PROGRAMMING MODEL EXAMPLES

DEMONSTRATION EXAMPLES OF VARIOUS PROGRAMMING MODELS

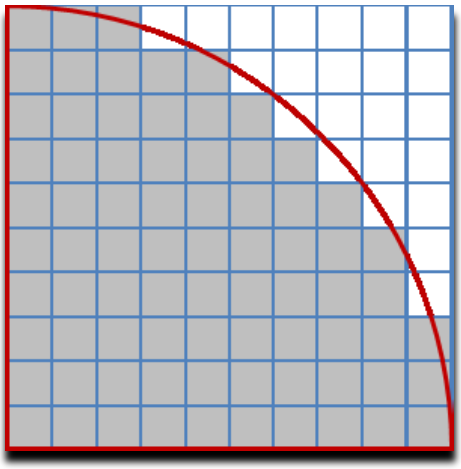
OVERVIEW

Building an application to use multiple processors (cores, cpus, nodes) can be done in various ways and in particular the High Performance Computing (HPC) community has a long experience in using multithreaded and multi-process programming models to develop fast scalable applications on a range of hardware platforms. Typical APIs in use are OpenMP (source threading markup) and MPI (message-passing). The examples provided and described here can be used to compare these models when used to tackle a very simple problem and as a platform to learn how to build and launch parallel applications on the Cray XC supercomputer.

The demonstrator problem was chosen for its simplicity and lack of subtle issues across the range of programming models.

THE SAMPLE PROBLEM AND ALGORITHM

The example we have chosen is to calculate π by piecewise approximation of the area of a circle. You could do this by drawing a quarter circle on graph paper and counting the number of squares inside and outside the circle. This approximates the area within the circle and hence π can be determined. A more complicated example might be to find the area/volume of a fractal structure; this would be much more computationally intensive and analytically complex. The algorithm covers the quarter circle with an N by N grid and uses a test in the centre to determine if the grid square is inside the circle (the error should average out somewhat). Each program loops over values of i and j indices to get the coordinates of the centre of each small square within the much larger unit square. The approximate value for π is then 4 times the number of squares within the quarter circle divided by the total number of squares. (We can of course do this is a much better way but not if we want to generalise to something like a fractal shape.)



CODE EXAMPLES PROVIDED

The algorithm previously mentioned was coded using various programming models. You will need to unpack Cray_pm_examples.tar or access a location provided to you. Once unpacked you will find a directory with a README, sample job scripts and subdirectories C and Fortran which contain source for multiple versions of the pi program. The following versions are available:

Programming Model	**Source File**
Basic Fortran	`pi_serial.f90`
Fortran using parallel language features	`pi_coarray.f90`
Basic Fortran with OpenMP threading	`pi_openmp.f90`
Fortran using MPI	`pi_mpi.f90`
Fortran using MPI and OpenMP (hybrid)	`pi_mpi_openmp.f90`
Fortran using SHMEM	`pi_shmem.f90`
Fortran using OpenACC	`pi_openacc.f90`
Basic C	`pi_serial.c`
C with pthreads	`Pi_pthreads.c`
C with OpenMP	`pi_openmp.c`
C with MPI	`pi_mpi.c`
C with MPI and OpenMP	`pi_mpi_openmp.c`
C with SHMEM	`pi_shmem.c`
C with OpenSHMEM	`pi_openshmem.c`
UPC	`pi_upc.c`
C++ using coarray implementation (Cray)	`pi_coarray.cpp`

Note that the pthreads version uses OMP_NUM_THREADS to pick up the number of threads to use so that it can be run from a job set up to run an OpenMP application.

Note in particular that no attempt has been made to optimize these examples as the goal was to provide the simplest possible code to illustrate the programming models. In some cases idioms are used that illustrate a feature of the programming model even if you would not normally code that way (for example the SHMEM version uses atomic update instead of reduction.)

In each language directory (Fortran and C) is a Makefile that will build most of the examples with the Cray CCE compiler. The SHMEM and OpenACC examples need specific modules to be loaded before they will compile. In addition a more complex version of the source is supplied (Fortran_timing and C_timing) with timer code added, this is more useful for scaling studies as the internal timing is the elapsed time of the computation only.

