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

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

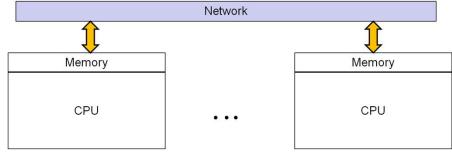


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mpi.pptx mjb – June 2, 2021

## 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

## **The Open MPI Consortium**









































































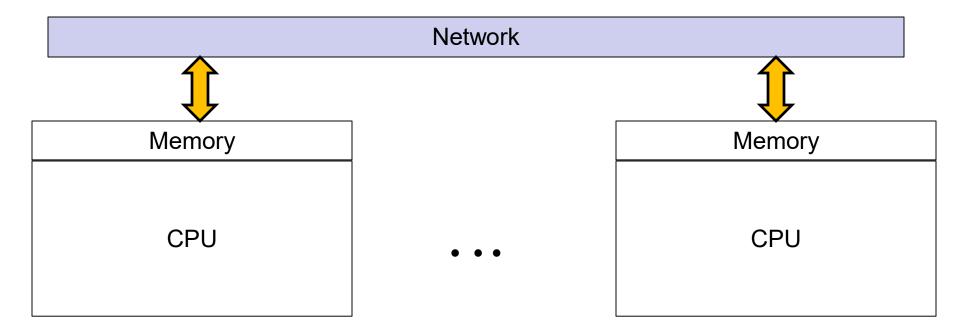








### **MPI: The Basic Idea**

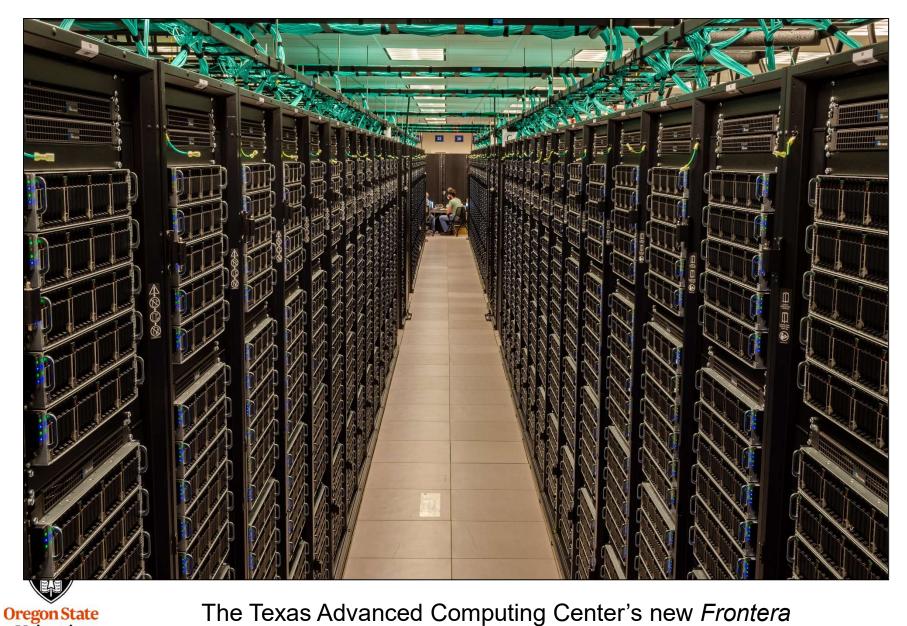


Programs on different CPUs coordinate computations by passing messages between each other

Note: Each CPU in the MPI "cluster" must be prepared ahead of time by having the MPI server code installed on it. 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!



The Texas Advanced Computing Center's new *Frontera* supercomputer, currently the 5<sup>th</sup> fastest in the word

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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/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

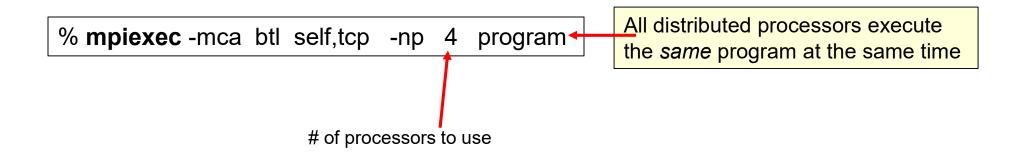
"The College of Engineering HPC cluster is a heterogeneous mix of 202 servers providing over 3600 CPU cores, over 130 GPUs, and over 31 TB total RAM. The systems are connected via gigabit ethernet, and most of the latest servers also utilize a Mellanox EDR InfiniBand network connection. The cluster also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

## **Compiling and Running from the Command Line**

```
% mpicc -o program program.c... ← C

or

% mpic++ -o program program.cpp... ← C++
```



Warning – use mpic++ and mpiexec!

