MPI and Collective Communication Patterns

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Last Updated:
Tue Feb 14 01:40:56 PM CST 2023

Logistics

Reading: Grama Ch 6 + 4

- Ch 6: MPI basics
- Ch 4: Communication patterns

Assignments

- A1 grading has commenced
- 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
- Exam at 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
- Send and Receive in MPI

```
MPI_Send(buf, len, MPI_INT, dest,   MPI_COMM_WORLD);
MPI_Recv(buf, len, MPI_INT, source, MPI_COMM_WORLD,
         MPI_STATUS_IGNORE);
```

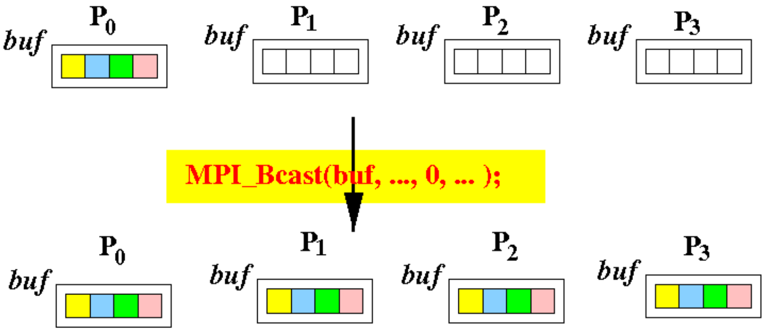
- Compile/Run

```
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



Source: Shun Yan Cheung Notes on MPI

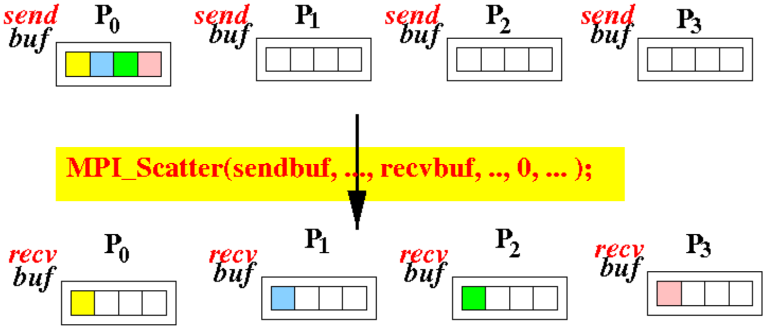
- Root processor wants to transmit `data` buffer to all processors
- Broadcast distributes to all procs
- Each proc gets same stuff in `data` buffer

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++){
    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



Source: Shun Yan Cheung Notes on MPI

- 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++){
    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];
  }
}
```

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

Answers: Scatter a Matrix

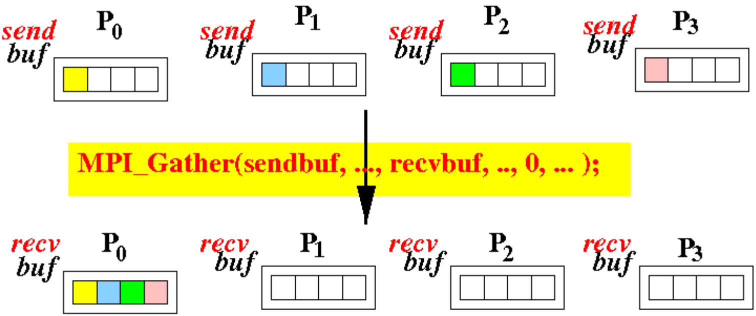
- Typically matrix must be allocated in **one block of memory** - single `malloc()`
- Allows a single `MPI_Scatter()` to scatter groups of rows

```
{
  // 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++){
    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



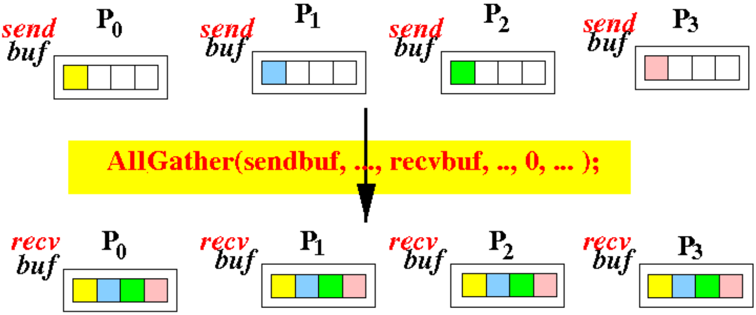
Source: Shun Yan Cheung Notes on MPI

- 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

