLE, rank+1,0, MPI_COMM_WORLD);
  /* receive from down */
  MPI_Recv(&a[1][M-1][1], N-2, MPI_DOUBLE, rank+1,0, MPI_COMM_WORLD,
            MPI_STATUS_IGNORE);
```

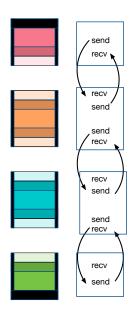
```
for (i=1;i<N-1; i++)
for(j=1;j<N-1;j++)
a[1-1][i][j]=0.25*(a[1][i-1][j]+a[1][i+1][j]+a[1][i][j-1]+a[1][i][j+1]);
l=1-1;</pre>
```

Deadlock is possible if send is not buffered



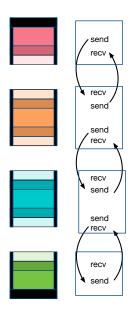
- Deadlock: situation where execution makes no progress.
- Typically due to a cycle of dependences: A waits for B to complete, B waits for C to complete, C waits for A to complete

Avoid deadlock, first solution



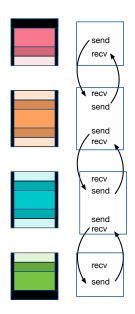
• Alternate the order of sends and receives

Avoid deadlock, first solution



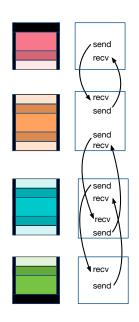
- Alternate the order of sends and receives
- Code is now deadlock-free

Avoid deadlock, first solution



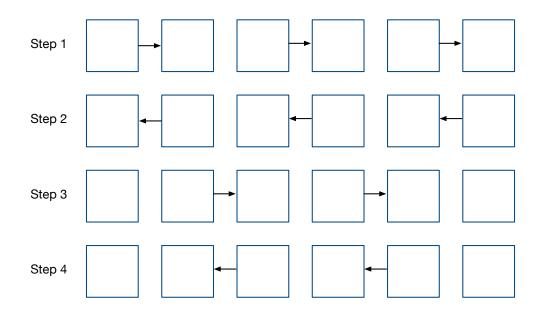
- Alternate the order of sends and receives
- Code is now deadlock-free
- But communications are serialized!

Avoid deadlock, second solution



Communicate in four rounds:

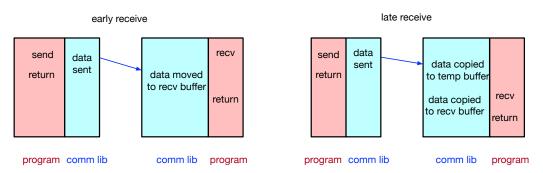
- 2i to 2i + 1
- 2i + 1 to 2i
- 2i 1 to 2i
- 2i to 2i 1

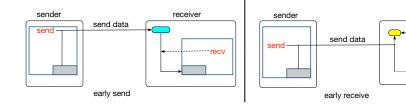


Communication Protocols

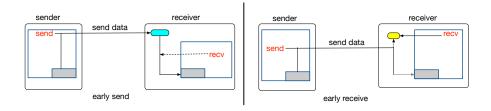
- Basic problem of send-receive communication (aka 2-sided communication): The processes have no common clock, so the send can occur before the receive or after the receive.
- If send data as soon as send occurs, then it may arrive before the receive is posted and needs to be buffered (eager protocol)
- If send data only after receive is posted, then additional communication is needed to inform the sender that the receive is posted (rendezvous protocol)

Eager protocol

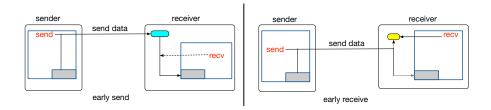




receiver



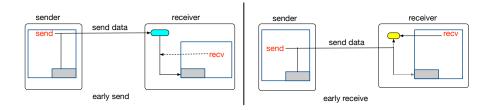
Good: Simple protocol; send completes rapidly



Good: Simple protocol; send completes rapidly

Bad: Extra copying; need extra buffer space and need to run protocol to prevent buffer overflow

Send returns before or after receive starts



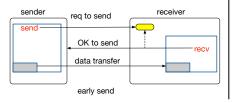
Good: Simple protocol; send completes rapidly

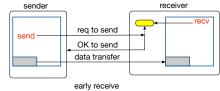
Bad: Extra copying; need extra buffer space and need to run protocol to prevent buffer overflow

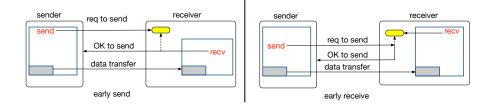
Send returns before or after receive starts

Best if receive is posted ahead of send

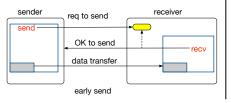
Rendezvous protocol late receive early receive request recv request send send to send to send ack send recv ack data return send data moved data to recv buffer return data moved return to recv buffer return program comm lib comm lib program comm lib comm lib program program







Good: Data moved once; need much less buffering

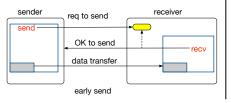


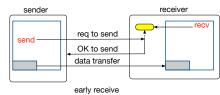


Good: Data moved once; need much less buffering

Bad: Extra protocol messages

Send returns only after receives start





Good: Data moved once; need much less buffering

Bad: Extra protocol messages

Send returns only after receives start

Best if receive is posted ahead of send

Typical implementation

- Uses eager protocol for short messages
- Uses rendezvous protocol for long message, when overhead of extra copy larger than overhead of extra messages .
- Always good to post receives ahead of matching sends

Back to Jacobi: Better – use nonblocking communication

Separate start of communication from completion of communication

