MPI and Collective Communication Patterns

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Logistics

Reading: Grama Ch 6 + 4

Ch 6: MPI basics

Ch 4: Communication patterns

Assignments

A2 will go up soon, feature MPI Coding

Today

- ► More MPI programming
- Discuss Comm. Patterns

Thursday Lecture + Mini Exam 1

- 45-min lecture
- 30-min Mini-Exam 1

Beginning or End of Lecture??

Exercise: MPI Basics Review

- ► What are the two basic operations required for distributed memory parallel programming?
- Describe some variants for these operations.
- What is a very common library for doing distributed parallel programming?
- How do the two main operations look in that library?
- ▶ How does one compile/run programs with this library?

Answers: MPI Basics Review

- send(data,count,dest) and receive(data,count,source) are the two essential ops for distributed parallel programming
- send/receive can be
 - blocking: wait for the partner to link up and complete the transaction
 - non-blocking: don't wait now but check later to before using/changing the message data
 - buffered: a special area of memory is used to facilitate the sends more efficiently
- MPI: The Message Passing Interface, common distributed memory programming library
- Compile/Run
 mpicc -o prog parallel-program.c
 mpirun -np 8 prog

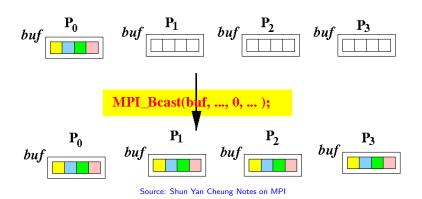
Patterns of Communication

- Common patterns exist in many algorithms
- Reasoning about algorithms easier if these are "primitives"
 - "I'll broadcast to all procs here and gather all results here" vs

"I'll use a loop here to send this data to every processor and a loop here for every processor to send its data to proc 0 which needs all of it."

- ► MPI provides a variety of collective communication operations which make these single function calls
- Vendors of super-computers usually implement those functions to run as quickly as possible on the network provided repeated halving/double if the network matches
- By making the function call, you get all the benefit the network can provide in terms of speed

Broadcasting One-to-All



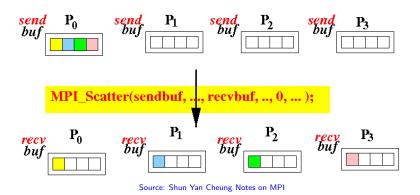
- Root processor wants to transmit data buffer to all processors
- Broadcast distributes to all procs
- Each proc gets same stuff in data buffer

6

Broadcast Example Code

```
In broadcast demo.c
// Everyone allocates
data = (int*)malloc(sizeof(int) * num_elements);
// Root fills data by reading from file/computation
if(procid == root_proc){
  for(i=0; i<num_elements; i++){</pre>
   data[i] = i*i;
// Everyone calls broadcast, root proc sends, others receive
MPI_Bcast(data, num_elements, MPI_INT, root_proc,
          MPI COMM WORLD);
// data[] now filled with same portion of root_data[] on each proc
```

Scatter from One To All



- Root processor has slice of data for each proc
- Scatter distributes to each proc
- Each proc gets an individualized message

Scatter Example

```
In scatter demo.c
// Root allocates/fills root_data by reading from file/computation
if(procid == root_proc){
 root_data = malloc(sizeof(int) * total_elements);
  for(i=0; i<total_elements; i++){</pre>
   root_data[i] = i*i;
// Everyone allocates for their share of data including root
data = malloc(sizeof(int) * elements_per_proc);
// Everyone calls scatter, root proc sends, others receive
MPI_Scatter(root_data, elements_per_proc, MPI_INT,
            data,
                       elements_per_proc, MPI_INT,
            root_proc, MPI_COMM_WORLD);
// data[] now filled with unique portion from root_data[]
```

Exercise: Scatter a Matrix

Often have Matrix and Vector data in HPC / Parallel Computing

```
// mat vec multiply
double **mat = ...;
...;
mat[i][j] = ...;
double *vec = ...;
double *out = ...;
for(int i=0; i<rows; i++){
   for(int j=0; j<cols; j++){
      out[i] = mat[i][j]*vec[j];
   }
}</pre>
```

- How can one MPI_Scatter() the rows of a matrix?
- What assumptions must be true about the matrix data?

