The Message Passing Interface (MPI): Parallelism on Distributed CPUs

http://mpi-forum.org
https://www.open-mpi.org/

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Why Two URLs?

http://mpi-forum.org
This is the definitive reference for the MPI standard. Go here if you want to read the official specification, which, BTW, continues to evolve.

https://www.open-mpi.org/
This consortium formed later. This is the open source version of MPI. If you want to start using MPI, I recommend you look here. This is the MPI that the COE systems use.

https://www.open-mpi.org/doc/v4.0/
This URL is also really good – it is a link to all of the MPI man pages.
Network

CPU

Memory

CPU

Memory

Note: Each CPU in the MPI "cluster" must be prepared ahead of time by having the MPI server code installed on it. Each MPI CPU must also have an integer ID assigned to it (called its rank).
This paradigm is how modern supercomputers work!

The Texas Advanced Computing Center’s new Frontera supercomputer, currently the 5th fastest in the world

**How to SSH to the COE MPI Cluster**

- `flip3` 151% `ssh` submit-c.hpc.engr.oregonstate.edu
- `submit-c` 142% module load slurm
- `submit-c` 143% module load openmpi/3.1

Type these two lines right away to set your paths correctly

BTW, you can find out more about the COE cluster here: [https://it.engineering.oregonstate.edu/hpc](https://it.engineering.oregonstate.edu/hpc)

“The College of Engineering HPC cluster is a heterogeneous mix of 202 servers providing over 3600 CPU cores, over 130 GPUs, and over 31 TB total RAM. The systems are connected via gigabit ethernet, and most of the latest servers also utilize a Mellanox EDR InfiniBand network connection. The cluster also has access to 100TB global scratch from the College of Engineering’s Dell/EMC Isilon enterprise storage.”
Compiling and Running

\begin{align*}
\text{% mpiexec -mca btl self,tcp -np 4 program} \\
\text{or} \\
\text{% mpic++ -o program program.cpp . . .}
\end{align*}

\text{All distributed processors execute} \\
\text{the same program at the same time}

\text{# of processors to use}

Warning – use mpic++ and mpiexec!

Don’t use g++ and don’t run by just typing the name of the executable!

So, a \textit{bash} Batch Script Would Look Like This

\texttt{
#!/bin/bash
#SBATCH -J Heat
#SBATCH -A cs475-575
#SBATCH -p class
#SBATCH -N 8  # number of nodes
#SBATCH -n 8  # number of tasks
#SBATCH -o heat.out
#SBATCH -e heat.err
#SBATCH --mail-type=END,FAIL
#SBATCH --mail-user=mjb@cs.oregonstate.edu
mpic++ heat.cpp -o heat -lm
mpiexec -mca btl self,tcp -np 4 heat
}

\texttt{submit-c 143\% sbatch submit.bash}

Submitted batch job 258759
Auto-Notifications via Email

#SBATCH --mail-user=joeparallel@oregonstate.edu

You don’t have to ask for email notification, but if you do, please, please be sure you get your email address right!

The IT people are getting real tired of fielding the bounced emails when people spell their own email address wrong.

Use slurm’s `scancel` if your Job Needs to Be Killed

```
submit-c 143% sbatch submit.bash
Submitted batch job 258759
```

```
submit-c 144% scancel 258759
```
Setting Up and Finishing

```c
#include <mpi.h>
int main( int argc, char *argv[] )
{
    MPI_Init( &argc, &argv );
    ...
    MPI_Finalize( );
    return 0;
}
```

You don’t need to process command line arguments if you don’t need to. You can also call it as:

```c
MPI_Init( NULL, NULL );
```

Getting information about our place in the communicator:

```c
int numCPUs;     // total # of cpus involved
int me;          // which one I am
MPI_Comm_size( MPI_COMM_WORLD, &numCPUs );
MPI_Comm_rank( MPI_COMM_WORLD, &me );
```

It is then each CPU’s job to figure out what piece of the overall problem it is responsible for and then go do it.

