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

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



Oregon State University

Mike Bailey

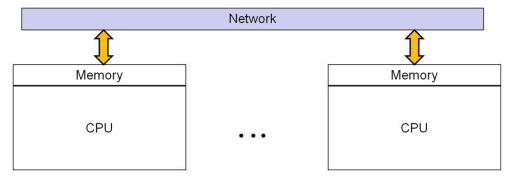
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Why Two URLs?



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/



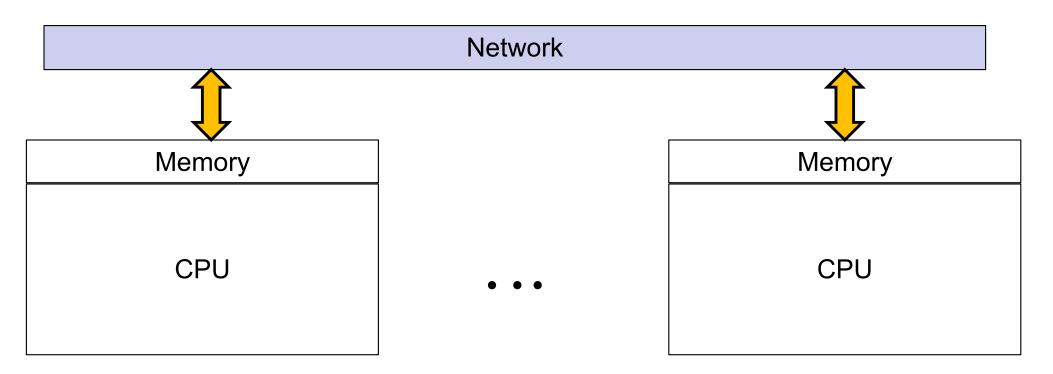
University Computer Graphics This URL is also really good – it is a link to all of the MPI man pages

The Open MPI Consortium





MPI: The Basic Idea



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

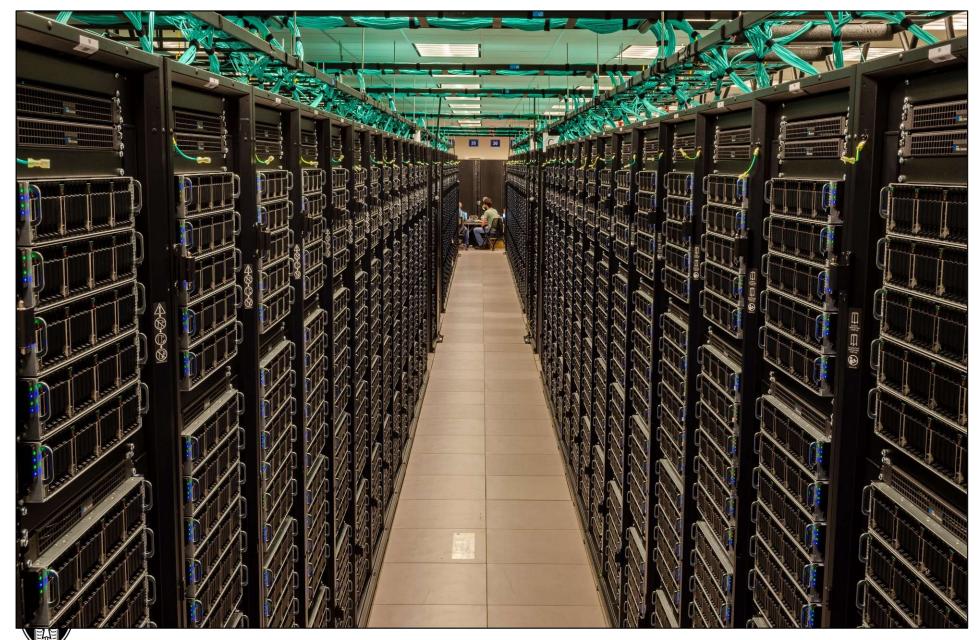
Note: Each CPU in the MPI "cluster" must be prepared ahead of time by having the MPI server code installed on it. It must then have that server code running and listening on its socket connection.

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

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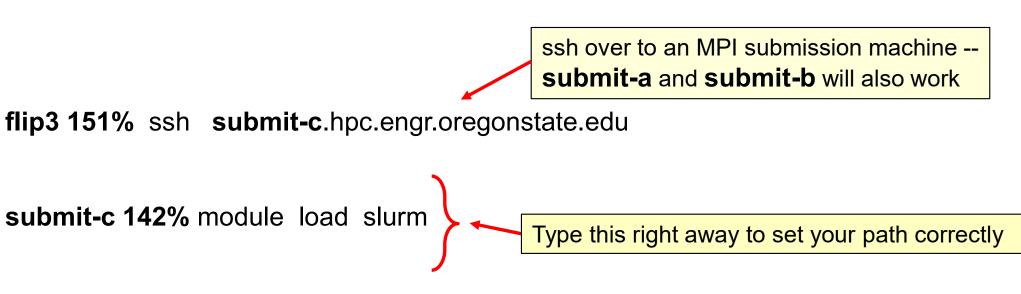
This paradigm is how modern supercomputers work!



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The Texas Advanced Computing Center's Frontera supercomputer

How to SSH to the COE MPI Cluster



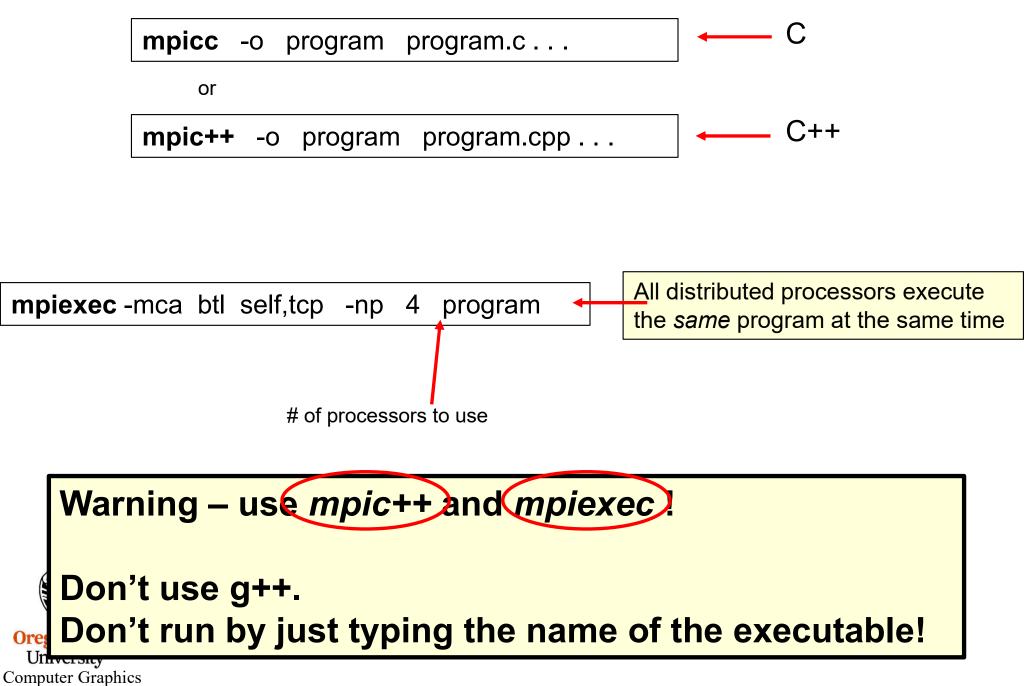
BTW, you can find out more about the COE cluster here: <u>https://it.engineering.oregonstate.edu/hpc</u>

"The College of Engineering HPC cluster is a heterogeneous mix of about 130 servers providing nearly 4000 CPU cores, over 200 GPUs, and over 43 TB 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 150TB global scratch from the College of Engineering's Dell/EMC Isilon enterprise storage. The CoE HPC Cluster is rated at over 1700 peak TFLOPS (double-precision)."

