PHYS52015 Core Ib: Introduction to High Performance Computing (HPC)

Session II: OpenMP (1/3)

Christopher Marcotte

Michaelmas term 2023

Outline

OpenMP
Loop scheduling

pollev.com/christophermarcotte820

OpenMP is a . . .

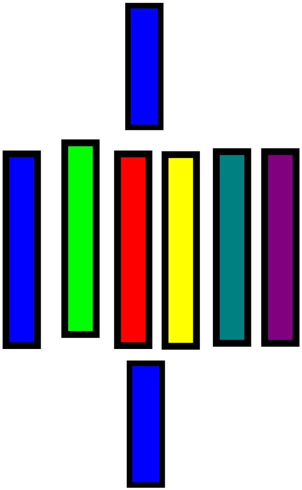
- abbreviation for *Open Multi Processing*
- allows programmers to annotate their C/FORTRAN code with parallelism specs
- portability stems from compiler support
- standard defined by a consortium (`www.openmp.org`)
- driven by AMD, IBM, Intel, Cray, HP, Nvidia, . . .
- "old" thing currently facing its fifth (5.2) generation (1st: 1997, 2nd: 2000; 3rd: 2008; 4th: 2013, 5th: 2018)
- standard to program embarrassingly parallel accelerators – i.e., GPGPU
  We've come a long way from manual loop unrolls in OpenCL...
- Way to iteratively parallelise serial code by identifying opportunities for concurrency

A first example

```c
const int size = ...
int a[size];
#pragma omp parallel for
for( int i=0; i<size; i++ ) {
        a[i] = i;
}
```

- OpenMP for C is a preprocessor(pragma)-based extension (annotations, not API)
  - Implementation is up to the compiler (built into recent GNU and Intel compilers; before additional precompiler required)
  - Implementations internally rely on libraries (such as pthreads)
  - Annotations that are not understood should be ignored (don't break old code)
- Syntax conventions
  - OpenMP statements always start with `#pragma omp`
  - Before GCC 4, source-to-source compiler replaced only those lines
- OpenMP originally written for BSP/Fork-Join applications
- OpenMP usually abstracts from machine characteristics
  (number of cores, threads, ...)

A first example



```
const int size = ...
int a[size];
#pragma omp parallel for
for( int i=0; i<size; i++ ) {
  a[i] = i;
}
```

Compilation and execution:

- GCC: `-fopenmp`
- Intel: `-openmp`
- Some systems require `#include <omp.h>`
- Set threads: `export OMP_NUM_THREADS=2`

What happens — usage

```c
const int size = ...
int a[size];
#pragma omp parallel for
for( int i=0; i<size; i++ ) {
  a[i] = i;
}
```

```
$ gcc -fopenmp test.c
$ export OMP_NUM_THREADS=4
$ ./a.out
```

- Code runs serially until it hits the `#pragma`
- System splits up for loop into chunks (we do not yet know how many)
- Chunks then are deployed among the available (four) threads
- All threads wait until loop has terminated on all threads, i.e. *it synchronises the threads* ⇒ bulk synchronous processing (bsp)
- Individual threads may execute different instructions from the loop concurrently (designed for MIMD machines)

OpenMP execution model

Explicit scoping:

```
#pragma omp parallel
{
  for( int i=0; i<size; i++ ) {
    a[i] = i;
  }
}
```

Implicit scoping:

```
#pragma omp parallel
for( int i=0; i<size; i++ ) {
  a[i] = i;
}
```

- Manager thread vs. worker threads
- Fork/join execution model with implicit synchronisation (barrier) at end of scope
- Nested parallel loops possible (though sometimes very expensive)
- Shared memory paradigm (everybody may access everything)

Some OMP functions

```
int numberOfThreads = omp_get_num_procs();

#pragma omp parallel for
for( int i=0; i<size; i++ ) {

  int thisLineCodeIsRunningOn = omp_get_thread_num();

}
```

- No explicit initialisation of OpenMP required in source code
- Abstracted from hardware threads—setting thread count is done by OS
- Error handling (to a greater extent) not specified by standard
- Functions almost never required (perhaps for debugging)

OpenMP function example

Durham University

```c
#include <stdio.h>
#include <omp.h>
int main(void)
{
  int mthread = omp_get_max_threads();
  int nthread = omp_get_num_threads();
int thread;
#pragma omp parallel private(thread) shared(mthread,nthread)
  {
    thread = omp_get_thread_num();
    printf("Hello, World! I am thread %d of %d of %d\n",
            thread, nthread, mthread);
}
return 0;
}
```