This requires MPI server code getting installed on all those CPUs. Only an administrator can do this.

A `communicator` is a collection of CPUs that are capable of sending messages to each other.

This requires MPI server code getting installed on all those CPUs. Only an administrator can do this.

Oh, look, a communicator of deer! Oh, look, a communicator of turkeys!

It is then each CPU’s job to figure out what piece of the overall problem it is responsible for and then go do it.
A First Test of MPI

```c
#include <stdio.h>
#include <math.h>
#include <mpi.h>

#define BOSS 0

int main( int argc, char *argv[] )
{
    MPI_Init( &argc, &argv );

    int numCPUs;       // total # of cpus involved
    int me;            // which one I am

    MPI_Comm_size( MPI_COMM_WORLD, &numCPUs );
    MPI_Comm_rank( MPI_COMM_WORLD, &me );

    if( me == BOSS )
        fprintf( stderr, "Rank %d says that we have a Communicator of size %d\n", BOSS, numCPUs );
    else
        fprintf( stderr, "Welcome from Rank %d\n", me );

    MPI_Finalize( );

    return 0;
}
```

submit-c 165% mpiexec -np 16 ./first
Welcome from Rank 13
Welcome from Rank 15
Welcome from Rank 3
Welcome from Rank 7
Welcome from Rank 5
Welcome from Rank 8
Welcome from Rank 9
Welcome from Rank 11
Rank 0 says that we have a Communicator of size 16
Welcome from Rank 1
Welcome from Rank 12
Welcome from Rank 14
Welcome from Rank 6
Welcome from Rank 2
Welcome from Rank 10
Welcome from Rank 4

submit-c 166% mpiexec -np 16 ./first
Welcome from Rank 1
Welcome from Rank 5
Welcome from Rank 7
Welcome from Rank 11
Welcome from Rank 13
Welcome from Rank 15
Rank 0 says that we have a Communicator of size 16
Welcome from Rank 3
Welcome from Rank 4
Welcome from Rank 6
Welcome from Rank 8
Welcome from Rank 12
Welcome from Rank 14
Welcome from Rank 10

submit-c 167% mpiexec -np 16 ./first
Welcome from Rank 9
Welcome from Rank 11
Welcome from Rank 13
Welcome from Rank 7
Welcome from Rank 1
Welcome from Rank 3
Welcome from Rank 10
Welcome from Rank 15
Welcome from Rank 4
Welcome from Rank 5
Rank 0 says that we have a Communicator of size 16
Welcome from Rank 2
Welcome from Rank 6
Welcome from Rank 8
Welcome from Rank 14
Welcome from Rank 12

submit-c 168% mpiexec -np 16 ./first
Welcome from Rank 13
Welcome from Rank 15
Welcome from Rank 7
Welcome from Rank 3
Welcome from Rank 5
Welcome from Rank 9
Welcome from Rank 11
Welcome from Rank 1
Welcome from Rank 2
Welcome from Rank 10
Welcome from Rank 14
Welcome from Rank 6
So, we have a group (a “communicator”) of distributed processors. How do they communicate about what work they are supposed to do?

Who am I?  
Where am I?  
What am I supposed to be doing?  
Hello? Is anyone listening?

Example: You could coordinate the units of our DGX system using MPI

A Good Place to Start:  
MPI Broadcasting

```c
MPI_Bcast( array, count, type, src, MPI_COMM_WORLD );
```

Address of data to send from if you are the src node;  
Address of the data to receive into if you are not

- `MPI_CHAR`  
- `MPI_INT`  
- `MPI_LONG`  
- `MPI_FLOAT`  
- `MPI_DOUBLE`  

# elements  
rank of the CPU doing the sending

Broadcast

Both the sender and receivers need to execute `MPI_Bcast` – there is no separate receive function
This is our heat transfer equation from before. Clearly, every CPU will need to know this value.

