Single Node Optimisation

OpenMP Performance

Reusing this material

A common scenario.....

"So I wrote my OpenMP program, and I checked it gave the right answers, so I ran some timing tests, and the speedup was, well, a bit disappointing really. Now what?".

Most of us have probably been here.

Where did my performance go?

It disappeared into overheads.....

The six (and a half) evils...

- There are six main sources of overhead in OpenMP programs:
  - sequential code
  - idle threads
  - synchronisation
  - scheduling
  - communication
  - hardware resource contention

- and another minor one:
  - compiler (non-)optimisation

- Let’s take a look at each of them and discuss ways of avoiding them.

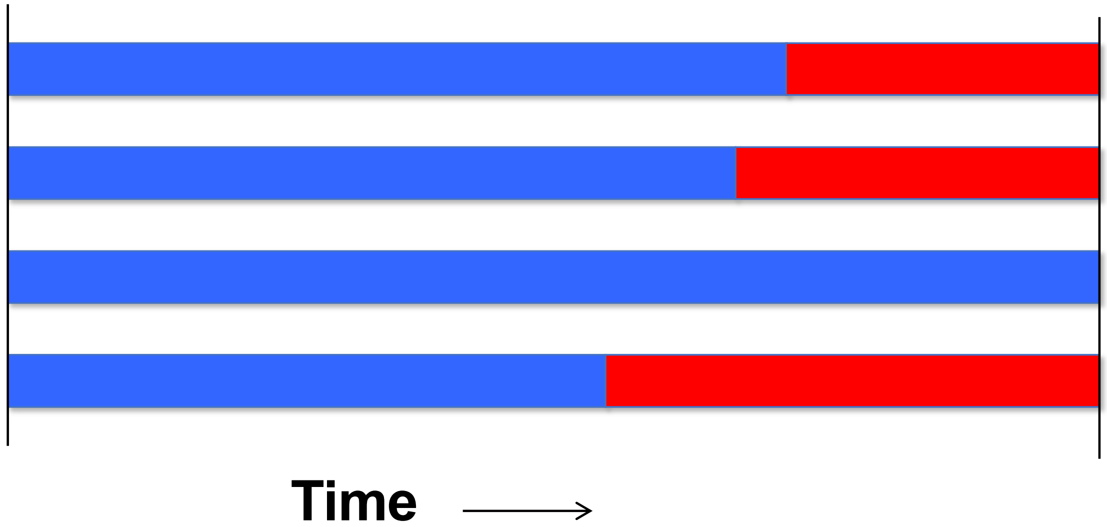
Sequential code

- In OpenMP, all code outside parallel regions, or inside MASTER and SINGLE directives is sequential.
- Time spent in sequential code will limit performance (that’s Amdahl’s Law).
- If 20% of the original execution time is not parallelised, I can never get more that 5x speedup.
- Need to find ways of parallelising it!

Idle threads

- Some threads finish a piece of computation before others, and have to wait for others to catch up.

- e.g. threads sit idle in a barrier at the end of a parallel loop or parallel region.



Avoiding load imbalance

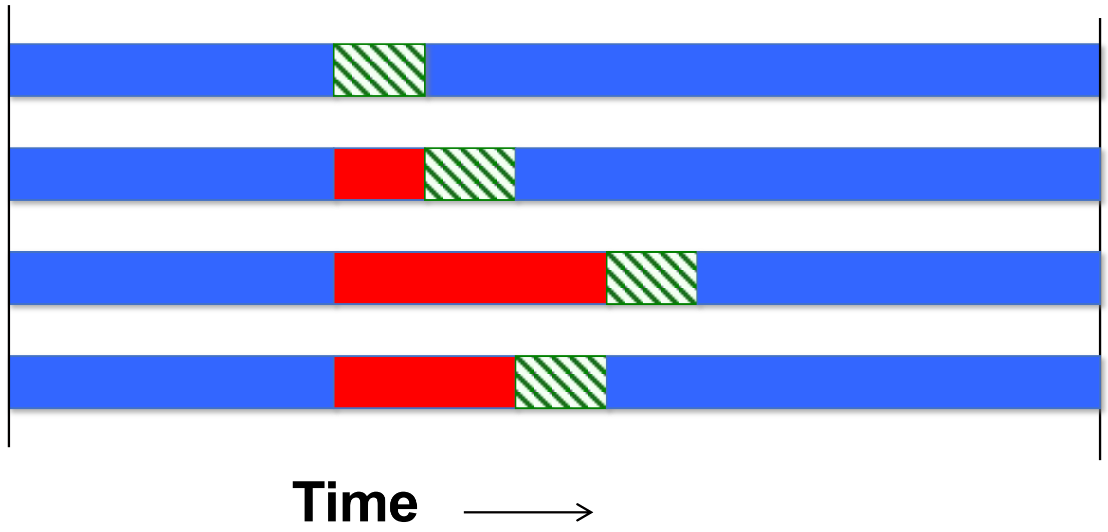
- It's a parallel loop, experiment with different schedule kinds and chunksizes
  - can use **`SCHEDULE(RUNTIME)`** to avoid recompilation.