```
int a[1000], b[1000];
MPI_Request req[2];
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Isend(a,1000,MPI_INT,rank+1,0,
MPI_COMM_WORLD,&req[0])
MPI_IRecv(b,1000,MPI_INT,rank-1,0,
MPI_COMM_WORLD,&req[1]);
MPI_Wait(&req[0],MPI_STATUS_IGNORE);
MPI_Wait(&req[1],MPI_STATUS_IGNORE);
```

- A nonblocking send returns (does not block), even if matching receive has not occurred
- The *request* object identifies the started communication
- MPI_WAIT blocks until the communication identified by the request is complete.
- Once both send and receive are started, the communication will complete – no further MPI call is needed.

Better

```
int a[1000], b[1000];
MPI_Request req[2];
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Isend(a,1000,MPI_INT,rank+1,0,
MPI_COMM_WORLD,&req[0])
MPI_IRecv(b,1000,MPI_INT,rank-1,0,
MPI_COMM_WORLD,&req[1]);
MPI_Waitall(2,req,MPI_STATUSES_IGNORE);
```

- Can wait for the completion of a set of communications (sends or receives)
- Also have MPI_Wait_any, MPI_Wait_some

Jacobi

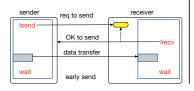
```
double a[2][M][N];
MPI Request req[4];
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Comm_size(MPI_COMM_WORLD,&size);
/* assume (M-2)*size=N */
for(iter=0;iter<MAX;iter++) {</pre>
/* up */
 if(rank>0) {
  MPI_Isend(&a[1][1][1], N-2, MPI_DOUBLE, rank-1,0, MPI_COMM_WORLD, &req[0]);
  MPI_Irecv(&a[1][0][1], N-2, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &req[1]);
```

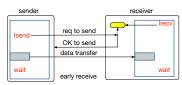
```
/*d.own */
 if(rank<size-1) {
  MPI_Isend(&a[1][M-2][1], N-2, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD, &req[2]);
  MPI_Irecv(&a[1][M-1][1], N-2, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD, &req[3]);
 if(rank==0) MPI_Waitall(2,&req[2],MPI_STATUSES_IGNORE);
 else if(rank==(size-1)) MPI_Waitall(2,&req[0],MPI_STATUSES_IGNORE);
 else MPI_Waitall(4,req,MPI_STATUSES_IGNORE);
 for (i=1; i < N-1; i++)
  for(j=1;j<N-1;j++)
   a[1-1][i][j]=0.25*(a[1][i-1][j]+a[1][i+1][j]+a[1][i][j-1]+a[1][i][j+1]);
1 = 1 - 1:
```

Nonblocking communication

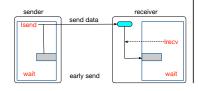
- If wait is too early, process blocks until communication is complete.
- Start communication as soon as possible and wait as late as possible

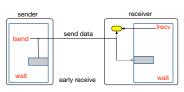
Rendezvous





Eager





Back to Jacobi

```
double a[2][M][N];
MPI Request req[4];
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Comm_size(MPI_COMM_WORLD,&size);
/* assume (M-2)*size=N */
for(iter=0;iter<MAX;iter++) {</pre>
/* up */
 if(rank>0) {
  MPI_Isend(&a[1][1][1], N-2, MPI_DOUBLE, rank-1,0, MPI_COMM_WORLD, &req[0]);
  MPI_Irecv(&a[1][0][1],N-2,MPI_DOUBLE,rank-1,0,MPI_COMM_WORLD,&req[1]);
```

```
/*d.own */
 if(rank<size-1) {
  MPI_Isend(&a[1][M-2][1], N-2, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD, &req[2]);
  MPI_Irecv(&a[1][M-1][1], N-2, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD, &req[3]);
 if(rank==0) MPI_Waitall(2,&req[2],MPI_STATUSES_IGNORE);
 else if(rank==(size-1)) MPI_Waitall(2,&req[0],MPI_STATUSES_IGNORE);
 else MPI_Waitall(4,req,MPI_STATUSES_IGNORE);
 for (i=1; i < N-1; i++)
  for(j=1;j<N-1;j++)
   a[1-1][i][j]=0.25*(a[1][i-1][j]+a[1][i+1][j]+a[1][i][j-1]+a[1][i][j+1]);
1 = 1 - 1:
```

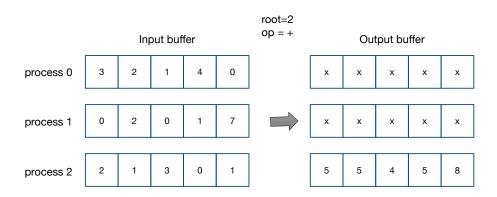
Reduction

- Convergence check: Need to compute the max of the local errors.
- Can use collective communication

```
int rank, maxrank, sumrank, size;
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Reduce(&rank,&maxrank,1,MPI_INT,MPI_MAX,0,MPI_COMM_WORLD);
MPI_Reduce(&rank,&sumrank,1,MPI_INT,MPI_SUM,0,MPI_COMM_WORLD);
if(rank==0) printf('' %d %d \n'', maxrank,sumrank);
...
```

