

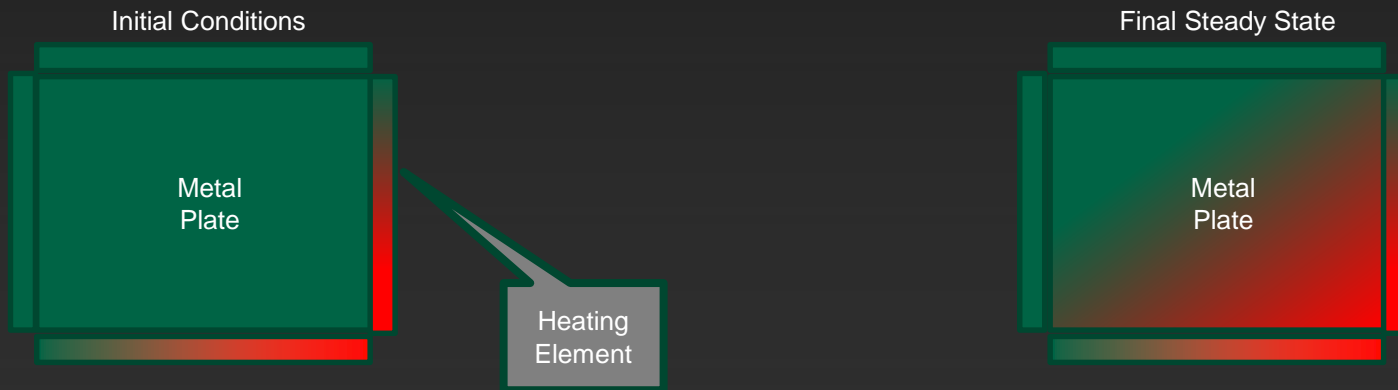
Laplace Exercise

John Urbanic

Parallel Computing Scientist
Pittsburgh Supercomputing Center

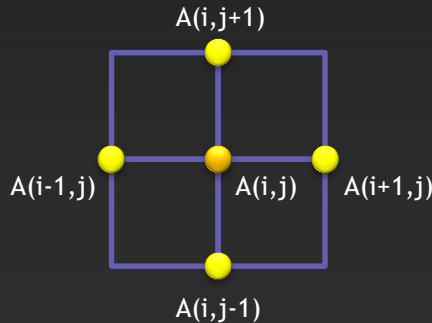
Our Foundation Exercise: Laplace Solver

- I've been using this for MPI, OpenMP and now OpenACC. It is a great simulation problem, not rigged for MPI.
- In this most basic form, it solves the Laplace equation: $\nabla^2 f(x, y) = 0$
- The Laplace Equation applies to many physical problems, including:
 - Electrostatics
 - Fluid Flow
 - Temperature
- For temperature, it is the Steady State Heat Equation:



Exercise Foundation: Jacobi Iteration

- The Laplace equation on a grid states that each grid point is the average of its neighbors.
- We can iteratively converge to that state by repeatedly computing new values at each point from the average of neighboring points.
- We just keep doing this until the difference from one pass to the next is small enough for us to tolerate.



$$A_{k+1}(i, j) = \frac{A_k(i-1, j) + A_k(i+1, j) + A_k(i, j-1) + A_k(i, j+1)}{4}$$

Serial Code Implementation

```
for(i = 1; i <= ROWS; i++) {  
    for(j = 1; j <= COLUMNS; j++) {  
        Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] + Temperature_last[i-1][j] +  
                                     Temperature_last[i][j+1] + Temperature_last[i][j-1]);  
    }  
}
```

```
do j=1,columns  
    do i=1,rows  
        temperature(i,j)= 0.25 * (temperature_last(i+1,j)+temperature_last(i-1,j) + &  
                                   temperature_last(i,j+1)+temperature_last(i,j-1) )  
    enddo  
enddo
```

Serial C Code (kernel)

```
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {
```

```
    for(i = 1; i <= ROWS; i++) {  
        for(j = 1; j <= COLUMNS; j++) {  
            Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] + Temperature_last[i-1][j] +  
                                         Temperature_last[i][j+1] + Temperature_last[i][j-1]);  
        }  
    }
```

```
    dt = 0.0;
```

```
    for(i = 1; i <= ROWS; i++){  
        for(j = 1; j <= COLUMNS; j++){  
            dt = fmax( fabs(Temperature[i][j]-Temperature_last[i][j]), dt);  
            Temperature_last[i][j] = Temperature[i][j];  
        }  
    }
```

```
    if((iteration % 100) == 0) {  
        track_progress(iteration);  
    }
```

```
    iteration++;
```

```
}
```



Done?



Calculate



Update
temp
array and
find max
change



Output

Serial C Code Subroutines

```
void initialize(){  
    int i,j;  
  
    for(i = 0; i <= ROWS+1; i++){  
        for (j = 0; j <= COLUMNS+1; j++){  
            Temperature_last[i][j] = 0.0;  
        }  
    }  
  
    // these boundary conditions never change throughout run  
  
    // set left side to 0 and right to a linear increase  
    for(i = 0; i <= ROWS+1; i++) {  
        Temperature_last[i][0] = 0.0;  
        Temperature_last[i][COLUMNS+1] = (100.0/ROWS)*i;  
    }  
  
    // set top to 0 and bottom to linear increase  
    for(j = 0; j <= COLUMNS+1; j++) {  
        Temperature_last[0][j] = 0.0;  
        Temperature_last[ROWS+1][j] = (100.0/COLUMNS)*j;  
    }  
}
```

```
void track_progress(int iteration) {  
    int i;  
  
    printf("-- Iteration: %d --\n", iteration);  
    for(i = ROWS-5; i <= ROWS; i++) {  
        printf("[%d,%d]: %5.2f ", i, i, Temperature[i][i]);  
    }  
    printf("\n");  
}
```

BCs could run from 0 to ROWS+1 or from 1 to ROWS. We chose the former.

