Programming OpenMP

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Based on materials developed by Evan Lee Turner and Luke Wilson at TACC
Overview

• Parallel processing
  – MPP vs. SMP platforms  
  – Motivations for parallelization
  
• What is OpenMP?
• How does OpenMP work?
  – Architecture
  – Fork-join model of parallelism
  – Communication
• OpenMP constructs
  – Directives
  – Runtime Library API
  – Environment variables
MPP platforms

- Clusters are distributed memory platforms in which each processor has its own local memory; use MPI on these systems.
SMP platforms

- In each Ranger node, the 16 cores share access to a common pool of memory; likewise for the 8 cores in each node of CAC’s v4 cluster
What is OpenMP?

- De facto open standard for scientific parallel programming on Symmetric MultiProcessor (SMP) systems
  - Allows fine-grained (e.g., loop-level) and coarse-grained parallelization
  - Can express both data and task parallelism
- Implemented by:
  - Compiler directives
  - Runtime library (an API, Application Program Interface)
  - Environment variables
- Standard specifies Fortran and C/C++ directives and API
- Runs on many different SMP platforms
- Find tutorials and description at [http://www.openmp.org/](http://www.openmp.org/)
Advantages/disadvantages of OpenMP

• Pros
  – Shared Memory Parallelism is easier to learn
  – Parallelization can be incremental
  – Coarse-grained or fine-grained parallelism
  – Widely available, portable

• Cons
  – Scalability limited by memory architecture
  – Available on SMP systems only

• Benefits
  ➢ Helps prevent CPUs from going idle on multi-core machines
  ➢ Enables faster processing of large-memory jobs
OpenMP architecture

- Application
- Compiler directives
- Runtime library
- Threads in operating system
- User
- Environment variables
OpenMP fork-join parallelism

- Parallel regions are basic “blocks” within code
- A master thread is instantiated at run time and persists throughout execution
- The master thread assembles teams of threads at parallel regions
How do threads communicate?

- Every thread has access to “global” memory (shared) and its own stack memory (private)
- Use shared memory to communicate between threads
- Simultaneous updates to shared memory can create a race condition: the results change with different thread scheduling
- Use mutual exclusion to avoid race conditions
  - But understand that “mutex” serializes performance wherever it is used
  - By definition only one thread at a time can execute that section of code
OpenMP constructs

OpenMP language extensions

parallel control structures
  • governs flow of control in the program
    parallel directive

work sharing
  • distributes work among threads
    do/parallel do and section directives

data scope
  • specifies variables as shared or private
    shared and private clauses

synchronization
  • coordinates thread execution
    critical and atomic directives
    barrier directive

runtime functions, environment variables
  • sets or queries runtime environment
    omp_set_num_threads()
    omp_get_thread_num()
    OMP_NUM_THREADS
    OMP_SCHEDULE
OpenMP directives

- OpenMP directives are comments in source code that specify parallelism for shared-memory (SMP) machines
- FORTRAN compiler directives begin with one of the sentinels `!$OMP`, `C$OMP`, or `*$OMP` – use `!$OMP` for free-format F90
- C/C++ compiler directives begin with the sentinel `#pragma omp`

<table>
<thead>
<tr>
<th>Fortran</th>
<th>C/C++</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>!$OMP parallel</code></td>
<td><code># pragma omp parallel</code></td>
</tr>
<tr>
<td><code>...</code></td>
<td><code>{...}</code></td>
</tr>
<tr>
<td><code>!$OMP end parallel</code></td>
<td><code># pragma omp parallel</code></td>
</tr>
<tr>
<td></td>
<td><code>for</code></td>
</tr>
<tr>
<td></td>
<td><code>for(...) {...}</code></td>
</tr>
<tr>
<td><code>!$OMP parallel do</code></td>
<td></td>
</tr>
<tr>
<td><code>DO ...</code></td>
<td></td>
</tr>
<tr>
<td><code>!$OMP end parallel do</code></td>
<td></td>
</tr>
</tbody>
</table>
Directives and clauses

- **Parallel regions** are marked by the `parallel` directive
- **Work-sharing loops** are marked by
  - `parallel do` directive in Fortran
  - `parallel for` directive in C
- Clauses control the behavior of a particular OpenMP directive
  1. Data scoping (Private, Shared, Default)
  2. Schedule (Guided, Static, Dynamic, etc.)
  3. Initialization (e.g., COPYIN, FIRSTPRIVATE)
  4. Whether to parallelize a region or not (if-clause)
  5. Number of threads used (NUM_THREADS)
Parallel region and work sharing