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



## Running with a bash Batch Script

```
submit.bash:
#!/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=joeparallel@cs.oregonstate.edu
module load openmpi/3.1
mpic++ heat.cpp -o heat -lm
mpiexec -mca btl self,tcp -np 4 heat
```



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

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

You don't have to ask for email notification, but if you do, please, 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.



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

**submit-c 144%** scancel 258759



## **Setting Up and Finishing**

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



MPI\_Init( NULL, NULL );

## 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 deer!



Oh, look, a communicator of turkeys!



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

Getting information about our place in the **communicator**:

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.

**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 BOSS 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 == 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 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 166% mpiexec -np 16 ./first

Welcome from Rank 1

Welcome from Rank 5

Welcome from Rank 7

Welcome from Rank 9

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 2

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 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 12

Welcome from Rank 14

Welcome from Rank 4

Welcome from Rank 2

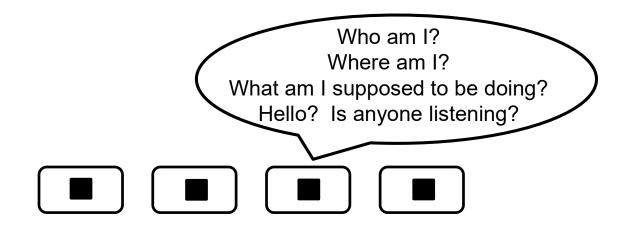
Rank 0 says that we have a Communicator of size 16

Welcome from Rank 8

Welcome from Rank 10

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?