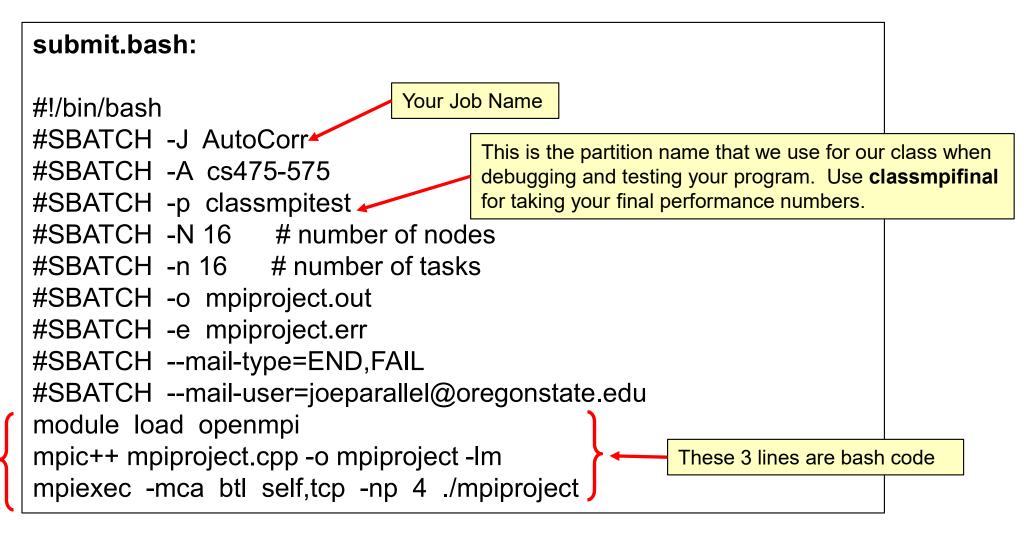
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Compiling and Running



Running with a bash Batch Script





University Computer Graphics **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.



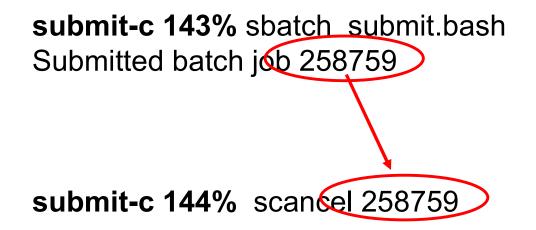
#SBATCH --mail-user=joeparallel@oregonstate.edu

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

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



Use slurm's scancel if your Job Needs to Be Killed





Setting Up and Finishing MPI

```
#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 want to. You can just call MPI_Init() as:

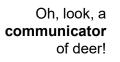


MPI_Init(NULL, NULL);

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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



int **me**;



Oh, look, a communicator of 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 // which one I am

MPI Comm size(MPI COMM WORLD, &numCPUs);

MPI_Comm_rank(MPI_COMM_WORLD, &me_);

Size, i.e., how many altogether?



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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.

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

A First Test of MPI

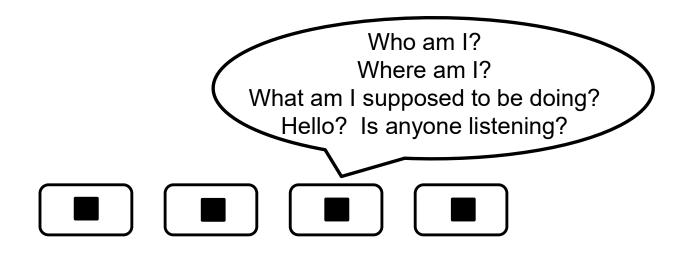
```
#include <stdio.h>
#include <math.h>
#include <mpi.h>
#define THEBOSS 0
int
main( int argc, char *argv[])
    MPI Init( & argc, & argv );
    int numCPUs; // total # of cpus involved
                       // which one I am
    int me;
    MPI Comm size(MPI COMM WORLD, &numCPUs);
    MPI Comm rank( 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	submit-c 168% mpiexec -np 16 ./first	
Welcome from Rank 9	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 3	
Welcome from Rank 1	Welcome from Rank 5	
Welcome from Rank 3	Welcome from Rank 9	
Welcome from Rank 10	Welcome from Rank 11	
Welcome from Rank 15	Welcome from Rank 1	
Welcome from Rank 4	Welcome from Rank 12	
Welcome from Rank 5	Welcome from Rank 14	
	Welcome from Rank 4	
Rank 0 says that we have a Communicator of size 16		
Welcome from Rank 2	Welcome from Rank 2	
Welcome from Rank 2 Welcome from Rank 6	Rank 0 says that we have a Communicator of size 16	
Welcome from Rank 2 Welcome from Rank 6 Welcome from Rank 8	Rank 0 says that we have a Communicator of size 16 Welcome from Rank 8	
Welcome from Rank 2 Welcome from Rank 6	Rank 0 says that we have a Communicator of size 16	

