Assignment 4 OpenMP and hybrid OpenMP/MPI Programming Assignment

B. Wilkinson and C Ferner: Modification date Nov 5, 2013 (Minor clarifications)

Overview

This assignment explores using OpenMP alone and with MPI.

Part 1 provides basic practice in coding, compiling and running OpenMP programs, covering hello world program, timing, using work sharing for, and sections constructs. OpenMP code is given. You are also asked to parallelize matrix multiplication using the work sharing **for** construct and draw conclusions. Code for sequential matrix multiplication is given.

Part 2 asks you to write a sequential program for the astronomical *n*-body problem. You are to add graphical output. Then convert the sequential program to an OpenMP program. A template for the sequential program is given.

Part 3 is for graduate students only (extra credit for undergraduates). You are to re-write the program in Part 2 to have both OpenMP threads and MPI message-passing routines. A sample hybrid OpenMP/MPI program is given.

Preliminaries

For this assignment, we will use the UNCC **cci-grid0x.uncc.edu** cluster. First carefully read the separate instructions on using this cluster.¹ We will use **coit-grid05** for OpenMP – four quad-core processor (16) core) shared memory system. You cannot ssh directly into this computer. First log onto the UNCC cluster using the gateway **cci-gridgw.uncc.edu.** From **cci-gridgw.uncc.edu**, ssh into **cci-grid05** with the command:

[<username@cci-gridgw ~]\$ ssh cci-grid05

Create a directory called **Assign4** to hold all the files for this assignment and **cd** into this directory*.*

Part 1 – OpenMP Tutorial (undergraduates 40%, graduates 30%)

The purpose of this part is to become familiar with OpenMP constructs and programs.

Task 1 – Compile a "hello world" program

An OpenMP hello world program is given below:

```
#include <omp.h> 
#include <stdio.h> 
#include <stdlib.h>
```
¹You may use your own computer with an OpenMP compiler installed instead.

```
int main (int argc, char *argv[]) { 
   int nthreads, tid; 
   /* Fork a team of threads giving them their own copies of variables */ 
   #pragma omp parallel private(nthreads, tid) 
\{tid = omp qet thread num(); \frac{1}{2} // Obtain thread number
    printf("Hello World from thread = d\n\cdot t tid);
      if (tid == 0) { // Only master thread does this 
        nthreads = omp_get_num_threads(); 
          printf("Number of threads = d\n\times n", nthreads);
      } 
   } // All threads join master thread and disband 
}
```
This program has the basic **parallel** construct for defining a single parallel region for multiple threads. It also has a **private** clause for defining a variable local to each thread. *Remember that OpenMP constructs such as parallel have their opening braces on the next line and not on the same line.*

Create this program and call it **omp_hello.c**. Compile the program with the regular gcc compiler (version 4.2 onwards) using the command:

cc –fopenmp –o omp_hello omp_hello.c

Execute the program with the command:

./omp_hello

You should get a listing showing a number of threads such as:

```
Hello World from thread = 0 
Number of threads = 4 
Hello World from thread = 3 
Hello World from thread = 2 
Hello World from thread = 1
```
The number of threads will depend upon the particular computer system. Explain your output.

Alter the number of threads to 8. There are three ways to do this and you should try all three (separately).

Method 1:

Altering the environment variable with the command (at the command prompt):

export OMP_NUM_THREADS=8

Check value is correct with the command:

echo \$OMP_NUM_THREADS

Re-execute the program.

Method 2:

Undo method 1 using the command:

unset OMP_NUM_THREADS

Add the following function *BEFORE* the parallel region **pragma**:

omp_set_num_threads(8);

Re-execute the program.

Method 3:

Undo method 2 by removing the omp_set_num_threads() function. Add the following clause to the parallel region **pragma** statement:

```
num_threads(8)
```
Re-execute the program.

What to submit from this task

Your submission document should include the following:

- 1) A copy of the hello world source program;
- 2) Screenshot from compiling and running your hello world program;
- 3) Screenshots from using the three above methods to alter the number of threads (this should include evidence of the modification as well as the output from running the program).