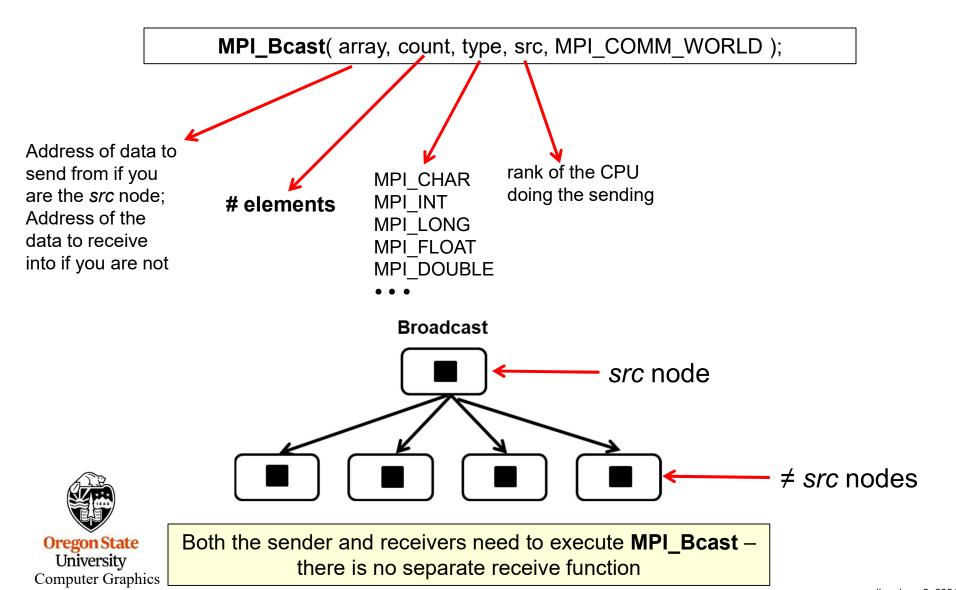


Example: You could coordinate the units of our DGX system using MPI





# A Good Place to Start: MPI Broadcasting



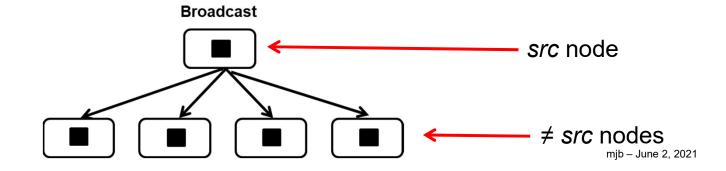
## **MPI Broadcast Example**

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

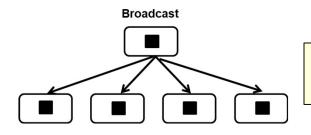
$$\Delta T_{i} = \left(\frac{k}{\rho C}\right) \left(\frac{T_{i-1} - 2T_{i} + T_{i+1}}{\left(\Delta x\right)^{2}}\right) \Delta t$$

```
numCPUs;
int
int
     me;
                                   // the BOSS node will know this value, the others won't (yet)
float k_over_rho_c;
#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 ) 
                                                         I am the BOSS: this identifies this call as a send
    << 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

Executable code k\_over\_rho\_c (set)

#### Node #BOSS:

MPI\_Bcast &k\_over\_rho\_c 1, MPI\_FLOAT, BOSS, MPI\_COMM\_WORLD ); // send if BOSS, and receive if not

### All Nodes that are *not* #BOSS:

Executable code	*	k_over_rho_c (being set)	
Executable code		k_over_rho_c (being set)	
Executable code		k_over_rho_c (being set)	
Executable code	1	k_over_rho_c (being set)	



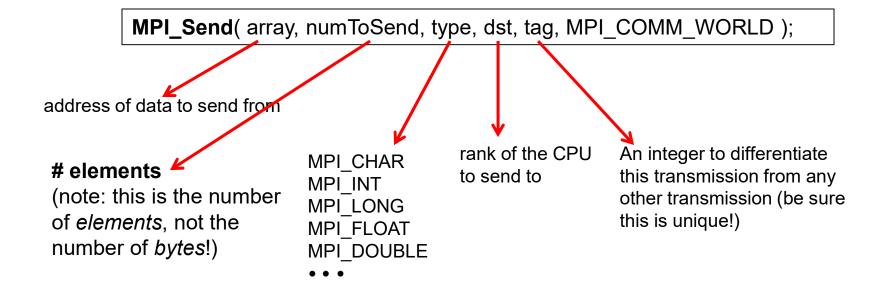
# How Does this Work? Think Star Trek Wormholes!







## Sending Data from One Source CPU to One Destination CPU



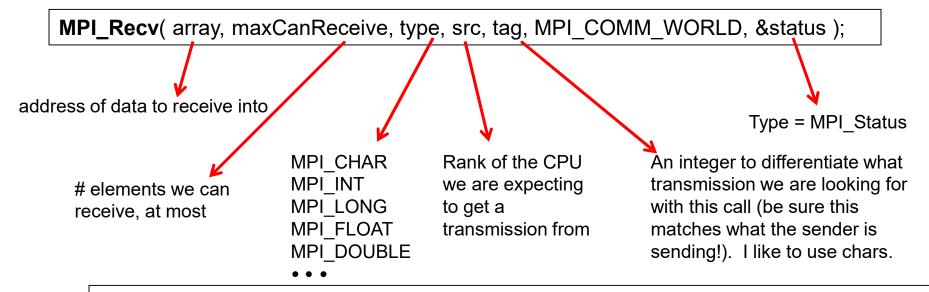
#### Rules:

- 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 .



src node dst node

### Receiving Data in a Destination CPU from a Source CPU



#### 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

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src node dst node

## **Example**

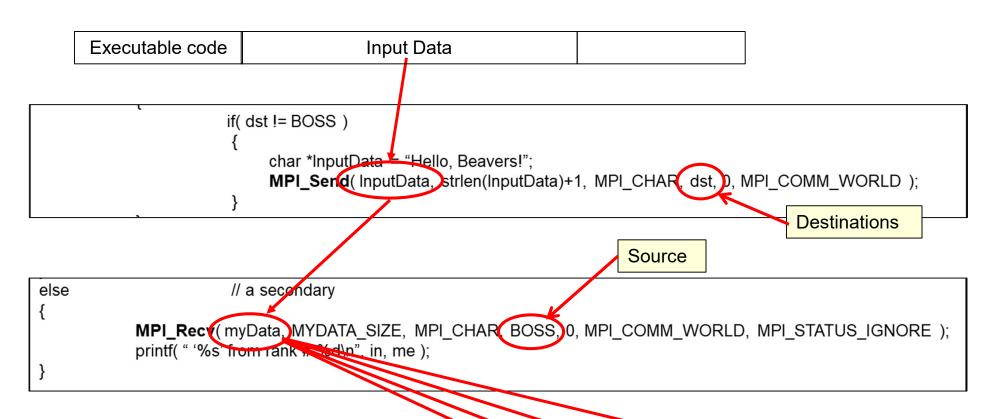
Remember, this *identical code* runs on all CPUs:

```
int numCPUs;
int me;
#define MYDATA SIZE
char mydata[ MYDATA SIZE ];
#define BOSS
MPI Comm size(MPI COMM WORLD, &numCPUs);
MPI Comm rank( MPI COMM WORLD, &me );
if( me == BOSS )
                       // the primary
                                                                      Be sure the receiving tag matches
                                                                      the sending tag
           for int dst = 0; dst < numCPUs; dst++1
                      if( dst != BOSS
                           char *InputData = "Hello, Beavers!";
                           MPI Send(InputData, strlen(InputData)+1, MPI CHAR (dst, 'B', MPI COMM WORLD);
                                                                                       The tag to send
                       // a secondary
else
                                                                      The tag to expect
           MPI Recv(myData, MYDATA SIZE, MPI CHAR, BOSS, 'B', MPI COMM WORLD, MPI STATUS IGNORE);
           printf( " '%s' from rank # %d\n", 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.

