OpenMP: Open Multiprocessing

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Outline

1. Basic concepts, hardware architectures
2. OpenMP Programming
3. How to parallelise an existing code
4. Advanced OpenMP constructs
OpenMP: Basic Concepts, Hardware Architecture

• Parallel programming is much harder than serial programming; we use it (only) because it improves performance

• Possible performance of a code is ultimately defined by the computing architecture on which it runs

• Need to have at least passing knowledge of hardware architectures
Parallel Computer Memory Architectures

Shared Memory

Distributed Memory

Hybrid Distributed Shared Memory
Relation to Parallel Programming Models

- **OpenMP**: Multi-threaded calculations occur within shared-memory components of systems, with different threads working on the same data.

- **MPI**: Based on a distributed-memory model, data associated with another processor must be communicated over the network connection.

- **GPUs**: Graphics Processing Units (GPUs) incorporate many (hundreds) of computing cores with single Control Unit, so this is a shared-memory model.

- **Processors vs. Cores**: Most common parallel computer, each processor can execute different instructions on different data streams
  - Often constructed of many SIMD subcomponents
MPI vs. OpenMP

• MPI: Difficult to use, but makes it *possible* (not easy!) to write highly efficient code
  • like writing machine code
• OpenMP: Easy to use
• 90/10 rule: Compared to MPI, OpenMP gives 90% of the performance with 10% of the effort
  • OpenMP requires shared memory system
### Single Image View vs. Communicating Processes

<table>
<thead>
<tr>
<th>Programming difficulty</th>
<th>Shared memory (small systems)</th>
<th>Distributed memory (large systems)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single image (one program) (easy)</td>
<td>OpenMP</td>
<td>e.g. HPF, CAF</td>
</tr>
<tr>
<td>Communicating processes (difficult)</td>
<td>e.g. pthreads</td>
<td>MPI</td>
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Multi-Threading

- Threading involves a single process that can have multiple, concurrent execution paths
- Works in a shared memory architecture
- Most common implementation is **OpenMP** (Open Multi-Processing)

```c
serial code
    ...
    ...
    ...

!$OMP PARALLEL DO
  do i = 1,N
    A(i)=B(i)+C(i)
  enddo

!$OMP END PARALLEL DO
serial code
    ...
    ...
    ...
```

- Relatively easy to make inner loops of a serial code parallel and achieve substantial speedups with modern multi-core processors
OpenMP Design Principle

- Parallel code has same semantics as serial code (and looks very similar)
- Parallelisation via *directives*, which are comments inserted into the code
- Parallel code remains also a serial code
- Main advantage: Can parallelise a code incrementally, starting with most expensive parts
More Information:

- http://www.openmp.org/
- Many tutorials available on the web, standard definition freely available
- Built into nearly every C/C++/Fortran compiler, including GNU
- available everywhere, easy to use, there is no excuse for not using it (except if your algorithm is not parallel)
Current CPU/Memory Hardware Architecture

• Today’s CPU/memory hardware architecture is surprisingly complex

• nearly impossible to precisely predict performance, even for experts

• Most systems have several processors, multiple cores, and several memory elements (!) on each node

• Relevant for performance: Flop/s (computations) and GB/s (memory accesses)
<table>
<thead>
<tr>
<th>Machine (24GB)</th>
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<tbody>
<tr>
<td>NUMANode P#0 (12GB)</td>
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<tr>
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<td>L2 (256KB)</td>
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<td>Core P#0</td>
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<td>PU P#0</td>
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<td>Core P#0</td>
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<td>PU P#6</td>
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</table>

Indexes: physical
Date: Wed 06 Jun 2012 11:12:29 AM CDT
Helium, Head node
First Steps in OpenMP

- Fortran:

```fortran
program hello
  implicit none
  integer :: i
  print '("Hello, world!")'
  !$omp parallel do
  do i=1,10
    print '("iteration: ",i4)\', i
  end do
  !$omp end parallel do
end program hello
```
First Steps in OpenMP

• C/C++:

```c
#include <stdio.h>
int main()
{
    printf("Hello, world!\n");
    #pragma omp parallel for
    for (int i=0; i<10; ++i) {
        printf("iteration %d\n", i);
    }
    return 0;
}
```
No Plumbing Necessary!

• Different from MPI code, it is generally not necessary to look at the thread number ("rank"), or at the total number of threads.

• Easy to combine serial and parallel parts of an algorithm.

