Supercomputing in Plain English

Distributed Multiprocessing

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Outline

- The Desert Islands Analogy
- Distributed Parallelism
- MPI

The Desert Islands Analogy

An Island Hut

Imagine you're on a desert island in a little hut.

Inside the hut is a desk and a chair.

On the desk is:

- a **phone;**
- a **pencil;**
- a **calculator;**
- a piece of paper with **instructions**;
- a piece of paper with **numbers**.

Instructions

The **instructions** are split into two kinds:

- **Arithmetic/Logical**: e.g.,
  - Add the 27th number to the 239th number
  - Compare the 96th number to the 118th number to see whether they are equal
- **Communication**: e.g.,
  - dial 555-0127 and leave a voicemail containing the 962nd number
  - call your voicemail box and collect a voicemail from 555-0063 and put that number in the 715th slot

Is There Anybody Out There?

If you're in a hut on an island, you aren't specifically aware of anyone else.

Especially, you don't know whether anyone else is working on the same problem as you are, and you don't know who's at the other end of the phone line.

All you know is what to do with the voicemails you get, and what phone numbers to send voicemails to.

Someone Might Be Out There

Now suppose that Julie is on another island somewhere, in the same kind of hut, with the same kind of equipment.

Suppose that she has the same list of instructions as you, but a different set of numbers (both data and phone numbers).

Like you, she doesn't know whether there's anyone else working on her problem.

Even More People Out There

Now suppose that Lloyd and Jerry are also in huts on islands.

Suppose that each of the four has the **exact same list of instructions**, but **different lists of numbers**.

And suppose that the phone numbers that people call are each others'. That is, your instructions have you call Julie, Lloyd and Jerry, Julie's has her call Lloyd, Jerry and you, and so on.

Then you might **all be working together** on the same problem, even though you're not aware of it.

All Data Are Private

Notice that you can’t see Julie’s or Lloyd’s or Jerry’s numbers, nor can they see yours or each other’s.

Thus, everyone’s numbers are **private**: there’s no way for anyone to share numbers, **except by leaving them in voicemails**.

Long Distance Calls: 2 Costs

When you make a long distance phone call, you typically have to pay two costs:

- **Connection charge**: the **fixed** cost of connecting your phone to someone else's, even if you're only connected for a second
- **Per-minute charge**: the cost per minute of talking, once you're connected

If the connection charge is large, then you want to make **as few calls as possible**.

Distributed Parallelism

Like Desert Islands

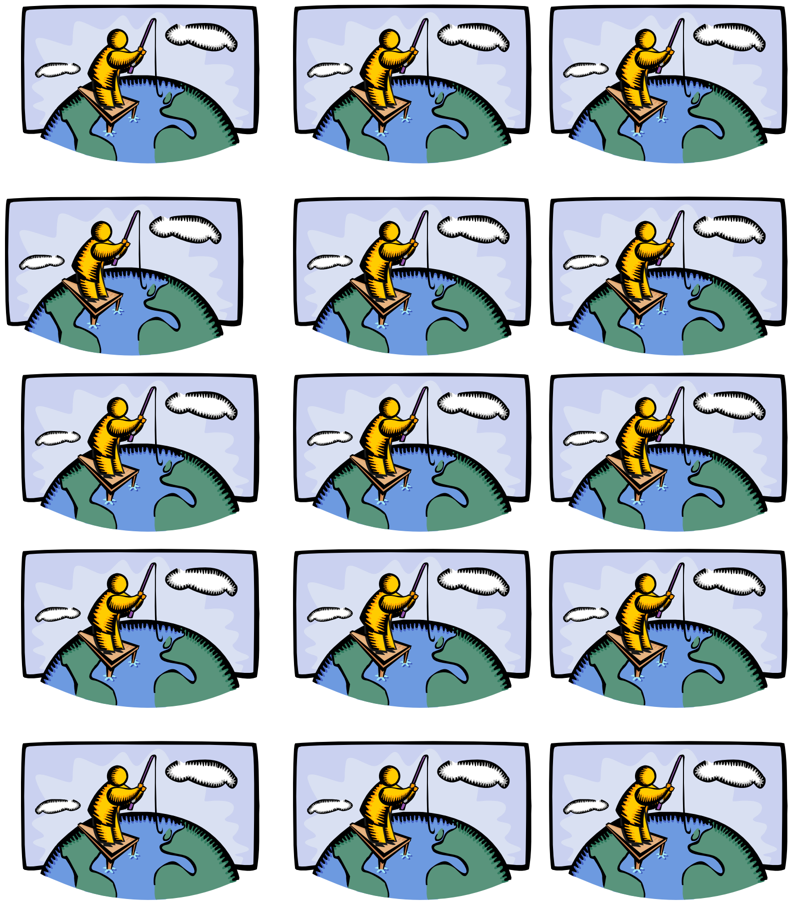
Distributed parallelism is very much like the Desert Islands analogy:

- processes are **independent** of each other.
- All data are **private**.
- Processes communicate by **passing messages** (like voicemails).
- The cost of passing a message is split into:
  - ***latency*** (connection time)
  - ***bandwidth*** (time per byte)

Parallelism

Parallelism means doing multiple things at the same time: you can get more work done in the same amount of time.

Less fish …



More fish!

What Is Parallelism?

Parallelism is the use of multiple processing units – either processors or parts of an individual processor – to solve a problem, and in particular the use of multiple processing units operating concurrently on different parts of a problem.

The different parts could be different tasks, or the same task on different pieces of the problem’s data.

Kinds of Parallelism

- Shared Memory Multithreading (our topic last time)
- Distributed Memory Multiprocessing (today)
- Hybrid Shared/Distributed

Why Parallelism Is Good

- **The Trees**: We like parallelism because, as the number of processing units working on a problem grows, we can solve **the same problem in less time**.
- **The Forest**: We like parallelism because, as the number of processing units working on a problem grows, we can solve **bigger problems**.

Parallelism Jargon

- ***Threads***: execution sequences that share a single memory area ("***address space***")
- ***Processes***: execution sequences with their own independent, private memory areas

… and thus:

- ***Multithreading***: parallelism via multiple threads
- ***Multiprocessing***: parallelism via multiple processes

As a general rule, **Shared Memory Parallelism** is concerned with **threads**, and **Distributed Parallelism** is concerned with **processes**.

Jargon Alert

In principle:

- "shared memory parallelism" ➔ "multithreading"
- "distributed parallelism" ➔ "multiprocessing"

In practice, these terms are often used interchangeably:

- Parallelism
- ***Concurrency*** (not as popular these days)
- Multithreading
- Multiprocessing

Typically, you have to figure out what is meant based on the context.

Load Balancing

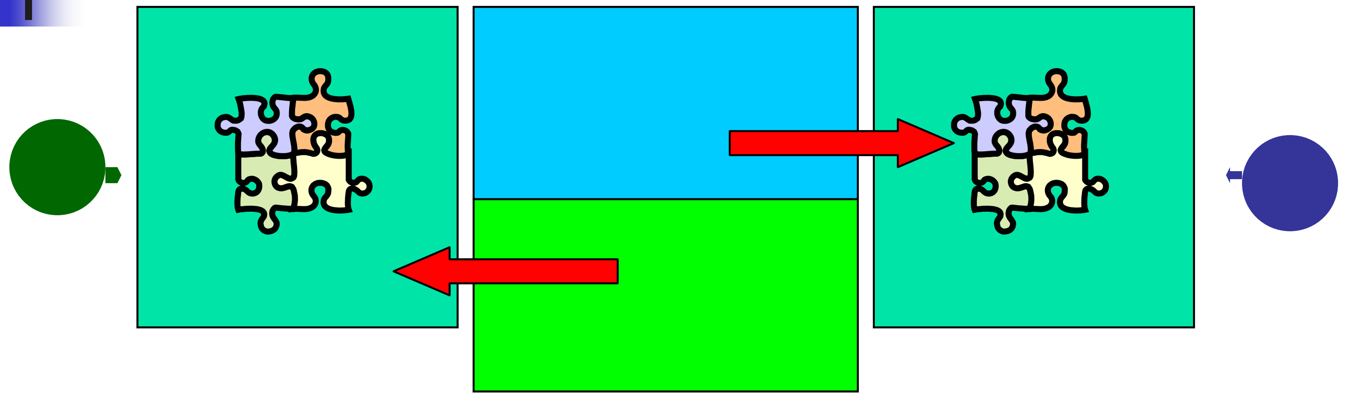
Suppose you have a distributed parallel code, but one process does 90% of the work, and all the other processes share 10% of the work.