Task 2– Work sharing with the for construct

This task explores the use of the **for** work-sharing construct. The following program adds two vectors together using a work-sharing approach to assign work to threads:

```
#include <omp.h> 
#include <stdio.h> 
#include <stdlib.h> 
#define CHUNKSIZE 10 
#define N 100 
int main (int argc, char *argv[]) { 
   int nthreads, tid, i, chunk; 
  float a[N], b[N], c[N];
  for (i=0; i < N; i++)
```

```
a[i] = b[i] = i * 1.0; // initialize arrays
  chunk = CHUNKSIZE; #pragma omp parallel shared(a,b,c,nthreads,chunk) private(i,tid) 
\{tid = omp\_get\_thread\_num();
     if (tid == 0) {
        nthreads = omp_get_num_threads(); 
       printf("Number of threads = d\n\times n", nthreads);
 } 
    printf("Thread %d starting...\n\timesn",tid);
       #pragma omp for schedule(dynamic,chunk) 
    for (i=0; i<N; i++)c[i] = a[i] + b[i];printf("Thread d: c[kd] = f\infty, tid, i, c[i]);
 } 
   } /* end of parallel section */
```
This program has an overall **parallel** region within which there is a work-sharing **for** construct. Compile and execute the program. Depending upon the scheduling of work different threads might add elements of the vector. It may be that one thread does all the work. Execute the program several times to see any different thread scheduling. In the case that multiple threads are being used, observe how they may interleave.

Experimenting with Scheduling:

Alter the code from **dynamic** scheduling to **static** scheduling and repeat. What are your conclusions?

Alter the code from **static** scheduling to **guided** scheduling (chunk size is irrelevant) and repeat. What are your conclusions?

Time of execution

}

Measure the execution time by instrumenting the MPI code with the OpenMP routine **omp_get_wtime()** at the beginning and end of the program and finding the elapsed in time. The function **omp_get_wtime()** returns a **double**.

What to submit from this task

Your submission document should include the following:

- 1) A copy of the source program;
- 2) Screenshot from compiling and running the program;
- 3) Screenshots from of running the program with dynamic and static scheduling;
- 4) Screenshot of output of execution time from instrumenting the program;

5) Your conclusions about the different scheduling approaches.

Task 3– Work-sharing with the sections construct

This task explores the use of the **sections** construction. The program below adds elements of two vectors to form a third and also multiplies the elements of the arrays to produce a fourth vector.

```
#include <omp.h> 
#include <stdio.h> 
#include <stdlib.h> 
#define N 50 
int main (int argc, char *argv[]) { 
   int i, nthreads, tid; 
  float a[N], b[N], c[N], d[N];
  for (i=0; i< N; i++) \{ // Some initializations, arbitrary values
     a[i] = i * 1.5;b[i] = i + 22.35ic[i] = d[i] = 0.0; } 
   #pragma omp parallel shared(a,b,c,d,nthreads) private(i,tid) 
\{ tid = omp_get_thread_num(); 
     if (tid == 0) {
           nthreads = omp_get_num_threads(); 
          printf("Number of threads = d\n\cdot", nthreads);
 } 
     printf("Thread %d starting...\n\timesn", tid);
      #pragma omp sections nowait 
      { 
           #pragma omp section 
        { 
            printf("Thread %d doing section 1\pi,tid);
            for (i=0; i<N; i++) {
               c[i] = a[i] + b[i];printf("Thread d: c[8d] = f\n", tid, i, c[i]);
 } 
 } 
           #pragma omp section 
       \{printf("Thread %d doing section 2\n",tid);
             for (i=0; i<N; i++) {
               d[i] = a[i] * b[i];printf("Thread d: d[zd] = tf\n",tid,i,d[i]);
 } 
 } 
        } // end of sections 
      printf("Thread d done.\n",tid);
```
}

This program has a parallel region but now with variables declared as shared among the threads as well as private variables. Also there is a sections work sharing construct. Within the sections construct, there are individual section blocks that are to be executed once by one member of the team of threads. *Remember that OpenMP constructs such as sections and section have their opening braces on the next line and not on the same line.*

Compile and execute the program and make conclusions on its execution.

What to submit from this task

Your submission document should include the following:

- 1) A copy of the source program;
- 2) Screenshot from compiling and running the program;
- 3) Your conclusions.