• If you need to execute certain operations in order, just don’t parallelise the loop.
Fortran vs. C/C++

• In Fortran, OpenMP directives begin with !$omp, and are usually paired with a corresponding end directive

• In C or C++, OpenMP directives begin with #pragma omp, and apply to the next statement or { } block
Important OpenMP Directives

- `parallel/end parallel`: define a parallel region
- `do/end do`: parallelise a do loop
- `critical/end critical`: serialise a region within a parallel region

- Clauses for parallel regions:
  - `private`: list variables that should not be shared between threads
  - `reduction`: list variables that should be reduced (their values “combined”)

Thursday, 7 June, 12
omp do
(omp for in C/C++)

• To parallelise a loop, the number of iterations must be known before the loop begins

• The loop iterations must also be independent

• OpenMP will split iterations automatically over all available threads

• The parallelised loop may be executed in an arbitrary order
Example: Fibonacci Series

The Fibonacci series is defined by:

\[ f(k + 2) = f(k + 1) + f(k) \quad \text{with} \quad f(1) = f(2) = 1 \]

The Fibonacci series is therefore \( (1, 1, 2, 3, 5, 8, 13, 21, \ldots) \)

The Fibonacci series can be calculated using the loop

\[
\begin{align*}
\text{f(1)} &= 1 \\
\text{f(2)} &= 1 \\
\text{do } i &= 3, N \\
& \quad \text{f(i)} = \text{f(i-1)} + \text{f(i-2)} \\
\text{enddo}
\end{align*}
\]

How do we do this computation in parallel?

This calculation cannot be made parallel.
- We cannot calculate \( f(k + 2) \) until we have \( f(k + 1) \) and \( f(k) \)
- This is an example of data dependence that results in a non-parallelizable problem
Example: `omp do`

- alpha = 0.24
  
  ```c
  !$omp parallel do
do i=2,N-1
  anew(i) = alpha * (aold(i-1) + aold(i+1))
  end do
  !$omp end parallel do
  ```
omp critical

- A **critical region** is a section of code (within a parallel region) that must not be executed simultaneously by multiple threads.
  - example: modifying a global variable, writing something to the screen.
- Critical regions are slow; use them only if necessary, e.g. to handle exceptional cases.
Example: \texttt{omp critical}

- \texttt{errcount = 0}
  \texttt{!$omp parallel do}
  \texttt{do i=2,N-1}
    \texttt{if (anew(i) < 0) then}
      \texttt{!$omp critical}
      \texttt{print '("error: anew<0 at ",i4), i}
      \texttt{errcount = errcount + 1}
      \texttt{!$omp end critical}
    \texttt{end if}
  \texttt{end do}
\texttt{!$omp end parallel do}
private

• By default, all variables are *shared* between all threads, i.e. there is a single instance of the variable

• Variables can be declared *private*, which means that each thread has its own, independent instance of the variable

• Rule of thumb:
  • read-only variables can be shared
  • temporary variables should be private
  • other variables can only be accessed in critical sections
Example: private

- **alpha = 0.24**
  
  ```
  !$omp parallel do private(i, j, tmp)
  do j=2,N-1
  do i=2,N-1
    tmp = aold(i-1,j) + aold(i+1,j) + &
    aold(i,j-1) + aold(i,j+1)
    anew(i) = alpha * tmp
  end do
  end do
  !$omp end parallel do
  ```
Reduction

- Reduction clauses allow reducing values (i.e. combining values) from multiple threads

- For example: sum, min, max, ...

- Much more efficient than critical regions – try to rewrite critical regions as reductions, if possible
Example: reduction

- errcount = 0
  !$omp parallel do reduction(sum: errcount)
  do i=2,N-1
    if (anew(i) < 0) then
      errcount = errcount + 1
    end if
  end do
  !$omp end parallel do
  print ‘(“error count:“,i4)’, errcount
Applying OpenMP to an Existing Program

- Adding MPI parallelism to a serial program typically requires much surgery, and needs to be done all at once
  - however, MPI can speed up a program by 100,000

- Adding OpenMP parallelism is much easier, and can be done incrementally
  - OpenMP can speed up a program maybe by a factor of 10
How to Parallelise a Code
(How to Modify a Code)

1. Understand the structure of the program
2. Define a simple test case, record its output
3. Find out which parts take a long time
   (this requires timing measurements)
4. Look for loops, examine data dependencies, add
   OpenMP directives
5. Check correctness (see 2.)
6. Compare performance
Loops

• General observation: the code inside a loop is executed (much) more often than the code outside of a loop

• Therefore, optimising and parallelising loops is likely to lead to the largest performance improvements

• Parallelising via OpenMP usually means adding `omp parallel do` statements around do loops
Compiler Optimisations

• When measuring performance, it is necessary to use good compiler options to optimise the executable

• typical flags: -O2, -O3, Intel: -fast, GNU: -Ofast, etc.

• It pays off to optimise for the particular hardware architecture (Intel: -xHOST, GNU: -march=native)

• Do not measure performance for a non-optimised executable; performance can differ significantly
Profiling

• *Profiling* means recording for each function how often it is called and how much time it takes during execution

• All compilers support adding profiling code to executables (“instrumenting”)

• Note: Instrumented code may run slower

• After running the instrumented executable, the profiling results can be analysed, e.g. with gprof (see Cheat Sheet)
Sample Profiling Output

Flat profile:

Each sample counts as 0.01 seconds.