Is it a big win to run on 1000 processes?

Now, suppose that each process gets exactly 1/N_p of the work, where N_p is the number of processes.

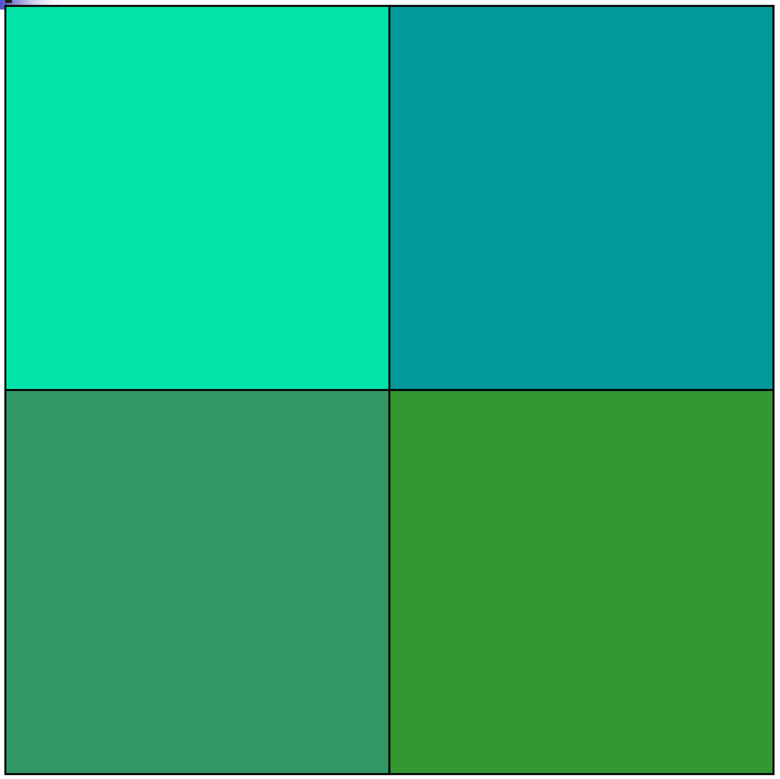
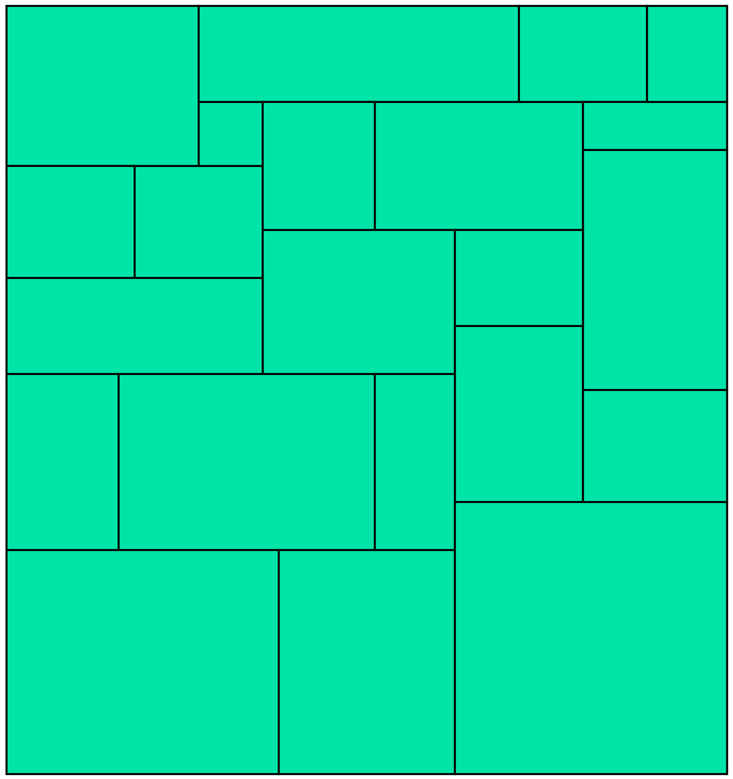
Now is it a big win to run on 1000 processes?