Answers: Scatter a Matrix

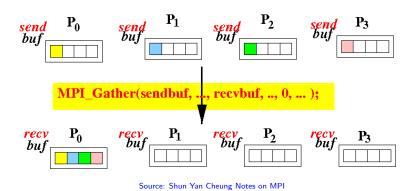
- Typically matrix must be allocated in one block of memory single malloc()
- ▶ Allows a single MPI_Scatter() to scatter groups of rows

```
// allocate data for all of matrix
double *all = malloc(rows*cols * sizeof(double));
// allocate / assign row pointers within single block
double **mat = malloc(rows * sizeof(double*));
for(int i=0; i<rows; i++){</pre>
  mat[i] = &all[i*cols];
}
mat[i][j] = 5.5;
                               // assign via row pointer
```

```
Answers: Scatter a Matrix
     double *all = NULL;
     // root reads in matrix rows
     if(rank == root proc){
       all = malloc(rows*cols * sizeof(double));
       fread(all, sizeof(double), rows*cols, infile);
     // set up and perform scatter
     int rows per_proc = rows / nprocs;
     int elems_per_proc = rows_per_proc * cols;
     double *myrows = malloc(sizeof(double) * elems_per_proc)
     MPI Scatter(all, elements per proc, MPI INT,
                 myrows, elements_per_proc, MPI_INT,
```

root proc, MPI COMM WORLD);

Gather from All to One

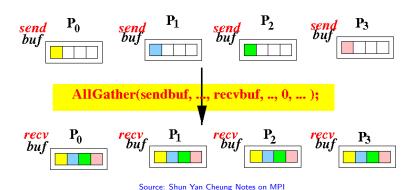


- Every processor has data in send buffer
- Root processor needs all data ordered by proc_id
- ▶ Root ends with all data in a receive buffer

Gather Example

```
// gather demo.c
int total elements = 16;
int elements per proc = total elements / total procs;
// Everyone allocates for their share of data including root
data = malloc(sizeof(int) * elements_per_proc);
// Each proc fills data[] with "unique" values
int x = 1;
for(i=0; i < elements per proc; i++){</pre>
 data[i] = x;
 x *= (procid+2);
// data[] now filled with unique values on each proc
// Root allocates root data to be filled with gathered data
if(procid == root_proc){
 root data = malloc(sizeof(int) * total elements):
// Everyone calls gather, root proc receives, others send
MPI_Gather(data, elements_per_proc, MPI_INT,
           root_data, elements_per_proc, MPI_INT,
           root_proc, MPI_COMM_WORLD);
// root data[] now contains each procs data[] in order
```

All Gather: Everyone to Everyone

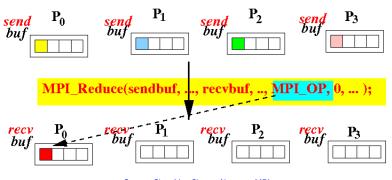


- Every processor has data in send buffer
- All processors need all data ordered by proc_id
- All procs end with all data in receive buffer

All-Gather Example

```
// allgather_demo.c
// Everyone allocates for their share of data including root
data = malloc(sizeof(int) * elements_per_proc);
// Each proc fills data[] with "unique" values
int x = 1:
for(i=0; i<elements_per_proc; i++){</pre>
 data[i] = x:
 x *= (proc_id+2);
// data[] now filled with unique values on each proc
// Everyone allocates all_data to be filled with gathered data
all_data = malloc(sizeof(int) * total_elements);
// Everyone calls all-gather, everyone sends and receives
MPI_Allgather(data, elements_per_proc, MPI_INT,
              all_data, elements_per_proc, MPI_INT,
              MPI_COMM_WORLD);
// all_data[] now contains each procs data[] in order on
// all procs
```

Reduction: All to One



Source: Shun Yan Cheung Notes on MPI

- Every processor has data in send buffer
- Root processor needs all data reduced
 - Reduction operation is transitive
 - Several pre-defined via constants
 - ► Common: MPI_MAX, MPI_MIN, MPI_SUM, MPI_PROD
- Root ends with reduced data in receive buffer

Reduce Example

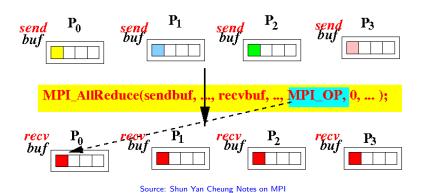
```
// reduce demo.c
{ // Each proc fills data[] with unique values
  int x = 1:
  for(i=0; i<total_elements; i++){</pre>
   data[i] = x:
    x *= (procid+2);
  // data[] now filled with unique values on each proc
  // Root allocates root_data to be filled with reduced data
  if(procid == root_proc){
    root_data = malloc(sizeof(int) * total_elements);
  // Everyone calls reduce, root proc receives,
  // others send and accumulate
  MPI_Reduce(data, root_data, total_elements, MPI_INT,
             MPI_SUM, // operation to perform on each element
             root_proc, MPI_COMM_WORLD);
  // root_data[] now contains each procs data[] summed up
```

Note: Reduction's Array Argument

- ▶ MPI_Reduce() works on a data[] argument like others
- Reduction happens for each element so that

► To get a single sum, Procs should iterate on their own array THEN MPI_Reduce() on a single value