Job scripts are provided in the jobscripts directory which you can use as templates to create your own scripts. They work with one particular installation of PBS and the PBS headers and directory definition may need changed for your environment. These scripts are…

JOB SCRIPT	**SCENARIO**
`pi.job`	Serial run (use also for OpenACC)
`pi_threads.job`	Multithreaded run (OMP_NUM_THREADS)
`pi_pes.job`	Multi process run (MPI,coarrays,SHMEM)
`pi_hybrid.job`	Hybrid (for example MPI/OpenMP)

In the following sections there is more information concerning the programming environment which you can use if you need it. There is also some very basic information about the programming models covered.

Have a look over those sections or alternatively just dive in or work as suggested by your instructor or guided by your own interests.

You might wish to consider the following activities:

- Decide on your area of interest
- Learn how to compile and run some of the examples. You can choose serial, threaded, many processes or hybrid.
- Compare the source code to get a feel for each programming model although note that these examples only use the most basic features available.
- Look at scalability as you increase the number of processes or threads. Does the code run 2 times faster as you double the resources available? Does it matter how large (or small) a problem size you pick?

BASIC NOTES ON THE PROGRAMMING MODELS

Various programming models are covered by the examples. If you do not have much background in High Performance Computing these could seem daunting. The models are all attempting to provide the HPC programmer with a platform to decompose some problem efficiently onto complex distributed hardware that can range from a multi-core processor to thousands of complex nodes in a supercomputer.

MULTITHREADED MODELS

The model familiar to a C Systems programmer would be pthreads but this does not have much traction with the HPC community due to the requirement to explicitly manage thread creation and requirement for C. More prevalent is the approach to add compiler directives that advise the compiler how to target computation to a set of threads. OpenMP is the example we choose and only one OpenMP directive/pragma is shown which parallelizes the outer I loop.

COOPERATING PROCESS MODELS

These form a family where normally the same binary is run multiple times encapsulated as a Linux process. The model allows the programmer to organize computation by providing a way to determine how many processes are executing and by enumerating each process instance. There will also be a mechanism to communicate data between processes (message-passing) either point-to-point operations or collective operations (for example a sum over all processes). Traditional message-passing APIs are two-sided (a send on one process is matched by a receive on the other), it is also possible to have single-sided communication where only one process is involved in a *put* or *get* operations without explicit involvement of the other process.

Examples here are MPI and SHMEM.

If you look at the examples they follow the same pattern. The API is used to determine the number of processes/ranks/PEs (npes,size) and which one is executing (mype,rank). The API is

also used to coordinate the processes (barriers and synchronization) and to add up the contribution to the final count from each process.

PGAS MODELS

These models are more complex and are typically languages that support access to local and remote data directly (this is why we put SHMEM in the previous section because it is an explicit API).

Examples are Fortran Coarrays, UPC and Chapel.

Fortran coarrays is the simplest, UPC allows data distribution across "threads" and provides special syntax to operate collectively on distributed (or shared) variables and Chapel is the most featured with advanced support a range of parallel programming paradigms.

MANIPULATING YOUR PROGRAMMING ENVIRONMENT

The Cray Programming Environment is designed to simplify the process of building parallel applications for the Cray XC30. It supports multiple different underlying tool chains (compilers) from different vendors (Cray, Intel and GNU).

Only one on the available tool chains, or Programming Environments (PrgEnvs), can be active at any one time; to see the list of currently loaded modules type:

```
module list
```

A list will be displayed on screen, one of which will be of the form `PrgEnv-*`, e.g.

```
20) PrgEnv-cray/5.2.14
```

To see which other modules are available to load run the command

```
module avail
```

On most systems this may be a very long list, to be more selective, run:

```
module avail PrgEnv
```

which will list all available modules that start with `PrgEnv`.

To swap from the current `PrgEnv` to another `PrgEnv` (e.g. to select a different tool chain), run:

```
module swap PrgEnv-cray PrgEnv-intel
```

This will unload the Cray `PrgEnv` and replace it with the Intel `PrgEnv`.