Load Balancing



Load balancing means giving everyone roughly the same amount of work to do.

Load Balancing

Load balancing can be easy, if the problem splits up into chunks of roughly equal size, with one chunk per process. Or load balancing can be very hard.

Load Balancing Is Good

- When every process gets the same amount of work, the job is ***load balanced***.
- We like load balancing, because it means that our speedup can potentially be linear: if we run on N_p processes, it takes $1/N_p$ as much time as on one.
- For some codes, figuring out how to balance the load is trivial (e.g., breaking a big unchanging array into sub-arrays).
- For others, load balancing is very tricky (e.g., a dynamically evolving collection of arbitrarily many blocks of arbitrary size).

Parallel Strategies

- ***Client-Server***: One worker (the server) decides what tasks the other workers (clients) will do; e.g., Hello World, Monte Carlo.
- ***Data Parallelism***: Each worker does exactly the same tasks on its unique subset of the data; e.g., distributed meshes (weather etc).
- ***Task Parallelism***: Each worker does different tasks on exactly the same set of data (each process holds exactly the same data as the others); e.g., N-body.
- ***Pipeline:*** Each worker does its tasks, then passes its set of data along to the next worker and receives the next set of data from the previous worker.

MPI: The Message-Passing Interface

Most of this discussion is from [1] and [2].

What Is MPI?

- The ***Message-Passing Interface*** (MPI) is a standard for expressing distributed parallelism via message passing.
- MPI consists of a ***header file***, a ***library of routines*** and a ***runtime environment***.
- When you compile a program that has MPI calls in it, your compiler links to a local implementation of MPI, and then you get parallelism; if the MPI library isn't available, then the compile will fail.
- MPI can be used in Fortran, C and C++.

MPI Calls

MPI calls in **Fortran** look like this:

```
CALL MPI_Funcname(…, errcode)
```

In C, MPI calls look like:

```
errcode = MPI_Funcname(…)
```

In C++, MPI calls look like:

```
errcode = MPI::Funcname(…)
```

Notice that **`errcode`** is returned by the MPI routine **`MPI_Funcname`**, with a value of **`MPI_SUCCESS`** indicating that **`MPI_Funcname`** has worked correctly.

MPI is an API

- MPI is actually just an ***Application Programming Interface*** (API).
- An API specifies what a call to each routine should look like, and how each routine should behave.
- An API does not specify how each routine should be implemented, and sometimes is intentionally vague about certain aspects of a routine's behavior.
- Each platform has its own MPI implementation.

Example MPI Routines

- `MPI_Init` starts up the MPI runtime environment at the beginning of a run.
- `MPI_Finalize` shuts down the MPI runtime environment at the end of a run.
- `MPI_Comm_size` gets the number of processes in a run, N_p (typically called just after `MPI_Init`).
- `MPI_Comm_rank` gets the process ID that the current process uses, which is between 0 and N_p-1 inclusive (typically called just after `MPI_Init`).

More Example MPI Routines

- **`MPI_Send`** sends a message from the current process to some other process (the ***destination***).
- **`MPI_Recv`** receives a message on the current process from some other process (the ***source***).
- **`MPI_Bcast`** **broadcasts** a message from one process to all of the others.
- **`MPI_Reduce`** performs a reduction (e.g., sum, maximum) of a variable on all processes, sending the result to a single process.

MPI Program Structure (F90)

```
PROGRAM my_mpi_program
  IMPLICIT NONE
  INCLUDE "mpif.h"
  [other includes]
  INTEGER :: my_rank, num_procs, mpi_error_code
  [other declarations]
  CALL MPI_Init(mpi_error_code)     !! Start up MPI
  CALL MPI_Comm_Rank(my_rank,   mpi_error_code)
  CALL MPI_Comm_size(num_procs, mpi_error_code)
  [actual work goes here]
  CALL MPI_Finalize(mpi_error_code) !! Shut down MPI
END PROGRAM my_mpi_program
```

Note that MPI uses the term "***rank***" to indicate process identifier.