```
MPI_Reduce(&rank,&maxrank,1,MPI_INT,MPI_MAX,0,MPI_COMM_WORLD);
int MPI Reduce(sendbuf, recvbuf, count, datatype, op, root, comm)
   sendbuf: the location where my input comes from
    recybuf: the location where the result goes to
     count: the length of the vector being reduced element-wise
  datatype: the type of each vector element
        op: the reduction operation
       root: the rank of the process that is gathering the result
     comm: the group of processes involved in the reduction
```

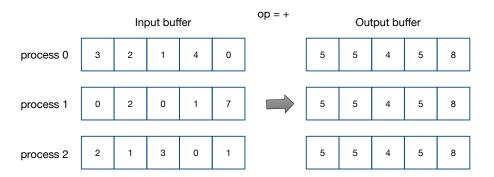
MPI_Reduce



MPI_Allreduce

- With reduce one process gets the result of the reduction and can decide whether the iteration converged. But we need *all* processes to break out of the loop.
- Use allreduce, instead: The result of the reduction is broadcast to all participating processes
- MPI_Allreduce(sendbuf,recvbuf,count,datatype,op,comm)
- Same as MPI_Reduce, except that there is no root argument

MPI_Allreduce

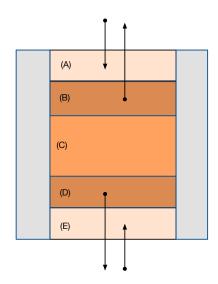


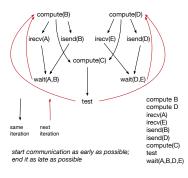
Jacobi, again

```
double a[2][M][N];
double local_err,global_err;
MPI_Request req[4];
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI Comm size (MPI COMM WORLD, & size);
. . .
/* assume (M-2)*size=N */
do {
/* up */
 if(rank>0) {
  MPI_Isend(&a[1][1][1], N-2, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &req[0]);
  MPI_Irecv(&a[0][1], N-2, MPI_DOUBLE, rank-1,0, MPI_COMM_WORLD, &req[1]);
/*down */
 if(rank < size-1) {
  MPI_Isend(&a[1][M-1][1], N-2, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD, &req[2]);
  MPI_Irecv(&a[1][M-1][1], N-2, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD, &req[3]);
```

```
if(rank == 0) MPI_Waitall(2,&req[2],MPI_STATUSES_IGNORE);
else if(rank==(size-1)) MPI_Waitall(2,&req[0],MPI_STATUSES_IGNORE);
else MPI_Waitall(4,req,MPI_STATUSES_IGNORE);
local err=0;
for (i=1; i<N-1; i++)
 for(j=1;j<N-1;j++) {
  a[1-1][i][j]=0.25*(a[1][i-1][j]
      +a[l][i+1][j]+a[l][i][j-1]+a[l][i][j+1]);
 local_err = fmax(local_err,fabs(a[1][i][j]-a[0][i][j]));
1=1-1:
MPI_Allreduce(&local_err, &global_err, 1, MPI_DOUBLE, MPI_MAX, MPI_COMM_WORLD);
} while(global_err>maxerr);
```

Optimize: overlap computation and communication





Optimized jacobi

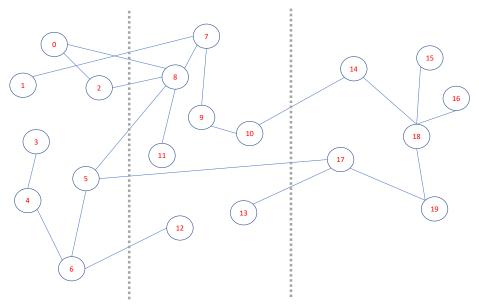
```
MPI_Request req[5];
/* loop */
do {
 local err=0: l=1-1:
/* compute top, bottom rows */
 for(j=1;j<N-1;j++) {
  a[1-1][1][j]=0.25*(a[1][0][j]
     +a[1][2][j]+a[1][1][j-1]+a[1][1][j+1]);
  local_err = fmax(local_err, fabs(a[1][1][j]-a[0][1][j]));
 for (j=1; j<N-1; j++) {
  a[1-1][M-2][j]=0.25*(a[1][M-3][j]
   +a[1][M-1][j]+a[1][M-2][j-1]+a[1][M-2][j+1]);
  local_err = fmax(local_err,fabs(a[1][M-2][j]-a[0][M-2][j]));
  }
```

```
/* start communications */
if(rank>0) {
 MPI_Isend(&a[1][1][1], N-2, MPI_DOUBLE, rank-1,0, MPI_COMM_WORLD, &req[0]);
 MPI_Irecv(&a[0][1], N-2, MPI_DOUBLE, rank-1,0, MPI_COMM_WORLD,&req[1]);
if(rank < size-1) {
 MPI_Isend(&a[1][M-1][1], N-2, MPI_DOUBLE, rank+1,0, MPI_COMM_WORLD,&req[2]);
 MPI_Irecv(&a[1][M-1][1],N-2, MPI_DOUBLE,rank+1,0,MPI_COMM_WORLD,&req[3]);
/* compute interior */
for (i=2; i<M-2; i++)
 for(j=1;j<N-1;j++) {
  a[1-1][i][i]=0.25*(a[1][i-1][i]
        +a[1][i+1][j]+a[1][i][j-1]+a[1][i][j+1]);
   local_err = fmax(local_err,fabs(a[1][i][i]-a[0][i][j]));
```

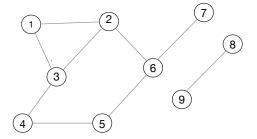
Shared memory vs. distributed memory Jacobi

- Computation partitioned in similar ways (tiling)
- Dynamic partitioning and overpartitioning seldom used for distributed memory
- Distributed memory (with MPI) adds the burden of
 - Distributing data, and using local indices/pointers
 - Communicating data (ghost cells)
 - Replicating sequential code

Distributed memory graph traversal



Distributed memory graph traversal



- 1 2 3
- 2 | 1 | 3 | 6
- 3 1 2 4
- 4 3 5
- 5 4 6
- 6 2 5 7
- 7 | 6 |
- 8 9
- 9 8

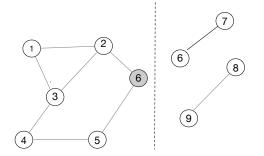
Distributed graph representation

- Nodes are distributed across processes
- If node u owned by a process connects to a node v owned by another process then a "ghost copy" of v is stored at the first process

Algorithm:

- Process 0 starts by traversing its nodes, starting from node 0
- If traversal encounters a ghost node, then a request is send to node owner to start a traversal from that node

Distributed graph representation (2 processes)







Partial, inefficient and incomplete traversal code

