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

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



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Mike Bailey

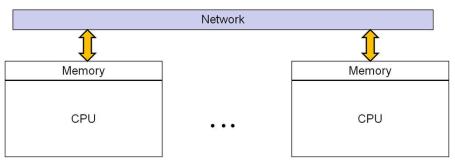
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Why Two URLs?



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/



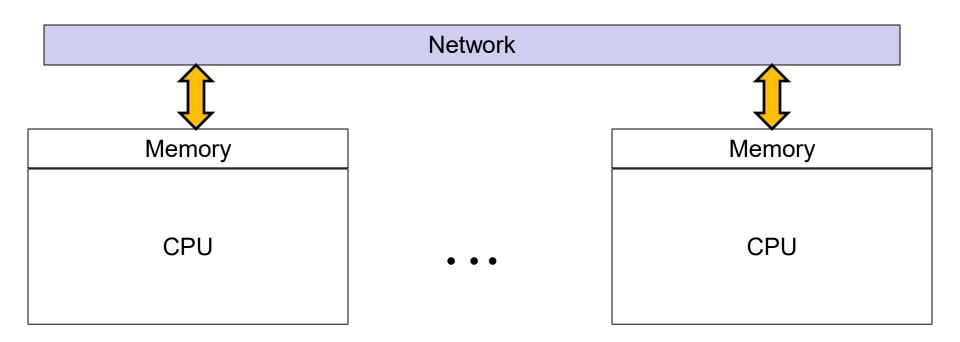
This URL is also really good – it is a link to all of the MPI man pages

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The Open MPI Consortium



MPI: The Basic Idea



Programs on different CPUs coordinate computations by passing messages between each other

Note: Each CPU in the MPI "cluster" must be prepared ahead of time by having the MPI server code installed on it. It must then have that server code running and listening on its socket connection.

Each MPI CPU must also have an integer ID assigned to it (called its **rank**).

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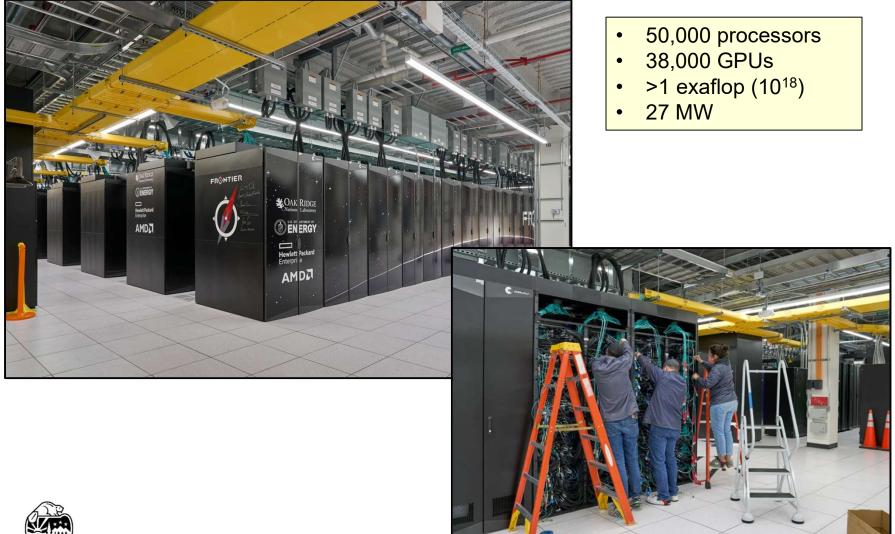
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This is how modern supercomputers work!



The Texas Advanced Computing Center's Frontera supercomputer University Computer Graphics

This is how modern supercomputers work!

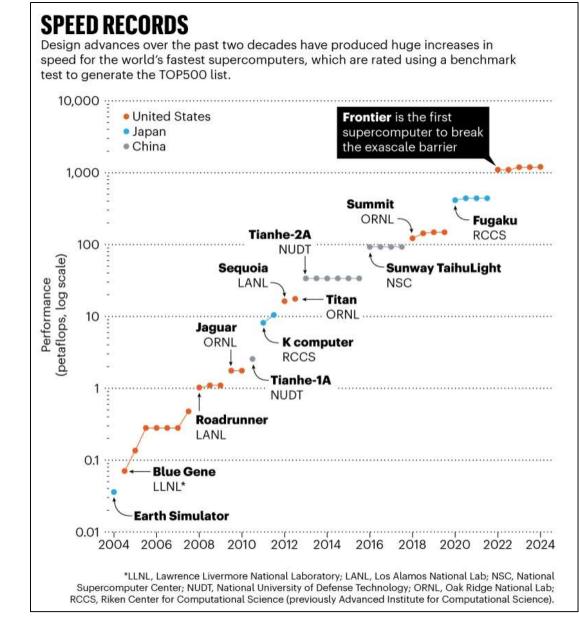




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The Oakridge National Lab Frontier supercomputer

This paradigm is how modern supercomputers work!





How to SSH to the COE MPI Cluster

ssh over to an MPI submission machine -submit-a and submit-b will also work

flip3 151% ssh submit-c.hpc.engr.oregonstate.edu

submit-c 142% module load slurm
submit-c 143% module load openmpi

Type these right away to set your path correctly

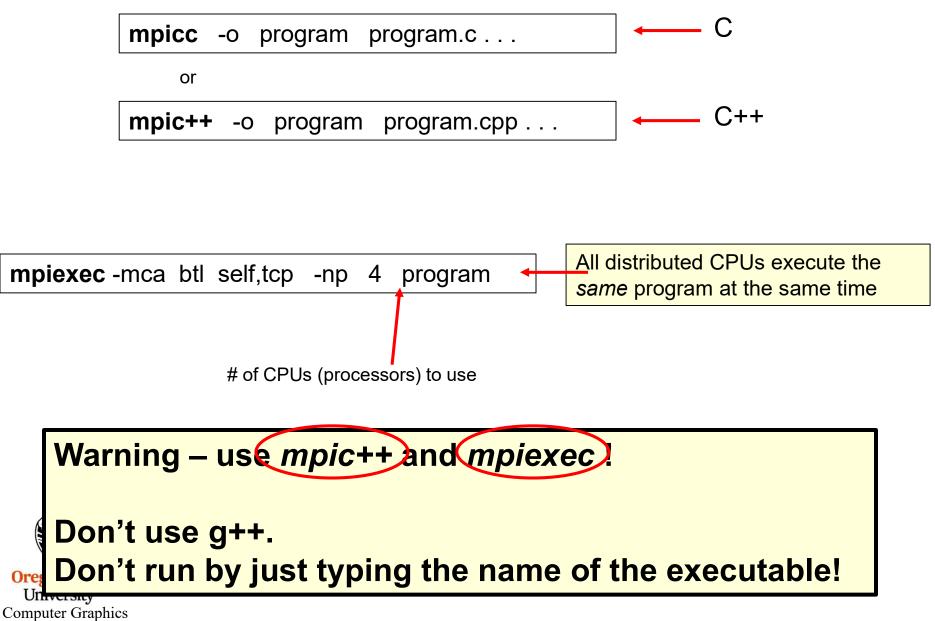
BTW, you can find out more about the COE cluster here: <u>https://it.engineering.oregonstate.edu/hpc</u>

The College of Engineering HPC cluster is a heterogeneous mix of over 130 servers providing 4,800 CPU cores, over 230 GPUs, and over 50 TB of total RAM. The systems are connected via gigabit ethernet and Infiniband. Most of the latest servers utilize Mellanox EDR or HDR InfiniBand network connection. The cluster also has access to 500TB global scratch space. The CoE HPC Cluster is rated at over 2,200 peak TFLOPS (double-precision).