$$\Delta T_i = \frac{k}{\rho C} \left( \frac{T_{i+1} - 2T_i + T_{i-1}}{(\Delta x)^2} \right) \Delta t$$

```c
int numCPUs;
int me;
float k_over_rho_c; // the BOSS node will know this value, the others won't (yet)
#define BOSS 0
MPI_Comm_size( MPI_COMM_WORLD, &numCPUs ); // how many are in this communicator
MPI_Comm_rank( MPI_COMM_WORLD, &me ); // which one am I?

if( me == BOSS )
{
    // << read k_over_rho_c from the data file >>
}
MPI_Bcast( &k_over_rho_c, 1, MPI_FLOAT, BOSS, MPI_COMM_WORLD ); // send if BOSS, and receive if not
```

Confused? Look at this Diagram

Both the sender and receivers need to execute `MPI_Bcast` -- there is no separate receive function.
How Does this Work?
Think Star Trek Wormholes!

Sending Data from One Source CPU to One Destination CPU

MPI_Send( array, numToSend, type, dst, tag, MPI_COMM_WORLD );

address of data to send from

# elements
(note: this is the number of elements, not the number of bytes!)

MPI_CHAR
MPI_INT
MPI_LONG
MPI_FLOAT
MPI_DOUBLE

• • •

rank of the CPU to send to

An integer to differentiate this transmission from any other transmission (be sure this is unique!)

Rules:

• One message from a specific src to a specific dst cannot overtake a previous message from the same src to the same dst.

• MPI_Send() blocks until the transfer is far enough along that array can be destroyed or re-used.

• There are no guarantees on order from different src's.

src node ———— dst node
Receiving Data in a Destination CPU from a Source CPU

```c
MPI_Recv( array, maxCanReceive, type, src, tag, MPI_COMM_WORLD, &status );
```

**Rules:**

- The receiver blocks waiting for data that matches what it declares to be looking for.
- One message from a specific `src` to a specific `dst` cannot overtake a previous message from the same `src` to the same `dst`.
- There are no guarantees on the order from different `src`'s.
- The order from different `src`'s could be implied in the `tag`.
- `status` is type `MPI_Status` – the "]status" can be replaced with `MPI_STATUS_IGNORE`.

Example

```c
int numCPUs;
int me;
#define MYDATA_SIZE 128
char mydata[ MYDATA_SIZE ];
#define BOSS 0
MPI_Comm_size( MPI_COMM_WORLD, &numCPUs );
MPI_Comm_rank( MPI_COMM_WORLD, &me );
if( me == BOSS ) // the primary
{
    for( int dst = 0; dst < numCPUs; dst++ )
    {
        if( dst != BOSS )
        {
            char *InputData = "Hello, Beavers!";
            MPI_Send( InputData, strlen(InputData)+1, MPI_CHAR, dst, 'B', MPI_COMM_WORLD );
        }
    }
}
else // a secondary
{
    MPI_Recv( myData, MYDATA_SIZE, MPI_CHAR, BOSS, 'B', MPI_COMM_WORLD, MPI_STATUS_IGNORE );
    printf( " '%s' from rank # %d
", in, me );
}
```

You are highly discouraged from sending to yourself. Because both the send and receive are capable of blocking, the result could be deadlock.
How does MPI let the Sender perform an MPI_Send( ) even if the Receivers are not ready to MPI_Rcv( )?