Whole C Code

```
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include <sys/time.h>

// size of plate
#define COLUMNS 1000
#define ROWS 1000

// largest permitted change in temp (This value takes about 3400 steps)
#define MAX_TEMP_ERROR 0.01

double Temperature[ROWS+2][COLUMNS+2]; // temperature grid
double Temperature_last[ROWS+2][COLUMNS+2]; // temperature grid from last iteration

// helper routines
void initialize();
void track_progress(int iter);

int main(int argc, char *argv[]) {
    int i, j; // grid indexes
    int max_iterations; // number of iterations
    int iteration=1; // current iteration
    double dt=100; // largest change in t
    struct timeval start_time, stop_time, elapsed_time; // timers

    printf("Maximum iterations [100-4000]? \n");
    scanf("%d", &max_iterations);

    gettimeofday(&start_time, NULL); // Unix timer

    initialize(); // initialize Temp_last including boundary conditions

    // do until error is minimal or until max steps
    while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {
        // main calculation: average my four neighbors
        for(i = 1; i <= ROWS; i++) {
            for(j = 1; j <= COLUMNS; j++) {
                Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] + Temperature_last[i-1][j] +
                Temperature_last[i][j+1] + Temperature_last[i][j-1]);
            }
        }

        dt = 0.0; // reset largest temperature change

        // copy grid to old grid for next iteration and find latest dt
        for(i = 1; i <= ROWS; i++){
            for(j = 1; j <= COLUMNS; j++){
                dt = fmax( fabs(Temperature[i][j]-Temperature_last[i][j]), dt);
                Temperature_last[i][j] = Temperature[i][j];
            }
        }

        // periodically print test values
        if((iteration % 100) == 0) {
            track_progress(iteration);
        }

        iteration++;
    }
}
```

```
gettimeofday(&stop_time, NULL);
timersub(&stop_time, &start_time, &elapsed_time); // Unix time subtract routine

printf("\nMax error at iteration %d was %f\n", iteration-1, dt);
printf("Total time was %f seconds.\n", elapsed_time.tv_sec+elapsed_time.tv_usec/1000000.0);
}

// initialize plate and boundary conditions
// Temp_last is used to to start first iteration
void initialize(){
    int i,j;

    for(i = 0; i <= ROWS+1; i++){
        for (j = 0; j <= COLUMNS+1; j++){
            Temperature_last[i][j] = 0.0;
        }
    }

    // these boundary conditions never change throughout run

    // set left side to 0 and right to a linear increase
    for(i = 0; i <= ROWS+1; i++) {
        Temperature_last[i][0] = 0.0;
        Temperature_last[i][COLUMNS+1] = (100.0/ROWS)*i;
    }

    // set top to 0 and bottom to linear increase
    for(j = 0; j <= COLUMNS+1; j++) {
        Temperature_last[0][j] = 0.0;
        Temperature_last[ROWS+1][j] = (100.0/COLUMNS)*j;
    }
}

// print diagonal in bottom right corner where most action is
void track_progress(int iteration) {

    int i;

    printf("----- Iteration number: %d ----- \n", iteration);
    for(i = ROWS-5; i <= ROWS; i++) {
        printf("[%d,%d]: %5.2f ", i, i, Temperature[i][i]);
    }
    printf("\n");
}
```

Serial Fortran Code (kernel)

```
do while ( dt > max_temp_error .and. iteration <= max_iterations)
```

```
  do j=1,columns
    do i=1,rows
      temperature(i,j)=0.25*(temperature_last(i+1,j)+temperature_last(i-1,j)+ &
        temperature_last(i,j+1)+temperature_last(i,j-1) )
    enddo
  enddo
```

```
  dt=0.0
```

```
  do j=1,columns
    do i=1,rows
      dt = max( abs(temperature(i,j) - temperature_last(i,j)), dt )
      temperature_last(i,j) = temperature(i,j)
    enddo
  enddo
```

```
  if( mod(iteration,100).eq.0 ) then
    call track_progress(temperature, iteration)
  endif
```

```
  iteration = iteration+1
```

```
enddo
```



Done?