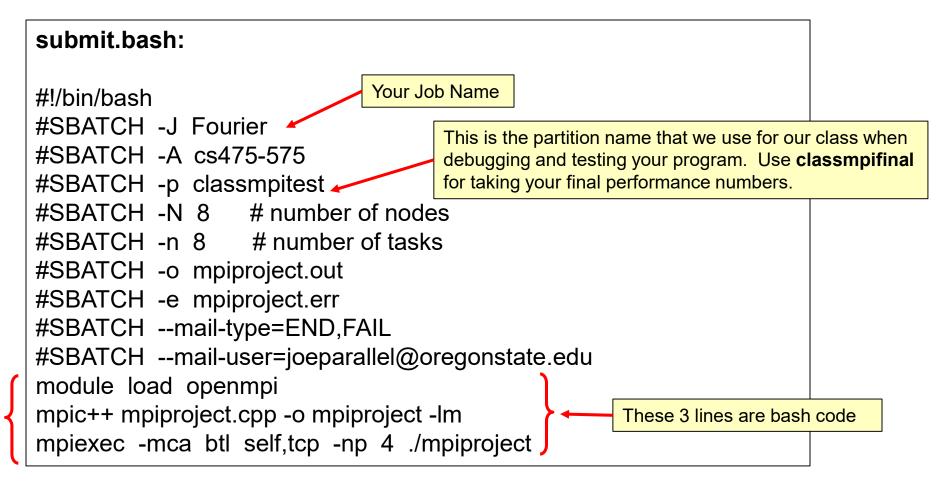
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Compiling and Running



Running with a bash Batch Script





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

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What is the Difference Between the Partitions classmpitest and classmpifinal?

classmpitest lets your program get into the system sooner, but it might be running alongside other jobs, so its performance might suffer. But, you don't care because you are just compiling and debugging, not taking performance numbers for your report.

classmpifinal makes your program wait in line until it can get dedicated resources so that you get performance results that are much more representative of what the machines can do, and thus are worthy to be listed in your report.



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

You don't have to ask the system to email information to you, but if you do, please be sure you spell your own email address correctly!

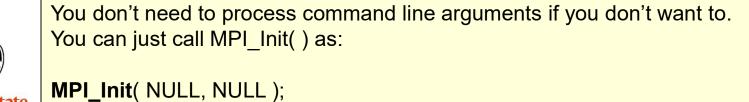
Our IT people are getting *really* tired of fielding the bounced emails when people misspell their own email address.



submit-c 143% sbatch submit.bash Submitted batch job 258759 submit-c 144% scance 258759



Setting Up and Finishing MPI



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mjb - March 26, 2025

MPI Follows a Single-Program-Multiple-Data (SPMD) Model

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

Oh, look, a communicator of Corvallis deer!

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Oh, look, a communicator of Corvallis turkeys!



This requires MPI server code getting installed on all those CPUs. That code then needs to be running and listening on a socket connection. Only an administrator can do this.

Getting information about our place in the communicator:

 int numCPUs;
 // total # of cpus involved
 Or

 int me;
 // which one I am
 Ca

 MPI_Comm_size(MPI_COMM_WORLD, &numCPUs);
 MPI_Comm_rank(MPI_COMM_WORLD, &me);
 Size, i.e.,

 It is then each CPU's job to figure out
 It is then each CPU's job to figure out
 Size, i.e.,

what piece of the overall problem it is

responsible for and then go do it.

Size, i.e., how many altogether?

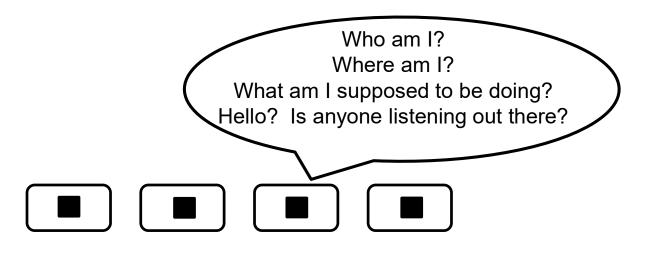
Rank, i.e., which one am I?

A First Test of MPI

```
#include <stdio.h>
#include <math.h>
#include <mpi.h>
#define THEBOSS 0
int
main( int argc, char *argv[ ] )
{
    MPI_Init( &argc, &argv );
    int numCPUs; // total # of cpus involved
                       // which one I am
    int me;
    MPI_Comm_size( MPI_COMM_WORLD, &numCPUs );
    MPI_Comm_rank( MPI_COMM_WORLD, &me );
    if( me == THEBOSS )
         fprintf( stderr, "Rank %d says that we have a Communicator of size %d\n", THEBOSS, numCPUs );
    else
         fprintf( stderr, "Welcome from Rank %d\n", me );
    MPI Finalize();
    return 0;
}
```

submit-c 165% mpiexec -np 16 ./first	submit-c 166% mpiexec -np 16 ./first
Welcome from Rank 13	Welcome from Rank 1
Welcome from Rank 15	Welcome from Rank 5
Welcome from Rank 3	Welcome from Rank 7
Welcome from Rank 7	Welcome from Rank 9
Welcome from Rank 5	Welcome from Rank 11
Welcome from Rank 8	Welcome from Rank 13
Welcome from Rank 9	Welcome from Rank 15
Welcome from Rank 11	Rank 0 says that we have a Communicator of size 16
Rank 0 says that we have a Communicator of size 16	Welcome from Rank 2
Welcome from Rank 1	Welcome from Rank 3
Welcome from Rank 12	Welcome from Rank 4
Welcome from Rank 14	Welcome from Rank 6
Welcome from Rank 6	Welcome from Rank 8
Welcome from Rank 2	Welcome from Rank 12
Welcome from Rank 10	Welcome from Rank 14
Welcome from Rank 4	Welcome from Rank 10
submit-c 167% mpiexec -np 16 ./first Welcome from Rank 9	submit-c 168% mpiexec -np 16 ./first Welcome from Rank 13
-	
Welcome from Rank 11	Welcome from Rank 15
Welcome from Rank 13	Welcome from Rank 7
Welcome from Rank 7 Welcome from Rank 1	Welcome from Rank 3 Welcome from Rank 5
Welcome from Rank 1 Welcome from Rank 3	Welcome from Rank 9
Welcome from Rank 3	Welcome from Rank 1
Welcome from Rank 15	Welcome from Rank 1
Welcome from Rank 4	Welcome from Rank 12
Welcome from Rank 5	Welcome from Rank 12
Rank 0 says that we have a Communicator of size 16	Welcome from Rank 4
Welcome from Rank 2	Welcome from Rank 2
	Rank 0 says that we have a Communicator of size 16
Welcome from Rank 6	
Welcome from Rank 6 Welcome from Rank 8	
	Welcome from Rank 8 Welcome from Rank 10

So, we have a group (a "communicator") of distributed CPUs. How do they communicate about what work they are supposed to do?