- `omp_get_max_threads()` – maximum number of threads, in this case reads `OMP_NUM_THREADS`
- `omp_get_num_threads()` – current number of threads, in this case 1
- `omp_get_thread_num()` – current thread index, in this case between 1 & `OMP_NUM_THREADS`

OpenMP function example

```c
#include <stdio.h>
#include <omp.h>
int main(void)
{
  int mthread = omp_get_max_threads();
  int nthread;
  int thread;
#pragma omp parallel private(thread,nthread) shared(mthread)
  {
    thread = omp_get_thread_num();
    nthread = omp_get_num_threads();
    printf("Hello, World! I am thread %d of %d of %d\n",
            thread, nthread, mthread);
}
return 0;
}
```

- What is the output of running this example with `OMP_NUM_THREADS=2`?

Parallel loops in action

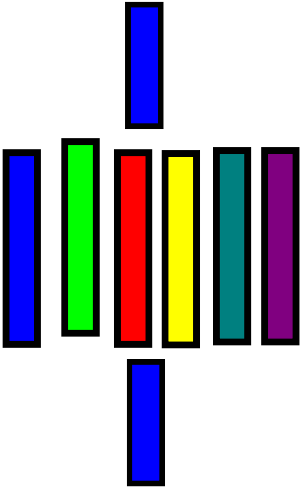
```
#pragma omp parallel        // parallel, but doesn't split the work!
{
  for( int i=0; i<size; i++ ) {
    a[i] = a[i]*2;
  }
}


#pragma omp parallel for   // splits work to be done in parallel
{
  for( int i=0; i<size; i++ ) {
    a[i] = a[i]*2;
  }
}
```

Observations:

- Global loop count is either `size` or *threads*·`size`
- We may run into race conditions
- These result from dependencies (read-write, write-read, write-write) on `a[i]`

Parallel loops and BSP



```
#pragma omp parallel
{
  #pragma omp for
  for( int i=0; i<size; i++ ) {
    a[i] = a[i]*2;
  }
}
```

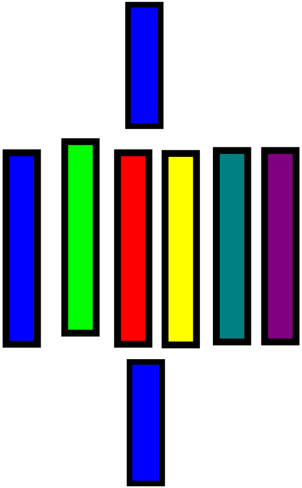
- `omp parallel` triggers fork technically, i.e. spawns the threads
- `for` decomposes the iteration range (logical fork part)
- `omp parallel for` is a shortcut
- BSP's join/barrier is done implicitly at end of the parallel section

Requirements for parallel loops

```
#pragma omp parallel for
{
  for( int i=0; i<size; i++ ) {
    a[i] = a[i]*2;
  }
}
```

- Loop has to follow plain initialisation-condition-increment pattern:
  - Only integer counters
  - Only plain comparisons
  - Only increment and decrement (no multiplication or any arithmetics)
- Loop has be countable (otherwise splitting is doomed to fail).
- Loop has to follow single-entry/single-exit pattern.

Data consistency in OpenMP's BSP model



```
#pragma omp parallel
{
  #pragma omp for
  for( int i=0; i<size; i++ ) {
    a[i] = a[i]*2;
  }
}
```

- No assumptions which statements run technically concurrent
- Shared memory without any consistency model
- No inter-thread communication (so far)

$\Rightarrow$ Data consistency is developer's responsibility

Concept of building block: OpenMP Introduction

- Content
  - OpenMP syntax basics
  - OpenMP runtime model
  - OpenMP functions
- Expected Learning Outcomes
  - The student can *translate* and use an application with OpenMP support
  - The student can *explain* with the OpenMP execution model
- Further Reading:
  - We will not talk about vectorisation (using OpenMP or otherwise) in this course, but a good resource for an introduction (and many other topics!) is here: *Algorithmica* `https://en.algorithmica.org/hpc/`

Remaining agenda

Starting point:

- Data analysis allows us to identify candidates for data parallelism/BSP
- Concurrency analysis plus speedup laws determine potential real-world speedup
- OpenMP allows us to annotate serial code with BSP logic

Open questions:

- How is work technically split?
- How is work assigned to compute cores?
- What speedup can be expected in practice?