MPI Program Structure (in C)

```
#include <stdio.h>
#include "mpi.h"
 [other includes]

int main (int argc, char* argv[])
{ /* main */
  int my_rank, num_procs, mpi_error;
  [other declarations]
  mpi_error = MPI_Init(&argc, &argv); /* Start up MPI  */
  mpi_error = MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
  mpi_error = MPI_Comm_size(MPI_COMM_WORLD, &num_procs);
  [actual work goes here]
  mpi_error = MPI_Finalize();         /* Shut down MPI */
} /* main */
```

Example: Hello World

1. Start the MPI system.
2. Get the rank and number of processes.
3. If you're **not** the server process:
    1. Create a "hello world" string.
    2. Send it to the server process.
4. If you **are** the server process:
    1. For each of the client processes:
        1. Receive its "hello world" string.
        2. Print its "hello world" string.
5. Shut down the MPI system.

hello_world_mpi.c

```
#include <stdio.h>
#include <string.h>
#include "mpi.h"

int main (int argc, char* argv[])
{ /* main */
  const int  maximum_message_length = 100;
  const int  server_rank            =   0;
  char       message[maximum_message_length+1];
  MPI_Status status;      /* Info about receive status  */
  int        my_rank;     /* This process ID            */
  int        num_procs;   /* Number of processes in run */
  int        source;      /* Process ID to receive from */
  int        destination; /* Process ID to send to      */
  int        tag = 0;     /* Message ID                 */
  int        mpi_error;   /* Error code for MPI calls   */
```

  [work goes here]

```
} /* main */
```

Hello World Startup/Shut Down

```
[header file includes]
int main (int argc, char* argv[])
{ /* main */
  [declarations]
  mpi_error = MPI_Init(&argc, &argv);
  mpi_error = MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
  mpi_error = MPI_Comm_size(MPI_COMM_WORLD, &num_procs);
  if (my_rank != server_rank) {
    [work of each non-server (worker) process]
  } /* if (my_rank != server_rank) */
  else {
    [work of server process]
  } /* if (my_rank != server_rank)…else */
  mpi_error = MPI_Finalize();
} /* main */
```

Hello World Client’s Work

```
[header file includes]
int main (int argc, char* argv[])
{ /* main */
  [declarations]
  [MPI startup (MPI_Init etc)]
  if (my_rank != server_rank) {
    sprintf(message, "Greetings from process #%d!“,
        my_rank);
    destination = server_rank;
    mpi_error =
      MPI_Send(message, strlen(message) + 1, MPI_CHAR,
        destination, tag, MPI_COMM_WORLD);
  } /* if (my_rank != server_rank) */
  else {
    [work of server process]
  } /* if (my_rank != server_rank)…else */
  mpi_error = MPI_Finalize();
} /* main */
```

Hello World Server's Work

[header file includes]

```
int main (int argc, char* argv[])
{ /* main */
```

[declarations, MPI startup]

```
  if (my_rank != server_rank) {
```

[work of each client process]

```
  } /* if (my_rank != server_rank) */
  else {
    for (source = 0; source < num_procs; source++) {
      if (source != server_rank) {
        mpi_error =
          MPI_Recv(message, maximum_message_length + 1,
            MPI_CHAR, source, tag, MPI_COMM_WORLD,
            &status);
        fprintf(stderr, "%s\n", message);
      } /* if (source != server_rank) */
    } /* for source */
  } /* if (my_rank != server_rank)…else */
  mpi_error = MPI_Finalize();
} /* main */
```

How an MPI Run Works

- Every process gets a copy of the executable: ***Single Program, Multiple Data*** (SPMD).
- They all start executing it.
- Each looks at its own rank to determine which part of the problem to work on.
- Each process works **completely independently** of the other processes, except when communicating.

Compiling and Running

```
% mpicc  -o  hello_world_mpi  hello_world_mpi.c
% mpirun  -np  1  hello_world_mpi
% mpirun  -np  2  hello_world_mpi
Greetings from process #1!
% mpirun  -np  3  hello_world_mpi
Greetings from process #1!
Greetings from process #2!
% mpirun  -np  4  hello_world_mpi
Greetings from process #1!
Greetings from process #2!
Greetings from process #3!
```

Note: the compile command and the run command vary from platform to platform.

