Introduction to High-Performance Computing

Session 05

Introduction to OpenMP

Parallel Programming Models

- two dominating programming models:
  - OpenMP: uses directives to define work decomposition
  - MPI: standardized message-passing interface
- other programming models
  - HPF (high-performance Fortran)
  - PGAS (Partitioned Global Address Space), e.g. Co-Array Fortran
    UPC (Unified Parallel C)
- programming models for compute devices
  - CUDA
  - OpenCL
  - OpenACC

What is OpenMP and why use it?

- OpenMP is a standard programming model for shared memory parallelization
  - portable across different shared memory architectures
  - allows incremental parallelization
  - based on compiler directives and a few library routines
  - supports Fortran and C/C++

- easy approach to multi-threaded programming
  - allows to exploit modern multi-core CPUs
  - good performance gain for invested effort
  - hybrid-parallelization with MPI-OpenMP

OpenMP Programming Model

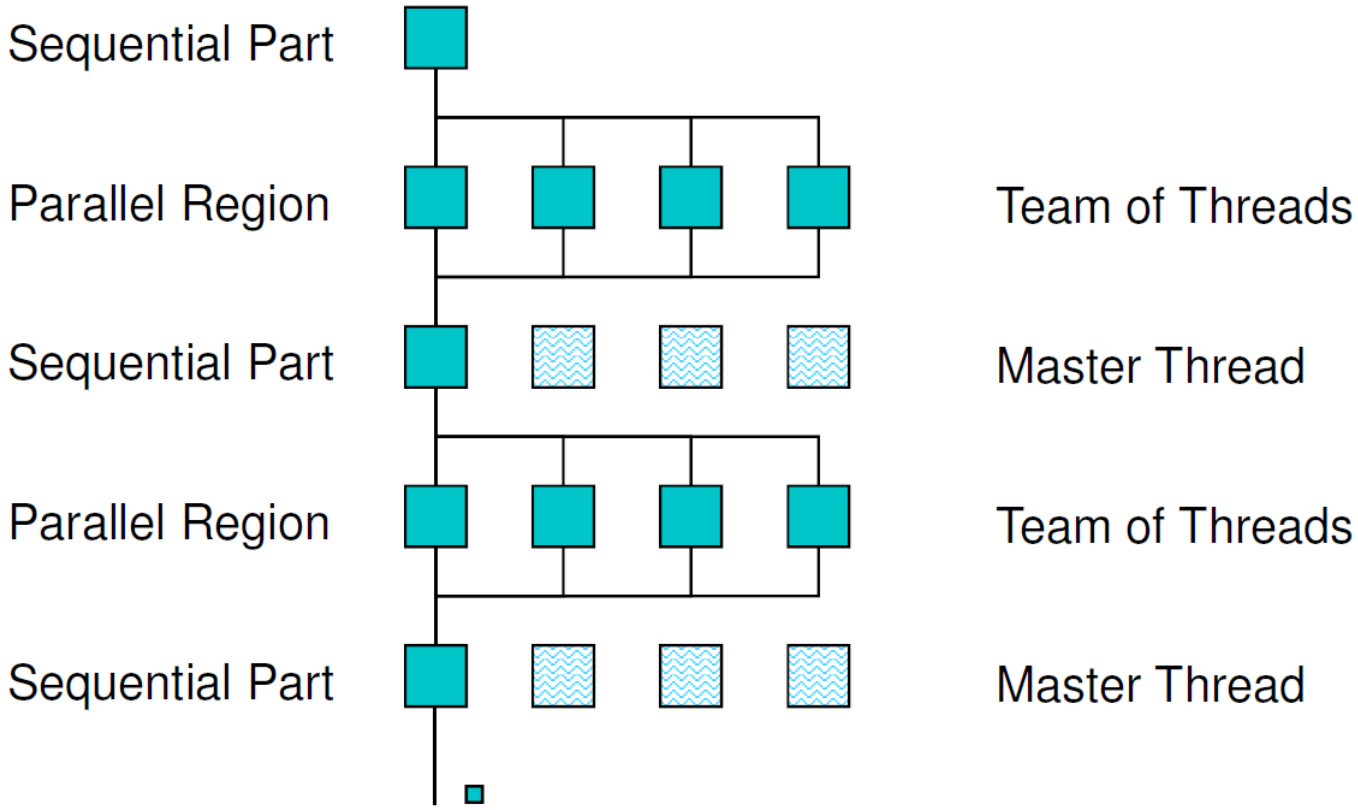
- OpenMP ist a shared memory model
- workload is distributed among threads
- variables can be
  - shared among all threads
  - duplicated for each thread (private)
- threads communicate by sharing variables
  - unintended sharing can lead to race condition
- synchronization for execution control and to avoid data conflicts