Calculate



**Update
temp
array and
find max
change**



Output

Serial Fortran Code Subroutines

```
subroutine initialize( temperature_last )
  implicit none

  integer, parameter      :: columns=1000
  integer, parameter      :: rows=1000
  integer                 :: i,j

  double precision, dimension(0:rows+1,0:columns+1) :: temperature_last

  temperature_last = 0.0

  !these boundary conditions never change throughout run

  !set left side to 0 and right to linear increase
  do i=0,rows+1
    temperature_last(i,0) = 0.0
    temperature_last(i,columns+1) = (100.0/rows) * i
  enddo

  !set top to 0 and bottom to linear increase
  do j=0,columns+1
    temperature_last(0,j) = 0.0
    temperature_last(rows+1,j) = ((100.0)/columns) * j
  enddo

end subroutine initialize
```

```
subroutine track_progress(temperature, iteration)
  implicit none

  integer, parameter      :: columns=1000
  integer, parameter      :: rows=1000
  integer                 :: i,iteration

  double precision, dimension(0:rows+1,0:columns+1) :: temperature

  print *, '----- Iteration number: ', iteration, ' -----'
  do i=5,0,-1
    write (*, '('( "i4," ", "i4," "):",f6.2," " )',advance='no'), &
      rows-i,columns-i,temperature(rows-i,columns-i)
  enddo
  print *
```

Whole Fortran Code

```

program serial
  implicit none

  !Size of plate
  integer, parameter      :: columns=1000
  integer, parameter      :: rows=1000
  double precision, parameter :: max_temp_error=0.01

  integer                :: i, j, max_iterations, iteration=1
  double precision       :: dt=100.0
  real                   :: start_time, stop_time

  double precision, dimension(0:rows+1,0:columns+1) :: temperature, temperature_last

  print*, 'Maximum iterations [100-4000]?'
  read*,   max_iterations

  call cpu_time(start_time)      !Fortran timer

  call initialize(temperature_last)

  !do until error is minimal or until maximum steps
  do while ( dt > max_temp_error .and. iteration <= max_iterations)

    do j=1,columns
      do i=1,rows
        temperature(i,j)=0.25*(temperature_last(i+1,j)+temperature_last(i-1,j)+ &
                               temperature_last(i,j+1)+temperature_last(i,j-1) )
      enddo
    enddo

    dt=0.0

    !copy grid to old grid for next iteration and find max change
    do j=1,columns
      do i=1,rows
        dt = max( abs(temperature(i,j) - temperature_last(i,j)), dt )
        temperature_last(i,j) = temperature(i,j)
      enddo
    enddo

    !periodically print test values
    if( mod(iteration,100).eq.0 ) then
      call track_progress(temperature, iteration)
    endif

    iteration = iteration+1

  enddo

  call cpu_time(stop_time)

  print*, 'Max error at iteration ', iteration-1, ' was ',dt
  print*, 'Total time was ',stop_time-start_time, ' seconds.'

end program serial

```

```

! initialize plate and boundary conditions
! temp_last is used to to start first iteration
subroutine initialize( temperature_last )
  implicit none

  integer, parameter      :: columns=1000
  integer, parameter      :: rows=1000
  integer                 :: i,j

  double precision, dimension(0:rows+1,0:columns+1) :: temperature_last

  temperature_last = 0.0

  !these boundary conditions never change throughout run

  !set left side to 0 and right to linear increase
  do i=0,rows+1
    temperature_last(i,0) = 0.0
    temperature_last(i,columns+1) = (100.0/rows) * i
  enddo

  !set top to 0 and bottom to linear increase
  do j=0,columns+1
    temperature_last(0,j) = 0.0
    temperature_last(rows+1,j) = ((100.0)/columns) * j
  enddo

end subroutine initialize

!print diagonal in bottom corner where most action is
subroutine track_progress(temperature, iteration)
  implicit none

  integer, parameter      :: columns=1000
  integer, parameter      :: rows=1000
  integer                 :: i, iteration

  double precision, dimension(0:rows+1,0:columns+1) :: temperature

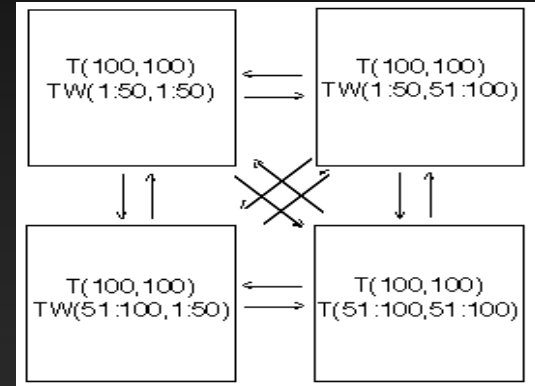
  print *, '----- Iteration number: ', iteration, ' -----'
  do i=5,0,-1
    write (*,('("i4,"",",i4,"):" ",f6.2," " )',advance='no'), &
           rows-i,columns-i,temperature(rows-i,columns-i)

    enddo
    print *
  end subroutine track_progress

```

First Things First: Domain Decomposition

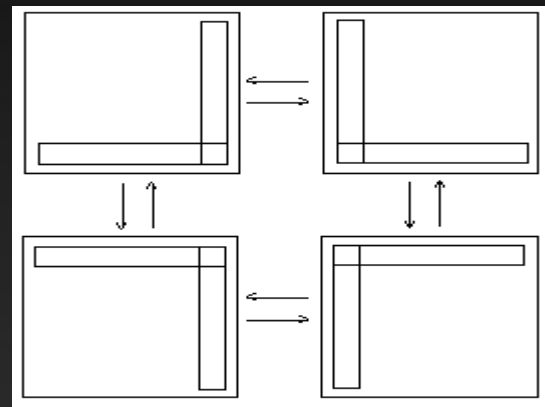
- All processors have entire T array.
- Each processor works on TW part of T.
- After every iteration, all processors broadcast their TW to all other processors.
- Increased memory. **NOT SCALABLE!**
- Global (message passing) variables are ALWAYS bad!