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

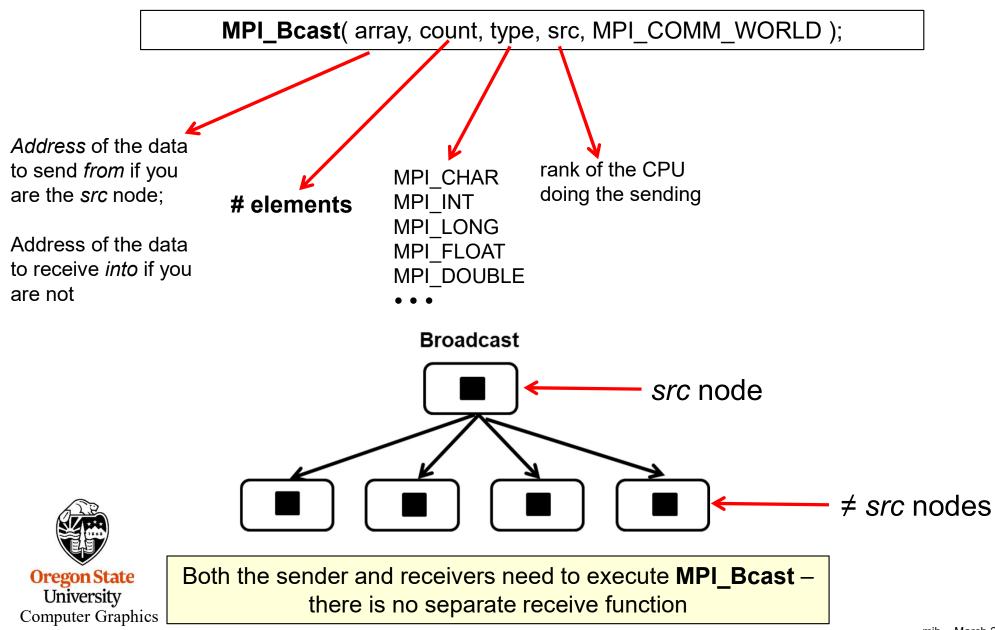


Example: You could coordinate the units of our DGX system using MPI



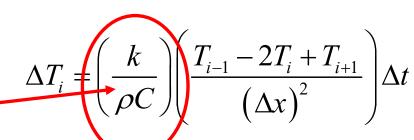


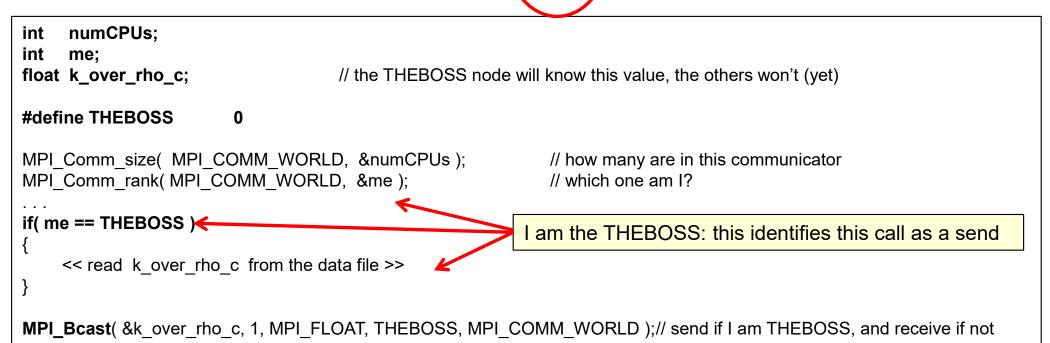
A Good Place to Start: MPI Broadcasting

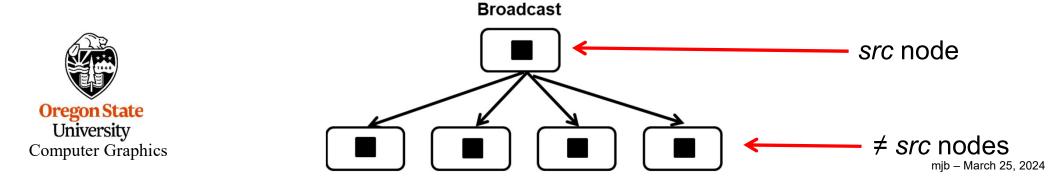


MPI Broadcast Example

This is our heat transfer equation from before. Clearly, every CPU will need to know this value.







How Does this Work? Think Star Trek Wormholes!

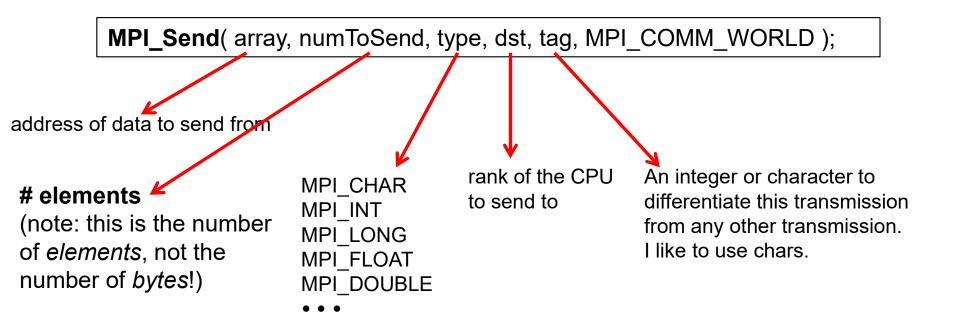




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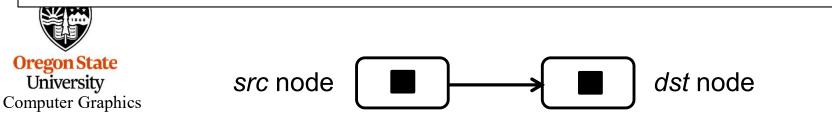


Sending Data from One Source CPU to Just One Destination CPU



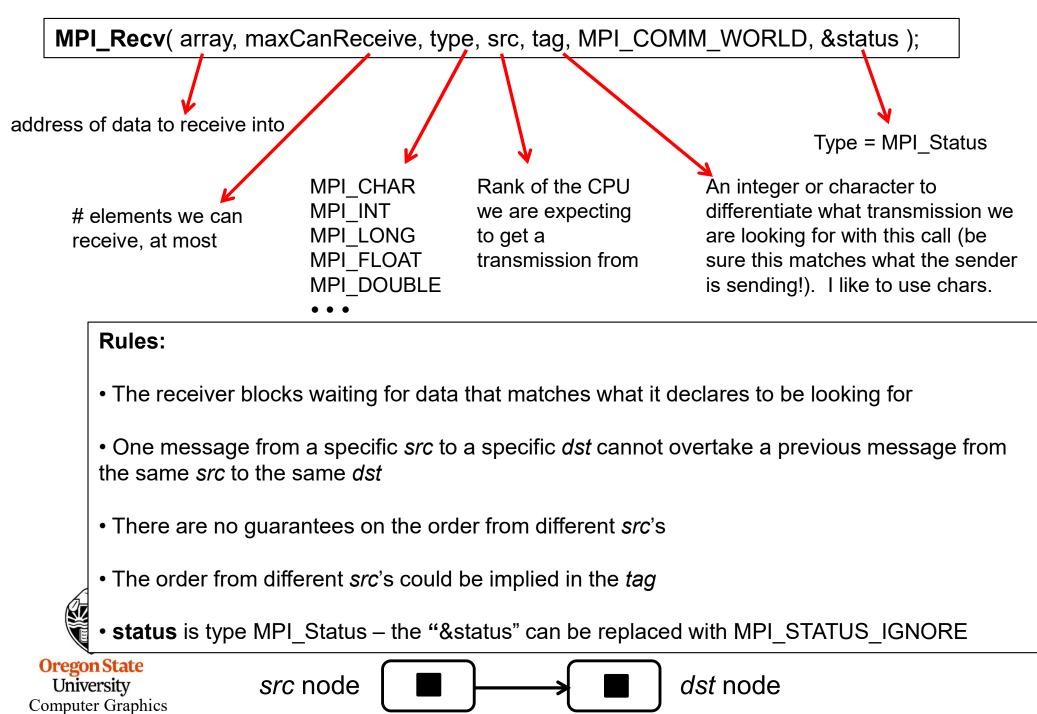
Rules:

- 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 .



20

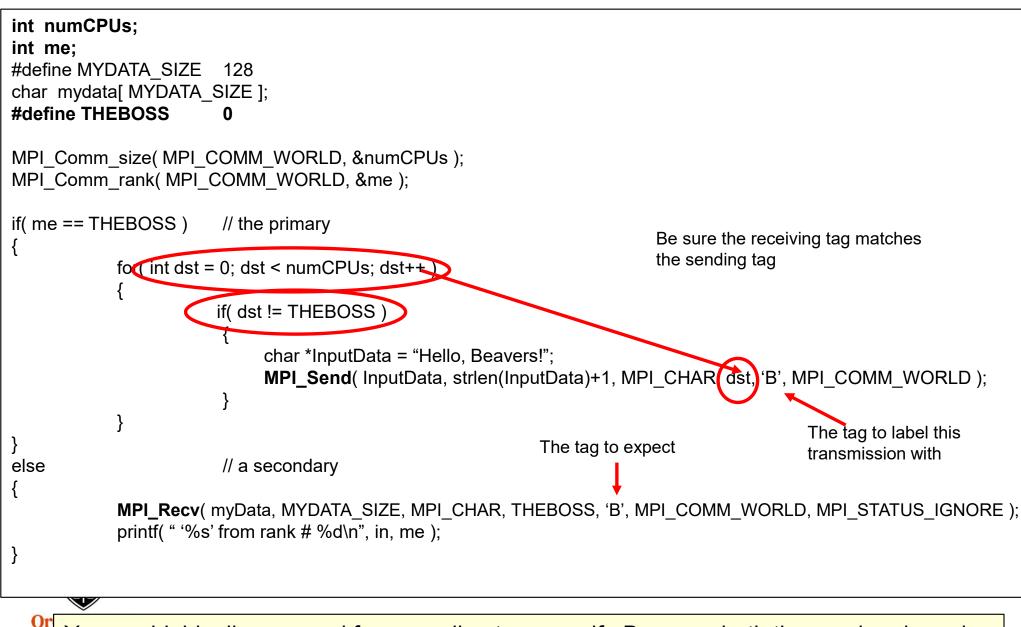
Receiving Data in a Destination CPU from a Source CPU