Why is Rank #0 the server?

```
const int server_rank = 0;
```

By convention, the server process has rank (process ID) #0. Why?

A run must use at least one process but can use multiple processes.

Process ranks are 0 through N_p-1, $N_p \geq 1$.

Therefore, every MPI run has a process with rank #0.

Note: every MPI run also has a process with rank N_p-1, so you could use N_p-1 as the server instead of 0 … but no one does.

Why “Rank?”

Why does MPI use the term ***rank*** to refer to process ID?

In general, a process has an identifier that is assigned by the operating system (e.g., Unix), and that is unrelated to MPI:

```
% ps
        PID TTY      TIME CMD
   52170812 ttyq57   0:01 tcsh
```

Also, each processor has an identifier, but an MPI run that uses fewer than all processors will use an arbitrary subset.

The rank of an MPI process is neither of these.

Compiling and Running

Recall:

```
% mpicc  -o  hello_world_mpi  hello_world_mpi.c
% mpirun  -np  1  hello_world_mpi
% mpirun  -np  2  hello_world_mpi
Greetings from process #1!
% mpirun  -np  3  hello_world_mpi
Greetings from process #1!
Greetings from process #2!
% mpirun  -np  4  hello_world_mpi
Greetings from process #1!
Greetings from process #2!
Greetings from process #3!
```

Deterministic Operation?

```
% mpirun  -np  4  hello_world_mpi
Greetings from process #1!
Greetings from process #2!
Greetings from process #3!
```

The order in which the greetings are printed is deterministic. **Why?**

```
for (source = 0; source < num_procs; source++) {
  if (source != server_rank) {
    mpi_error =
      MPI_Recv(message, maximum_message_length + 1,
        MPI_CHAR, source, tag, MPI_COMM_WORLD,
        &status);
    fprintf(stderr, "%s\n", message);
  } /* if (source != server_rank) */
} /* for source */
```

This loop **ignores the receive order**.

Message = Envelope+Contents

```
MPI_Send(message, strlen(message) + 1,
     MPI_CHAR, destination, tag,
     MPI_COMM_WORLD);
```

When MPI sends a message, it doesn’t just send the contents; it also sends an “envelope” describing the contents:

- **Size** (number of elements of data type)
- **Data type**
- **Source**: rank of sending process
- **Destination**: rank of process to receive
- **Tag** (message ID)
- **Communicator** (e.g., `MPI_COMM_WORLD`)

MPI Data Types

C		Fortran 90	
char	**MPI_CHAR**	CHARACTER	**MPI_CHARACTER**
int	**MPI_INT**	INTEGER	**MPI_INTEGER**
float	**MPI_FLOAT**	REAL	**MPI_REAL**
double	**MPI_DOUBLE**	DOUBLE PRECISION	**MPI_DOUBLE_PRECISION**

MPI supports several other data types, but most are variations of these, and probably these are all you'll use.

Message Tags

```
for (source = 0; source < num_procs; source++) {
  if (source != server_rank) {
    mpi_error =
      MPI_Recv(message, maximum_message_length + 1,
        MPI_CHAR, source, tag, MPI_COMM_WORLD,
        &status);
    fprintf(stderr, "%s\n", message);
  } /* if (source != server_rank) */
} /* for source */
```

The greetings are **printed** in deterministic order not because messages are sent and received in order, but because each has a ***tag*** (message identifier), and **`MPI_Recv`** asks for a specific message (by tag) from a specific source (by rank).

Communicators

An MPI communicator is a collection of processes that can send messages to each other.

`MPI_COMM_WORLD` is the default communicator; it contains all of the processes. It's probably the only one you'll need.

Some libraries (e.g., PETSc) create special library-only communicators, which can simplify keeping track of message tags.

Broadcasting

What happens if one process has data that everyone else needs to know?

For example, what if the server process needs to send an input value to the others?

```
CALL MPI_Bcast(length, 1, MPI_INTEGER, &
 &        source, MPI_COMM_WORLD,
          error_code)
```

Note that **`MPI_Bcast`** doesn't use a tag, and that the call is the same for both the sender and all of the receivers.