Try Again:

Domain Decomposition II

- Each processor has sub-grid.
- Communicate boundary values only.
- Reduces memory.
- Reduces communications.
- Have to keep track of neighbors in two directions.
- But not too bad.



Simplest: Domain Decomposition III



- Only have to keep track of up/down neighbors, and no corner case.
- Scales, as below. How would we handle 5 PEs with the “square decomposition”?

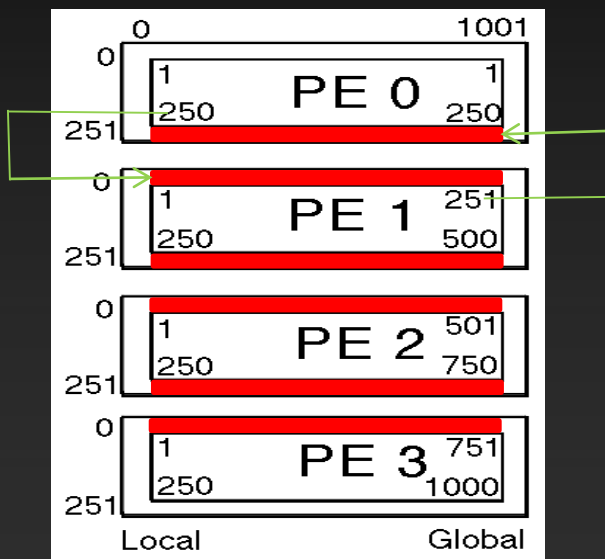


Simplest Decomposition for C Code

0		0																
	<table><tr><td>1</td><td>1</td></tr><tr><td>250</td><td>250</td></tr><tr><td>1</td><td>251</td></tr><tr><td>250</td><td>500</td></tr><tr><td>1</td><td>501</td></tr><tr><td>250</td><td>750</td></tr><tr><td>1</td><td>751</td></tr><tr><td>250</td><td>1000</td></tr></table>	1	1	250	250	1	251	250	500	1	501	250	750	1	751	250	1000	
1	1																	
250	250																	
1	251																	
250	500																	
1	501																	
250	750																	
1	751																	
250	1000																	
Local	Global	1001																

Simplest Decomposition for C Code

In the parallel case, we will break this up into 4 processors. There is only one set of boundary values. But when we distribute the data, each processor needs to have an extra row for data distribution, these are commonly called the “ghost cells”.



The program has a local view of data. The programmer has to have a global view of data. The ghost cells don't exist in the global dataset. They are only copies from the “real” data in the adjacent PE.

Sending Multiple Elements

- For the first time we want to send multiple elements. In this case, a whole row or column of data. That is exactly what the count parameter is for.
- The common use of the count parameter is to point the Send or Receive routine at the first element of an array, and then the count will proceed to strip off as many elements as you specify.
- This implies (and demands) that the elements are contiguous in memory. That will be true for one dimension of an array, but the other dimension(s) will have a stride.
- In C this is true for our rows. In Fortran this is true for our columns. This will give us a strong preference for the problem orientation in each language. Then we don't have to worry about strides in the strips that we send.
- However, it is very often necessary to send messages that are not contiguous data. Using defined data types, we can send other array dimensions, or even blocks or surfaces. We will talk about that capability in the Advanced talk.

Sending Multiple Elements

C: ← This last index is the one contiguous in memory.

```
int A[8][12];
```

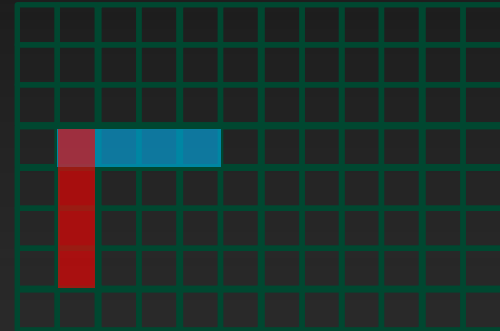
```
MPI_Send(&A[3][1], 4, MPI_INT, pe, tag, MPI_COMM_WORLD);
```

Fortran:

```
integer A(0:7,0:11)
```

```
MPI_Send(A(3,1), 4, MPI_INT, pe, tag, MPI_COMM_WORLD, err);
```

← This first index is the one contiguous in memory.



Array Ordering

- Once again, we will make this issue less critical from the MPI perspective once we learn about user defined datatypes in the advanced talk, but...
- this is extremely important to understand for general performance reasons. Notice how the C code iterates over the last (j) variable in the inner loop while the Fortran uses the first (i) in our serial code? This would kill our performance if it was the other way around. And I mean in the serial code. Go ahead and try...

```
for(i = 1; i <= ROWS; i++) {  
    for(j = 1; j <= COLUMNS; j++) {  
        Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] + Temperature_last[i-1][j] +  
                                     Temperature_last[i][j+1] + Temperature_last[i][j-1]);  
    }  
}
```