21

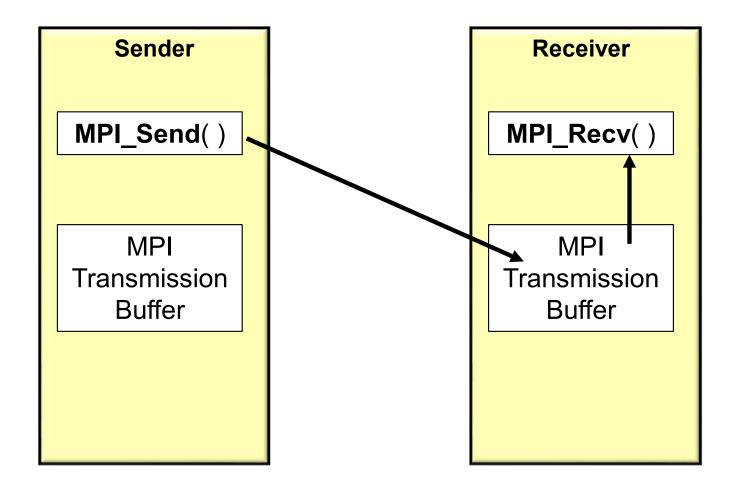
Example

Remember, this *identical code* runs on all CPUs:



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_Recv()?



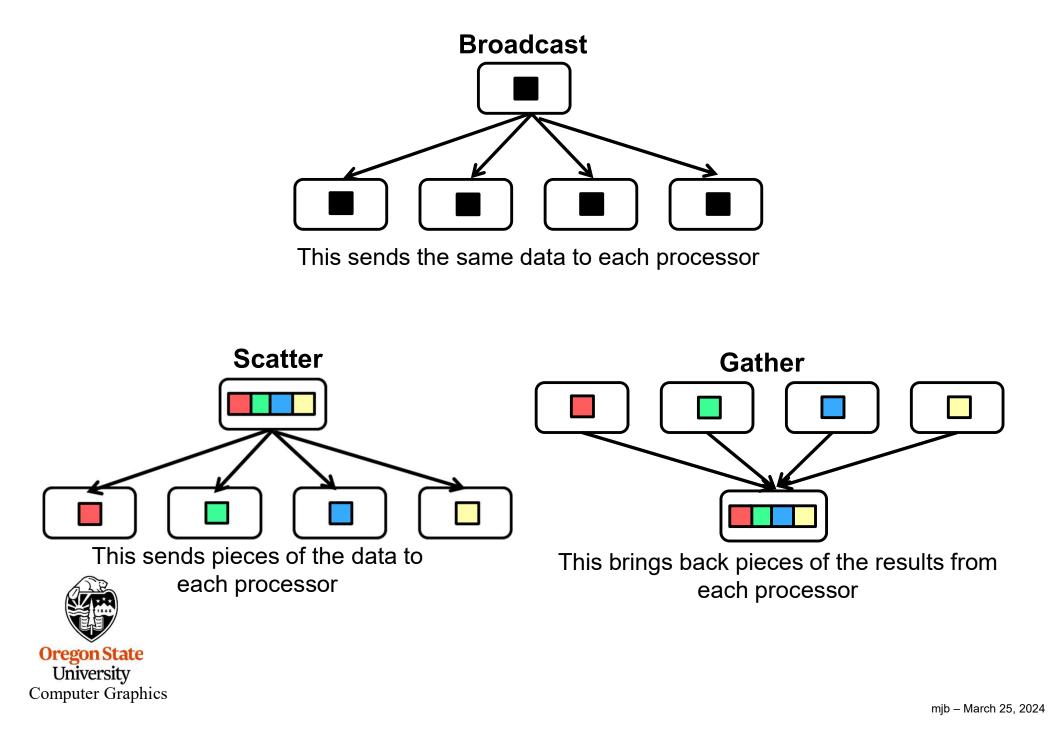


MPI_Send() blocks until the transfer is far enough along that the *array* can be destroyed or re-used.

