Laplace Exercise

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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

```c
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) )
endo
dndo
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++;
}
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.
```c
#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
    while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) { // do until error is minimal or until max steps
        // 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++){
                Temperature_last[i][j] = Temperature[i][j];
                dt = max( fabs(Temperature[i][j]-Temperature_last[i][j]), dt);
            }
        }
        // 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("Max 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]);
    }
   }
```
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
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

  write (*,'(a80)') '---------------- Iteration number: ', iteration, ' ------------------'

  do i=5,0,-1
    write (*,'(i4,i16,3f6.2)') rows-i,columns-i,temperature(rows-i,columns-i)
  enddo

print *
program serial
implicit none
!
Size of plate
!
integer, parameter :: columns=1000
integer, parameter :: rows=1000
integer, parameter :: max_iterations, iteration=1
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_last(i,j) = temperature(i,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) )

!
!
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
!
%temperature_last(i,j) = temperature(i,j)


dt = max( abs(temperature(i,j) - temperature_last(i,j)), dt )

!
!
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*, '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_last(i,j) = temperature(i,j)


dt = max( abs(temperature(i,j) - temperature_last(i,j)), dt )

!
!
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
!
%temperature_last(i,j) = temperature(i,j)


dt = max( abs(temperature(i,j) - temperature_last(i,j)), dt )

!
!
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*, '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_last(i,j) = temperature(i,j)


dt = max( abs(temperature(i,j) - temperature_last(i,j)), dt )

!
!
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
!
%temperature_last(i,j) = temperature(i,j)


dt = max( abs(temperature(i,j) - temperature_last(i,j)), dt )

!
!
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*, 'Total time was ',stop_time-start_time,' seconds.'
!
end program serial
All processors have an entire Temperature array.
Each processor works on its part of Temperature.
After every iteration, all processors broadcast their pieces to all other processors.

No! Preserving any large shared data structures is bad.
Increased memory. Not Scalable.
Large messages. Not Scalable.
Each processor has only its own sub-grid. 
1000x1000 array not longer exists (except on paper). 
Communicate boundary values only. 
Reduces memory. 
Reduces communications. 
Have to keep track of neighbors in two directions. 
But not bad.
Simplest: Domain Decomposition III

- Only have to keep track of up/down neighbors, and no corner case.
- Easiest with our simple message passing experience.
- Scales, as below. How would we handle 5 PEs with the “square decomposition”?
### Simplest Decomposition for C Code

![Graph showing decomposition](image)

<table>
<thead>
<tr>
<th>Local</th>
<th>Global</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1001</td>
</tr>
<tr>
<td>250</td>
<td>250</td>
</tr>
<tr>
<td>1</td>
<td></td>
</tr>
<tr>
<td>250</td>
<td>500</td>
</tr>
<tr>
<td>1</td>
<td></td>
</tr>
<tr>
<td>250</td>
<td>750</td>
</tr>
<tr>
<td>1</td>
<td></td>
</tr>
<tr>
<td>250</td>
<td>1000</td>
</tr>
</tbody>
</table>

- **Local** values range from 1 to 250.
- **Global** values range from 1001 to 1000.

---

**Note:** The diagram and values are illustrative and may not correspond directly to any specific C code implementation. The focus is on the concept of decomposition rather than the actual 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:

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 last index is the one contiguous in memory.

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…

```c
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]);
    }
}
```

```fortran
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
endo
```
Sending Multiple Elements

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

Alternatively (and there are many ways to do this):

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

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

Alternatively (and there are many ways to do this):

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

while (dt > MAX_TEMP_ERROR && iteration <= max_iterations)
    Calculate new Temperature
    Copy into temp array
    ...

Compute Phase
(almost unchanged)

Communicate Phase
(all new)

while (dt > MAX_TEMP_ERROR && iteration <= max_iterations)
    Calculate new Temperature
    Copy into temp array
    ...

Send values down (Temperature or Temperature_last?)
Send values up
Receive values from above into ghost zone (Temperature or Temperature_last?)
Receive values from below into ghost zone
Find max change
Synchronize?
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[]) {
    int i, j;
    int max_iterations;
    int iteration=1;

    // the usual MPI startup routines
    >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
    // verify only NPES PEs are being used
    >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
    // PE 0 asks for input
    >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
    // bcast max iterations to other PEs
    >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
    if (my_PE_num==0) gettimeofday(&start_time,NULL);
    initialize(npes, my_PE_num);

    while ( dt_global > 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]);
            }
        }

        // COMMUNICATION PHASE: send and receive ghost rows for next iteration
        >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
        dt = 0.0;
    }
}

MPI Template for C
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
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?

Both converge at 3372 steps!
All the action is here.
```c
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);
    }
}
```

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

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

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

- 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.**
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/

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