## **Look at this Diagram**

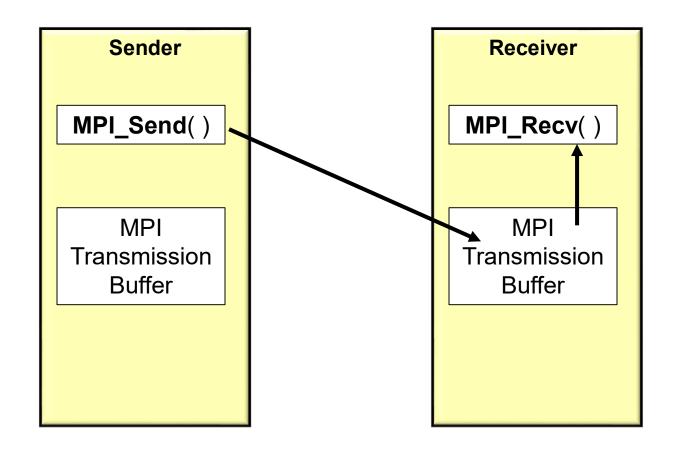






Executable code	→ MyData
Executable code	MyData
Executable code	MyData
Executable code	MyData

# 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.

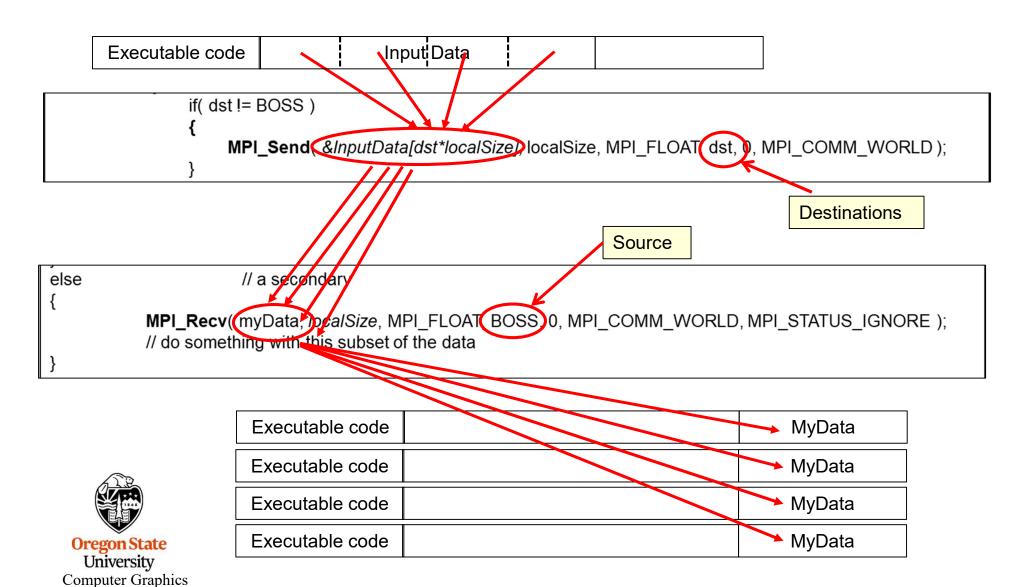
## **Another Example**

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

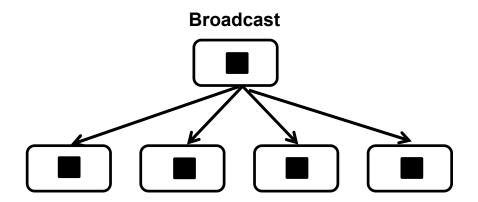
```
#define NUMELEMENTS
                         22222
int numCPUs;
int me;
#define BOSS
                      0
MPI Comm size( MPI COMM WORLD, &numCPUs );
MPI Comm rank( MPI COMM WORLD, &me );
int localSize = NUMELEMENTS / numCPUs;
                                             // assuming it comes out 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 );
                      // a receiver
else
           MPI_Recv( myData, localSize, MPI FLOAT, BOSS, 0, MPI COMM WORLD, MPI STATUS IGNORE );
           // do something with this subset of the data
```

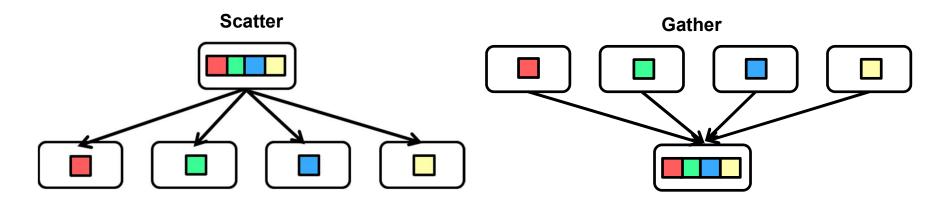
## **Another Example**

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



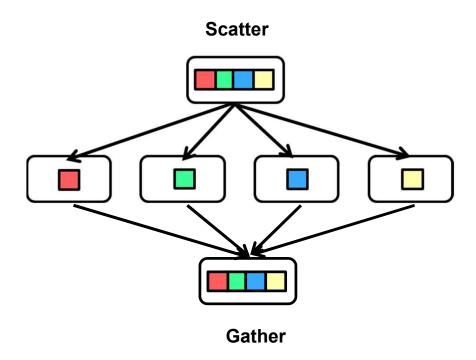
# In Distributed Computing, You Often Hear About These Design Patterns 27