```
typedef struct {
  bool visited;
  int degree; // number of neighbors
  int neighbor[]; // indices of neighbors; use reversed sign to mark ghosts
} Node;

Node *node; // local array of nodes
int nnodes; // number of nodes
MPI_Requests reqs[max];
int reqcount // index for requests;

void graph_init() {}
```

```
void visit(int i) {
 int j,k,m;
 if (!node[i]->visited) {
  node[i] -> visited=true;
  for(j=0;j<node[i]->degree;j++) {
   k=node[i]->neighbor[j];
   if(isGhostCopy(k))
    MPI_Isend(k, 1, MPI_INT,
      k*size/nnodes, 0, MPI_COMM_WORLD, reqs[reqcount++]);
   else
    visit(k)}
```

```
int main(int argc, char **argv) {
 int i, j;
 MPI_Request recvreq;
 MPI_Init(&argc, &argv);
 MPI_Comm_rank(MPI_COMM_WORLD, &rank);
 MPI Comm size (MPI COMM WORLD, &size);
 graph_init();
 MPI_Irecv(&i, 1, MPI_INT, MPI_ANY_SOURCE,O, MPI_COMM_WORLD, &recvreq);
 if(rank==0)
  visit(0);
 while(notdone) {
  MPI_Wait(&recvreq, MPI_STATUS_IGNORE);
  j=i;
  MPI_Irecv(&i, 1, MPI_INT, MPI_ANY_SOURCE,0, MPI_COMM_WORLD, &recvreq);
  visit(j);
 // complete all sends of visit
  MPI_Waitall(reqs, reqcount, MPI_STATUSES_IGNORE);
  reqcount=0;
MPI Finalize():
```

Problems

- Correctness: How do we know computation has completed?
 - Need to periodically test for completion; i.e., that all processes are done
- Performance: Sending too many small messages
 - Need to aggregate messages and send them in bulk

Bulk-synchronous code

- Computation proceeds in phases, with communication at end of each phase
- At each phase do as much work as possible without communicating

```
typedef struct {
  bool visited;
  int degree;
  int neighbor[]; // mark qhost cell with negative index
} Node:
Node *node[nnodes]:
void graph_init() {}
int rank, size;
int **out; // send buffers (one per destination)
int *out_ptr; // points to first empty slot in output buffer
int *in; // receive buffer
int in_ptr; // points to first empty slot in input buffer
MPI_Request *reqs;
MPI_Status status;
MPI_Request *reqs;
MPI_Status status;
 . . .
```

```
void visit(int i) {
  int j,k,m;
  if (!node[i]->visited) {
    node[i]->visited=true;
    for(j=0;j<node[i]->degree;j++) {
      k= node[i]->neighbor[j];
      if(isGhostCopy(k)) { // ghost node; append to appropriate output list
        m = k*size/nnodes; // destination
        out [m] [out_ptr[m]++]=k;
      else
      visit(k);
```

```
int main(int argc, char **argv) {
  int i,j,k;
  bool done, global_done;
  MPI_Init(&argc, &argv);
 MPI_Comm_rank(MPI_COMM_WORLD, &rank);
 MPI_Comm_size(MPI_COMM_WORLD, &size);
  graph init();
  for(i=0;i<size;i++) out[size] = (int*)malloc(max*sizeof(int));</pre>
  in = (int *)malloc(max*size*sizeof(int));
 reqs = (MPI_Request *)malloc(size*sizeof(MPI_Request));
  out_ptr = (int *)malloc(size*sizeof(int));
  if(rank==0)
     in[in ptr++] = 0;
```

```
while (1) {
 for(i=0;i<size;i++)
  out_ptr[i]=0;
// visit all newly marked nodes
 for(i=0; i<in_ptr ;i++)</pre>
 visit(in[i]);
 in_ptr=0;
// send out marked ghost nodes
k=0:
 for(i=0;i<size;i++)
 if (i!=rank)
 MPI_Isend(out[i],out_ptr[i], MPI_INT, i, 0, MPI_COMM_WORLD, &reqs[k++]);
```

```
// receive marked ghost nodes
 done=true:
 for(i=0:i<size:i++)
  if(i !=rank) {
   MPI_Recv(&in[in_ptr], max, MPI_INT, MPI_ANY_SOURCE, 0,
   MPI_COMM_WORLD, &status);
   MPI_Get_count(&status, MPI_INT,&j);
   if(j>0) done=false;
   in_ptr+=j;
// complete sends
 MPI_Waitall(regs, size-1, MPI_STATUSES_IGNORE)
// test for completion
 MPI_Allreduce(&done,&global_done, 1, MPI_C_BOOL, MPI_LAND, MPI_COMM_WORLD);
 if(global_done) break;
```

New Constructs

- MPI_ANY_SOURCE wildcard source
- Also have MPI_ANY_TAG
- status object, of type MPI_Status
- MPI_Get_count(status, datatype, count)
- Also can directly access status.MPI_SOURCE and status.MPI_TAG

Graph traversal Possible Improvements

- All processes first send to process 0 then to process 1, etc.;
- Communication not overlapped optimally
- Better: Process i sends to $i + 1, i + 2, \ldots$ and receives from $i 1, i 2, \ldots$