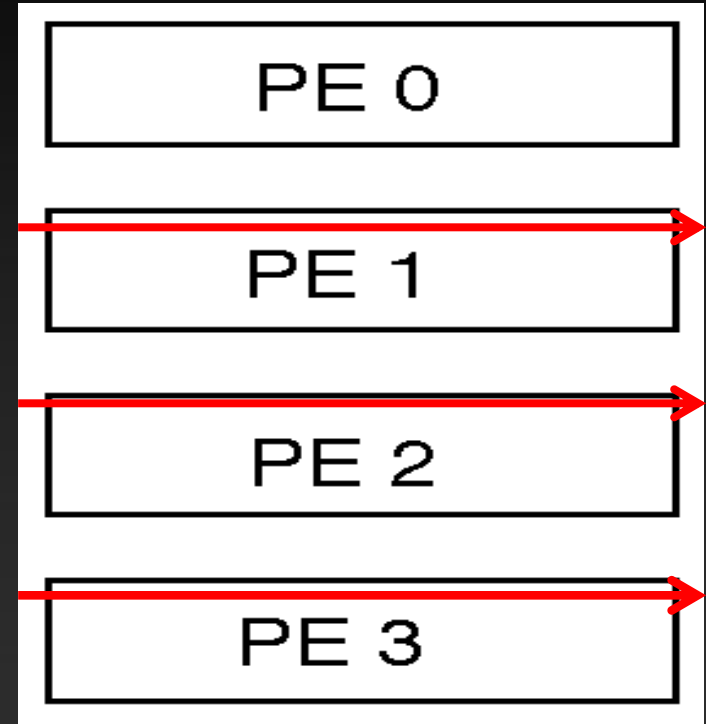
```
do j=1,columns  
    do i=1,rows  
        temperature(i,j)= 0.25 * (temperature_last(i+1,j)+temperature_last(i-1,j) + &  
                                   temperature_last(i,j+1)+temperature_last(i,j-1) )  
    enddo  
enddo
```

Sending Multiple Elements

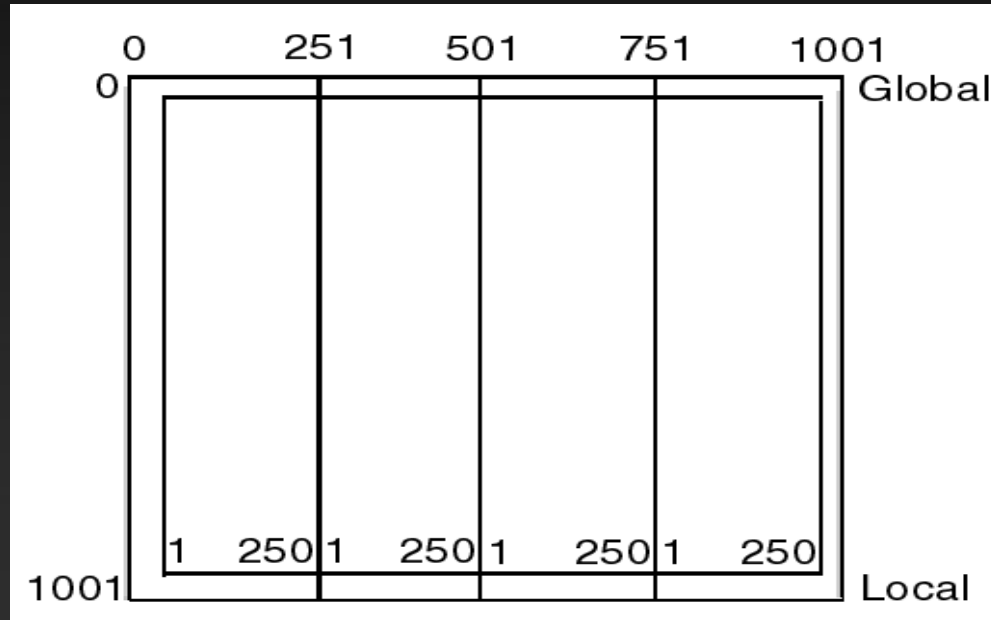
```
if ( mype != 0 ){  
    up = mype - 1  
    MPI_Send( t, COLUMNS, MPI_FLOAT, up, UP_TAG, comm);  
}
```

Alternatively

```
up = mype - 1  
if ( mype == 0 ) up = MPI_PROC_NULL;  
MPI_Send( t, COLUMNS, MPI_FLOAT, up, UP_TAG, comm);
```

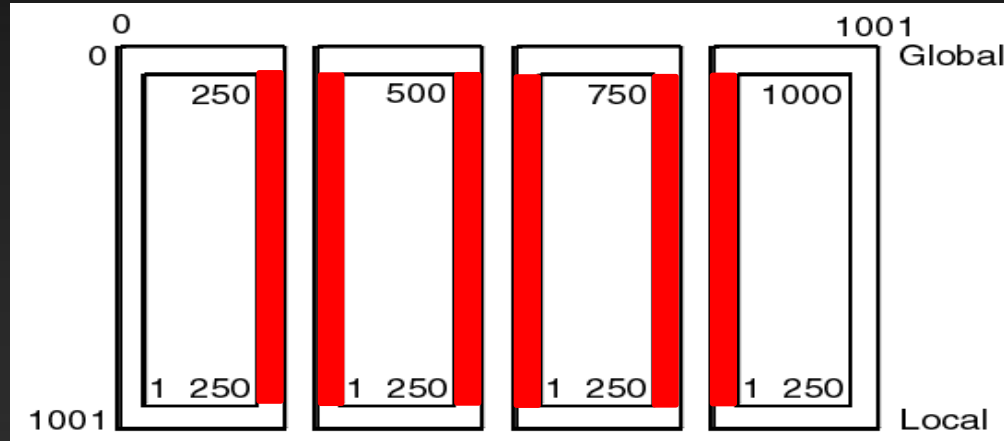


Simplest Decomposition for Fortran Code



Simplest Decomposition for Fortran Code

Then we send strips to ghost zones like this:



Same **ghost cell** structure as the C code, we have just swapped rows and columns.