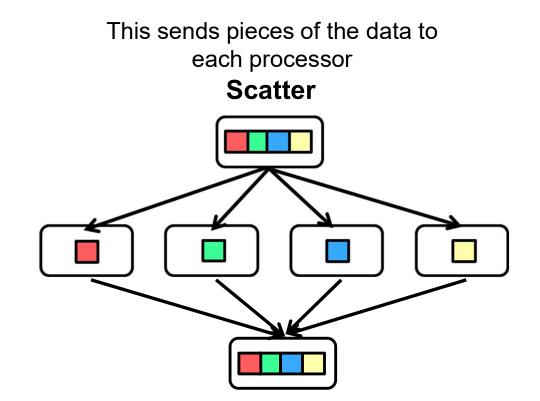
You typically don't send the entire workload to each dst – you just send part of it, like this:

```
#define NUMELEMENTS
                        22222
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
else
                      // a receiver
           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 Patterns²⁵



Scatter and Gather Usually Go Together



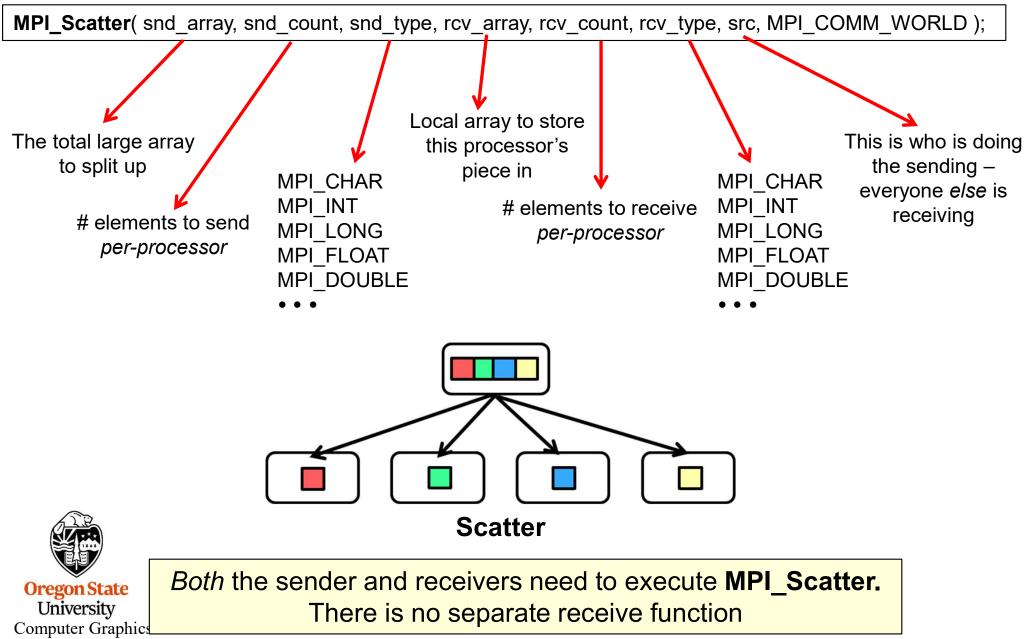
Gather This brings back pieces of the results from each processor



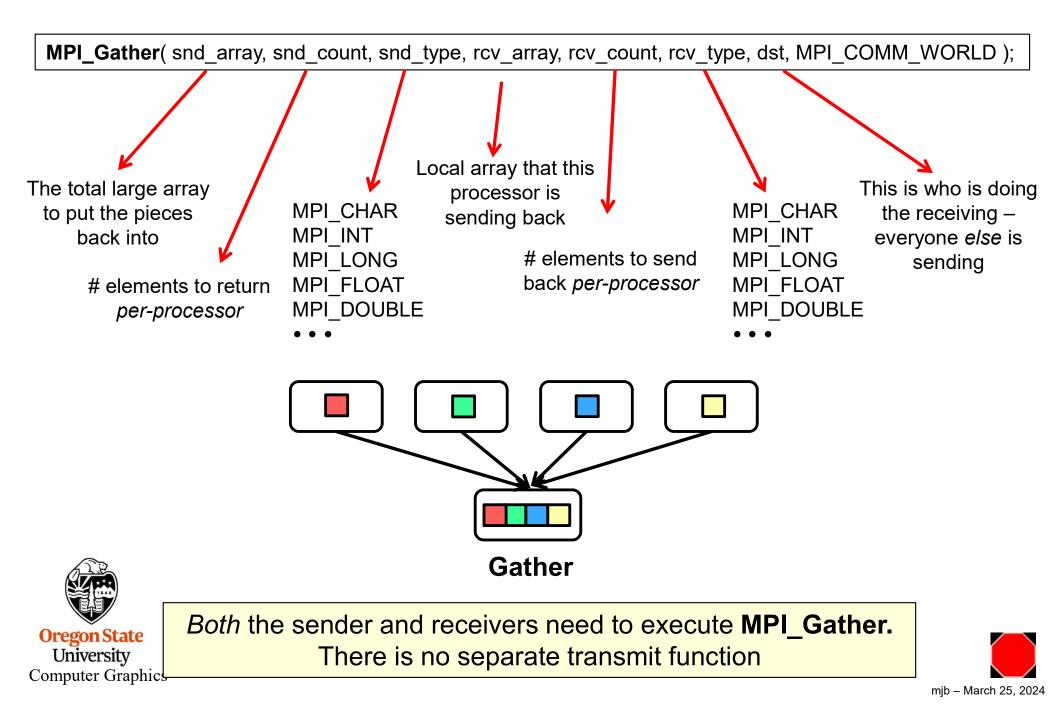
Oregon State University Computer Graphics Note surprisingly, this is referred to by the combined term *Scatter/Gather*

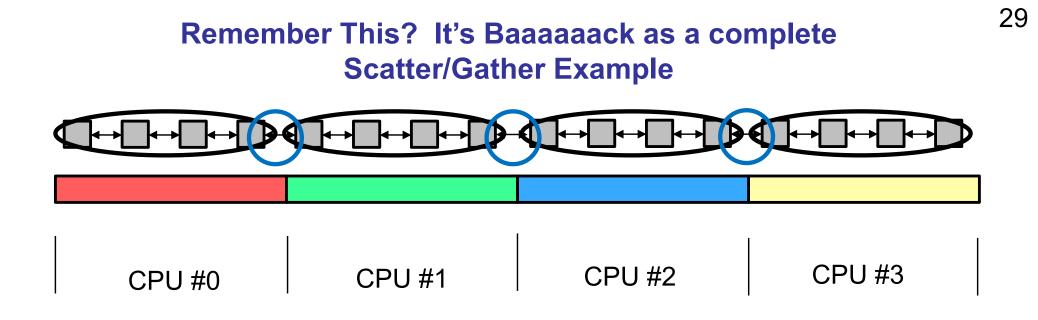
MPI Scatter

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 const float float k_ove	RHO = 8050.; C = 0.466; K = 20.; er_rho_c = K / (RHO*C 0*C) = 5.33x10^-6 m^2/s	
	const float const float	DX = 1.0; DT = 1.0;	
	#define Th	HEBOSS 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)	• •

heat.cpp, II

int main(int argc, char *argv[])

{

```
MPI_Init( &argc, &argv );
```

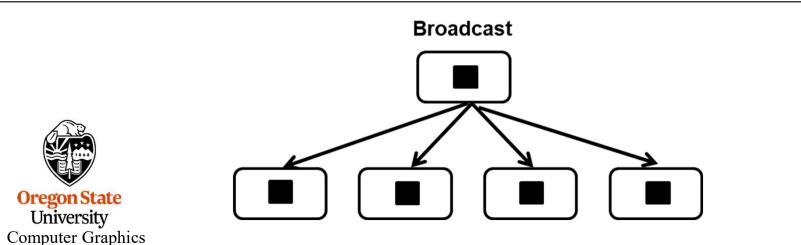
int me; // which one I am

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

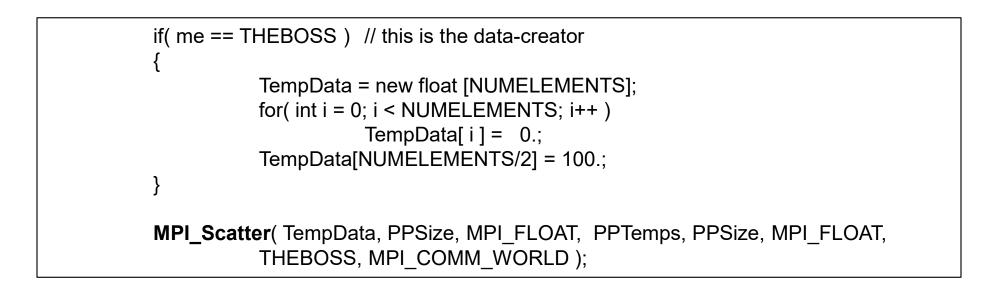
// decide how much data to send to each processor:

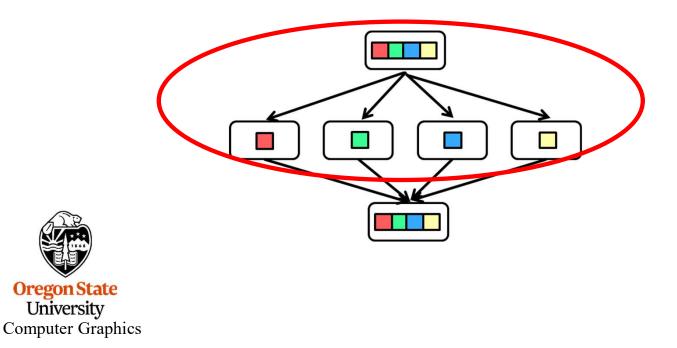
PPSize = NUMELEMENTS / NumCpus; // assuming it comes out evenly PPTemps = new float [PPSize]; // all processors now have this uninitialized Local array NextTemps = new float [PPSize]; // all processors now have this uninitialized local array too

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



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 25, 2024
```

heat.cpp, V

```
if( me == THEBOSS )
{
    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\n", NumCpus, NUMELEMENTS, performance );
}
MPI_Finalize( );
return 0;
```