Broadcast Example: Setup

```
PROGRAM broadcast
  USE mpi
  IMPLICIT NONE
  INTEGER,PARAMETER :: server = 0
  INTEGER,PARAMETER :: source = server
  INTEGER,DIMENSION(:),ALLOCATABLE :: array
  INTEGER :: length, memory_status
  INTEGER :: num_procs, my_rank, mpi_error_code

  CALL MPI_Init(mpi_error_code)
  CALL MPI_Comm_rank(MPI_COMM_WORLD, my_rank,   &
 &       mpi_error_code)
  CALL MPI_Comm_size(MPI_COMM_WORLD, num_procs, &
 &       mpi_error_code)
  [input]
  [broadcast]
  CALL MPI_Finalize(mpi_error_code)
END PROGRAM broadcast
```

Broadcast Example: Input

```
PROGRAM broadcast
  USE mpi
  IMPLICIT NONE
  INTEGER,PARAMETER :: server = 0
  INTEGER,PARAMETER :: source = server
  INTEGER,DIMENSION(:),ALLOCATABLE :: array
  INTEGER :: length, memory_status
  INTEGER :: num_procs, my_rank, mpi_error_code
```

[MPI startup]

```
  IF (my_rank == server) THEN
    OPEN (UNIT=99,FILE="broadcast_in.txt")
    READ (99,*) length
    CLOSE (UNIT=99)
    ALLOCATE(array(length), STAT=memory_status)
    array(1:length) = 0
  END IF !! (my_rank == server)...ELSE
```

[broadcast]

```
  CALL MPI_Finalize(mpi_error_code)
END PROGRAM broadcast
```

Broadcast Example: Broadcast

```
PROGRAM broadcast
  USE mpi
  IMPLICIT NONE
  INTEGER,PARAMETER :: server = 0
  INTEGER,PARAMETER :: source = server
  [other declarations]

  [MPI startup and input]
  IF (num_procs > 1) THEN
    CALL MPI_Bcast(length, 1, MPI_INTEGER, source, &
 &          MPI_COMM_WORLD, mpi_error_code)
    IF (my_rank /= server) THEN
      ALLOCATE(array(length), STAT=memory_status)
    END IF !! (my_rank /= server)
    CALL MPI_Bcast(array, length, MPI_INTEGER, source, &
            MPI_COMM_WORLD, mpi_error_code)
    WRITE (0,*) my_rank, ": broadcast length = ", length
  END IF !! (num_procs > 1)
  CALL MPI_Finalize(mpi_error_code)
END PROGRAM broadcast
```

Broadcast Compile & Run

```
% mpif90 -o broadcast broadcast.f90
% mpirun -np 4 broadcast
 0 : broadcast length =  16777216
 1 : broadcast length =  16777216
 2 : broadcast length =  16777216
 3 : broadcast length =  16777216
```

Reductions

A ***reduction*** converts an array to a scalar: e.g., sum, product, minimum value, maximum value, Boolean AND, Boolean OR, etc.

Reductions are so common, and so important, that MPI has two routines to handle them:

- **`MPI_Reduce`**: sends result to a single specified process
- **`MPI_Allreduce`**: sends result to all processes (and therefore takes longer)

Reduction Example

```
PROGRAM reduce
  USE mpi
  IMPLICIT NONE
  INTEGER,PARAMETER :: server = 0
  INTEGER :: value, value_sum
  INTEGER :: num_procs, my_rank, mpi_error_code

  CALL MPI_Init(mpi_error_code)
  CALL MPI_Comm_rank(MPI_COMM_WORLD, my_rank,   mpi_error_code)
  CALL MPI_Comm_size(MPI_COMM_WORLD, num_procs, mpi_error_code)
  value_sum = 0
  value     = my_rank * num_procs
  CALL MPI_Reduce(value, value_sum, 1, MPI_INT, MPI_SUM, &
 &       server, MPI_COMM_WORLD, mpi_error_code)
  WRITE (0,*) my_rank, ": reduce  value_sum = ", value_sum
  CALL MPI_Allreduce(value, value_sum, 1, MPI_INT, MPI_SUM, &
 &      MPI_COMM_WORLD, mpi_error_code)
  WRITE (0,*) my_rank, ": allreduce value_sum = ", value_sum
  CALL MPI_Finalize(mpi_error_code)
END PROGRAM reduce
```

Compiling and Running

```
% mpif90 -o reduce reduce.f90
% mpirun -np 4 reduce
 3 : reduce  value_sum =  0
 1 : reduce  value_sum =  0
 2 : reduce  value_sum =  0
 0 : reduce  value_sum =  24
 0 : allreduce value_sum =  24
 1 : allreduce value_sum =  24
 2 : allreduce value_sum =  24
 3 : allreduce value_sum =  24
```

Why Two Reduction Routines?

