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.

\[ A_{k+1}(i, j) = \frac{A_k(i - 1, j) + A_k(i + 1, j) + A_k(i, j - 1) + A_k(i, j + 1)}{4} \]
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++;
}
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.
```c
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include <sys/time.h>

#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 iteration);

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

    for(; dt > MAX_TEMP_ERROR && iteration <= max_iterations ; iteration++) {

        // 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];
                Temperature[i+1][j] = Temperature_last[i][j];
                Temperature[i-1][j] = Temperature_last[i][j];
                Temperature[i][j+1] = Temperature_last[i][j];
                Temperature[i][j-1] = Temperature_last[i][j];
            }
        }

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

    gettimeofday(&stop_time,NULL);
    timersub(&stop_time, &start_time, &elapsed_time); // Unix timer 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 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;
                Temperature_last[i][0] = 0.0;
                Temperature_last[i][COLUMNS+1] = (100.0/ROWS)*i;
                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]);
            print("\n");
        }
    }

    return 0;
}
```

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 )
  !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)
  !these boundary conditions never change throughout run
  !set left side to 0 and right to linear increase
  do i=5,0,-1
    write (*,'("("i4",",i4,"):",f6.2," ")',advance='no'), &
    rows-i,columns-i,temperature(rows-i,columns-i)
  enddo
end subroutine track_progress
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
real :: 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
 outside of do loop:
!
! print* for progress
!
!
!
!
!
!
!

end subroutine initialize

! print diagonal in bottom corner where most action is
!
!
!
!
!
!
!

end subroutine track_progress

end program serial
First Things First: Domain Decomposition

- 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”? 

```
1000
```

```
1000
```

```
1000
```
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:

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

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

This last index is the one contiguous in memory.

Fortran:

```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...

```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
enddo
```
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.
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
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?
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;
    }
}

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.
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.*
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/](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 4Pes: “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