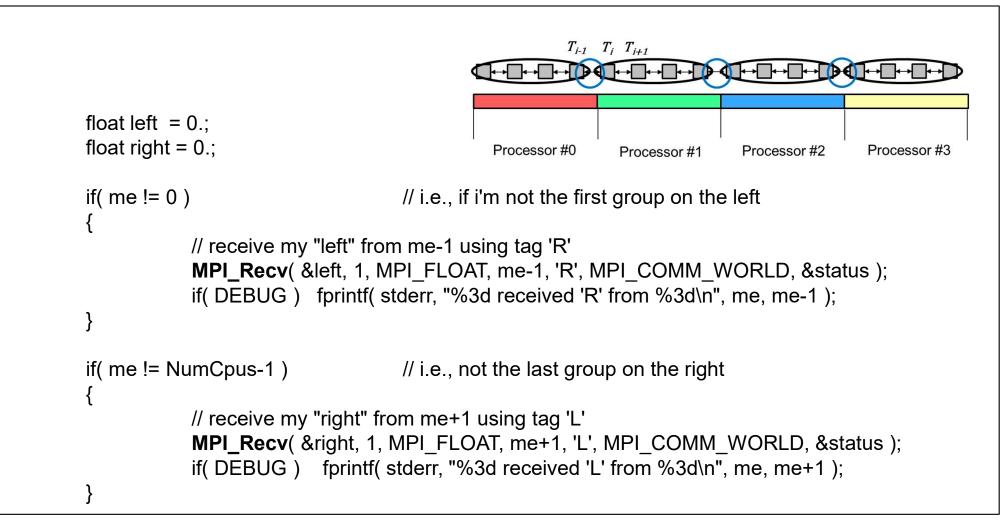
}

DoOneTimeStep, I

```
// read from PerProcessorData[ ], write into NextTemps[ ]
                                                                 T_{i-1} T_i T_{i+1}
void
DoOneTimeStep( int me )
           MPI Status status;
                                                         Processor #0
                                                                       Processor #1
                                                                                     Processor #2
                                                                                                  Processor #3
           // 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 );
```



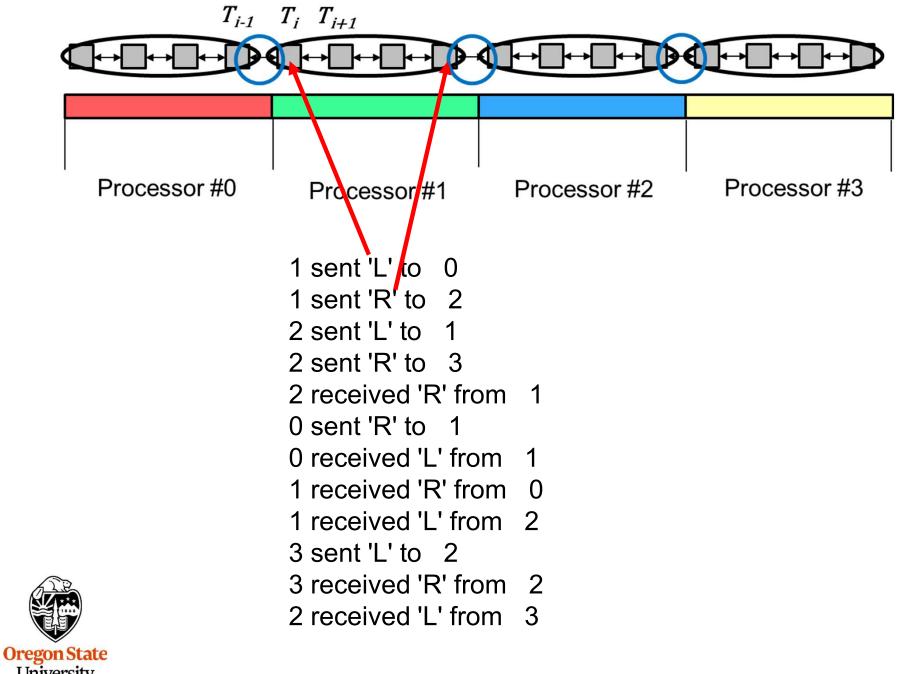
DoOneTimeStep, II



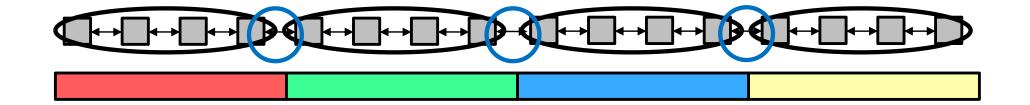


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Sharing Values Across the Boundaries



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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