Reduction for All: All-Reduce



- Every processor has data in send buffer
- ► All processors need all data **reduced**
- All procs end with reduced data in a receive buffer

Allreduce Example

```
{ // Each proc fills data[] with unique values
  int x = 1:
  for(i=0; i<total elements; i++){</pre>
   data[i] = x;
    x *= (procid+2);
  // data[] now filled with unique values on each proc
  // Everyone allocates reduced data to be filled with reduced data
  reduced_data = malloc(sizeof(int) * total_elements);
  // Everyone calls reduce, everyone sends and receives
  MPI_Allreduce(data, reduced_data, total_elements, MPI_INT,
                MPI_SUM, // operation to perform on each element
                MPI COMM WORLD):
  // reduced_data[] now contains each procs data[] summed up
```

In-place Reduction

- Occasionally want to do reductions in-place: send and receive buffers are the same.
- May be useful in upcoming assignment
- Use MPI_IN_PLACE for the send buffer

Summary of Communications

Operation	MPI Function	Synopsis
		Individual
Send	MPI_Send	One-to-one send
Receive	MPI_Recv	One-to-one receive
Send/Receive	MPI_Sendrecv	One-to-one send/receive
		Collective
Barrier	MPI_Barrier	All wait for stragglers
Broadcast	MPI_Bcast	Root to all, all data copied
Scatter	MPI_Scatter	Root to all, slices of data copied
Gather	MPI_Gather	All to root, slices ordered on Root
Reduce	MPI_Reduce	All to root, data reduced on Root
All-Gather	MPI_Allgather	All to all, data ordered
All-Reduce	MPI_Allreduce	All to all, data reduced
		Not Discussed
Prefix	MPI_Prefix	All-to-all, data ordered/reduced
All-to-AllP	MPI_Alltoall	All-to-all, personal messages

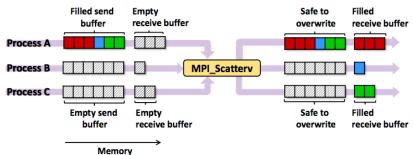
Vector Versions

- Collective comm ops like MPI_Scatter assume same amount of data to/from each processor
- Not a safe, general assumption (e.g. len % P != 0)
- Vector¹ versions of each comm op exist which relax these assumptions, allow arbitrary data counts per proc
- Provide additional arguments indicating
 - counts: How many elements each proc has
 - displs: Offsets elements are/will be stored in master array

Operation	Equal counts	Different counts
Broadcast	MPI_Bcast	
Scatter	MPI_Scatter	MPI_Scatterv
Gather	MPI_Gather	MPI_Gatherv
All-Gather	MPI_Allgather	MPI_Allgatherv
Reduce	MPI_Reduce	
All-Reduce	MPI_Allreduce	

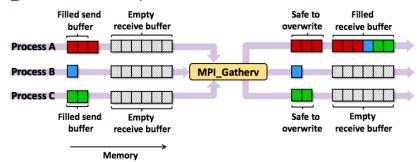
^{1&}quot;Vector" here means extra array arguments, NOT hardware-level parallelism like "Vector Instruction"

MPI_Scatterv Example



Source: SKIRT Docs

MPI_Gatherv Example



Source: SKIRT Docs

Dynamic Count and Displacements for Vector Comm Ops

- Common prob: # of procs does not evenly divide data size
- ▶ Use the vector versions of collective ops
- To calculate counts and displacements and spread work evenly, use a pattern like the below (see scatterv_demo.c)

```
int total_elements = 16;
int *counts = malloc(total_procs * sizeof(int));
int *displs = malloc(total_procs * sizeof(int));
// Divide total_elements as evenly as possible: lower numbered
// processors get one extra element each.
int elements_per_proc = total_elements / total_procs;
int surplus
                      = total_elements % total_procs;
for(i=0; i<total_procs; i++){</pre>
  counts[i] = (i < surplus) ? elements_per_proc+1 : elements_per_proc;</pre>
  displs[i] = (i == 0) ? 0 : displs[i-1] + counts[i-1];
// counts[] and displs[] now contain relevant data for a scattery,
// gatherv, all-gatherv calls
```

Barriers

```
MPI_Barrier(MPI_COMM_WORLD);
```

- Causes all processors to synchronize at the given line of code
- Early arrivers idle while other procs catch up
- ▶ To be avoided if possible as it almost always incurs idle time
- Unavoidable in some select scenarios
- Can be useful in debugging to introduce barriers

Basic Debugging Discpline

- Q: How do I debug Open MPI processes in parallel?

 A: This is a difficult question...

 OpenMPI FAQ on Debugging
- Commercial Parallel Debuggers exist, TotalView is popular
- For small-ish programs...
 Debug Printing + Valgrind + Effort + Patience
 will usually suffice
- > mpirun -v -np 4 valgrind ./my_program arg1 arg2