## **Scatter and Gather Usually Go Together**

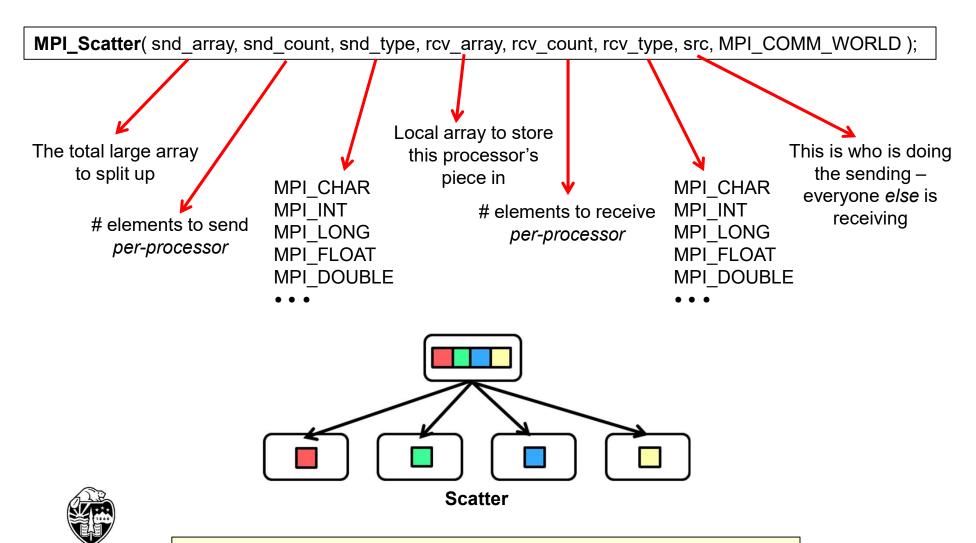


Note surprisingly, this is referred to as Scatter/Gather



#### **MPI Scatter**

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



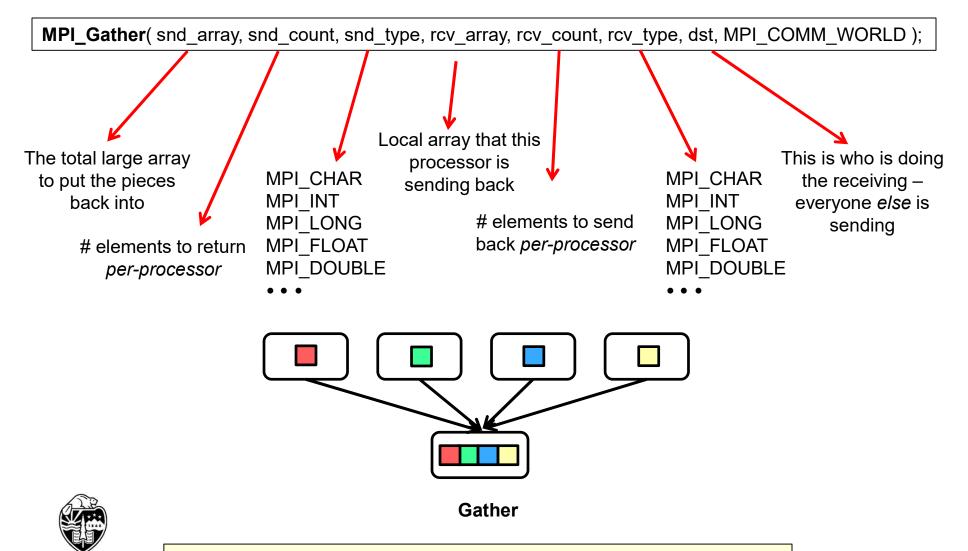
Both the sender and receivers need to execute MPI\_Scatter.

There is no separate receive function

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### **MPI** Gather



Both the sender and receivers need to execute MPI\_Gather.

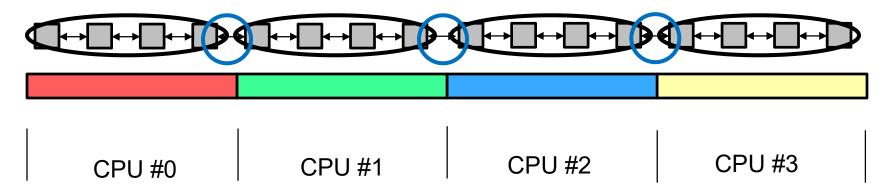
There is no separate receive function

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# 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.