**MPI_Send( )** blocks until the transfer is far enough along that the array can be destroyed or re-used.
Another Example

You typically don't send the entire workload to each dst – you just send part of it, like this:

```c
#define NUMELEMENTS ???
int numCPUs;
int me;
#define BOSS 0
MPI_Comm_size( MPI_COMM_WORLD, &numCPUs );
MPI_Comm_rank( MPI_COMM_WORLD, &me );
int localSize = NUMELEMENTS / numCPUs; // assuming it comes out evenly
float *myData = new float [ localSize ];

if( me == BOSS ) // the sender
{
    float *InputData = new float [ NUMELEMENTS ];
    << read the full input data into InputData from disk >>
    for( int dst = 0; dst < numCPUs; dst++ )
    {
        if( dst != BOSS )
        {
            MPI_Send( &InputData[dst*localSize], localSize, MPI_FLOAT, dst, 0, MPI_COMM_WORLD );
        }
    }
}
else // a receiver
{
    MPI_Recv( myData, localSize, MPI_FLOAT, BOSS, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE );
    // do something with this subset of the data
}
```
In Distributed Computing, You Often Hear About These Design Patterns

- **Broadcast**
- **Scatter**
- **Gather**

Scatter and Gather Usually Go Together

Note surprisingly, this is referred to as Scatter/Gather
MPI Scatter

Take a data array, break it into ~equal portions, and send it to each CPU

MPI_Scatter( snd_array, snd_count, snd_type, rcv_array, rcv_count, rcv_type, src, MPI_COMM_WORLD );

Both the sender and receivers need to execute MPI_Scatter.
There is no separate receive function

MPI Gather

MPI_Gather( snd_array, snd_count, snd_type, rcv_array, rcv_count, rcv_type, dst, MPI_COMM_WORLD );

Both the sender and receivers need to execute MPI_Gather.
There is no separate receive function
Remember This? It’s Baaaaaack as a complete Scatter/Gather Example

The Compute : Communicate Ratio still applies, except that it is even more important now because there is much more overhead in the Communicate portion.

This pattern of breaking a big problem up into pieces, sending them to different CPUs, computing on the pieces, and getting the results back is very common. That’s why MPI has its own scatter and gather functions.

heat.cpp, I

#include <stdio.h>
#include <math.h>
#include <mpi.h>

const float RHO = 8050.;
const float C   = 0.466;
const float K   = 20.;
float k_over_rho_c = K / (RHO*C); // units of m^2/sec  
// K / (RHO*C) = 5.33x10^-6 m^2/sec

const float DX    = 1.0;
const float DT    = 1.0;

#define BOSS 0
#define NUMELEMENTS (8*1024*1024)
#define NUM_TIME_STEPS 4
#define DEBUG false

float * NextTemps; // per-processor array to hold computer next-values
int NumCpus; // total # of cpus involved
int PPSize; // per-processor local array size
float * PPTemps; // per-processor local array temperature data
float * TempData; // the overall NUMELEMENTS-big temperature data

void DoOneTimeStep( int );
# Heat Simulation with MPI

```c
int main( int argc, char *argv[] )
{
    MPI_Init( &argc, &argv );
    int me; // which one I am
    MPI_Comm_size( MPI_COMM_WORLD, &NumCpus );
    MPI_Comm_rank( MPI_COMM_WORLD, &me );

    // decide how much data to send to each processor:
    PPSize = NUMELEMENTS / NumCpus; // assuming it comes out evenly
    PPTemps = new float [PPSize];   // all processors now have this uninitialized Local array
    NextTemps = new float [PPSize]; // all processors now have this uninitialized local array too

    // broadcast the constant:
    MPI_Bcast( (void *)&k_over_rho_c, 1, MPI_FLOAT, BOSS, MPI_COMM_WORLD );

    if( me == BOSS ) // this is the data-creator
    {
        TempData = new float [NUMELEMENTS];
        for( int i = 0; i < NUMELEMENTS; i++ )
            TempData[i] = 0.;
        TempData[NUMELEMENTS/2] = 100.;

        MPI_Scatter( TempData, PPSize, MPI_FLOAT, PPTemps, PPSize, MPI_FLOAT, BOSS, MPI_COMM_WORLD );
    }
```
// all the PPTemps arrays have now been filled
// do the time steps:

double time0 = MPI_Wtime();

for( int steps = 0; steps < NUM_TIME_STEPS; steps++ )
{
    // do the computation for one time step:
    DoOneTimeStep( me );