COMPILING AN APPLICATION

To build applications to run on the XC30 users should always use the Cray compiler driver wrappers, ftn (Fortran), cc (C) and CC (C++) to compile their applications. These wrappers

interface with the Cray Programming Environment and make sure the correct libraries and flags are supplied to the underlying library.

When compiling an application make sure that the appropriate modules are loaded before starting to compile, then modify the build system to call the appropriate wrapper scripts in place of the direct compilers.

If you wish to try other compilers you may need to add compiler flags, for example to enable OpenMP.

SUBMITTING JOBS TO THE BATCH SYSTEM

Nearly all XC30 system will run some form of batch scheduling system to fairly manage the nodes of the system between all the users. Therefore, users must submit all their work in the form of batch job scripts for the scheduler to run in the future.

Example scripts for the PBS Pro (version 12+) batch scheduler plus very simple ECMWF job directives are provided in the example directory,

```
./jobscripts/
```

They are called

```
pi.job – Runs a program in serial on a compute node
pi_pes.job - Runs a non-threaded program on multiple PEs
pi_threads.job – Runs a threaded program on one PE with threads
pi_hybrid.job – Run a hybrid program on a mixture of PEs and threads
```

You will need to edit these scripts.

These scripts includes special #PBS comments which are used to provide information to the batch system about the job resource requirements, e.g.

```
#PBS -N pi
```

specifies the name of the job (displayed in queues etc).

```
#PBS -l EC_nodes=1
```

specifies the number of nodes that are required (in this case just one node).

```
#PBS -l walltime=0:05:00
```

specifies the length of time the job will take (no longer than five minutes).

Some systems, like ECMWF, may require additional queue information, e.g.

```
#PBS –q np
```

Jobs are then submitted for execution using the qsub command:

```
qsub jobscripts/pi.job
```

which will return a job id that uniquely identifies the job. Any of the #PBS settings contained within a file can be overridden at submission time, e.g.

```
qsub –l EC_nodes=2 jobscripts/pi_pes.job
```

changes the number of nodes requested for the job.

To view the status of all the jobs in the system use the qstat command. To find information about a specific job using the jobid:

```
qstat <jobid.sdb>
```

To find information about jobs belonging to a specific user run:

```
qstat –u <username>
```

By default, when a run has completed, the output from the run is left in the run directory in the form:

```
<jobname>.o<jobid>
```

for stdout and

```
<jobname>.e<jobid>
```

for stderr.

LAUNCHING APPLICATIONS ON THE CRAY XC30

A while after a job is submitted, the scheduler will assign the resources the job requested and start the job script running. At this point the supplied script will begin to execute on a PBS MOM node, and it is important to understand that at this stage most of the programs in the script are not yet running in parallel on the Cray XC30 compute nodes.

So for example a simple statement like this:

```
cd ${PBS_O_WORKDIR}
```

(which changes the current working directory to the same directory that the original qsub command was executed) is actually run in serial on the PBS MOM node.

Only programs/commands that are preceded by an aprun statement will run in parallel on the XC30 compute nodes, e.g.

```
aprun –n 16 –N 16 ./pi_mpi
```

Therefore users should take care that long or computationally intensive jobs are only ever run inside an appropriate aprun command.

Each batch job may contain multiple programs with aprun statements, as long as:

- An individual parallel program does not request more resources than have been allocated by the batch scheduler
- The program does not exceed the wall clock time limit specified in the submission script.

See the lecture notes and the manual page, man aprun for a full explanation of the command line arguments to aprun.

LAUNCHING HYBRID MPI/OPENMP APPLICATIONS

The aprun command cannot launch application threads directly. This is done by the application itself, commonly via the OpenMP runtime. However, the aprun can reserve space on the CPUs for threads to execute via the `-d` parameter.

For a typical OpenMP application the script should include the following settings:

```
export OMP_NUM_THREADS=4
aprun -n ${NPROC} -N ${NTASK} -d ${OMP_NUM_THREADS} ./pi_mpi_openmp
```