MPI has two reduction routines because of the high cost of each communication.

If only one process needs the result, then it doesn't make sense to pay the cost of sending the result to all processes.

But if all processes need the result, then it may be cheaper to reduce to all processes than to reduce to a single process and then broadcast to all.

Example: Monte Carlo

Monte Carlo methods are approximation methods that randomly generate a large number of examples (***realizations***) of a phenomenon, and then take the average of the examples' properties.

When the realizations' average converges (i.e., doesn't change substantially if new realizations are generated), then the Monte Carlo simulation stops.

Monte Carlo simulations are sometimes known as ***embarrassingly parallel***.

Serial Monte Carlo

Suppose you have an existing serial Monte Carlo simulation:

```
PROGRAM monte_carlo
  CALL read_input(…)
  DO WHILE (average_properties_havent_converged(…))
    CALL generate_random_realization(…)
    CALL calculate_properties(…)
    CALL calculate_average(…)
  END DO
END PROGRAM monte_carlo
```

How would you parallelize this?

Parallel Monte Carlo

```
PROGRAM monte_carlo
  [MPI startup]
  IF (my_rank == server_rank) THEN
    CALL read_input(…)
  END IF !! (my_rank == server_rank)
  CALL MPI_Bcast(…)
  DO WHILE (average_properties_havent_converged(…))
    CALL generate_random_realization(…)
    CALL calculate_properties(…)
    IF (my_rank == server_rank) THEN
      [collect properties]
    ELSE   !! (my_rank == server_rank)
      [send properties]
    END IF !! (my_rank == server_rank)…ELSE
    CALL calculate_average(…)
  END DO !! WHILE (average_properties_havent_converged(…))
  [MPI shutdown]
END PROGRAM monte_carlo
```

Asynchronous Communication

MPI allows a process to start a send, then go on and do work while the message is in transit.

This is called ***asynchronous*** or ***non-blocking*** or ***immediate*** communication. (Here, "immediate" refers to the fact that the call to the MPI routine returns immediately rather than waiting for the send to complete.)

Immediate Send

```
CALL MPI_Isend(array, size, MPI_FLOAT,          &
 &     destination, tag, communicator, request, &
 &     mpi_error_code)
```

Likewise:

```
CALL MPI_Irecv(array, size, MPI_FLOAT,     &
 &     source, tag, communicator, request, &
 &     mpi_error_code)
```

This call starts the send/receive, but the send/receive won’t be complete until:

```
CALL MPI_Wait(request, status)
```

What’s the advantage of this?

Communication Hiding

In between the call to `MPI_Isend/Irecv` and the call to `MPI_Wait`, both processes can do work!

If that work takes at least as much time as the communication, then the cost of the communication is effectively zero, since the communication won't affect how much work gets done.

This is called ***communication hiding***.

Communication Hiding in MC

In our Monte Carlo example, we could use communication hiding by, for instance, sending the properties of each realization asynchronously.

That way, the sending process can start generating a new realization while the old realization’s properties are in transit.

The server process can collect the other processes’ data when it’s done with its realization.

Rule of Thumb for Hiding

When you want to hide communication:

- as soon as you calculate the data, send it;
- don't receive it until you need it.

That way, the communication has the maximal amount of time to happen in ***<u>background</u>*** (behind the scenes).

Next Time

Part VII:

Grab Bag:

I/O, Visualization, etc

References

[1] P.S. Pacheco, *Parallel Programming with MPI*, Morgan Kaufmann Publishers, 1997.

[2] W. Gropp, E. Lusk and A. Skjellum, *Using MPI: Portable Parallel Programming with the Message-Passing Interface*, 2nd ed. MIT Press, 1999.