> Scheduling: Assign work (loop fragments) to threads.

> Pinning: Assign thread to core.

Technical remarks

On threads:

- A thread is a logically independent application part, i.e. it has its own call stack (local variables, local function history, . . .)
- All threads share one common heap (pointers are replicated but not the area they are pointing two)
- OpenMP literally starts new threads when we hit `parallel for` $\Rightarrow$ overhead
- OpenMP hides the scheduling from user code

On cores:

- Unix cores can host more than one thread though more than two (hyperthreading) becomes inefficient
- Unix OS may reassign threads from one core to the other $\Rightarrow$ overhead
- Unix OS can restrict cores-to-thread mapping (task affinity)
- Unix OS can be forced to keep cores-to-thread mapping (pinning)

Grain size

Grain size: Minimal size of piece of work (loop range, e.g.).

- Concurrency is a theoretical metric, i.e. machine concurrency might/should be smaller
- Multithreading environment thus wrap up multiple parallel tasks into one job
- Grain size specifies how many tasks may be fused

Technical mapping of tasks

- Each thread has a queue of tasks (jobs to do)
- Each job has at least grain size
- Each thread processes tasks of its queues (dequeue)
- When all task queues are empty, BSP joins

Static scheduling

Definition:

1. Cut problem into pieces (constrained by prescribed grain size)
2. Distribute work chunks among queues
3. Disable any work stealing

In OpenMP:

- Default behaviour of `parallel for`
- Trivial grain size of 1 if not specified differently
- Problem is divided into `OMP_NUM_THREADS` chunks $\Rightarrow$ at most one task per queue

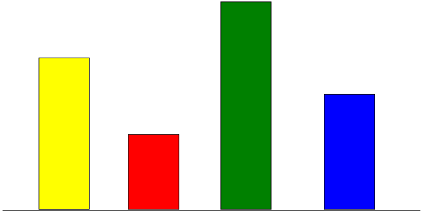
```
#pragma omp parallel for schedule(static,14)
```

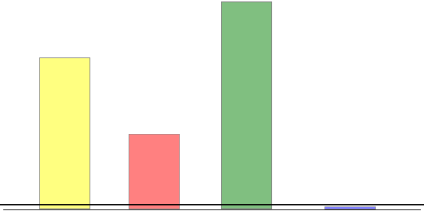
Properties:

- Overhead
- Balancing
- Inflexibility w.r.t. inhomogeneous computations

Work stealing

Work stealing: When one thread runs out of work (work queue become empty), it tries to grab (steal) work packages from other threads.





Dynamic scheduling

Definition:

1. Cut problem into pieces of prescribed grain size
2. Distribute all work chunks among queues
3. Enable work stealing

In OpenMP:

- To be explicitly enabled in `parallel for`
- Trivial grain size of 1 if not specified differently
- Set of chunks is divided among `OMP_NUM_THREADS` queues first

```
#pragma omp parallel for schedule(dynamic)
...
#pragma omp parallel for schedule(dynamic,14)
...
```

Properties:

- Overhead
- Balancing
- Flexibility w.r.t. inhomogeneous computations

Guided scheduling

Definition:

1. Cut problem into chunks of size N/p constrained by grain size and with $p =$ `OMP_NUM_THREADS`
2. Cut remaining tasks into pieces of $(N/(2p))$ constrained by grain size
3. Continue cut process iteratively
4. Distribute all work chunks among queues; biggest jobs first
5. Enable work stealing

In OpenMP:

- To be explicitly enabled in `parallel for`
- Trivial grain size of 1 if not specified differently
- Set of chunks is divided among `OMP_NUM_THREADS` queues first

```
#pragma omp parallel for schedule(guided)
...
#pragma omp parallel for schedule(guided,14)
...
```

Properties:

- Overhead
- Balancing
- Requires domain knowledge

Concept of building block: Loop scheduling

- Content
  - Introduce terminology
  - Discuss work stealing
  - Study OpenMP's scheduling mechanisms
  - Study OpenMP's two variants of dynamic scheduling
  - Conditional parallelisation
- Expected Learning Outcomes
  - The student **knows** technical terms tied to scheduling
  - The student can **explain** how work stealing conceptually works
  - The student can **identify problems** arising from poor scheduling/too small work packages
  - The student can **use** proper scheduling in OpenMP applications