<table>
<thead>
<tr>
<th>% cumulative</th>
<th>time</th>
<th>% cumulative seconds</th>
<th>self</th>
<th>% cumulative seconds</th>
<th>self</th>
<th>total</th>
<th>self</th>
<th>total</th>
<th>name</th>
</tr>
</thead>
<tbody>
<tr>
<td>72.48</td>
<td>0.79</td>
<td>0.79</td>
<td>10001</td>
<td>0.00</td>
<td>0.00</td>
<td>0.79</td>
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<td>0.00</td>
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</tr>
<tr>
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<td>1.08</td>
<td>0.29</td>
<td>10000</td>
<td>0.00</td>
<td>0.00</td>
<td>1.08</td>
<td>0.00</td>
<td>0.00</td>
<td>potential_mp_step_</td>
</tr>
<tr>
<td>0.92</td>
<td>1.09</td>
<td>0.01</td>
<td>1</td>
<td>0.01</td>
<td>1.09</td>
<td>1.09</td>
<td>0.00</td>
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<td>MAIN__</td>
</tr>
<tr>
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<td>1.09</td>
<td>0.00</td>
<td>1</td>
<td>0.00</td>
<td>0.00</td>
<td>1.09</td>
<td>0.00</td>
<td>0.00</td>
<td>potential_mp_initial_</td>
</tr>
</tbody>
</table>

- Here, most of the time is spent in “residual” and “step”
- Parallelising the main program or the initial data routine is pointless
Manual Timing Measurements

- The Unix `time` command can be used to measure execution time:
  - `time ./calcpi`

- Alternatively, you can time specific code section via `omp_get_wtime()`:
  - `use omp_lib`
  - `double precision :: t0, t1`
  - `t0 = omp_get_wtime()`
  - `! parallel section`
  - `t1 = omp_get_wtime()`
  - `print "("elapsed time:\",f20.15)", t1-t0`
Compiling OpenMP Code

- By default, compilers will ignore all OpenMP directives, and will produce a serial executable

- note: this serial executable will run correctly, it will only run more slowly

- see the compiler documentation (or the Cheat Sheet) for enabling OpenMP
Running OpenMP Code

• You should explicitly choose the number of OpenMP threads when running a code
• the default choice may be inefficient (it is unlikely to use a single thread)
• Unfortunately it’s slightly complicated, see the cheat sheet for details
• use qlogin to run on a compute node; timing measurements on the head node will be unpredictable
• by default, the operating system likes to shift threads between cores, which is bad for performance
Advanced OpenMP Programming

• The current standard is OpenMP 3.1

• However, some compilers only support version 3.0 or 2.x

• Future versions will likely add support for defining memory locality for variables (for NUMA architectures, maybe even for GPUs and other accelerators)
Other OpenMP Directives

- OpenMP offers a range of other directives:
  - atomic: a fast version of critical
  - barrier: wait for other threads
  - master: execute only on the master thread
  - single: execute only once
  - workshare: parallelise array operations
  - sections: MPMD, functional decomposition
  - task: low-level task management
Other OpenMP Clauses

- OpenMP offers a range of other clauses:
  - **collapse**: parallelise nested do loops
  - **schedule**: choose strategy for splitting loops
  - **nowait**: disable some implicit barriers
  - **copyin, copyprivate, firstprivate, lastprivate**: manage private and shared variables
  - **if**: conditionally disable a parallel region
  - **num_threads**: choose number of threads
Other OpenMP Functions

- OpenMP also offers run-time functions that can be called:
  - Fortran: `use omp_lib`
  - C/C++: `#include <omp.h>`
  - `omp_get_thread_num()`: current thread id
  - `omp_get_num_threads()`: number of threads
  - `omp_get_max_threads()`: max number of threads
  - `omp_set_num_threads()`: set number of threads
  - `omp_get_num_procs()`: number of cores
Hybrid Parallelisation

• It makes sense to combine MPI and OpenMP:
  • MPI handles communication between nodes, OpenMP distributes the workload within a node

• This can help reduce overhead introduced by MPI:
  • MPI may require duplicating certain data structures for each process
  • there may be scaling problems for large numbers of MPI processes
Alternatives to OpenMP and MPI

- There is a large gap between OpenMP, which is rather easy to use, and MPI, which is quite difficult.

- A range of other, much less widely used programming standards exist, targeting parallel programming, distributed programming, accelerators, etc.
HPF

(High Performance Fortran)

• HPF uses concepts similar to OpenMP, but for distributed memory systems, not just shared memory

• HPF adds directives that specify which variables (arrays) should be distributed over processes

• Unfortunately, HPF is mostly dead, and there are no open-source implementations available

• However, HPF would otherwise be an ideal choice for many of the examples presented here
CAF (Co-Array Fortran)

- CAF is a proposed addition to the Fortran standard
- CAF takes the same “communicating processes” approach as MPI
- CAF allows distributing arrays over multiple processes, and provides a simple way to access remote array elements (much simpler than MPI)
  - Example: \texttt{a[myrank] = a[myrank+1]}
Remote Direct Memory Access

- MPI, as well as several low-level libraries on which MPI implementations are built, as well as most high-performance interconnects, support RDMA (called one-sided communication in MPI)
- This allows accessing memory of another node as if it was on the local node, except that it is slower
- much simpler to use than MPI_Send/ MPI_Recv (but not faster)