```
k=0;
m = rank;
for(i=0;i<size-1;i++) {
    m=(m+1)%size;
MPI_Isend(out[m],out_ptr[m], MPI_INT, m, 0, MPI_COMM_WORLD, &reqs[k++]);</pre>
```

- Use multiple receive buffers, so that all receives can be started at the same time
- But, then may need to allocate more space
- Check how much space each send needs, then allocate receive buffer

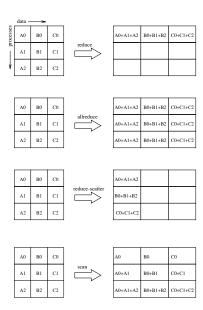
```
k=0;
m = rank;
for(i=0;i<size-1;i++) {
    m=(m-1)%size;
    MPI_Probe(m,0,MPI_COMM_WORLD,status);
    MPI_Get_count(&status, MPI_INT,&j);
    MPI_Irecv(in[in_ptr], j, MPI_INT, m, 0, MPI_COMM_WORLD, &reqs[k++]);
    int_ptr += j;
}</pre>
```

• MPI_Probe(source, tag, comm, status): Returns information about incoming message without actually receiving it

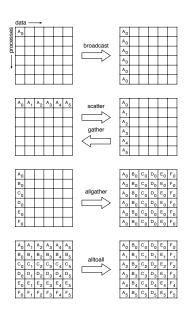
Collective communications

- Computation collectives: Reduce, Allreduce, Reducescatter
- Synchronization collective: Barrier
- Data movement collectives: broadcast, scatter, gather, allgather, alltoall

Computation collectives



Communication collectives



alltoall

MPI_Ialltoall(sendbuf, sendcount, sendtype, recvbuf, recvcount, recvtype, comm, request)

Each process send to every process (itself included) the same amount of data

- sendbuf send buffer
- sendcount number of elements sent to each process
- sendtype datatype of send buffer elements
- recybuf receive buffer
- recvcount number of elements received from any process
- recytype data type of receive buffer elements
- comm communicator
- request communication request



Alltoall

```
...
// run on 4 processes, each process has 2 elements, and the recv is filled
// with 2 elements from each process (including itself)
int send[2];
int recv[8];
MPI_Alltoall(&send, 2, MPI_INT, recv, 2, MPI_INT, MPI_COMM_WORLD);
```

MPI_Ialltoallv(sendbuf, sendcounts, sdispls, sendtype, recvbuf, recvcounts, rdispls, recvtype, comm, request)

Each process sends to every process different amounts of data

- sendbuf send buffer
- sendcounts array with number of elements sent to each process
- sdispls array with displacement from sendbuf start of each sent block
- sendtype datatype of send buffer elements
- recybuf receive buffer
- recvcounts array with number of elements received from each process
- rdispls array with displacement from recybuf start of each received block
- recvtype data type of receive buffer elements
- comm communicator
- request communication request

Alltoallv

```
. . .
/* run on 3 processes; p0 has 3 elements (a,b,c), p1 has 3 elements (d,e,f),
p2 has 5 elements (q,h,i,j,k);
after the call, the recv buffer at p0 contains (a,g), p1 contains (b,c,h),
and p3 contains (e,f) */
int rank:
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
int send_counts[3], recv_counts[3], send_displs[3], recv_displs[3];
int *send, *recv;
if (rank == 0) {
  send = (int *) malloc(3 * sizeof(int));
  recv = (int *) malloc(2 * sizeof(int));
  send[0] = 'a'; send[1] = 'b'; send[2] = 'c';
  send_counts[0] = 1; send_counts[1] = 2; send_counts[2] = 0;
  send_displs[0] = 0; send_displs[1] = 1; send_displs[2] = 3;
  recv_counts[0] = 1; recv_counts[1] = 0; recv_counts[2] = 1;
  recv_displs[0] = 0; recv_displs[1] = 1; recv_displs[2] = 1;
```

Alltoallv

```
else if (rank == 1) {
    send = (int *) malloc(3 * sizeof(int));
    recv = (int *) malloc(3 * sizeof(int));
    send[0] = 'd'; send[1] = 'e'; send[2] = 'f';
    send_counts[0] = 0; send_counts[1] = 0; send_counts[2] = 2;
    send_displs[0] = 0; send_displs[1] = 0; send_displs[2] = 1;
    recv_counts[0] = 2; recv_counts[1] = 0; recv_counts[2] = 1;
    recv_displs[0] = 0; recv_displs[1] = 2; recv_displs[2] = 2;
}
```

Alltoallv

```
else if (rank == 2) {
   send = (int *) malloc(5 * sizeof(int));
   recv = (int *) malloc(2 * sizeof(int));
   send[0] = 'g'; send[1] = 'h'; send[2] = 'i'; send[3] = 'j'; send[4] = 'k';
   send_counts[0] = 1; send_counts[1] = 1; send_counts[2] = 0;
   send_displs[0] = 0; send_displs[1] = 1; send_displs[2] = 0;
   recv_counts[0] = 0; recv_counts[1] = 2; recv_counts[2] = 0;
   recv_displs[0] = 0; recv_displs[1] = 0; recv_displs[2] = 0;
}
MPI_Alltoallv(send, send_counts, send_displs, MPI_INT,
   recv, recv_counts, recv_displs, MPI_INT, MPI_COMM_WORLD);
```

Example: graph traversal with Alltoally

First communicate size of messages, then communicate data Reminder:

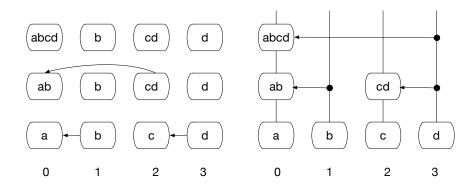
- out[i][] contains indices to be sent to process i. Each row has max elements
- out_ptr[i] contains number of indices to be sent to process i
- in[] is the receive buffer for all indices.