Task 4 – Matrix Multiplication

In this part, you are to add OpenMP constructs to the sequential program for matrix multiplication given here:

```
#include <omp.h> 
#include <stdio.h> 
#include <stdlib.h> 
#define M 500 
#define N 500 
int main(int argc, char *argv) { 
     omp_set_num_threads(8);//set number of threads here 
     int i, j, k; 
     double sum; 
    double start, end; \sqrt{2} // used for timing
     double **A, **B, **C; 
    A = \text{malloc}(M^* \text{sizeof}(double *)); B = malloc(M*sizeof(double *)); 
    C = \text{malloc}(M^* \text{sizeof}(double *));for (i = 0; i < M; i++) {
      A[i] = malloc(N*sizeof(double));B[i] = \text{malloc}(N^* \text{sizeof}(double));C[i] = malloc(N*sizeof(double));
       } 
      for (i = 0; i < M; i++) {
         for (j = 0; j < N; j++) {
               A[i][j] = j*1;
```

```
B[i][j] = i * j + 2;C[i][j] = j-<i>i</i>*2; } 
 } 
   start = omp_get_wtime(); //start time measurement 
    for (i = 0; i < M; i++) {
       for (j = 0; j < N; j++) {
         sum = 0;for (k=0; k < M; k++) {
                   sum += A[i][k]*B[k][j]; } 
            C[i][j] = sum; } 
     } 
  end = omp_get_wtime(); //end time measurement
   printf("Time of computation: %f\n", end-start);
```
You are to parallelize this algorithm in three different ways:

}

- 1. Add the necessary **pragma** to parallelize the outer **for** loop;
- 2. Remove the **pragma** for the outer **for** loop and create a pragma for the middle **for** loop;
- 3. Add the necessary **pragma**'s to parallelize both the outer and middle **for** loops.

and collect timing data given one thread, four threads, eight threads, and 16 threads and two matrix sizes, 50x50 and 500x500. You will find that when you run the same program several times, the timing values can vary significantly. Therefore for each set of conditions, collect ten data values and average them. You are encouraged to use a spreadsheet program either from MS Office or OpenOffice to store your data and perform the necessary calculations.

Here are the conditions you should collect data for:

- 1. No parallelization at all (that is, the given program)
- 2. Parallelizing the loops as above with 1, 4, 8, and 16 threads using matrix sizes 50x50 and 500x500

*Acknowledgement:*This part is derived from the OpenMP tutorial at https://computing.llnl.gov/tutorials/openMP/exercise.html

What to submit from this task

Your submission document should include the following:

- 1) Two copies of the source program: (outer loop 8 threads-500x500 and middle loop 8 threads-500x500);
- 2) Two screenshot from compiling and running the program: one for each of the two ways;
- 3) Results of your graphs of the average timings;
- 4) Your conclusions and explanations of the data.

Part 2 Astronomical *n***-Body Problem (60% undergraduates, 40% graduates)**

The Problem

The objective is to find the positions and movements of bodies in space (e.g., planets) that are subject to gravitational forces from other bodies using Newtonian laws of physics. The gravitational force between two bodies of masses m_a and m_b is given by:

$$
F = \frac{Gm_a m_b}{r^2}
$$

where G is the gravitational constant and Γ is the distance between the bodies. When there are multiple bodies, each body will feel the influence of each of the other bodies and the forces will sum together (taking into account the direction of each force). Subject to forces, a body will accelerate according to Newton's second law:

$$
F = ma
$$

where *m* is the mass of the body, *F* is the force it experiences, and *a* is the resultant acceleration. All the bodies will move to new positions due to these forces and have new velocities. Written as differential equations, we have:

> dv dt

 dx dt

 $F = m$

 $v =$

and

where
$$
v
$$
 is the velocity. For a computer simulation, we use values at particular times, t_0 , t_1 , t_2 , and so on, the time intervals being as short as possible to achieve the most accurate solution. Let the time interval be Δt . Then, for a particular body of mass m , the force is given by:

$$
F = \frac{m(v^{t+1} - v^t)}{\Delta t}
$$

$$
v^{t+1} = v^t + \frac{F\Delta t}{m}
$$

and a new velocity

where v^{t+1} is the velocity of the body at time $t + 1$, and v^t is the velocity of the body at time *t*. If a body is moving at a velocity *v* over the time interval Δt , its position changes by

$$
x^{t+1} - x^t = v\Delta t
$$

where x^{t+1} is its position at time $t+1$ and x^t is its position at time *t*. Once bodies move to new positions, the forces change and the computation has to be repeated. The velocity is not actually constant over the time interval, Δt , so only an approximate answer is obtained.