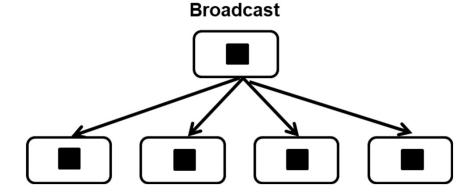
This pattern of breaking a big problem up into pieces, sending them to different CPUs, computing on the pieces, and getting the results back is *very* common. That's why MPI has its own scatter and gather functions.

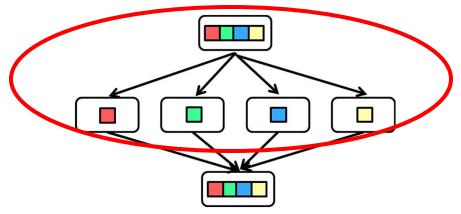


## heat.cpp, I

```
#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 NOTE: this cannot be a const!
// 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
#define DEBUG
                                false
float *
          NextTemps;
                                // per-processor array to hold computer next-values
          NumCpus;
PPSize;
PPTemps;
                                // total # of cpus involved
int
                                // per-processor local array size
int
float *
                                // per-processor local array temperature data
          TempData;
                                // the overall NUMELEMENTS-big temperature data
float *
void
           DoOneTimeStep( int );
```







### 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
                     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( );
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```



## DoOneTimeStep, I

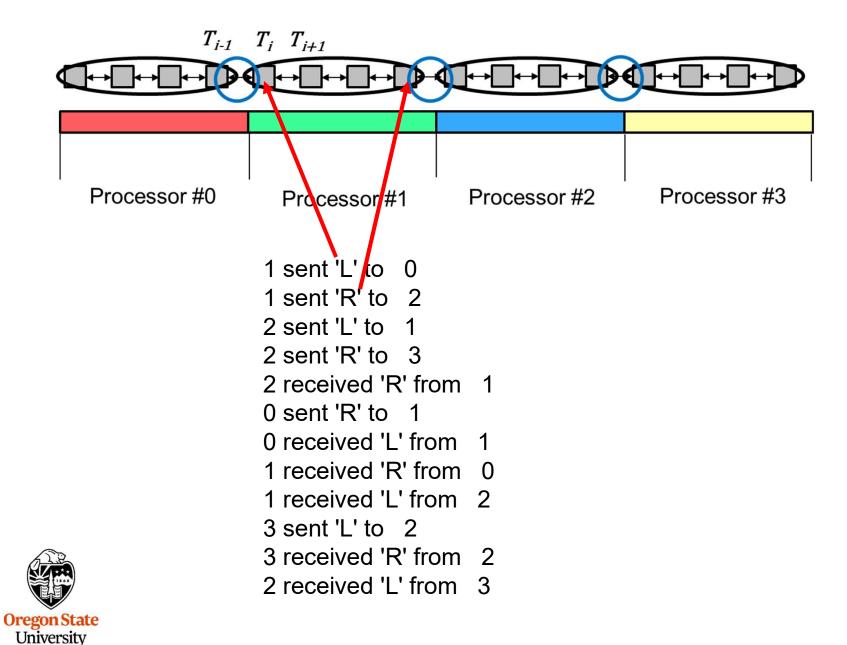
```
// read from PerProcessorData[ ], write into NextTemps[ ]
                                                                  T_{i-1} T_i T_{i+1}
void
DoOneTimeStep( int me )
           MPI Status status;
                                                         Processor #0
                       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



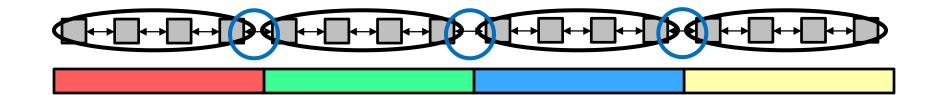
```
T_{i-1} T_i T_{i+1}
float left = 0.;
float right = 0.;
                                              Processor #0
                                                                          Processor #2
                                                                                         Processor #3
                                                            Processor #1
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 );
```

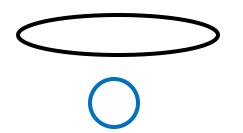


## **Sharing Values Across the Boundaries**



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**Intraprocessor** computing

**Interprocessor** communication

Compute : Communicate ratio = N : 2

where N is the number of compute cells per processor



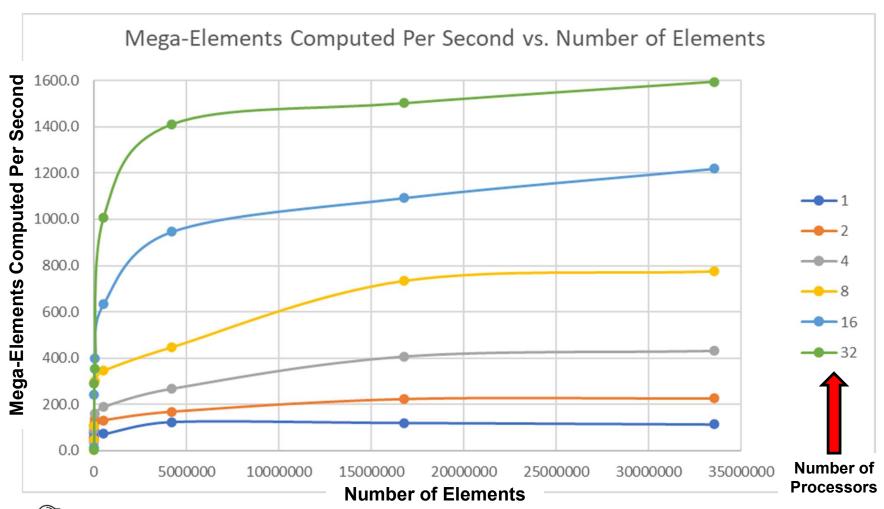
In the above drawing, Compute: Communicate is 4:2