    // ask for all the data:
    #ifdef WANT_EACH_TIME_STEPS_DATA
        MPI_Gather( PPTemps, PPSize, MPI_FLOAT, TempData, PPSize, MPI_FLOAT, BOSS, MPI_COMM_WORLD );
    #endif

    #ifndef WANT_EACH_TIME_STEPS_DATA
        MPI_Gather( PPTemps, PPSize, MPI_FLOAT, TempData, PPSize, MPI_FLOAT, BOSS, MPI_COMM_WORLD );
    #endif

    double time1 = MPI_Wtime();
}

if( me == BOSS )
{
    double seconds = time1 - time0;
    double performance =
        (double)NUM_TIME_STEPS * (double)NUMELEMENTS / seconds / 1000000.;
    // mega-elements computed per second
    fprintf( stderr, "%3d, %10d, %8.2lf
", NumCpus, NUMELEMENTS, performance );
}

MPI_Finalize( );
return 0;

void DoOneTimeStep( int me )
{

// send out the left and right end values:
// (the tag is from the point of view of the sender)
if( me != 0 ) // i.e., if i'm not the first group on the left
{

    // send my PPTemps[0] to me-1 using tag 'L'
    MPI_Send( &PPTemps[0], 1, MPI_FLOAT, me-1, 'L', MPI_COMM_WORLD );
    if( DEBUG ) fprintf( stderr, "%3d sent 'L' to %3d\n", me, me-1 );
}

if( me != NumCpus-1 ) // i.e., not the last group on the right
{

    // send my PPTemps[PPSize-1] to me+1 using tag 'R'
    MPI_Send( &PPTemps[PPSize-1], 1, MPI_FLOAT, me+1, 'R', MPI_COMM_WORLD );
    if( DEBUG ) fprintf( stderr, "%3d sent 'R' to %3d\n", me, me+1 );
}

}

float left = 0.;
float right = 0.;
if( me != 0 ) // i.e., if i'm not the first group on the left
{

    // receive my "left" from me-1 using tag 'R'
    MPI_Recv( &left, 1, MPI_FLOAT, me-1, 'R', MPI_COMM_WORLD, &status );
    if( DEBUG ) fprintf( stderr, "%3d received 'R' from %3d\n", me, me-1 );
}

if( me != NumCpus-1 ) // i.e., not the last group on the right
{

    // receive my "right" from me+1 using tag 'L'
    MPI_Recv( &right, 1, MPI_FLOAT, me+1, 'L', MPI_COMM_WORLD, &status );
    if( DEBUG ) fprintf( stderr, "%3d received 'L' from %3d\n", me, me+1 );
}
**Sharing Values Across the Boundaries**

1 sent 'L' to 0
1 sent 'R' to 2
2 sent 'L' to 1
2 sent 'R' to 3
2 received 'R' from 1
0 sent 'R' to 1
0 received 'L' from 1
1 received 'R' from 0
1 received 'L' from 2
3 sent 'L' to 2
3 received 'R' from 2
2 received 'L' from 3

---

**1D Compute-to-Communicate Ratio**

Intraprocessor computing

Interprocessor communication

Compute : Communicate ratio = N : 2

where N is the number of compute cells per processor

In the above drawing, Compute : Communicate is 4 : 2
DoOneTimeStep, III

// first element on the left (0):
{
    float dtemp = ( k_over_rho_c *
    ( left - 2.*PPTemps[0] +  PPTemps[1] ) / ( DX*DX ) ) * DT;
    NextTemps[0] = PPTemps[0] + dtemp;
}

// all the nodes in the middle:
for( int i = 1; i < PPSize-1; i++ )
{
    float dtemp = ( k_over_rho_c *
    ( PPTemps[i-1] - 2.*PPTemps[i] + PPTemps[i+1] ) / ( DX*DX ) ) * DT;
    NextTemps[i] = PPTemps[i] + dtemp;
}