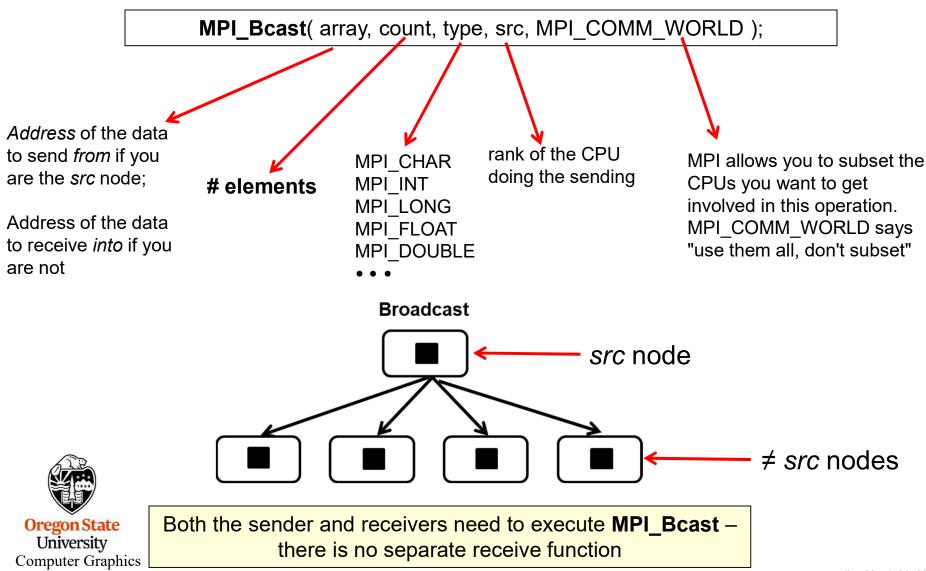


Example: You could coordinate the units of our DGX system using MPI

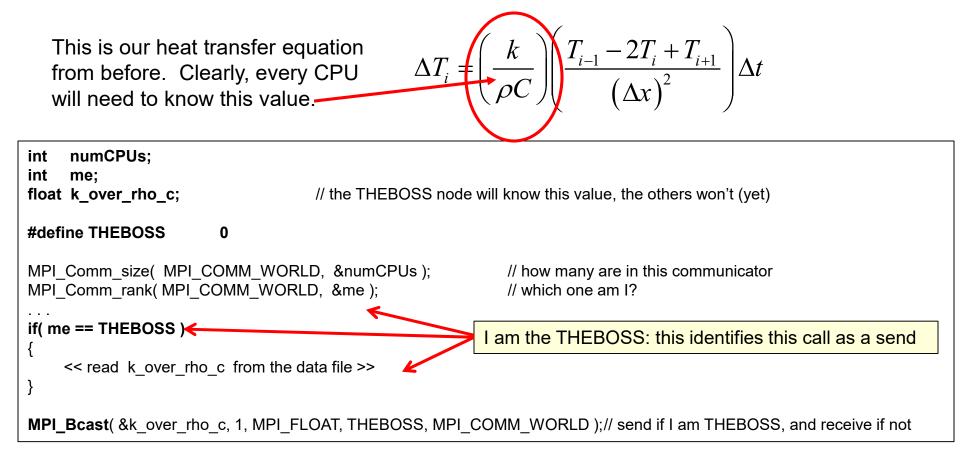


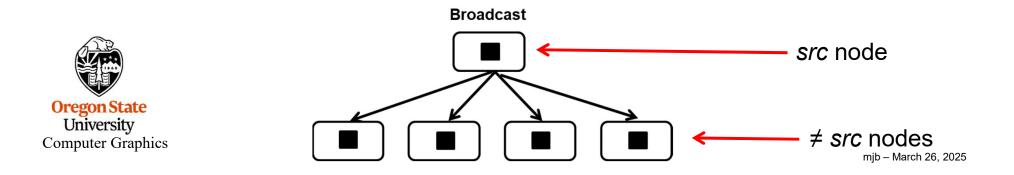


A Good Place to Start: MPI Broadcasting



MPI Broadcast Example





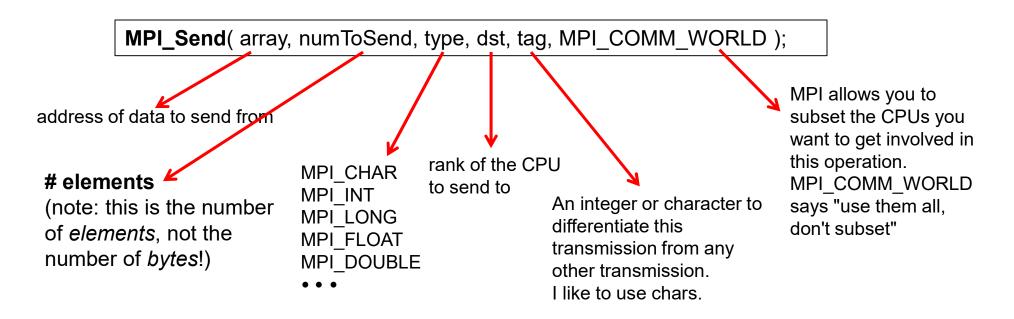
How Does this Work? Think Star Trek Wormholes!







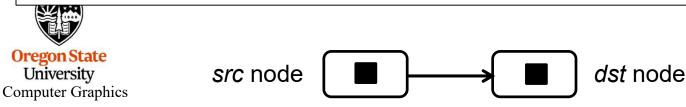
Sending Data from One Source CPU to Just One Destination CPU



Rules:

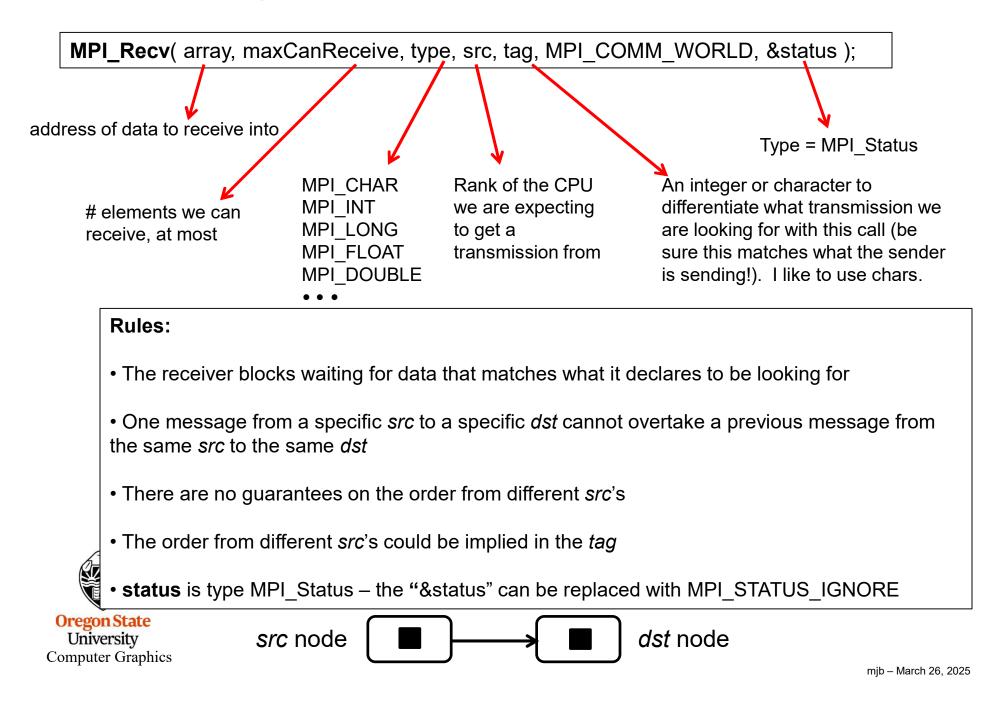
• One message from a specific *src* to a specific *dst* cannot overtake a previous message from the same *src* to the same *dst*.

