

Shared Memory Programming with OpenMP - Exercise Notes

OpenMP on ARCHER2

Compiling OpenMP programs

The Cray compilers (cc/ftn) are loaded by default.

To compile an OpenMP code, simply add the flag **-fopenmp** for the C compiler or **-h omp** for the Fortran compiler.

Using a Makefile

Makefiles are supplied with most of the exercise to help you build the code.

To build the code in a directory, just type **make**, and to remove all object and executable files, type **make clean**

Job Submission

Batch processing the only way of accessing the compute nodes on ARCHER2. For doing accurate timing runs you should use the compute nodes. To do this, you should submit a batch job as follows.

```
sbatch myjob.slurm
```

where **myjob.slurm** is the shell script supplied with each exercise.

You will have received a registration email letting you know the project code for this course. When you sign up for your machine account in this project, a personal budget for your user will be created. For example, if you are using project **ta123** and your username is **sam** then your personal budget will be **ta123-sam**. This is the budget code you should use in your submit scripts – you will need to edit the script to use your own budget code before you submit it.

To change the number of threads, edit the script and change the value assigned to the **OMP_NUM_THREADS** variable. You can monitor your job's status with the **squeue** command and queued or running jobs can be cancelled with **scancel**.

For further details please refer to the ARCHER2 User and Best Practice Guide at <https://docs.archer2.ac.uk/user-guide/>

Getting started

Copy the tar file containing the code to your account on ARCHER2 and unpack it with the commands:

```
cp /home/z19/shared/TP/TP.tar .
```

```
tar xvf TP.tar
```

Exercise 1: Hello World

This is a simple exercise to introduce you to the compilation and execution of OpenMP programs. The example code can be found in `*/HelloWorld/` where the `*` represents the language of your choice, i.e. `C`, or `Fortran90`.

Compile the code, making sure you use the appropriate flag to enable OpenMP. Before running it, set the environment variable `OMP_NUM_THREADS` to a number `n` between 1 and 4 with the command:

```
export OMP_NUM_THREADS=n
```

When run, the code enters a parallel region at the `!$OMP PARALLEL / #pragma omp parallel` directive. At this point `n` threads are spawned, and each thread executes the print command separately. The `OMP_GET_THREAD_NUM()` / `omp_get_thread_num()` library routine returns a number (between 0 and `n-1`) which identifies each thread.

Extra Exercise

Incorporate a call to `omp_get_num_threads()` into the code and print its value inside and outside the parallel region.

Exercise 2: Area of the Mandelbrot Set

The aim of this exercise is to use the OpenMP directives learned so far and apply them to a real problem. It will demonstrate some of the issues which need to be taken into account when adapting serial code to a parallel version.

The Mandelbrot Set

The Mandelbrot Set is the set of complex numbers c for which the iteration $z = z^2 + c$ does not diverge, from the initial condition $z = c$. To determine (approximately) whether a point c lies in the set, a finite number of iterations are performed, and if the condition $|z| > 2$ is satisfied, then the point is considered to be outside the Mandelbrot Set. What we are interested in is calculating the area of the Mandelbrot Set. There is no known theoretical value for this, and estimates are based on a procedure similar to that used here.

The Code

The method we shall use generates a grid of points in a box of the complex plane containing the upper of the (symmetric) Mandelbrot Set. Then each point is iterated using the equation above a finite number of times (say 2000). If within that number of iterations the threshold condition $|z| > 2$ is satisfied then that point is considered to be outside of the Mandelbrot Set. Then counting the number of points within the Set and those outside will lead to an estimate of the area of the Set.

Parallelise the serial code using the OpenMP directives and library routines that you have learned so far. The method for doing this is as follows:

1. Start a parallel region before the main loop, nest making sure that any private, shared or reduction variables within the region are correctly declared.
2. Distribute the outermost loop across the threads available so that each thread has an equal number of the points. For this you will need to use some of the OpenMP library routines.

Once you have written the code try it out using 1, 2, 3 and 4 threads. Check that the results are identical in each case, and compare the time taken for the calculations using different number of threads.

Extra Exercise

Is your solution well load balanced? Try different ways of mapping iterations to threads.