```
for(i=0;i<size;i++)
  sdispl[i] = rank*max;
out_ptr(rank) = 0;
    ...
MPI_Alltoall(out_ptr,1,MPI_INT,recvcounts,1,MPI_INT,MPI_COMM_WORLD)
rdipls[0]=0;
for (i=1; i<size; i++)
  rdispls[i]= rdispls[i-1]+recvcounts[i];
MPI_Ialltoallv(out,out_ptr,sdipls,MPI_INT,in,recvcounts,rdispls,MPI_INT,MPI_COM...</pre>
```

How is reduce implemented?

- Assume we reduce vector of length *n*
- Simple implementation: All processes send message to root; root sums them all.
- Assume receive of n words takes time $\ell + n/b$; only one receive at a time
- Communication time is $(p-1)(\ell+n/b) = \Theta(pn)$ not good

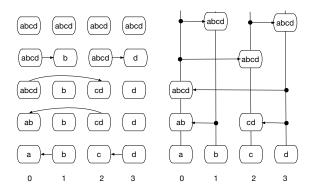
Binary reduction



- ullet Communication time is $\lg(p)(\ell+n/b)=\Theta(\log(p)\cdot n)$ much better
- Different processes exit collective operation at different times



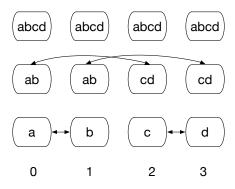
Allreduce – reduce followed by broadcast



• Communication time is $2 \lg(p)(\ell + n/b)$



Allreduce – alternative implementation

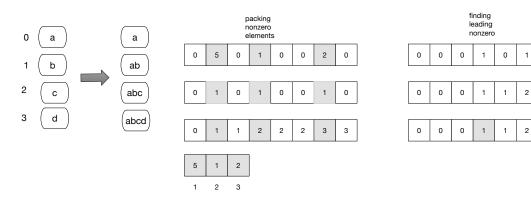


- Assume send and receive can be simultaneous: Communication time is $\lg(p)(\ell+n/b)$ half as much as previous algorithm
- Assume no overlap at all between send and receive; then the two algorithms take as much time.



Scan

Examples

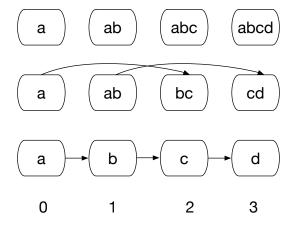


0

3 3

3 3

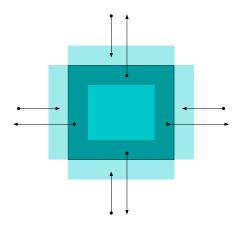
Scan evaluation



- Assuming simultaneous send and receive
- Time is $\lg(p)(\ell + n/b)$

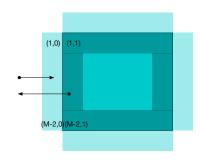
Good MPI implementation uses *polyalgorithm*: It chooses the right algorithm, based on machine properties (latency, bandwidth), number of involved processes, length of messages, etc.

Jacobi – 2D decomposition



- Problem: Columns are not stored in consecutive locations
- Solution 1: Pack to consecutive locations to send; unpack after receiving
- Solution 2: Define a suitable datatype for the send and receive locations
- Solution 2 is better if the MPI implementation does a good job

Option 1

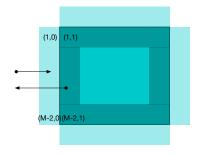


Derived datatypes

count=3 blocklength=2 stride=6

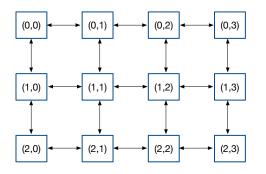
MPI Type vector(3,2,6,MPI DOUBLE,&vector-type); MPI_TYPE_VECTOR(count,blocklength,stride, oldtype, newtype count: number of blocks blocklength: number of elements per block (usually 1) stride: distance from start of block to start of next block oldtype: type of each element newtype: name of new derived datatype

Option 2



Cartesian grid of processes

- For the 2D Jacobi, it is convenient to think of the processes as organized in a 2D mesh
- Can do this with MPI_Cart_create



```
dims[0]=4; dims[1]=3;
periods[0]=false; periods[1]=false;
reorder= true;
ndim=2;
MPI_Cart_create(MPI_COMM_WORLD,ndim,
dims,periods,reorder,&comm2d);
```

- May want to know my Cartesian coordinates: MPI_Cart_Coords()
- May want to know my rank and the rank of one of my neighbors:
 MPI_Cart_shift(comm2d,direction,disp,&rank_source,&rank_dest)
- What happens if there is no neighbor in the chosen direction? The call returns
 MPI_PROC_NULL; a send to MPI_PROC_NULL or a receive from MPI_PROC_NULL is a noop.

2D Jacobi, in all its glory...

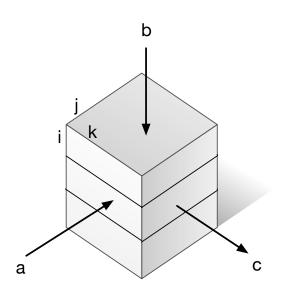
```
/* initialization */
MPI_Comm_size(MPI_Comm_World,&size)
/* pick grid dimensions */
MPI Dims create(size.2.dims)
/* dims [0]*dims [1] = size */
period[0]=period[1]=false;
MP_Cart_create(MPI_COMM_WORLD,2,dims,periods,true,&comm2d);
MPI Cart shift (comm2d, 0, -1, &myrank, &up);
MPI_Cart_shift(comm2d,0,1,&myrank,&down);
MPI Cart shift(comm2d,1,-1,&myrank,&left);
MPI_Cart_shift(comm2d,1,1,&myrank,&right);
MPI Type vector (M-2,1,N,MPI DOUBLE, &vector type);
MPI_Type_commit(&vector_type);
```