- Use OpenMP directives to specify Parallel Region and Work Sharing constructs

Parallel

Code block
DO
SECTIONS
SINGLE
CRITICAL

Each Thread Executes:
Work Sharing
Work Sharing
One Thread
One Thread at a Time

Parallel DO/for
Parallel SECTIONS

Stand-alone
parallel constructs
Parallel regions

1  !$OMP PARALLEL
2    code block
3    call work(...)
4  !$OMP END PARALLEL

Line  1  Team of threads is formed at parallel region
Lines  2-3  Each thread executes code block and subroutine call, no branching into or out of a parallel region
Line   4  All threads synchronize at end of parallel region (implied barrier)
Parallel work example

Speedup = \frac{\text{cputime}(1)}{\text{cputime}(N)}

If work is completely parallel, scaling is linear
Work sharing

1 !$OMP PARALLEL DO
2       do i=1,N
3            a(i) = b(i) + c(i)  !not much work
4       enddo
5 !$OMP END PARALLEL DO

Line  1   Team of threads is formed at parallel region
Lines  2-4 Loop iterations are split among threads, each loop iteration must be independent of other iterations
Line  5   (Optional) end of parallel loop (implied barrier at enddo)
Work-sharing example

Speedup = \frac{\text{cputime}(1)}{\text{cputime}(N)}

Scheduling, memory contention and overhead can impact speedup
Team overhead

- Increases roughly linearly with number of threads
OpenMP parallel constructs

- **Replicated**: executed by all threads
- **Work sharing**: divided among threads

```
PARALLEL
    {code}
END PARALLEL

PARALLEL DO
    do I = 1,N*4
        {code}
    end do
END PARALLEL
```

```
PARALLEL
    {code1}
DO
    do I = 1,N*4
        {code2}
    end do
    {code3}
END PARALLEL
```

```
I=1,N
    code
I=N+1,2N
    code2
I=2N+1,3N
    code2
I=3N+1,4N
    code2
I=1,N
    code
```

**Replicated**

**Work sharing**

**Combined**
Merging parallel regions

The !$OMP PARALLEL directive declares an entire region as parallel; therefore, merging work-sharing constructs into a single parallel region eliminates the overhead of separate team formations.

```c
!$OMP PARALLEL
  !$OMP DO
    do i=1,n
      a(i)=b(i)+c(i)
    enddo
  !$OMP END DO
  !$OMP DO
    do i=1,m
      x(i)=y(i)+z(i)
    enddo
  !$OMP END DO
!$OMP END PARALLEL
```

```c
!$OMP PARALLEL DO
  do i=1,n
    a(i)=b(i)+c(i)
  enddo
!$OMP END PARALLEL DO
!$OMP PARALLEL DO
  do i=1,m
    x(i)=y(i)+z(i)
  enddo
!$OMP END PARALLEL DO
```
Distribution of work: SCHEDULE clause

- !$OMP PARALLEL DO SCHEDULE(STATIC)
  - Default schedule: each CPU receives one set of contiguous iterations
  - Size of set is ~ (total_no_iterations / no_of_cpus)
- !$OMP PARALLEL DO SCHEDULE(STATIC,N)
  - Iterations are divided round-robin fashion in chunks of size N
- !$OMP PARALLEL DO SCHEDULE(DYNAMIC,N)
  - Iterations handed out in chunks of size N as threads become available
- !$OMP PARALLEL DO SCHEDULE(GUIDED,N)
  - Iterations handed out in pieces of exponentially decreasing size
  - N = minimum number of iterations to dispatch each time (default is 1)
  - Can be useful for load balancing (“fill in the cracks”)
OpenMP data scoping

- Data-scoping clauses control how variables are shared within a parallel construct
- These include the `shared`, `private`, `firstprivate`, `lastprivate`, `reduction` clauses
- Default variable scope:
  - Variables are shared by default
  - Global variables are shared by default
  - Automatic variables within a subroutine that is called from inside a parallel region are private (reside on a stack private to each thread), unless scoped otherwise
  - Default scoping rule can be changed with `default` clause
PRIVATE and SHARED data

- **SHARED** - Variable is shared (seen) by all processors
- **PRIVATE** - Each thread has a private instance (copy) of the variable
- Defaults: loop indices are private, other variables are shared

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

- All threads have access to the same storage areas for A, B, C, and N, but each loop has its own private copy of the loop index, i.
PRIVATE data example