38

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;
}
```

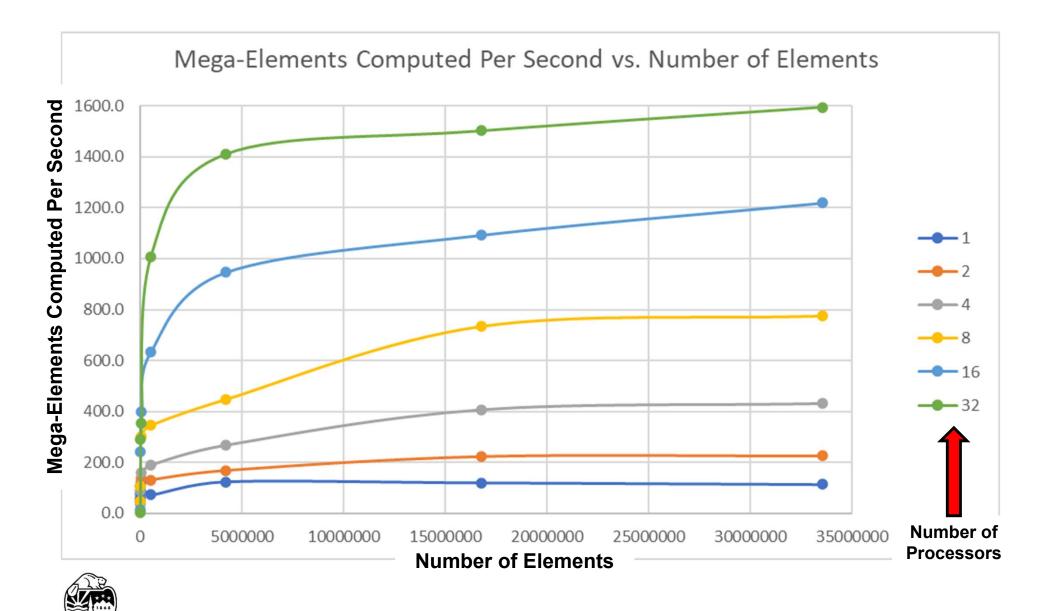


DoOneTimeStep, IV

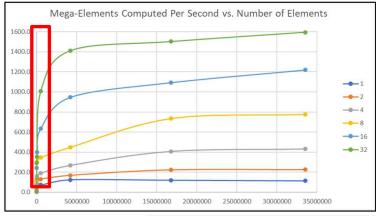
```
// update the local dataset:
for( int i = 0; i < PPSize; i++ )
{
PPTemps[ i ] = NextTemps[ i ];
}
}
```

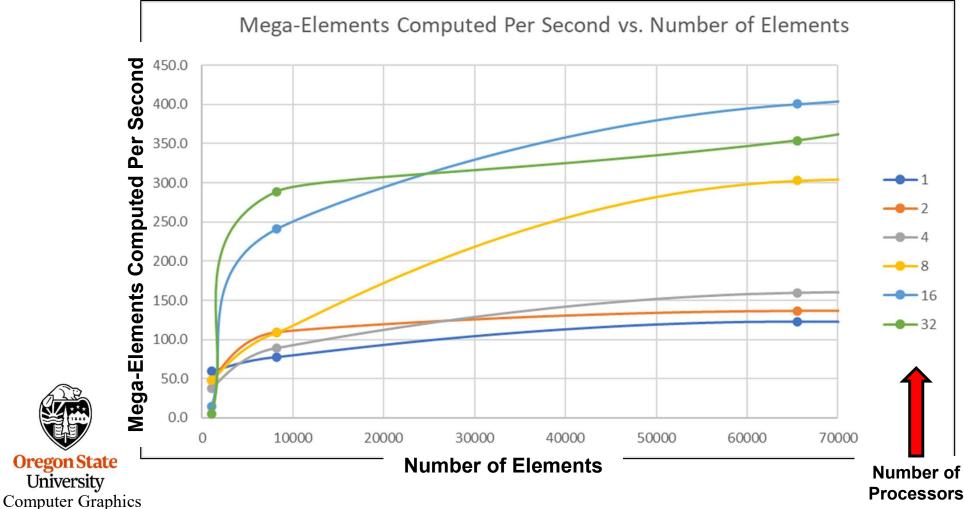


MPI Performance

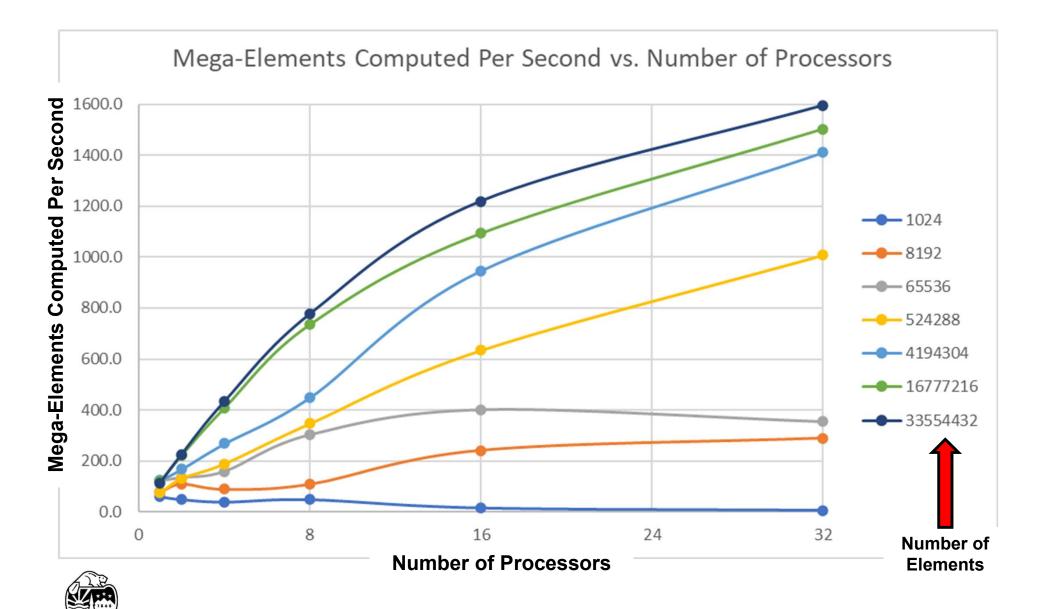




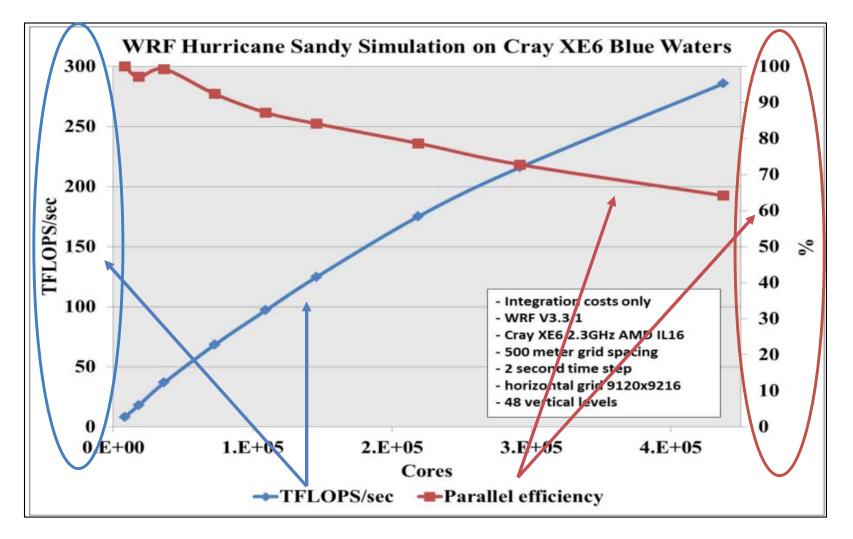




MPI Performance



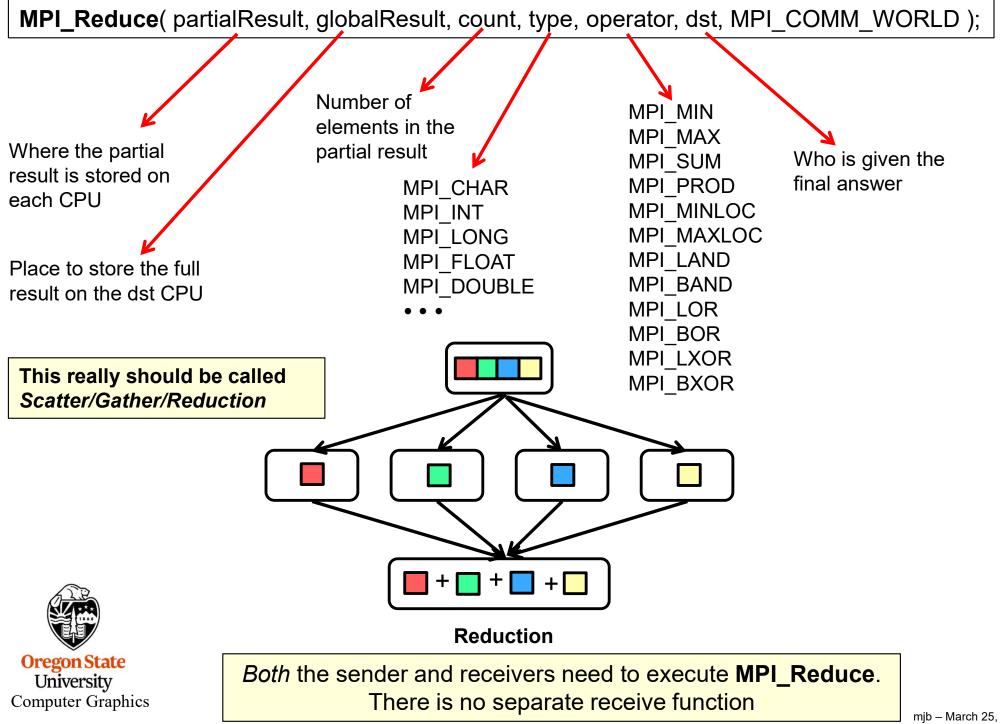
Using MPI and OpenMP on 13,680 nodes (437,760 cores) of the Cray XE6 at NCSA at the University of Illinois



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



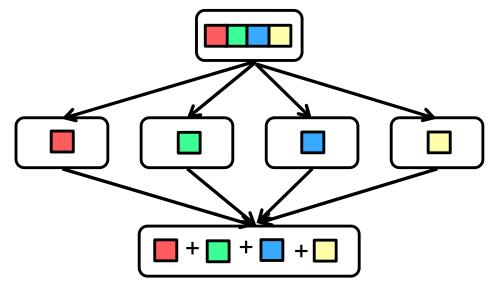
MPI Reduction



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MPI Reduction Example

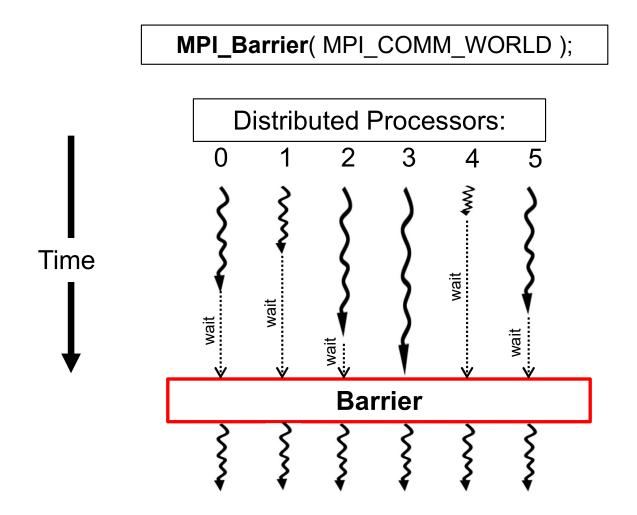
```
// gratuitous use of a reduce -- average all the temperatures:
float partialSum = 0.;
for( int i = 0; i < PPSize; i++ )
    partialSum += PPTemps[ i ];
float globalSum = 0.;
MPI_Reduce( &partialSum, &globalSum, 1, MPI_FLOAT, MPI_SUM, THEBOSS, MPI_COMM_WORLD );
if( me == THEBOSS )
    fprintf( stderr,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