- 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 .



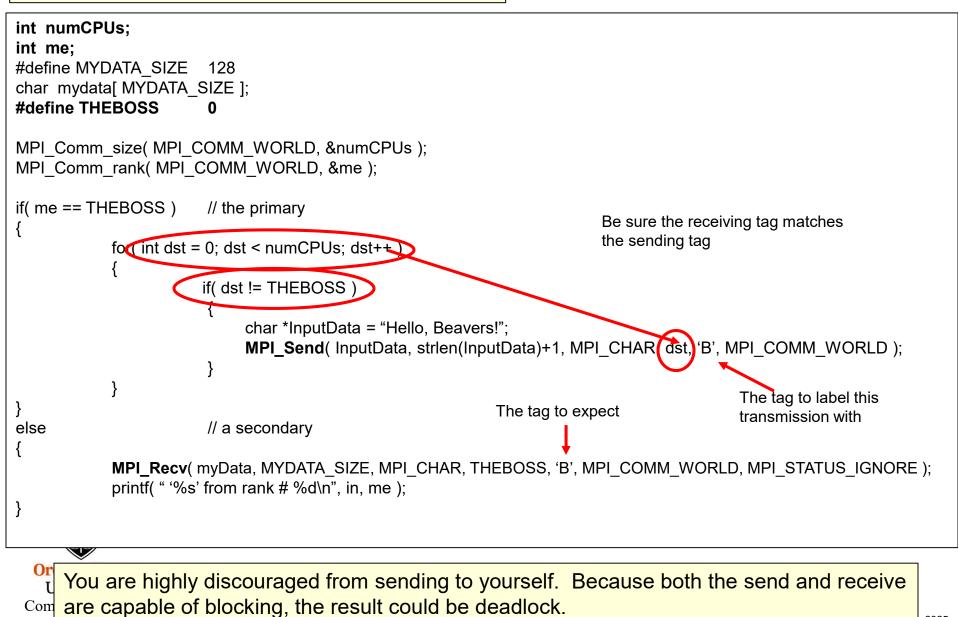
22

Receiving Data in a Destination CPU from a Source CPU

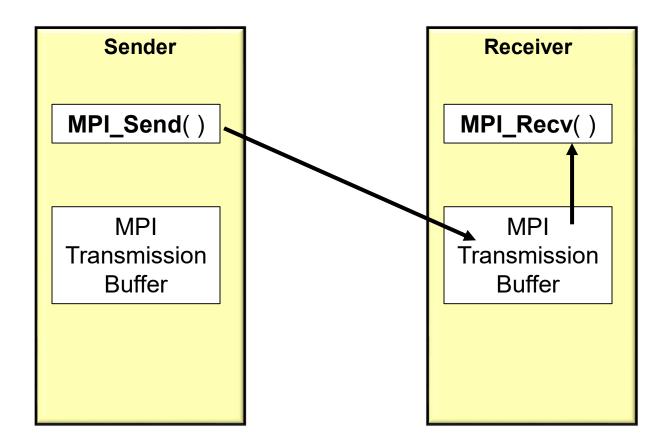


Example

Remember, this identical code runs on all CPUs:



How does MPI let the Sender perform an MPI_Send() even if the Receivers are not ready to MPI_Recv()?



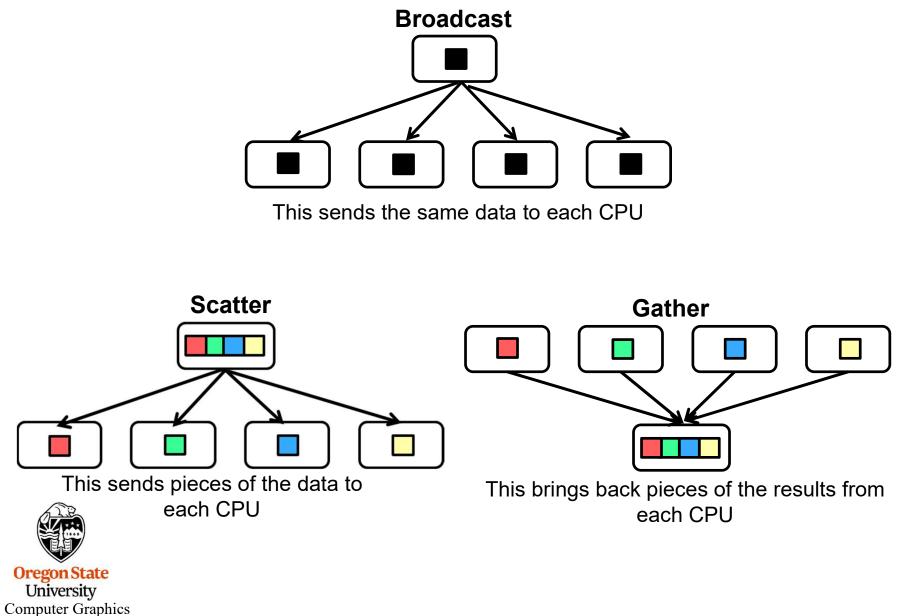
Oregon State University Computer Graphics **MPI_Send()** blocks until the transfer is far enough along that the *array* can be destroyed or re-used.

```
src node
```

Another Example

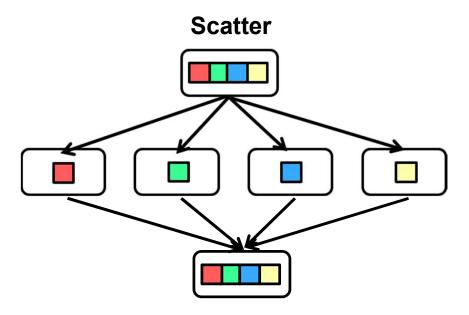
```
You typically don't send the entire workload to each dst – you just send part of it, like this:
#define NUMELEMENTS
                         ?????
int numCPUs:
int me;
#define THEBOSS
                      0
MPI Comm size( MPI COMM WORLD, &numCPUs );
MPI Comm rank( MPI COMM WORLD, &me );
int PPSize = NUMELEMENTS / numCPUs;
                                             // per-processor data size -- assuming it comes out evenly
float *myData = new float [ PPSize ];
if( me == THEBOSS )
                      // the sender
           float *InputData = new float [ NUMELEMENTS ];
           << read the full input data into InputData from disk >>
           for( int dst = 0; dst < numCPUs; dst++ )
           {
                                                     The address of node dst's share of the data to send
               if( dst != THEBOSS )
                {
                    MPI Send( &InputData[dst*PPSize], PPSize, MPI FLOAT, dst, 0, MPI COMM WORLD );
           }
}
                                      Each dst node will store its data in this array
                      // a receiver
else
ł
           MPI_Recv(myData, PPSize, MPI_FLOAT, THEBOSS, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
           // do something with this subset of the data
}
```