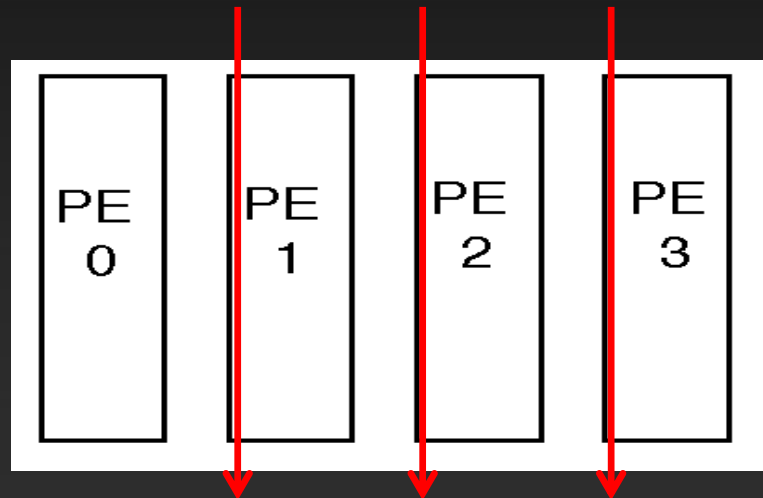
Sending Multiple Elements in Fortran

```
if( mype.ne.0 ) then
  left = mype - 1
  call MPI_Send( t, ROWS, MPI_REAL, left, L_TAG, comm, ierr)
endif
```

Alternatively

```
left = mype - 1
if( mype.eq.0 ) left = MPI_PROC_NULL
call MPI_Send( t, ROWS, MPI_REAL, left, L_TAG, comm, ierr)
endif
```

Note: You may also `MPI_Recv` from `MPI_PROC_NULL`



Main Loop Structure

```
for (iter=1; iter < NITER; iter++) {  
    Do averaging  
    Copy Temperature into Temperature_last
```

```
Send real values down
```

```
Temperature or Temperature_last?
```

```
Send real values up
```

```
Receive values from above into ghost zone
```

```
Receive values from below into ghost zone
```

```
Temperature or Temperature_last?
```

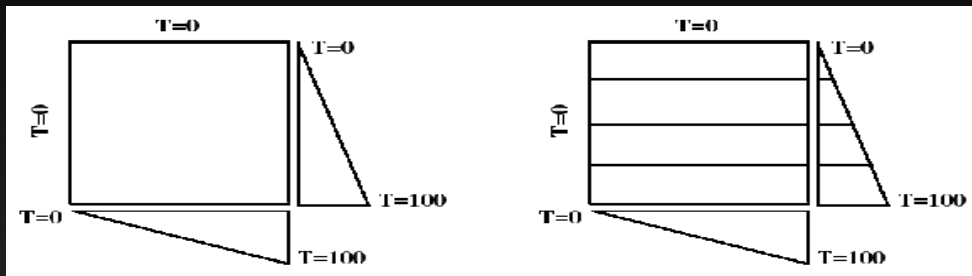
```
Find the max change
```

```
Synchronize?
```

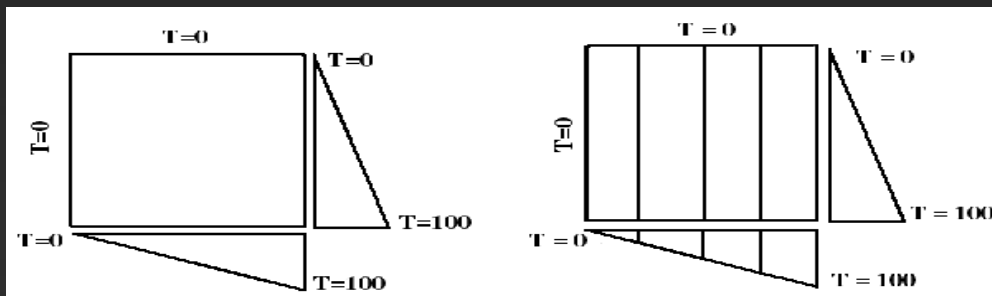
**Compute
Phase**
(almost unchanged)

**Communicate
Phase**
(all new)

Boundary Conditions



Both C and Fortran will need to set proper boundary conditions based upon the PE number.



Two ways to approach this exercise.