Three-Dimensional Space. If the bodies are in a three-dimensional space, all values (forces, velocities and distances) are vectors and have to be resolved into three directions, *x*, *y*, and *z*. The forces due to all the bodies on each body are added together in each dimension to obtain the final force on each body. Finally, the new position and velocity of each body are computed due to the forces. This then gives the velocity and positions in three directions. For a simple computer solution, we usually assume a threedimensional space with fixed boundaries. Actually, the universe is continually expanding and does not have fixed boundaries!

For this assignment, you will use two-dimensional space so the forces, velocities and distances need only be resolved into two directions, x and y.

Two-Dimensional Space. In a two-dimensional space having a coordinate system (x, y) , the distance between two bodies at (x_a, y_a) and (x_b, y_b) is given by:

$$
r = \sqrt{(x_b - x_a)^2 + (y_b - y_a)^2}
$$

The forces are resolved in the two directions, using:

$$
F_x = \frac{Gm_a m_b}{r^2} \left(\frac{x_b - x_a}{r}\right)
$$

$$
F_y = \frac{Gm_a m_b}{r^2} \left(\frac{y_b - y_a}{r}\right)
$$

It is convenient to store the position and velocities of the bodies in an array as shown in Table 1.

Table 1: Input data

Sequential Code. The overall gravitational *N*-body computation can be described by the following steps:

for $(t = 0; t < T; t+)$ { // for each time interval

for $(x = 0; x < N; x++)$ $\{\n\forall$ for body x, calculate force on body due to other bodies for $(i = 0; i < N; i++)$ { if $(a != i)$ { // for different bodies

```
x_{\text{diff}} = ...; // compute distance between body a and body i in x direction
          y diff = ... ; // compute distance between body a and body i in y direction
          r = ...; //compute distance r
          F = ...: // compute force on bodies
          Fx[x] += ...; // resolve and accumulate force in x direction
          Fy[x] += ...; // resolve and accumulate force in y direction
        } 
    } 
 } 
for (i = 0; i < N; i++) { // for each body, compute and update positions and velocity
   A[i][x_{\text{velocity}}] = ...; // new velocity in x direction, column 4 in Table 1
   \text{A[i]}[y_{\text{velocity}}] = ...; // new velocity in y direction, column 5 in Table 1
   A[i][x\_position] = ...; // new position in x direction, column 2 in Table 1
   \text{A[i]}[y\_position] = ...; // new position in y direction, column 3 in Table 1
    }
```
} // end of simulation

Task 1

Write a sequential C program that computes the movement on *N* bodies in two dimensions, where *N* is a constant. Set $N = 8$. Let the number of time intervals be another constant *T*. Set $T = 100$. Select a suitable value for the time interval Δt through experimentation. Use a value of G = 100 and an x-y resolution of 1000 x 1000 points. The program is to read the initial values for masses, initial positions, and velocities from a file. Store initial data in an array (Table 1). Update this array after each iteration and display the values. Demonstrate your program with the input data file provided on the course home page, and with your own input data file.

Task 2 Display movement of the bodies over time

Find a way to display the movement of the bodies over time. They are several ways this can be achieved. For example:

1. Display movement using X11 graphics dynamically while program is executing. Follow the separate notes on creating X11 graphical output posted on the home page to create X11 display of the bodies moving while the program is executing. Forward the X11 graphics to your PC as explained in those notes.

Alternatively:

2 Create graphical output or a video after program has executed. Modify the program to collect the 100 time steps of data. (Change the two-dimensional array holding the data in Table 1 to three dimensions (the third dimension being time.) At the end of executing the program for 100 time steps, store and download the 3-dimensional data array. Use this data to display the movement of the bodies over time (pictures of bodies or video). X11 graphics could be used.

Task 3

Re-write your program as an OpenMP program to execute on **cci-grid05** using all 4 processors (16 cores in total). Incorporate code to measure the time of execution.

What to submit from this part

Your submission document should include the following:

- 1) A listing of the sequential program
- 2) A screenshot of compiling and executing the sequential program
- 3) Pictures or video showing the movement of the bodies for the sequential program
- 4) A listing of the OpenMP program for the parallel program
- 5) Pictures or video showing the movement of the bodies
- 6) Comparison of the time of execution for sequential and parallel versions along with your conclusions and explanation of this data.