// last element on the right (PPSize-1):
{
    float dtemp = ( k_over_rho_c *
    ( PPTemps[PPSize-2] - 2.*PPTemps[PPSize-1] + right ) / ( DX*DX ) ) * DT;
    NextTemps[PPSize-1] = PPTemps[PPSize-1] + dtemp;
}

DoOneTimeStep, IV

// update the local dataset:
for( int i = 0; i < PPSize; i++ )
{
    PPTemps[ i ] = NextTemps[ i ];
}
### MPI Performance

#### Mega-Elements Computed Per Second vs. Number of Processors

- **Number of Processors**
- **Number of Elements**

![Graph showing the relationship between Mega-Elements Computed Per Second and Number of Processors.]

- 1024
- 8192
- 65536
- 524288
- 4194304
- 16777216
- 33554432

### MPI Reduction

**MPI_Reduce** function:

```c
MPI_Reduce( partialResult, globalResult, count, type, operator, dst, MPI_COMM_WORLD);
```

- **Where the partial result is stored on each CPU**
- **Place to store the full result on the dst CPU**
- **Who is given the final answer**

- **This really should be called Scatter/Gather/Reduction**

- **Both the sender and receivers need to execute MPI_Reduce.**

- **There is no separate receive function**
MPI Reduction Example

// gratuitous use of a reduce -- average all the temperatures:

float partialSum = 0.;
for (int i = 0; i < PPSize; i++)
    partialSum += PPTemps[i];

float globalSum = 0.;
MPI_Reduce( &partialSum, &globalSum, 1, MPI_FLOAT, MPI_SUM, BOSS, MPI_COMM_WORLD );

if ( me == BOSS )
    fprintf( stderr, "Average temperature = %f\n", globalSum/(float)NUMELEMENTS );

MPI Barriers

MPI_Barrier( MPI_COMM_WORLD );

All CPUs must execute the call to MPI_Barrier( ) before any of the CPUs can move past it. That is, each CPU's MPI_Barrier( ) blocks until all CPUs execute a call to MPI_Barrier( ).
**MPI Derived Types**

Idea: In addition to types MPI_INT, MPI_FLOAT, etc., allow the creation of new MPI types so that you can transmit an “array of structures”.

Reason: There is significant overhead with each transmission. Better to send one entire array of structures instead of sending several arrays separately.

```c
MPI_Type_create_struct(count, blocklengths, displacements, types, datatype);
```

```c
struct point {
    int pointSize;
    float x, y, z;
};
```

```c
MPI_Datatype MPI_POINT;
int blocklengths[ ] = {1, 1, 1, 1};
int displacements[ ] = {0, 4, 8, 12};
MPI_type types[ ] = {MPI_INT, MPI_FLOAT, MPI_FLOAT, MPI_FLOAT};
MPI_Type_create_struct(4, blocklengths, displacements, types, &MPI_POINT);
```

You can now use MPI_POINT everywhere you could have used MPI_INT, MPI_FLOAT, etc.

---

**MPI Timing**

```c
double MPI_Wtick();
```

Returns the resolution of the clock, in seconds.

```c
double MPI_Wtime();
```

Returns the time, in seconds, since “some time in the past”.

**Warning:** the clocks on the different CPUs are not guaranteed to be synchronized!
Autocorrelation – a Piece of the Original Signal

The Original Signal

Autocorrelation – More than Just a Scatter

NUMELEMENTS

Divide NUMELEMENTS into pieces for the NumCpus (this is what MPI_Scatter does)

But, in the Autocorrelation case, we need MAXSHIFTS more data values for each CPU
Autocorrelation – How the Shifting Works

Shift = 0

Shift = 1

Shift = 2

Shift = 3

Shift = MAXSHIFTS - 1