OpenMP Standard

http://www.openmp.org/

- standard since 1997 (Fortran version 1.0)
- current standard is 4.5 (Nov 2015)
  - supported in GCC 6.1, Intel 2017 and others
  - older versions of OpenMP have more compilers to choose from
- active development to improve performance and to adapt to new hardware technologies
  - support for SIMD parallelism was added
  - OpenMP on devices/accelerators (e.g. GPUs)

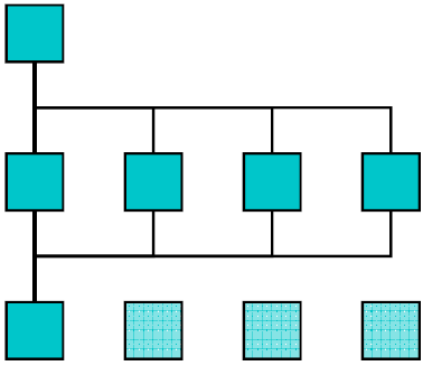
OpenMP Execution Model



OpenMP Parallel Region Construct

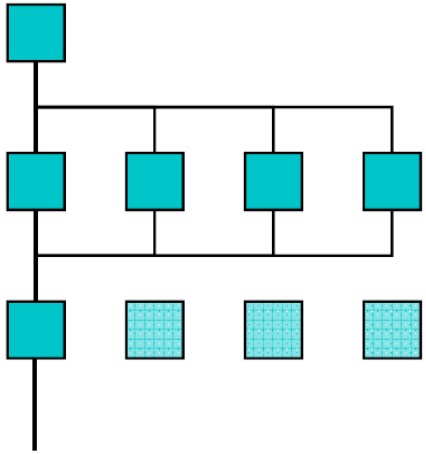
Fortran:

```
!$OMP PARALLEL
    block
!$OMP END PARALLEL
```



C / C++:

```
#pragma omp parallel
    structured block
/* omp end parallel */
```



Example: OMP_HelloWorld

- code available on HPC Wiki

```
#include <iostream>
#include <omp.h>

using namespace std;

int main () {

  #pragma omp parallel
  {
    cout << "Hello World from thread "
         << omp_get_thread_num() << endl;
  } /* end omp parallel */

}
```

Compiling and Running OpenMP Programs

- compilation with an extra option, e.g.

```
$ g++ -fopenmp OMP_HelloWorld.cpp -o OMP_HelloWorld
$ icpc -qopenmp OMP_HelloWorld.cpp -o OMP_HelloWorld
```

  - different compilers use different options

- before running may set environment for control

```
$ export OMP_NUM_THREADS=4
```

  - default is to use all available cores

- running the program as usual

```
$ ./OMP_HelloWorld
```

Running OpenMP Programs with SLURM

- basic job script

```
#!/bin/bash

#SBATCH -p carl.p
#SBATCH -n 1                    # single task with
#SBATCH -c 8                    # cpus-per-task

# execute code
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
srun ./OMP_HelloWorld
```

  - OpenMP programs as single task (and single node)
  - number of cores set by **`--cpus-per-task=<n>`** or **`-c <n>`**
  - environment variable **`SLURM_CPUS_PER_TASK`** available **`cpus-per-task`** has been set
  - **`srun`** may used to create a separate job step (better accounting)

OpenMP Programming

- include library

```
#include <omp.h>
```

- available library routines
  - setting number of threads
  - getting number of threads
  - getting thread ID
  - wall clock time

```
omp_set_num_threads()
omp_get_num_threads()
omp_get_thread_num()
omp_get_wtime()
```

OMP_HelloWorld2

- what will happen here?

```
int main () {

  int threadID, nthreads;
  #pragma omp parallel
  {
    threadID = omp_get_thread_num();
    cout << "Hello World from thread " << threadID << endl;

    // wait for all threads
    #pragma omp barrier
    if (threadID==0) {
      nthreads = omp_get_num_threads();
      cout << "Using " << nthreads << " threads!" << endl;
    }
  } /* end omp parallel */
}
```

Shared and Private Variables

- in OMP_HelloWorld2 threadID is shared among all threads
- race condition
  - every thread is writing to the same memory address
  - final value unpredictable

- solution is to make threadID private

```
#pragma omp parallel private(threadID)
```

Clauses for Parallel Regions

- private(variable list)
  - each thread has its own copy of the variables in the list
  - variables are not initialized (firstprivate does that)
  - no change to variable outside of parallel region (lastprivate does that)
- shared(variable list)
  - all threads shared the same variable
  - typically initialized outside of the parallel region
  - changes persist outside the parallel region
  - be careful to avoid race conditions

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