In Distributed Computing, You Often Hear About These Design Patterns²⁷



Scatter and Gather Usually Go Together

This sends pieces of the data to each CPU



Gather

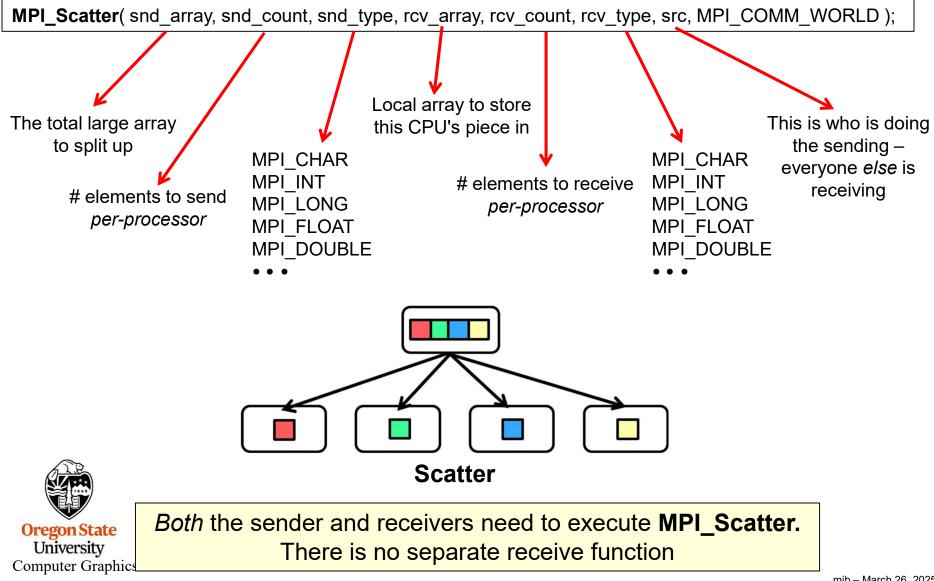
This brings back pieces of the results from each CPU



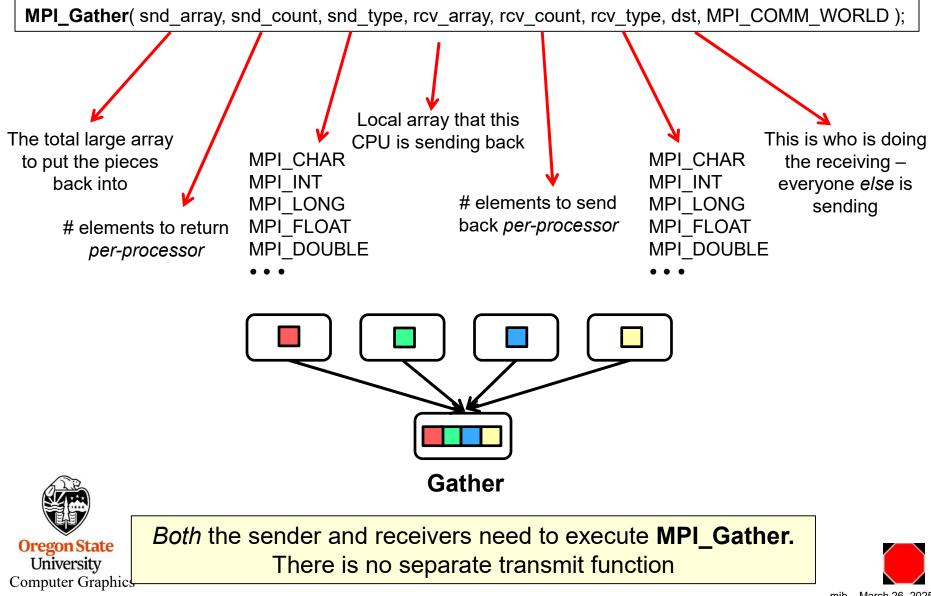
University Computer Graphics Note surprisingly, this is referred to by the combined term *Scatter/Gather*

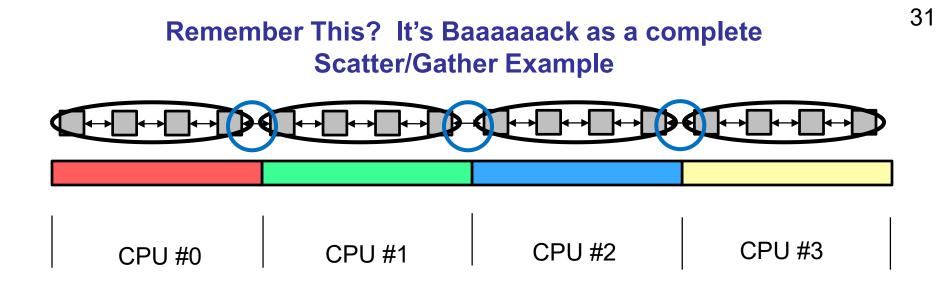
MPI Scatter

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



MPI Gather





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

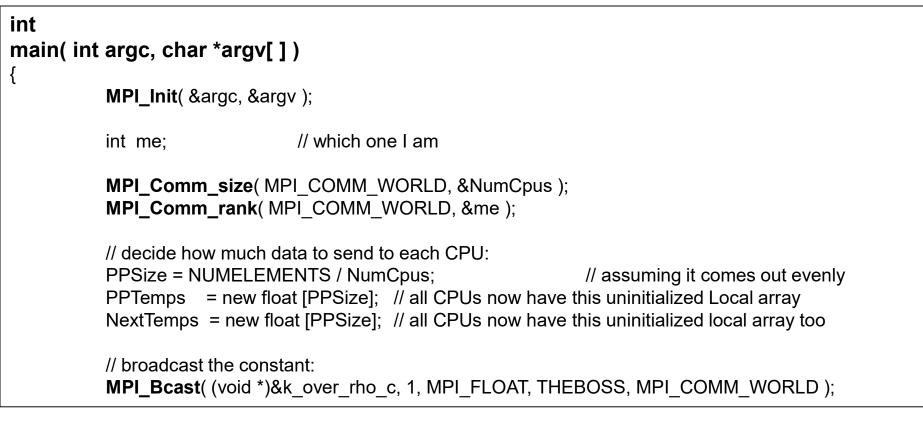
This pattern of breaking a big problem up into pieces, sending them to different CPUs, computing on the pieces, and getting the results back is *very* common. That's why MPI has its own scatter and gather functions.

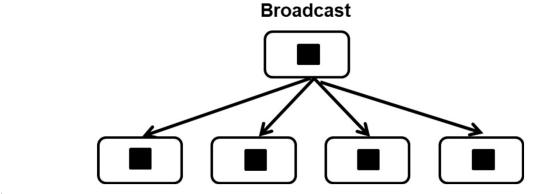


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heat.cpp, I

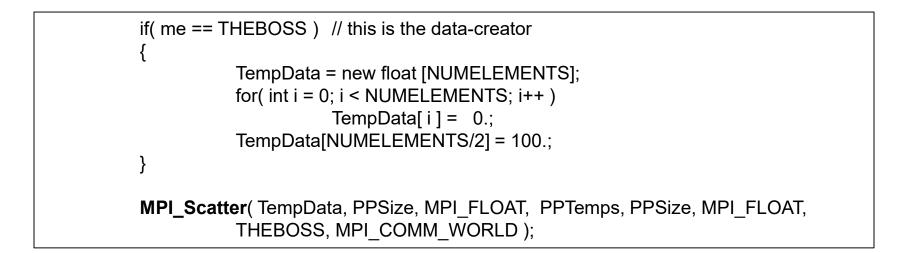
	#include < #include < #include <	math.h>		
const float RHO = 8050.; const float C = 0.466; const float K = 20.; float k_over_rho_c = K / (RHO*C); // K / (RHO*C) = 5.33x10^-6 m^2/sec				
		DX = 1.0; DT = 1.0;		
	#define Th	THEBOSS 0		
#define NUMELEMENTS #define NUM_TIME_STEPS #define DEBUG		UM_TIME_STEPS	(8*1024*1024) 4 false	
	float * int int float * float *	NextTemps; NumCpus; PPSize; PPTemps; TempData;	 // per-processor array to hold computer next-values // total # of cpus involved // per-processor local array size // per-processor local array temperature data // the overall NUMELEMENTS-big temperature data 	
(void	DoOneTimeStep(int);		