```
// 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;
```



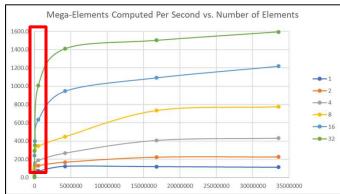


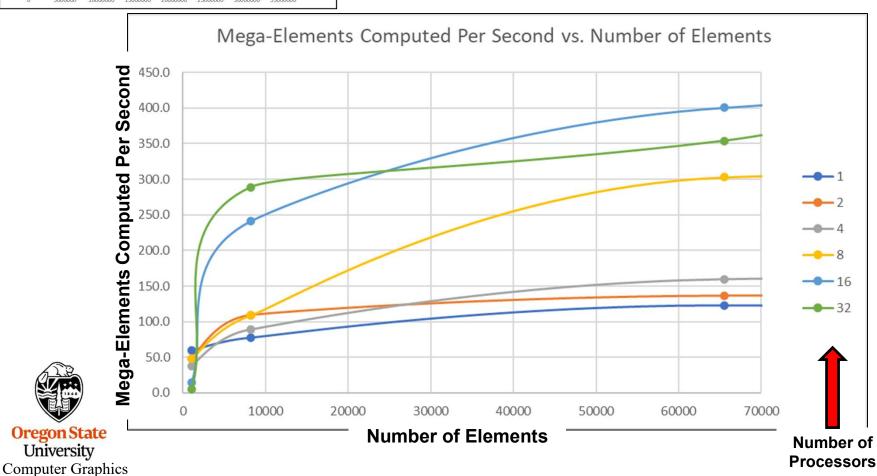
### **MPI Performance**



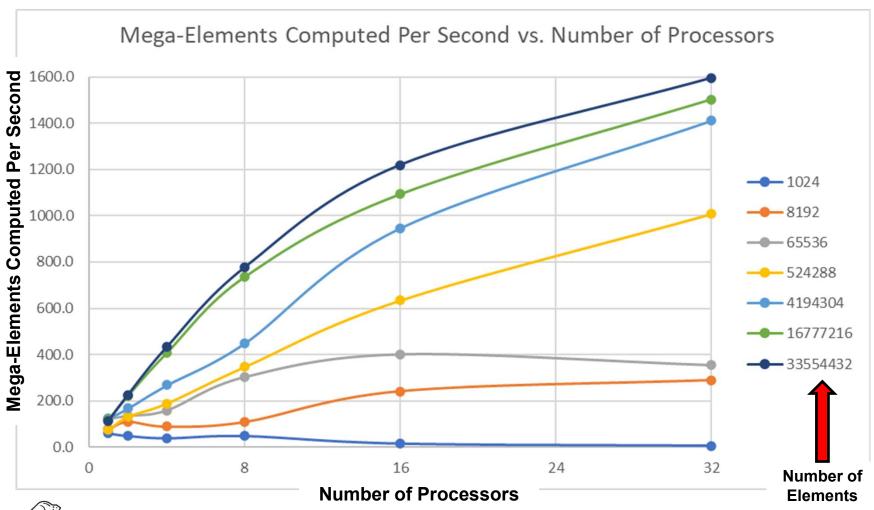


### **Low Dataset-Size MPI Performance**



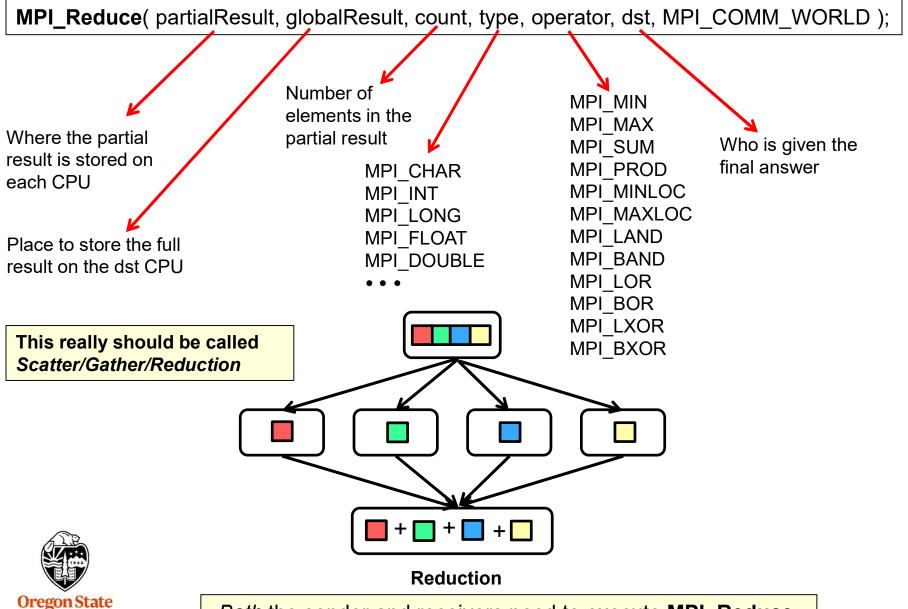


### **MPI Performance**





### **MPI** Reduction



Both the sender and receivers need to execute MPI\_Reduce.

There is no separate receive function

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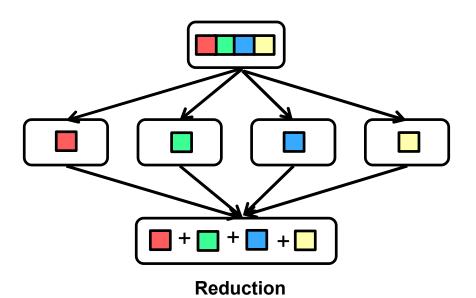
## **MPI Reduction Example**