```
/* loop */
do {
local err=0;
/* compute boundaries */
/* top */
for (j=1; j<N-1; j++) {
a[1-1][1][j]=0.25*(a[1][0][j]
   +a[1][2][j]+a[1][1][j-1]+a[1][1][j+1]);
 local_err = fmax(local_err,fabs(a[1][1][j]-a[0][1][j]));
/* bottom */
for(j=1;j<N-1;j++) {
a[1-1][M-2][j]=0.25*(a[1][M-3][j]
  +a[1][M-1][j]+a[1][M-2][j-1]+a[1][M-2][j+1]);
 local_err = fmax(local_err,fabs(a[1][M-2][j]-a[0][M-2][j]));
```

```
/* left */
for(i=1:i<M-1:i++) {
 a[1-1][i][1]=0.25*(a[1][i-1][1]
 +a[1][i+1][1]+a[1][i][0]+a[1][i][2]):
 local_err = fmax(local_err,fabs(a[1][i][1]-a[0][i][1]));
/* right */
for(i=1;i<M-1;i++) {
a[1-1][i][N-2]=0.25*(a[1][i-1][N-3]
  +a[1][i+1][N-1]+a[1][i][N-3]+a[1][i][N-1]);
 local_err = fmax(local_err,fabs(a[1][i][N-2]-a[0][i][N-2]));
/* start communications */
MPI_Irecv(&a[1][0][1],N-2,MPI_DOUBLE,up,0,MPI_COMM_WORLD,&req[1]);
MPI_Irecv(&a[1][M-1][1], N-2, MPI_DOUBLE, down, 0, MPI_COMM_WORLD, &req[2]);
MPI_Irecv(&a[1][1][0],1,vector_type,left,MPI_COMM_WORLD,&req[3]);
MPI_Irecv(&a[1][1][N-1],1,vector_type,right,MPI_COMM_WORLD,&req[4])
MPI_Isend(&a[1][1][1], N-2, MPI_DOUBLE, up, MPI_COMM_WORLD, &req[5]);
MPI_Isend(&a[1][M-2][1], N-2, MPI_DOUBLE, down, MPI_COMM_WORLD, &req[6]);
MPI_Isend(&a[1][1][1],1,vector_type,left,MPI_COMM_WORLD,&req[7]);
MPI_Isend(&a[1][1][N-2],1,vector_type,right,MPI_COMM_WORLD,&req[8]);
```

```
/* compute interior */
for (i=2;i<M-2; i++)
for (j=2; j<N-2; j++) {
  a[1-1][i][j]=0.25*(a[1][i-1][j]
   +a[l][i+1][j]+a[l][i][j-1]+a[l][i][j+1]);
  local_err = fmax(local_err,fabs(a[1][i][j]-a[0][i][j]));
1=1-1:
/* start convergence test */
MPI_Iallreduce(&local_err,&global_err,1,MPI_DOUBLE,MPI_MAX,
  MPI_COMM_WORLD,&req[9]);
/* end communications */
MPI_Waitall(9,req,MPI_STATUSES_IGNORE);
   while(global_err>maxerr);
```

Matrix product 1D tiling



Will parallelize with MPI, by assigning a tile to each process

Code

```
. . .
int matmult(int nra, int nca, int ncb, double a[nra][nca],
double b[nca][ncb], double c[nra][ncb], MPI_Comm comm) {
   /********
   Computes the product c = a*b using the processes in the group of
   communicator comm
   The three matrices are stored on the process with rank 0 in comm
   *********
                             /* number of processes in group */
   int numprocs,
                       /* a process identifier */
   procid,
   numworkers.
                        /* number of worker processes */
                        /* process id of message source */
   source.
                        /* process id of message destination */
   dest,
                        /* rows of matrix A sent to each worker */
   rows.
   averow, extra, offset, /* used to determine rows sent to each worker */
   i, j, k, rc;
                         /* misc */
   MPI_Comm_rank(comm,&procid);
   MPI_Comm_size(comm,&numprocs);
```

```
if (numprocs < 2 ) {
    /* run sequential code */
    for (i=0;i<nra;i++)
    for (j=0;j<ncb;j++)
    for(k=0;k<nca;k++)
    c[i][j] += a[i][k]*b[k][j];
    exit(1);
}</pre>
```

```
if(procid==0) {
/******* master process **********/
numworkers = numprocs-1;
/* Send matrix data to the worker tasks */
averow = nra/numworkers:
extra = nra%numworkers;
offset = 0:
for (dest=1; dest<=numworkers; dest++)</pre>
    rows = (dest <= extra) ? averow+1 : averow:
    MPI_Send(&offset, 1, MPI_INT, dest, 0, comm);
    MPI_Send(&rows, 1, MPI_INT, dest, 0, comm);
    MPI_Send(&a[offset][0], rows*nca, MPI_DOUBLE, dest, 0,
    comm):
    MPI_Send(b, nca*ncb, MPI_DOUBLE, dest, 0, comm);
    offset = offset + rows:
```

```
/* Receive results from worker processes */
for (source=1; source<=numworkers; source++)
{
MPI_Recv(&offset, 1, MPI_INT, source, 0, comm, MPI_STATUS_IGNORE);
MPI_Recv(&rows, 1, MPI_INT, source, 0, comm, MPI_STATUS_IGNORE);
MPI_Recv(&c[offset][0], rows*ncb, MPI_DOUBLE, source, 0, comm, MPI_STATUS_IGNORE);
}
</pre>
```