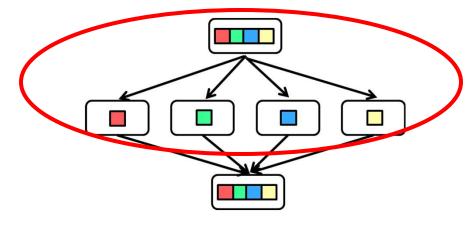




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heat.cpp, III



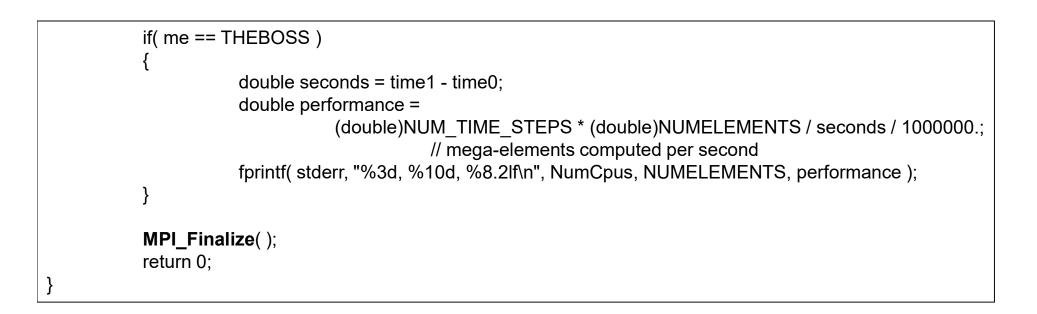




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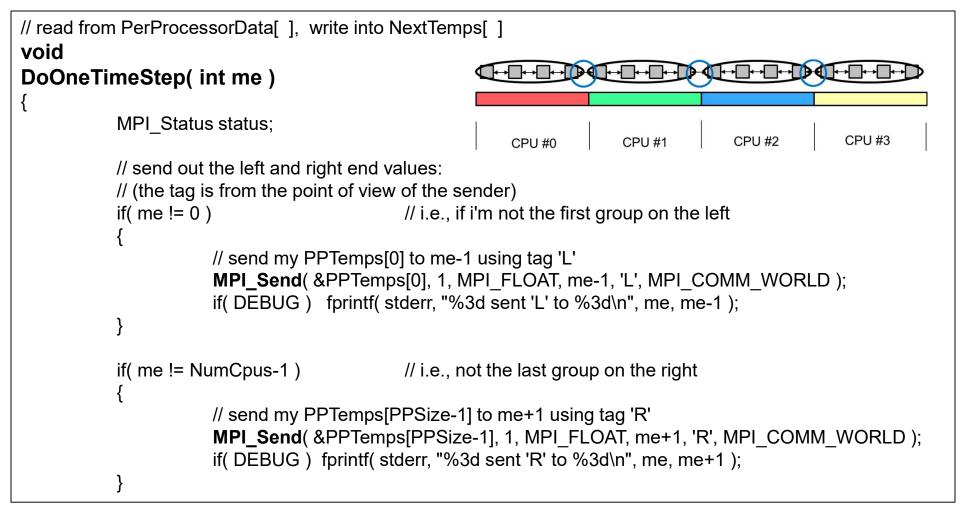
heat.cpp, IV

```
// 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 BACK
                      MPI_Gather( PPTemps, PPSize, MPI FLOAT, TempData, PPSize, MPI FLOAT,
                                 THEBOSS, MPI COMM WORLD );
#endif
           }
#ifndef WANT EACH TIME STEPS DATA BACK
           MPI Gather( PPTemps, PPSize, MPI FLOAT, TempData, PPSize, MPI FLOAT,
                      THEBOSS, MPI COMM WORLD );
#endif
           double time1 = MPI_Wtime( );
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                                                                                          mjb - March 26, 2025
```





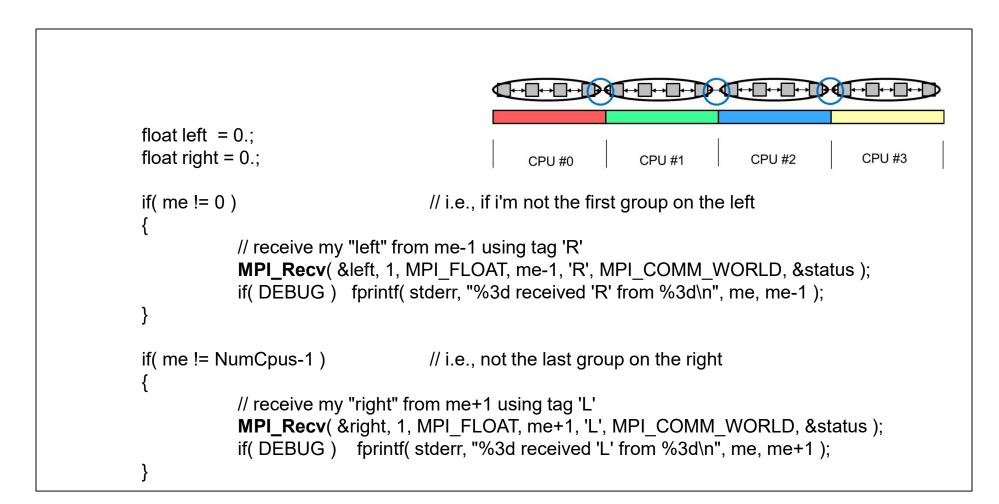
DoOneTimeStep, I



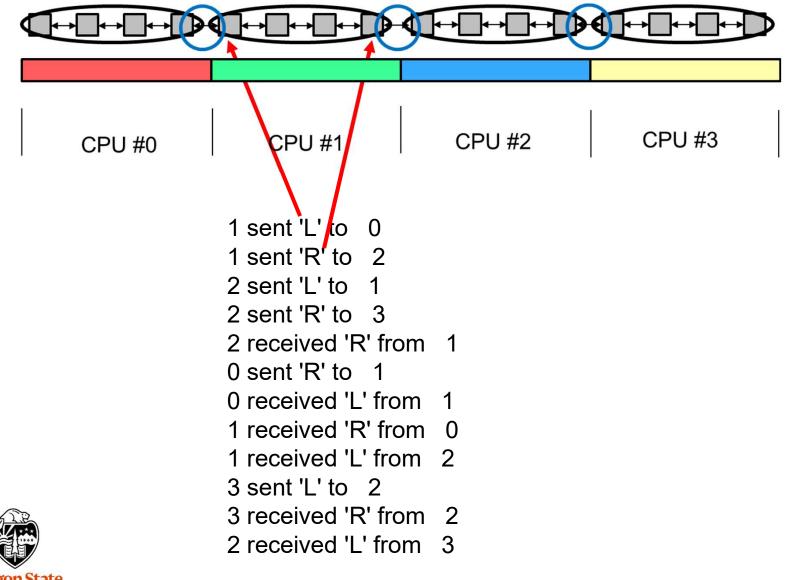


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DoOneTimeStep, II







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;
           }
     Oregon State
  University
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```