```
// 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, BOSS, MPI_COMM_WORLD );

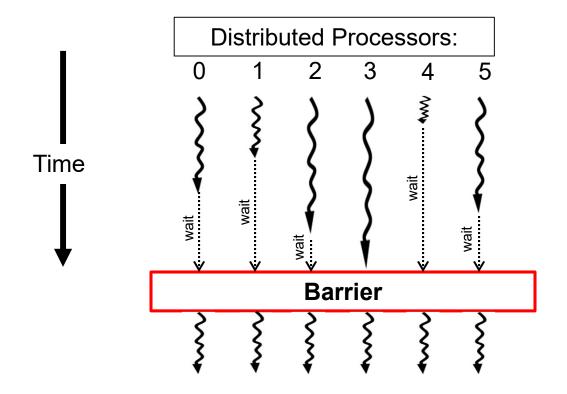
if( me == BOSS )
    fprintf( stderr, "Average temperature = %f\n", globalSum/(float)NUMELEMENTS );
```





### **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().

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## **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 );

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

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.

**Oregon State** 

## **MPI Timing**

double MPI\_Wtick( );

Returns the resolution of the clock, in seconds.

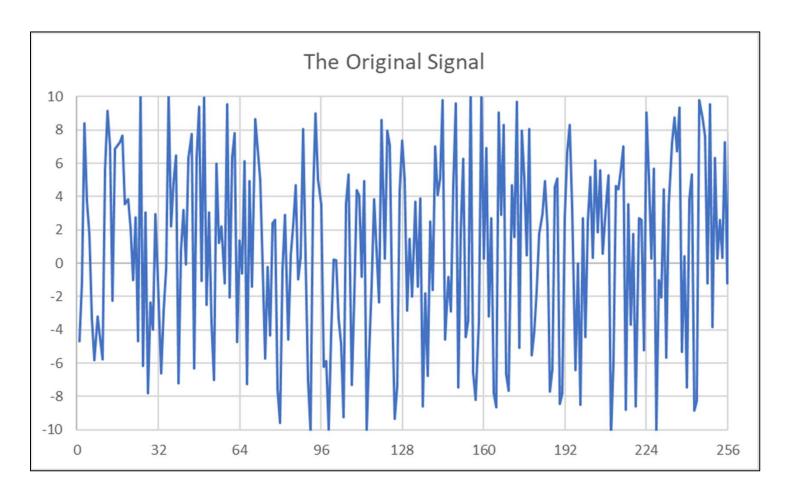
double MPI\_Wtime( );

Returns the time, in seconds, since "some time in the past".

Warning: the clocks on the different CPUs are not guaranteed to be synchronized!



# **Autocorrelation – a Piece of the Original Signal**





#### **Autocorrelation – More than Just a Scatter**

#### **NUMELEMENTS** Divide NUMELEMENTS into pieces for the NumCpus (this is what MPI Scatter does) NUMELEMENTS NUMELEMENTS NUMELEMENTS NUMELEMENTS NUMELEMENTS NUMELEMENTS NumCpus NumCpus NumCpus NumCpus NumCpus NumCpus But, in the Autocorrelation case, we need MAXSHIFTS more data values for each CPU NUMELEMENTS NumCpus



## **Autocorrelation – How the Shifting Works**