- For more irregular computations, using tasks can be helpful
  - runtime takes care of the load balancing

- Note that it's not always safe to assume that two threads doing the same number of computations will take the same time.
  - the time taken to load/store data may be different, depending on if/where it's cached.

Critical sections

- Threads can be idle waiting to access a critical section
  - In OpenMP, critical regions, atomics or lock routines



Avoiding waiting

- Minimise the time spent in the critical section

- OpenMP critical regions are a global lock
  - but can use critical directives with different names

- Use atomics if possible
  - allows more optimisation, e.g. concurrent updates to different array elements

- ... or use multiple locks

Synchronisation

- Every time we synchronise threads, there is some overhead, even if the threads are never idle.
  - threads must communicate somehow.....
- Many OpenMP codes are full of (implicit) barriers
  - end of parallel regions, parallel loops
- Barriers can be very expensive
  - depends on no. of threads, runtime, hardware, but typically 1000s to 10000s of clock cycles.
- Criticals, atomics and locks are not free either.
- ...nor is creating or executing a task

Avoiding synchronisation overheads

- Parallelise at the outermost level possible.
  - Minimise the frequency of barriers
  - May require reordering of loops and/or array indices.

- *Careful* use of NOWAIT clauses.
  - easy to introduce race conditions by removing barriers that are required for correctness

- Atomics *may* have less overhead that critical or locks
  - quality of implementation problem

Scheduling

- If we create computational tasks, and rely on the runtime to assign these to threads, then we incur some overheads
  - some of this is actually internal synchronisation in the runtime
- Examples: non-static loop schedules, task constructs

```
#pragma omp parallel for schedule(dynamic,1)
for (i=0;i<10000000;i++){
.......
}
```

- Need to get granularity of tasks right
  - too big may result in idle threads
  - too small results in scheduling overheads

Communication

- On shared memory systems, communication is "disguised" as increased memory access costs - it takes longer to access data in main memory or another processors cache than it does from local cache.
- Memory accesses are expensive! (O(100) cycles for a main memory access compared to 1-3 cycles for a flop).
- Communication between processors takes place via the cache coherency mechanism.
- Unlike in message-passing, communication is fine–grained and spread throughout the program
    - much harder to analyse or monitor.

Cache coherency in a nutshell

- If a thread writes a data item, it gets an exclusive copy of the data in its local cache
- Any copies of the data item in other caches get invalidated to avoid reading of out-of-date values.
- Subsequent accesses to the data item by other threads must get the data from the exclusive copy
  - this takes time as it requires moving data from one cache to another

(Caveat : this is a *highly* simplified description!)

Data affinity

- Data will be cached on the processors which are accessing it, so we must reuse cached data as much as possible.

- Need to write code with good *data affinity* - ensure that the same thread accesses the same subset of program data as much as possible.

- Try to make these subsets large, contiguous chunks of data

- Also important to prevent threads migrating between cores while the code is running.
  - use export OMP_PROC_BIND=true

Data affinity example 1

```
#pragma omp parallel for schedule(static)
for (i=0;i<n;i++){
   for (j=0; j<n; j++){
      a[i][j] = i+j;
   }
}

#pragma omp parallel for schedule(static,16)
for (i=0;i<n;i++){
   for (j=0; j<i; j++){
      b[j] += a[i][j];
   }
}
```

Balanced loop

Unbalanced loop

Different access patterns for `a` will result in extra communication

Data affinity example 2

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

for (i=0;i<n;i++){
      a[i] = 23;
}

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

a will be spread across multiple caches

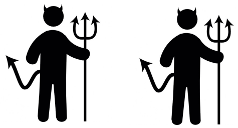
Sequential code!
a will be gathered into one cache

a will be spread across multiple caches again

Data affinity (cont.)

- Sequential code will take longer with multiple threads than it does on one thread, due to the cache invalidations
- Second parallel region will scale badly due to additional cache misses
- May need to parallelise code which does not appear to take much time in the sequential program!