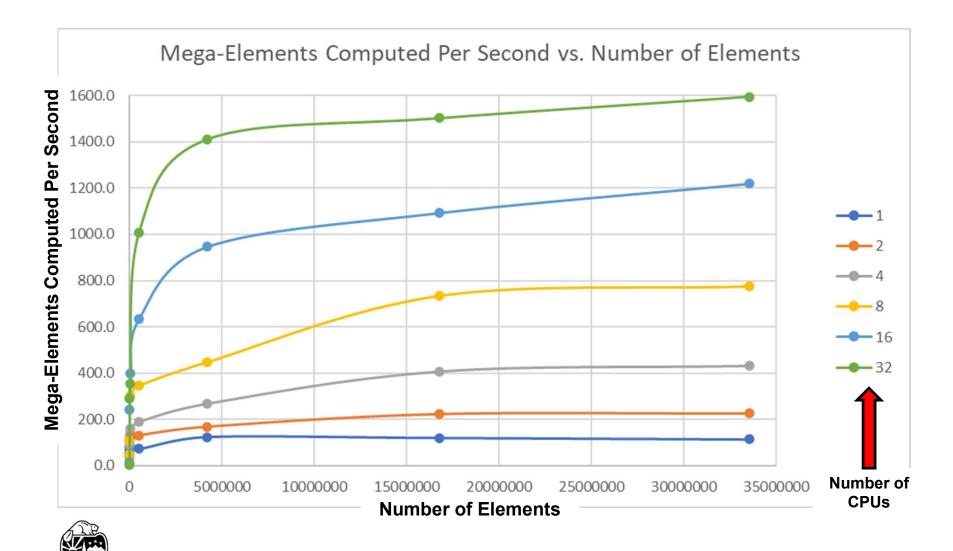
DoOneTimeStep, IV

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

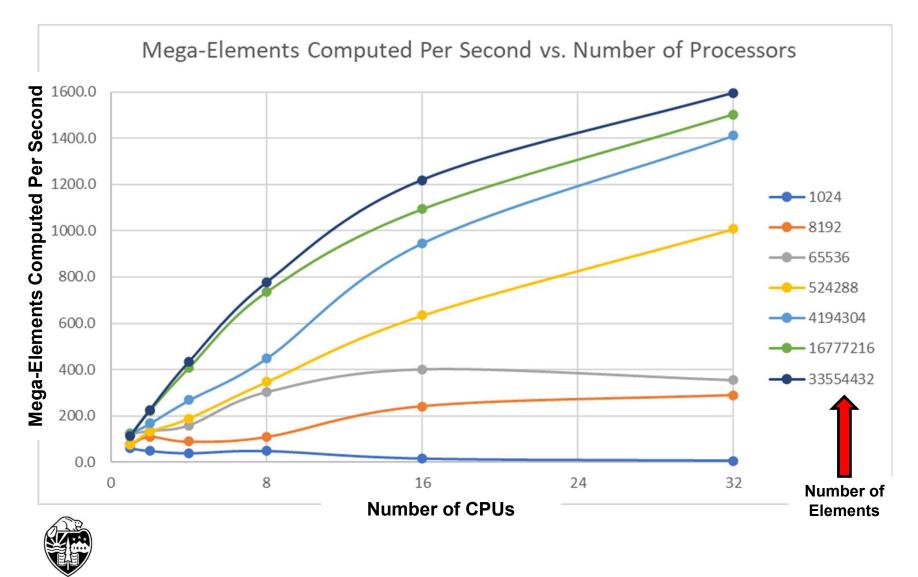


}

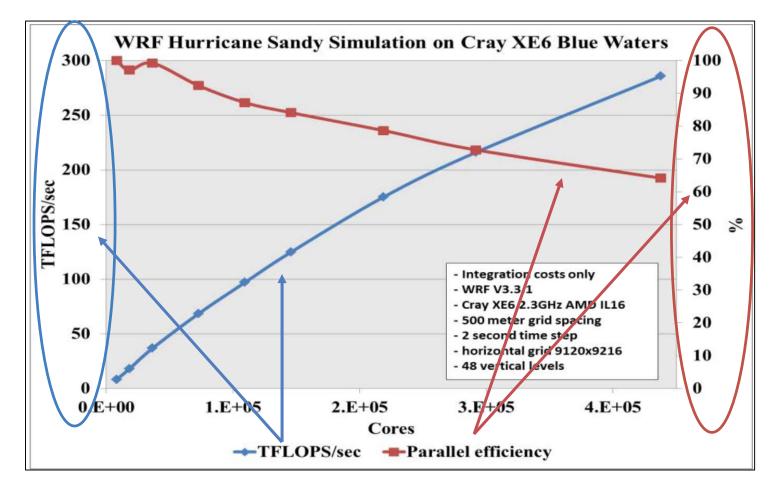
MPI Performance



MPI Performance



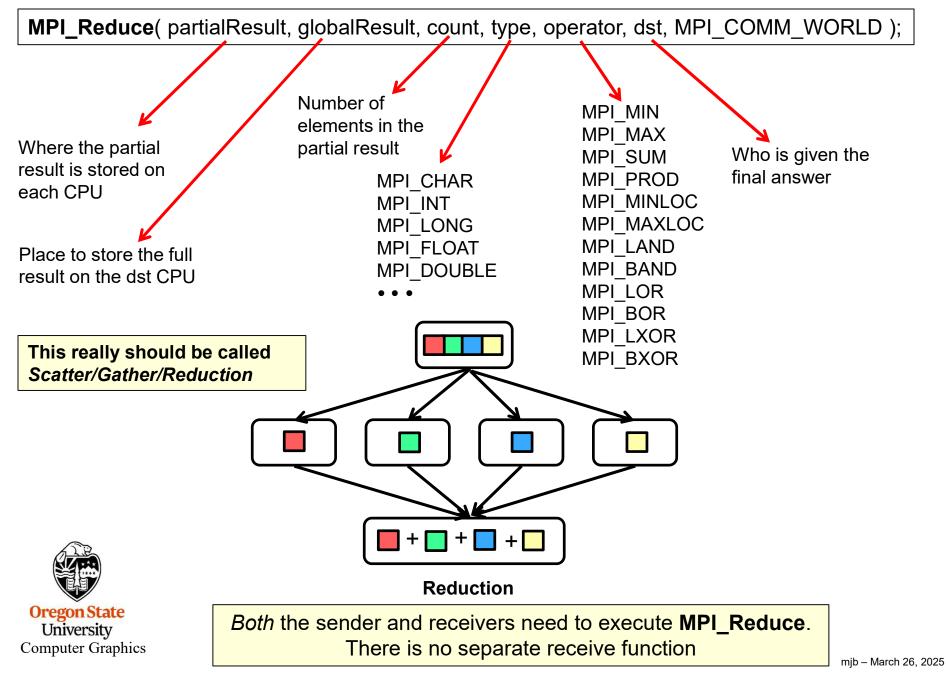
Using MPI and OpenMP on 13,680 nodes (437,760 cores) of the Cray XE6 at NCSA at the University of Illinois



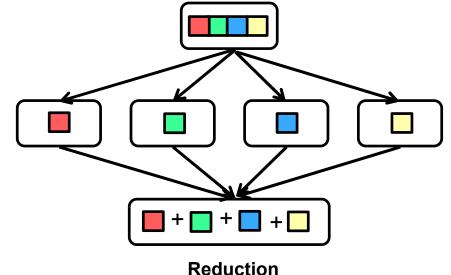
From: Peter Johnsen, Mark Straka, Melvyn Shapiro, Alan Norton, Thomas Galarneau, *Petascale WRF Simulation of Hurricane Sandy.*