- Start from the serial code
- Start from the template (“hint”) code

Starting files in Exercises/MPI:

laplace_serial.c

laplace_serial.f90

laplace_template.c

laplace_template.f90

You can peek at my answer in /Solutions

laplace_mpi.c

laplace_mpi.f90

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

[illegible][illegible][illegible]

```
initialize(npes, my_PE_num);
```

```
// main calculation: average my four neighbors
```

```
for(i = 1; i <= ROWS; i++) {
```

```
for(j = 1; j <= COLUMNS; j++) {
```

```
Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] + Temperature_last[i-1][j] +
    Temperature_last[i][j+1] + Temperature_last[i][j-1]);
```

}

}

[illegible]

```

program mpi
    implicit none
    include 'mpif.h'

```

```
!Size of plate
integer, parameter      :: columns_global=1000
integer, parameter      :: rows=1000
```

```
double precision, dimension(0:rows+1,0:columns+1) :: temperature, temperature_last
```

```
!usual mpi startup routines
```

```
!It is nice to verify that proper number of PEs are running
```

```
!Only one PE should prompt user
if( mype == 0 ) then
    print*, 'Maximum iterations [100-4000]?'
    read*, max_iterations
endif
```

!Other PEs need to receive this information

```
call cpu_time(start_time)
```

```
call initialize(temperature_last, npes, mype)
```

```
!do until global error is minimal or until maximum steps
do while ( dt_global > max_temp_error .and. iteration <= max_iterations)
```

```
do j=1,columns
  do i=1,rows
    temperature(i,j)=0.25*(temperature_last(i+1,j)+temperature_last(i-1,j)+ &
                           temperature_last(i,j+1)+temperature_last(i,j-1) )
  enddo
enddo
```

Some ways you might go wrong...

You have two main data structures

- Temperature
- Temperature_last

Each has

- Boundary Conditions (unchanged through entire run)
- Ghost zones (changing every timestep)

Each iteration

- Copying/calculating Temperature to/from Temperature_last
- Sending/receiving into/from ghost zones and data

It is easy to mix these things up. I suggest you step through at least the initialization and first time step for each of the above combinations of elements.

There are multiple reasonable solutions. Each will deal with the above slightly differently.

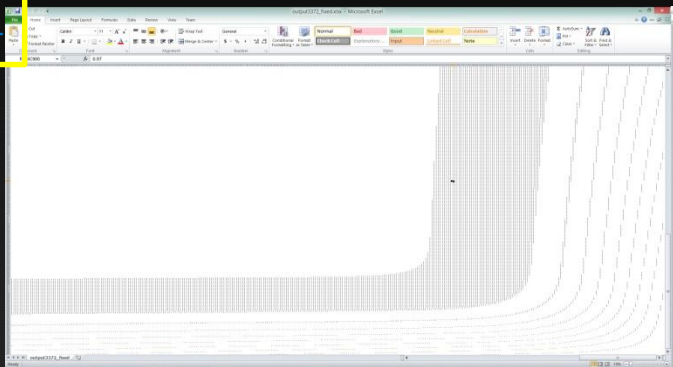
How do you know you are correct?



Your solution converges
at 3372 timesteps!

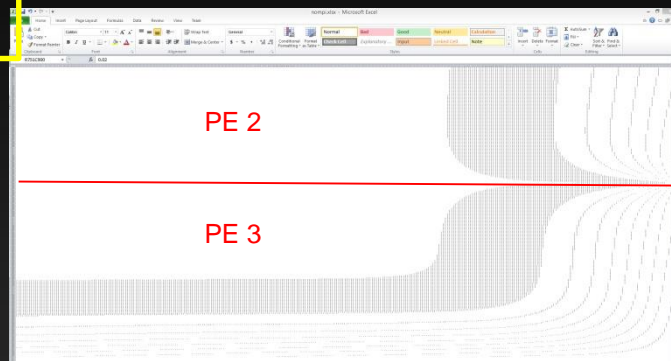
How do you know you are correct?