Data affinity: NUMA effects

- Very evil! 
- On multi-socket systems, the location of data in main memory is important.
  - Note: all current multi-socket x86 systems are NUMA!
- OpenMP has no support for controlling this.
- Common default policy for the OS is to place data on the processor which first accesses it (first touch policy).
- For OpenMP programs this can be the worst possible option
  - data is initialised in the master thread, so it is all allocated one socket
  - having all threads accessing data on the same socket becomes a bottleneck

Avoiding NUMA effects

- In some OSs, there are options to control data placement
  - e.g. in Linux, can use **`numactl`** change policy to round-robin
- First touch policy can be used to control data placement indirectly by parallelising data initialisation
  - even though this may not seem worthwhile in view of the insignificant time it takes in the sequential code
- Don’t have to get the distribution exactly right
  - some distribution is usually much better than none at all.
- Remember that the allocation is done on an OS page basis
  - typically 4KB to 16KB
  - beware of using large pages!

False sharing

- Very very evil!

- The units of data on which the cache coherency operations are done (typically 64 or 128 bytes) are always bigger than a word (typically 4 or 8 bytes).

- Different threads writing to *neighbouring words* in memory may cause cache invalidations!
  - still a problem if one thread is writing and others reading

False sharing patterns

- Worst cases occur where different threads repeatedly write neighbouring array elements.

```
count[omp_get_thread_num()]++;
```

```
#pragma omp parallel for schedule(static,1)
for (i=0;i<n;i++){
   for (j=0; j<i; j++){
      b[i] += a[j][i];
   }
}
```

Hardware resource contention 

- The design of shared memory hardware is often a cost vs. performance trade-off.
- There are shared resources which if all cores try to access at the same time, do not scale.
  - or, put another way, an application running on a single core can access more than its fair share of the resources
- In particular, cores (and hence OpenMP threads) can contend for:
  - memory bandwidth
  - cache capacity
  - functional units (if using SMT)

Memory bandwidth

- Codes which are very bandwidth-hungry will not scale linearly of most shared-memory hardware.

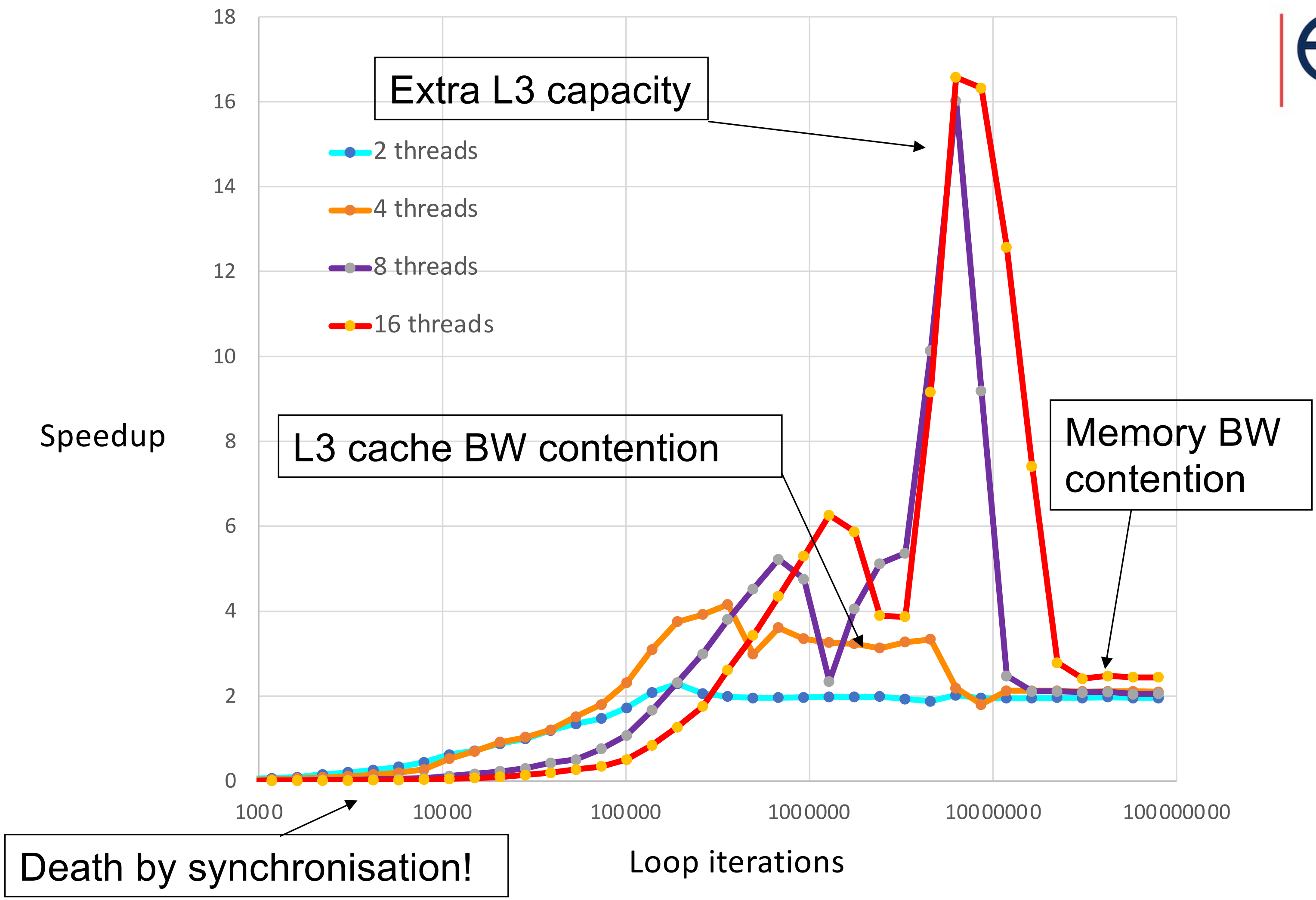
- Try to reduce bandwidth demands by improving locality, and hence the re-use of data in caches
  - will benefit the sequential performance as well.