```
else {
MPI_Recv(&offset, 1, MPI_INT, 0, 0, comm, MPI_STATUS_IGNORE);
MPI Recv(&rows, 1, MPI INT, 0, 0, comm, MPI STATUS IGNORE);
MPI Recv(a, rows*nca, MPI DOUBLE, 0, 0, comm, MPI STATUS IGNORE);
MPI_Recv(b, nca*ncb, MPI_DOUBLE, 0, 0, comm, MPI_STATUS_IGNORE);
for (i=0: i<rows: i++)
for (j=0; j<ncb; j++) {
c[i][i] = 0;
for (k=0; k<nca; k++)
c[i][j] += a[i][j] * b[j][k];
MPI Send(&offset. 1. MPI INT. 0. 0. comm):
MPI Send(&rows, 1, MPI INT, 0, 0, comm);
MPI_Send(&c, rows*ncb, MPI_DOUBLE, 0, 0, comm);
return(1);
```

- Matmult is invoked on all processes should be a collective invocation
- Matrices a,b and c are allocated on all processes not a big problem?
- (Usually matmult is invoked while matrices are already distributed)

Possible improvements:

- Involve process 0 in computation as well
- Avoid communicating offset and rows
- Use collective communications (scatter a, broadcast b, gather c)

uneven scatter-gather

Problem: Not each worker receives same number of rows; need to use scattery and gathery functions.

MPI_Scatterv(sendbuf, sendcounts, displs, sendtype, recvbuf, recvcount, recvtype, root, comm)

sendcounts Number of elements sent to each process

displs displs[i] is displacement from start of buffer to start of elements sent to process i

MPI_Gatherv(sendbuf, sendcount, sendtype, recvbuf, recvcounts, displs, recvtype, root, comm)

Arguments that are not needed can be NULL

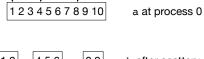
Example

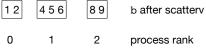
Assume 3 processes

```
int a[10] ={1,2,3,4,5,6,7,8,9,10};
int counts ={2,3,2}
int displs={0,3,7}]
int b[3];

MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Scatterv(&a, counts, displs, MPI_INT, &b, count[rank], MPI_INT,0, MPI_COMM_WORLD);
```

/* array arguments needed at root */





Improved code

```
int matmult(int nra, int nca, int ncb, double a[nra][nca],
double b[nca][ncb], double c[nra][ncb], MPI_Comm comm) {
                         /* number of processes in group */
int numprocs,
                     /* a process identifier */
procid,
                     /* process id of message source */
source.
                   /* process id of message destination */
dest,
averow, extra, offset, /* used to determine rows sent to each worker */
                      /* misc */
i, j, k;
MPI_Comm_rank(comm,&procid);
MPI_Comm_size(comm,&numprocs);
int rows[numprocs],
                            /* # rows sent to each process */
countsa[numprocs], /* # elements of a sent to each process */
countsc[numprocs], /* # elements of c received form each process */
displsa[numprocs], /* displacements in matrix a */
displsc[numprocs];  /* displacements in matrix c */
```

```
if (numprocs < 2 ) {</pre>
/* run sequential code */
for (i=0;i<nra;i++)
for (j=0;j<ncb;j++)
for (k=0; k<nca; k++)
c[i][j] += a[i][k]*b[k][j];
exit(1);
/* computed by all processes */
averow = nra/numprocs;
extra = nra%numprocs;
offset=0;
for (i=0; i<numprocs; i++) {</pre>
rows[i] = (i < extra) ? averow+1 : averow;</pre>
countsa[i] = rows[i]*nca;
countsc[i] = rows[i]*ncb;
displsa[i] = offset*nca;
displsc[i] = offset*ncb;
offset += rows[i];
```

```
/* Scatter matrix data to all processes */
double aa[rows[procid]][nca]; /* local tile of a */
double cc[rows[procid]][ncb]; /* local tile of c */
MPI_Scatterv(&a[0][0], countsa, displsa, MPI_DOUBLE, &aa[0][0],
countsa[procid], MPI_DOUBLE, 0, MPI_COMM_WORLD);
MPI_Bcast(&b[0][0], nca*ncb, MPI_DOUBLE, 0, MPI_COMM_WORLD);
/* local computation */
for (i=0; i<rows[procid]; i++)</pre>
for (j=0; j<ncb; j++) {
cc[i][j] = 0;
for (k=0; k < nca; k++)
cc[i][j] += aa[i][k] * b[k][j];
/* gather results */
MPI_Gatherv(&cc[0][0], countsc[procid], MPI_DOUBLE,
&c[0][0], countsc, displsc, MPI_DOUBLE, 0, MPI_COMM_WORLD);
return(1);
```

Consider two MPI processes, P1 and P2. Answer on the likelihood of the following program deadlocking:

P1:	P2:
MPI_Send(P2)	MPI_Send(P1)
MPI_Recv(P2)	MPI_Recv(P1)

- Never deadlocks
- May deadlock
- Always deadlocks

Consider two MPI processes, P1 and P2. Answer on the likelihood of the following program deadlocking:

P1:	P2:
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MPI_Recv(P2)	MPI_Recv(P1)

- Never deadlocks
- May deadlock
- Always deadlocks

Consider two MPI processes, P1, P2, and P3. Answer on the likelihood of the following program deadlocking:

P1:	P2:	P3:
MPI_Send(P2)	MPI_Send(P3)	MPI_Recv(P2)
MPI_Recv(P3)	MPI_Recv(P1)	MPI_Send(P1)

- Never deadlocks
- May deadlock
- Always deadlocks

Consider two MPI processes, P1, P2, and P3. Answer on the likelihood of the following program deadlocking:

P1:	P2:	P3:
MPI_Send(P2)	MPI_Send(P3)	MPI_Recv(P2)
MPI_Recv(P3)	MPI_Recv(P1)	MPI_Send(P1)

- Never deadlocks
- May deadlock
- Always deadlocks