Part 3 Hybrid OpenMP/MPI Program

(For graduate students only 30%, extra credit for undergraduates)

In this part, you are to write a hybrid program that has both MPI message-passing routines and OpenMP threads. This is a form of "hybrid programming" and extremely relevant for clusters of multiprocessor and multicore computer systems. The message-passing routines are used to pass messages between computer systems and the threads are run using the multiple cores on each system. The overall structure of the program is illustrated below:

Figure 1 Hybrid MPI message passing and OpenMP threads

Sample MPI/OpenMP program and compiling. A sample MPI/OpenMP program, **hybrid.c**, is given below:

```
#include <stdio.h> 
#include <string.h> 
#include <stddef.h> 
#include <stdlib.h> 
#include "mpi.h" 
#define CHUNKSIZE 10 
#define N 100 
void openmp_code(){ 
    int nthreads, tid, i, chunk; 
    float a[N], b[N], c[N]; 
   for (i=0; i < N; i++)a[i] = b[i] = i * 1.0; // initialize arrays
    chunk = CHUNKSIZE; 
    #pragma omp parallel shared(a,b,c,nthreads,chunk) private(i,tid) 
    { 
      tid = omp\_get\_thread\_num();
      if (tid == 0) {
          nthreads = omp_get_num_threads(); 
         printf("Number of threads = d\n\times n", nthreads);
       } 
      printf("Thread %d starting...\n",tid);
       #pragma omp for schedule(dynamic,chunk) 
      for (i=0; i<N; i++)c[i] = a[i] + b[i];printf("Thread d: c[d] = f\n", tid, i, c[i]);
       } 
    } /* end of parallel section */ 
} 
main(int argc, char **argv ) { 
    char message[20]; 
    int i,rank, size, type=99; 
   MPI Status status;
    MPI_Init(&argc, &argv); 
    MPI_Comm_size(MPI_COMM_WORLD,&size); 
    MPI_Comm_rank(MPI_COMM_WORLD, &rank); 
   if(rank == 0) {
       strcpy(message, "Hello, world"); 
      for (i=1; i< size; i++) MPI_Send(message, 13, MPI_CHAR, i, type, MPI_COMM_WORLD); 
    } 
    else 
       MPI_Recv(message, 20, MPI_CHAR, 0, type, MPI_COMM_WORLD, &status); 
    openmp_code(); //all MPI processes run OpenMP code, no message passing 
    printf( "Message from process =%d : %.13s\n", rank,message); 
   MPI Finalize();
}
```
Compile with:

 mpicc -fopenmp -o hybrid hybrid.c

Note this command invokes the regular cc compiler.

Execute as an MPI program on the UNCC cluster **cci-gridgw.uncc.edu2**

mpiexec.hydra -f *<machinesfile>* **-n** *<number of processes>* **./hybrid**

Task 2 Hybrid MPI/OpenMP program

Modify your OpenMP program in Part 2 to be an hybrid program using both OpenMP and MPI. Use both **cci-gridgw.uncc.edu** and **cci-grid05** with MPI message passing between them and OpenMP threads on each. Use the following approach:

- 1. The master process holds the array and broadcast the array to the slaves
- 2. Each slave presents 4 bodies and computes the new position for those bodies
- 3. All positions are gathered by the master process and the array is updated
- 4. Steps 1 3 are repeated

What to submit from this part

Your submission document should include the following:

- 1) Result for task 1 sample program with an explanation of the output
- 2) A copy of the source program to perform the *n*-body problem using both MPI and OpenMP
- 3) A screenshot of compiling and executing the program
- 4) Comparison of the time of execution for sequential and parallel versions along with your conclusions and explanation of this data.

Assignment Preparation and Submission

Produce a document that provides the following details:

- 1) Your name and school;
- 2) Whether you are a graduate or undergraduate student;
- 3) A full explanation of your code;
- 4) Code listing;
- 5) Sample output;
- 6) Insightful conclusions.

Submit to Moodle by the due date (see home page). Combine everything into one PDF file. *All students must work individually.* **Include all code, not as screen shots of the listings but as complete properly documented code listing.**

 ² VERY IMPORTANT -- NOT FROM **cci-grid05**