Exercise 3: Mandelbrot again

You can start from the code you have already, or another copy of the sequential code which can be found in `*/Mandelbrot2/`.

This time parallelise the outer loop using a **PARALLEL DO** / **parallel for** directive. Don't forget to use **default(none)** and declare the shared, private and reduction variables. Add a schedule clause and experiment with the different schedule kinds.

Exercise 4: Nested parallelism

Now parallelise *both* outer loops in the Mandelbrot example using nested parallel regions. To enable nested parallelism use

```
export OMP_NESTED=true
```

and set the number of threads at each level with, for example,

```
export OMP_NUM_THREADS=2,4
```

You will need to think carefully about the data scoping (i.e. shared/private/reduction). Experiment with different thread numbers – is the performance ever better than with one level of parallelism?

You can also try parallelising both loops using a parallel loop directive on the outer loop and a collapse clause.

Exercise 5: Molecular Dynamics

The aim of this exercise is to demonstrate how to use OpenMP critical constructs to parallelise a molecular dynamics code.

The Code

The code can be found in ***/MolDyn/**. The code is a molecular dynamics (MD) simulation of argon atoms in a box with periodic boundary conditions. The atoms are initially arranged as a face-centred cubic (fcc) lattice and then allowed to melt. The interaction of the particles is calculated using a Lennard-Jones potential. The main loop of the program is in the file **main.c / main.f90**. Once the lattice has been generated and the forces and velocities initialised, the main loop begins. The following steps are undertaken in each iteration of this loop:

1. The particles are moved based on their velocities, and the velocities are partially updated (call to **domove**)
2. The forces on the particles in their new positions are calculated and the virial and potential energies accumulated (call to **forces**)
3. The forces are scaled, the velocity update is completed and the kinetic energy calculated (call to **mkekin**)
4. The average particle velocity is calculated and the temperature scaled (call to **velavg**)
5. The full potential and virial energies are calculated and printed out (call to **prnout**)

Parallelisation

The parallelisation of this code is a little less straightforward. There are several dependencies within the program which will require use of the critical construct as well as the reduction clause. The instructions for parallelising the code are as follows:

1. Edit the subroutine/function in **forces.c / forces.f90**. Add a **!\$OMP PARALLEL DO / #pragma omp parallel for** directive to the outermost loop in this subroutine, identifying any private or reduction variables. Hint: There are 2 reduction variables.

2. Identify the variable within the loop which must be protected from possible race conditions and use `!$OMP CRITICAL / #pragma omp critical` to ensure this is the case.

Once this is done the code should be ready to run in parallel. Compare the output using 2, 3 and 4 threads with the serial output to check that it is working. Try adding the schedule clause with the kind `static,n` to the `DO/for` directive for different values of `n`. Does this have any effect on performance?

Exercise 6: Molecular Dynamics Part II

Following on from the previous exercise, we will update the molecular dynamics code to take advantage of orphaning and examine the performance issues of using critical regions.

Orphaning

To reduce the overhead of starting and stopping the threads, you can change the `PARALLEL DO / parallel for` directive to a `DO/for` directive and start the parallel region outside the main loop of the program. In `main.c / main.f90` enclose the main loop in a parallel region. Except for the forces routine, all the other work in this loop should be executed by one thread only. Ensure that this is the case using the single or master construct. Recall that any reduction variables updated in a parallel region but outside of the `DO/for` construct should be updated by one thread only. As before, check your code is still working correctly. Is there any difference in performance compared with the code without orphaning?

Extra exercise

Try using array reductions, or atomic directives, or lock routines (with one lock variable per particle) instead of critical regions.

Exercise 7: Mandelbrot with tasks

Redo the Mandelbrot exercise using OpenMP tasks. To begin with, make the computation of each point a task, and use one thread only to generate the tasks. Once this is working, measure the performance. Note that reduction variables cannot be used inside tasks – you will need to use an alternative mechanism to avoid the race condition on `numoutside`.

Now modify your code so that it treats each row of points as a task. Modify your code again, so that all threads generate tasks. Which version performs best? Is the performance better or worse than using a loop directive?