Memory bandwidth example

- AMD Rome processor
  - 1 NUMA region - 16 cores
  - L1 and L2 caches per core
  - 16 MB shared L3 cache per 4 cores
  - Cray compiler

```
#pragma omp parallel for reduction(+:sum)
for (i=0;i<n;i++){
   sum += a[i];
}
```

- Measure speedup for varying values of n and no. of threads


Extra L3 capacity
2 threads
4 threads
8 threads
16 threads
L3 cache BW contention
Memory BW contention
Speedup
18
16
14
12
10
8
6
4
2
0
1000
10000
100000
1000000
10000000
100000000
Loop iterations
Death by synchronisation!

Cache space contention

- On systems where cores share some level of cache (e.g. L3), codes may not appear to scale well because a single core can access the whole of the shared cache.

- Beware of tuning block sizes for a single thread, and then running multithreaded code
  - each thread will try to utilise the whole cache

Hardware threads

- When using hardware threads, OpenMP threads running on the same core contend for functional units as well as cache space and memory bandwidth.
- Tends to benefit codes where threads are idle because they are waiting on memory references
  - code with non-contiguous/random memory access patterns
- Codes which are bandwidth-hungry, or which saturate the floating point units (e.g. dense linear algebra) may not benefit from this
  - may actually run slower

Oversubscription

- Running more threads than hardware execution units (cores or hardware threads) is generally a bad idea.
- OS tries to give each thread a fair share of execution units
- Cost of stopping one thread and starting another is high (1000s of clock cycles)
- Ruins data locality!

Compiler (non-)optimisation

- Very rarely, the addition of OpenMP directives can inhibit the compiler from performing sequential optimisations.
- Symptoms: 1-thread parallel code has longer execution time than sequential code.
- Can be hard to find a workaround
- Can sometimes be cured by making shared data private, or making local copies of variables.

Minimising overheads

My code is giving poor speedup. I don’t know why.

What do I do now?

1.
   - Say “OpenMP is a heap of junk”.
   - Give up.
2.
   - Try to *classify* and *localise* the sources of overhead.
   - What type of problem is it, and where in the code does it occur?
   - Use any available tools to help you (e.g. timers, hardware counters, profiling tools).
   - Fix problems which are responsible for large overheads first.
   - Iterate.

Profilers

- Standard profilers (gprof, IDE profilers) can be confusing
  - they typically accumulate the time spent in functions across all threads.

- You can get a lot out of using timers (`omp_get_wtime()`)

- Add timers round every parallel region, and round the whole code.
  - work out which parallel regions have the worst speedup
  - don't assume the time spent outside parallel regions is independent of the number of threads.

Performance tools

- Vampir
  - timeline traces can be very useful for visualising load balance
- Intel Vtune
- TAU
- Arm MAP
- CrayPAT
- Scalasca
  - breaks down overheads into different categories
- ParaTools Threadspotter
  - very good for finding cache/memory problems, including false sharing.

Exercise

- Profile and optimise a not very efficient OpenMP version of the molecular dynamics (MD) code

- Separate source files:

```
tpo.tar
```