Reduction

MPI Barriers



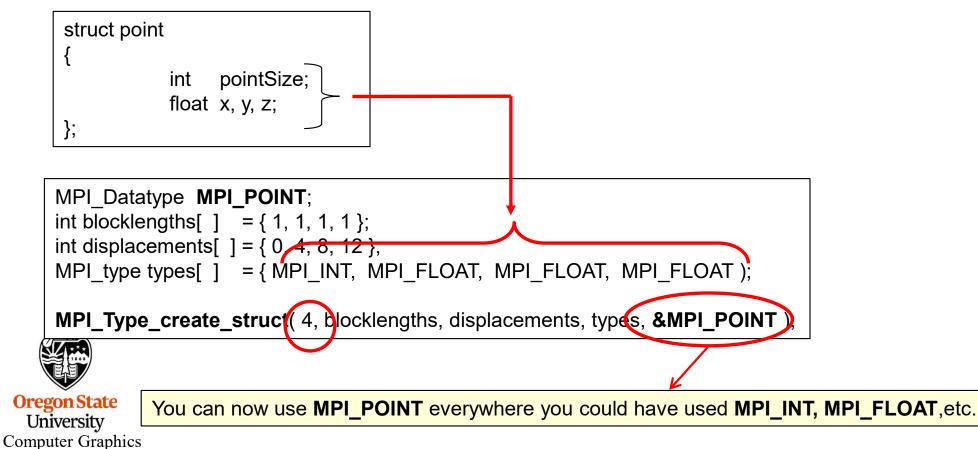
All CPUs must execute the call to MPI_Barrier() before any of the CPUs can move past it. That is, each CPU's MPI_Barrier() blocks until all CPUs execute a call to MPI_Barrier().

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!



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:

typedef struct {	_MPI_Status
int	MPI_SOURCE;
int	MPI_TAG;
int	MPI_ERROR;
} MPI_Status;	_

- 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

Example: MPI_Status status; MPI_Recv(myData, MYDATA_SIZE, MPI_CHAR, THEBOSS, **MPI_ANY_TAG**, MPI_COMM_WORLD, &status);



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

Univer MPI ERR 10

Computer MPI ERR LASTCODE

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 QUOTA MPI ERR READ ONLY MPI ERR FILE IN USE MPI ERR DUP DATAREP Oregon MPI ERR_CONVERSION

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 exists

Invalid file name (e.g., path name too long)

Permission denied

Not enough space

Quota exceeded

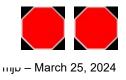
Read-only file or file system

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



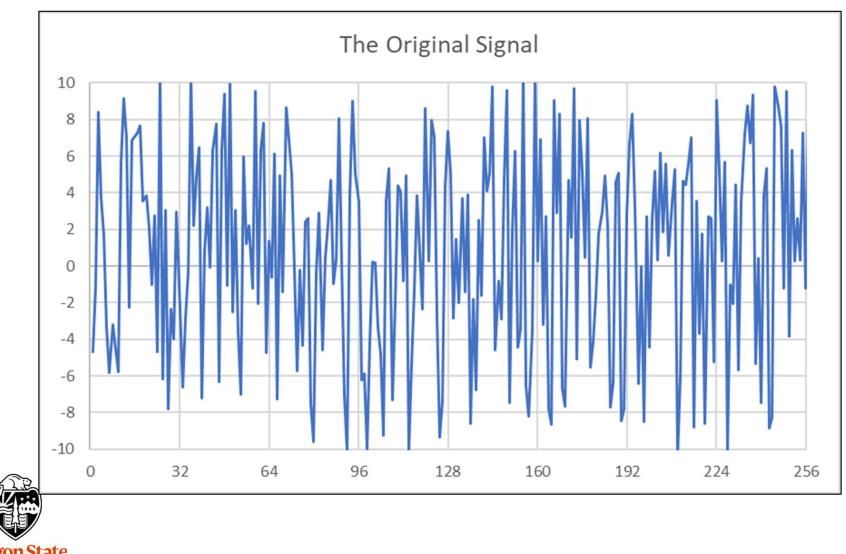
Invalid file handle

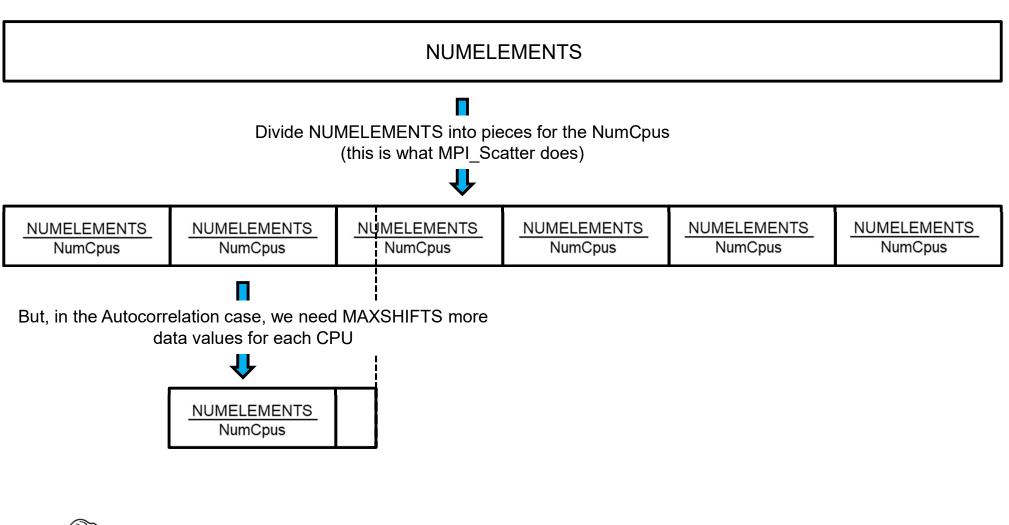
File does not exist





Example: Autocorrelation







Autocorrelation – How the Shifting Works