MPI Reduction

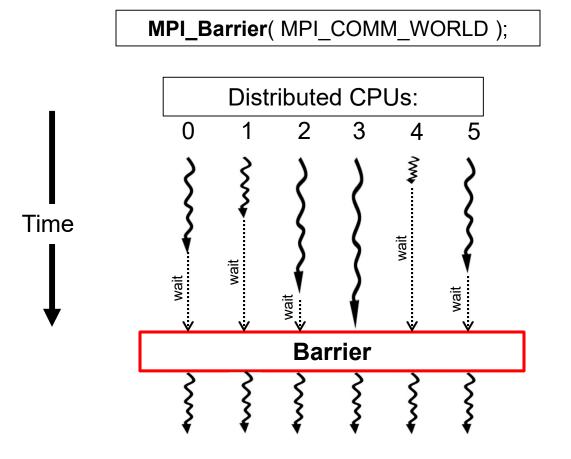


```
// gratuitous use of a reduce -- average all the temperatures:
    float partialSum = 0.;
    for( int i = 0; i < PPSize; i++ )
         partialSum += PPTemps[ i ];
    float globalSum = 0.;
    MPI_Reduce( &partialSum, &globalSum, 1, MPI_FLOAT, MPI_SUM, THEBOSS, MPI_COMM_WORLD );
     if( me == THEBOSS )
         fprintf( stderr, "Average temperature = %f\n", globalSum/(float)NUMELEMENTS );
```





MPI Barriers



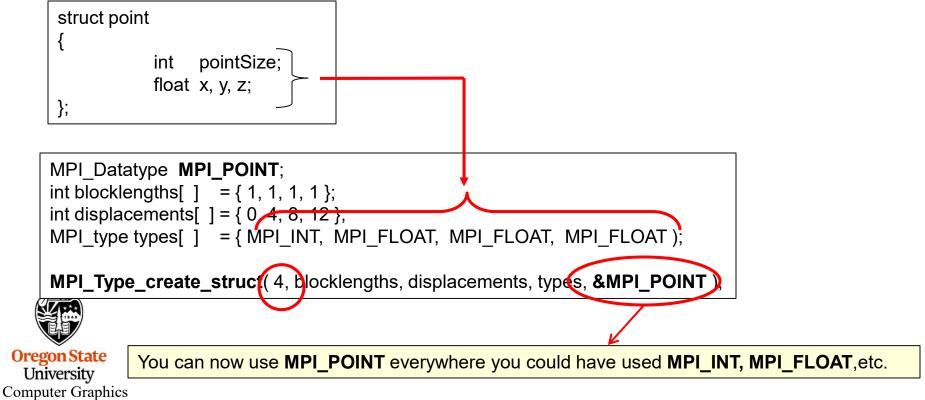
All CPUs must execute the call to MPI_Barrier() before any of the CPUs can move past it. That is, each CPU's MPI_Barrier() blocks until all CPUs execute a call to MPI_Barrier().

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.

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



MPI Timing

double MPI_Wtick();

Returns the resolution of the clock, in seconds.

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!

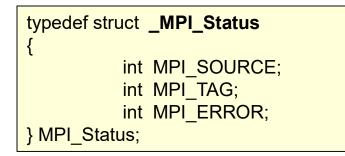


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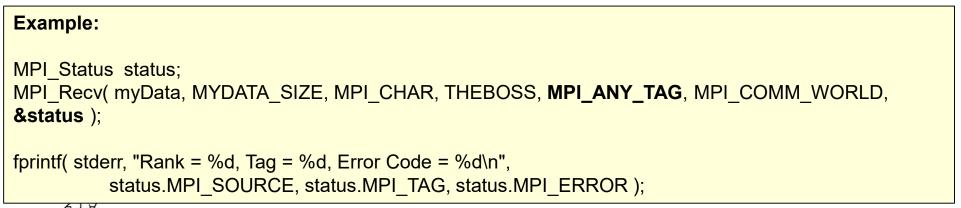
MPI Status-Checking

Some MPI calls have a **&status** in their argument list.

The **status** argument is declared to be of type **MPI_Status**, which is actually a struct:



- MPI_SOURCE is the rank of the node who sent this
- MPI_TAG is the tag used during the send
- MPI_ERROR is the error number that occurred





MPI Error Codes

MPI SUCCESS MPI ERR BUFFER MPI ERR COUNT MPI ERR TYPE MPI ERR TAG MPI ERR COMM MPI ERR RANK MPI ERR REQUEST MPI ERR ROOT MPI ERR GROUP MPI ERR OP MPI ERR TOPOLOGY MPI ERR DIMS MPI ERR ARG MPI ERR UNKNOWN MPI ERR TRUNCATE MPI_ERR_OTHER MPI ERR INTERN MPI ERR IN STATUS MPI ERR PENDING

No error Invalid buffer pointer Invalid count argument Invalid datatype argument Invalid tag argument Invalid communicator Invalid rank Invalid request (handle) Invalid root Invalid group Invalid operation Invalid topology Invalid dimension argument Invalid argument of some other kind Unknown error Message truncated on receive Known error not in this list Internal MPI (implementation) error Error code is in status Pending request

MPI ERR KEYVAL MPI ERR NO MEM MPI ERR BASE MPI ERR INFO KEY MPI_ERR_INFO_VALUE MPI ERR INFO NOKEY MPI ERR SPAWN MPI ERR PORT MPI ERR SERVICE MPI ERR NAME MPI ERR WIN MPI ERR SIZE MPI ERR DISP MPI ERR INFO MPI ERR_LOCKTYPE MPI ERR ASSERT MPI ERR RMA CONFLICT MPI ERR RMA SYNC

Invalid keyval has been passed MPI_ALLOC_MEM failed because memory is exhausted Invalid base passed to MPI_FREE_MEM Key longer than MPI_MAX_INFO_KEY Value longer than MPI_MAX_INFO_VAL Invalid key passed to MPI_INFO_DELETE Error in spawning processes Invalid port name passed to MPI_COMM_CONNECT Invalid service name passed to MPI_UNPUBLISH_NAME Invalid service name passed to MPI_LOOKUP_NAME Invalid win argument

Invalid size argument Invalid disp argument Invalid info argument Invalid locktype argument Invalid assert argument Conflicting accesses to window Wrong synchronization of RMA calls

MPI ERR FILE

MPI_ERR_NOT_SAME

MPI_ERR_AMODE MPI_ERR_UNSUPPORTED_DATAREP MPI_ERR_UNSUPPORTED_OPERATION MPI_ERR_NO_SUCH_FILE MPI_ERR_FILE_EXISTS MPI_ERR_BAD_FILE MPI_ERR_ACCESS MPI_ERR_NO_SPACE MPI_ERR_READ_ONLY MPI_ERR_FILE_IN_USE MPI_ERR_FILE_IN_USE MPI_ERR_DUP_DATAREP Oregon MPI_ERR_CONVERSION MPI_ERR_IO Computer MPI_ERR_LASTCODE

Invalid file handle Collective argument not identical on all processes, or collective routines called in a different order by different processes Error related to the amode passed to MPI FILE OPEN Unsupported datarep passed to MPI FILE SET VIEW Unsupported operation, such as seeking on a file which supports sequential access only File does not exist File exists Invalid file name (e.g., path name too long) Permission denied Not enough space Quota exceeded Read-only file or file system File operation could not be completed, as the file is currently open by some process Conversion functions could not be registered because a data representation identifier that was already defined was passed to MPI REGISTER DATAREP An error occurred in a user supplied data conversion function. Other I/O error Last error code



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