```c
// 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++){
  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



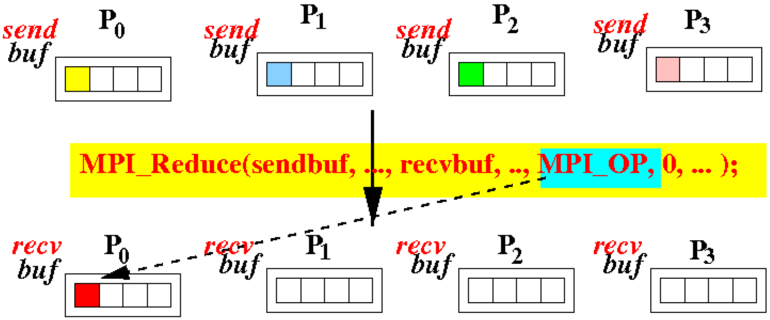
Source: Shun Yan Cheung Notes on MPI

- 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

```c
// 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++){
  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++){
    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
}
```

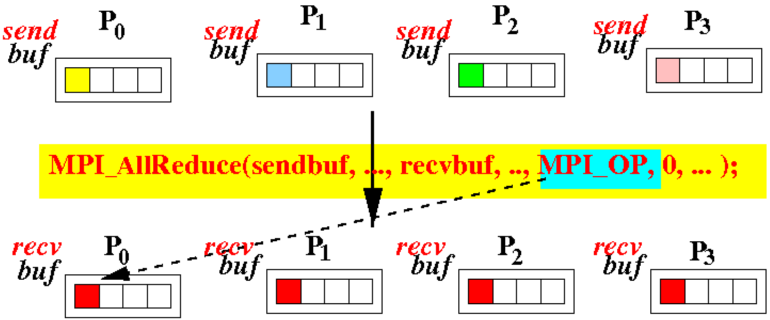
Note: Reduction's Array Argument

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

```
root_proc = 0;
MPI_Reduce(data, root_data, total_elements, MPI_INT,
           MPI_SUM, root_proc, MPI_COMM_WORLD);
// results in
P0.root_data[0] = P0.data[0] + P1.data[0] + P2.data[0] + ...
P0.root_data[1] = P0.data[1] + P1.data[1] + P2.data[1] + ...
P0.root_data[2] = P0.data[2] + P1.data[2] + P2.data[2] + ...
...
```

- To get a single sum, Procs should iterate on their own array THEN `MPI_Reduce()` on a single vlaue

Reduction for All: All-Reduce



Source: Shun Yan Cheung Notes on MPI

- 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++){
    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

```
{ // Everyone calls reduce, everyone sends and receives
  MPI_Allreduce(MPI_IN_PLACE,   // no destination buffer - use data
                data,            // reduction is placed here
                total_elements, MPI_INT,
                MPI_SUM,         // op to perform on each element
                MPI_COMM_WORLD);
  // data[] now contains each procs data[], min elements
}
```