Bottom
Right
Corner



Working MPI Solution

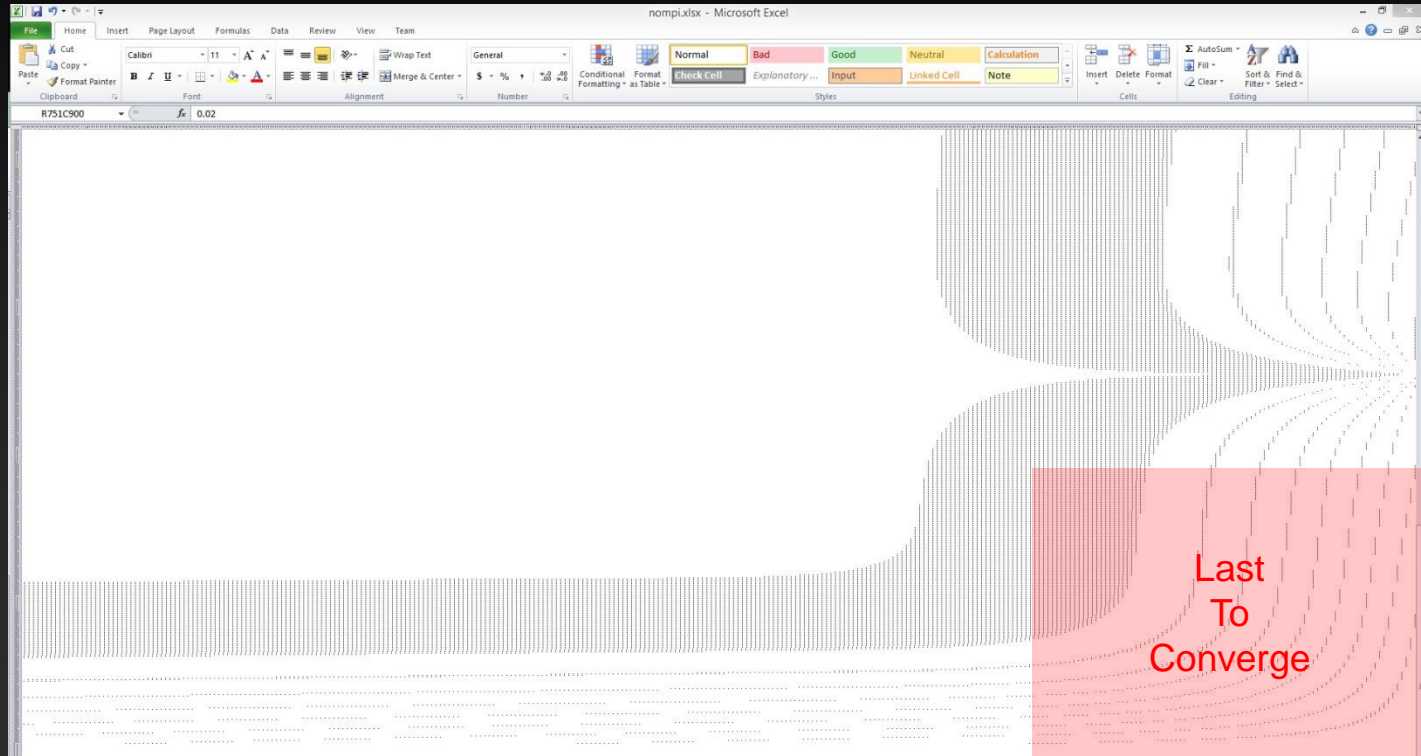
Bottom
Right
Corner



MPI Routines Disabled

Both converge at 3372 steps!

All the action is here.

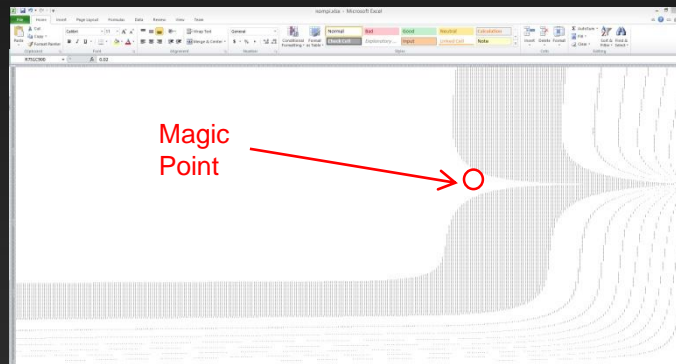


Check for yourself.

```
void output(int my_pe, int iteration) {  
    FILE* fp;  
    char filename[50];  
  
    sprintf(filename,"output%d.txt",iteration);  
  
    for (int pe = 0; pe<4; pe++){  
        if (my_pe==pe){  
  
            fp = fopen(filename, "a");  
  
            for(int y = 1; y <= ROWS; y++){  
                for(int x = 1; x <= COLUMNS; x++){  
                    fprintf(fp, "%5.2f ",Temperature[y][x]);  
                }  
                fprintf(fp,"\n");  
            }  
  
            fflush(fp);  
            fclose(fp);  
  
        }  
        MPI_Barrier(MPI_COMM_WORLD);  
    }  
}
```

```
C:  
if (my_PE_num==2)  
    printf("Global coord [750,900] is %f \n:", Temperature[250][900]);
```

```
Fortran:  
if (mype==2) then  
    print*, 'magic point', temperature(900,250)  
endif
```



- Human Readable
- 1M entries
- Visualize. I used Excel (terrible idea).

- If about 1.0, probably good
- Otherwise (like 0.02 here) probably not

A Quick Note About Our Pace Before We Start

This exercise is doable during the exercise session time allotted if all goes well.

That has been our historical standard.

However some of you may need a little more time. That is fine.

We will not “spoil” the exercise during the Laplace Exercise Review tomorrow.

Those of you that need additional time can use your accounts through next week.

Please take advantage of that. **If you complete this exercise, you understand MPI.**

Laplace Exercise

1. You copied a directory called Exercises/MPI into your home directory. Go there and you will see the files:

`laplace_template.c` and `laplace_serial.c`

or

`laplace_template.f90` and `laplace_serial.f90`

2. The templates are “hint” files with sections marked >>>> in the source code where you might add statements so that the code will run on 4 PEs. You can start from either these or from the serial code, whichever you prefer. A useful Web reference for this exercise is the Message Passing Interface Standard at:

<http://www.mpich.org/static/docs/latest/www3/>

3. To compile the program as it becomes an MPI code, execute:

```
mpicc laplace_your_mpi.c
```

```
mpif90 laplace_your_mpi.f90
```

4. In an interactive session (with at least 4 Pes: “interact -n 4”), you can just run these as:

```
mpirun -n 4 a.out
```

5. You can check your program against one possible solution in the Solutions directory:

```
laplace_mpi.c or laplace_mpi.f90
```

6. When you are done, let us know by hitting the survey button on the workshop page: bit.ly/XSEDE-Workshop