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

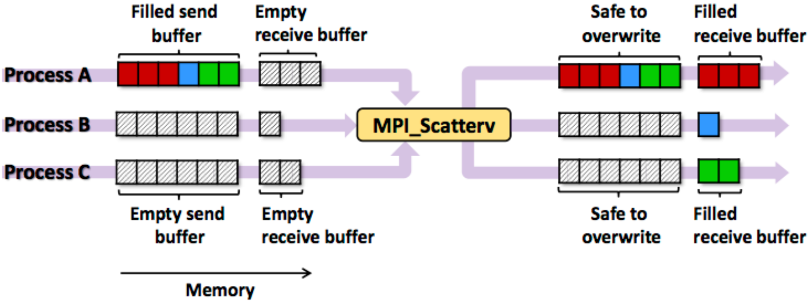
Vector Versions

- 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`)
- *Vector*[1] 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] "Vector" here means extra array arguments, NOT hardware-level parallelism like "Vector Instruction"

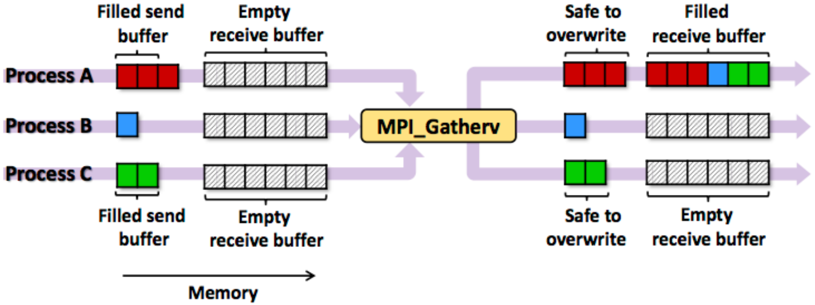
MPI_Scatterv Example



Source: SKIRT Docs

```c
//                P0 P1 P2
int counts[] = { 3, 1, 2};
int displs[] = { 0, 3, 4};
//                 P0  P0  P0  P1  P2  P2
int send[] =   { 10, 20, 30, 40, 50, 60 };
int *recv = malloc(counts[rank] * sizeof(int));
MPI_Scatterv(send, counts, displs, MPI_INT,
             recv, counts[rank], MPI_INT,
             0, MPI_COMM_WORLD);
```

MPI_Gatherv Example



Source: SKIRT Docs

```c
int total = 6;
int counts[] = { 3, 1, 2};
int displs[] = { 0, 3, 4};
int send[counts[rank]];
int *recv, i;
for(i=0; i<counts[rank]; i++){
  send[i] = rank*(i+1);
}
```

```c
recv = (rank!=0) ? NULL :
  malloc(total * sizeof(int));

MPI_Gatherv(
 send, counts[rank],   MPI_INT,
 recv, counts, displs, MPI_INT,
 0, MPI_COMM_WORLD);
```

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`)

```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++){
  counts[i] = (i < surplus) ? elements_per_proc+1 : elements_per_proc;
  displs[i] = (i == 0) ? 0 : displs[i-1] + counts[i-1];
}
// counts[] and displs[] now contain relevant data for a scatterv,
// 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

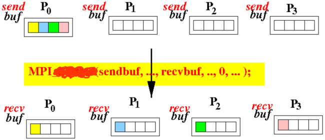
Basic Debugging Discpline

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
```

Exercise: MPI Collective Comm Review



1. Which MPI Collective Communication Operation does the above picture represent?
2. Draw a similar picture for MPI All-Gather
3. What are common operations work with a Reduction?
4. Which collective communication operations would be useful in the following settings:
   - At the beginning of a computation, the root processor needs to distribute rows of a matrix read from a data file to all other processors
   - After each processor finishes some computations using its own rows, all processors need the sum of all columns in the matrix

Answers: MPI Collective Comm Review

1. Which MPI Collective Communication Operation does the above picture represent?
   Scatter / `MPI_Scatter`
2. Draw a similar picture for MPI All-Gather
   See slide 15
3. What are common operations work with a Reduction?
   Addition/Sum, Multiply/Product, Min, Max
4. Which collective communication operations would be useful in the following settings:
   - At the beginning of a computation, the root processor needs to distribute rows of a matrix read from a data file to all other processors
     Scatter the rows
   - After each processor finishes some computations using its own rows, all processors need the sum of all columns in the matrix
     Local sum of columns, All-Reduce on local Column sums