• In the following loop, each thread needs a PRIVATE copy of temp
  – The result would be unpredictable if temp were shared, because each processor would be writing and reading to/from the same location

```c
!$OMP PARALLEL DO SHARED(A,B,C,N) PRIVATE(temp,i)
  do i=1,N
    temp = A(i)/B(i)
    C(i) = temp + cos(temp)
  enddo
!$OMP END PARALLEL DO
```

  – A “lastprivate(temp)” clause will copy the last loop (stack) value of temp to the (global) temp storage when the parallel DO is complete
  – A “firstprivate(temp)” initializes each thread’s temp to the global value
REDUCTION

- An operation that “combines” multiple elements to form a single result, such as a summation, is called a reduction operation.

```latex
!$OMP PARALLEL DO REDUCTION(+:asum) REDUCTION(*:aprod)
  do i=1,N
    asum = asum + a(i)
    aprod = aprod * a(i)
  enddo
!$OMP END PARALLEL DO
```

- Each thread has a private ASUM and APROD (declared as real*8, e.g.), initialized to the operator’s identity, 0 & 1, respectively.
- After the loop execution, the master thread collects the private values of each thread and finishes the (global) reduction.
**NOWAIT**

- When a work-sharing region is exited, a barrier is implied – all threads must reach the barrier before any can proceed.

- By using the NOWAIT clause at the end of each loop inside the parallel region, an unnecessary synchronization of threads can be avoided.

```plaintext
!$OMP PARALLEL
!$OMP DO
  do i=1,n
    work(i)
  enddo
!$OMP END DO NOWAIT
!$OMP DO schedule(dynamic,M)
  do i=1,m
    x(i)=y(i)+z(i)
  enddo
!$OMP END
!$OMP END PARALLEL
```
Mutual exclusion: atomic and critical directives

- When threads must execute a section of code serially (only one thread at a time can execute it), the region must be marked with CRITICAL / END CRITICAL directives
- Use the “!$OMP ATOMIC” directive if executing only one operation

```c
!$OMP PARALLEL SHARED(sum,X,Y)
...
!$OMP CRITICAL
  call update(x)
  call update(y)
  sum=sum+1
!$OMP END CRITICAL
...
!$OMP END PARALLEL

!$OMP PARALLEL SHARED(X,Y)
...
!$OMP ATOMIC
  sum=sum+1
...
!$OMP END PARALLEL
```
Mutual exclusion: lock routines

- When each thread must execute a section of code serially (only one thread at a time can execute it), locks provide a more flexible way of ensuring serial access than CRITICAL and ATOMIC directives.

```plaintext
call OMP_INIT_LOCK(maxlock)
!$OMP PARALLEL SHARED (X,Y)
...
call OMP_set_lock(maxlock)
call update(x)
call OMP_unset_lock(maxlock)
...
!$OMP END PARALLEL
call OMP_DESTROY_LOCK(maxlock)
```
Overhead associated with mutual exclusion

All measurements were made in dedicated mode

<table>
<thead>
<tr>
<th>Open MP exclusion routine/directive</th>
<th>cycles</th>
</tr>
</thead>
<tbody>
<tr>
<td>OMP_SET_LOCK/OMP_UNSET_LOCK</td>
<td>330</td>
</tr>
<tr>
<td>OMP_ATOMIC</td>
<td>480</td>
</tr>
<tr>
<td>OMP_CRITICAL</td>
<td>510</td>
</tr>
</tbody>
</table>
What you need to compile your OpenMP code

• A compiler plus library that can process OpenMP directives and function calls
  – Intel: icc or ifort, with option -openmp
  – GNU: gcc or gfortran, with option -fopenmp

• In C/C++, the header file for function prototypes
  – include <omp.h>
## Runtime library functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>omp_get_num_threads()</code></td>
<td>Number of threads in current team</td>
</tr>
<tr>
<td><code>omp_get_thread_num()</code></td>
<td>Thread ID, {0: N-1}</td>
</tr>
<tr>
<td><code>omp_get_max_threads()</code></td>
<td>Number of threads in environment</td>
</tr>
<tr>
<td><code>omp_get_num_procs()</code></td>
<td>Number of machine CPUs</td>
</tr>
<tr>
<td><code>omp_in_parallel()</code></td>
<td>True if in parallel region &amp; multiple threads executing</td>
</tr>
<tr>
<td><code>omp_set_num_threads(#)</code></td>
<td>Changes number of threads for parallel region</td>
</tr>
</tbody>
</table>
More functions and variables

- To enable dynamic thread count (*not* dynamic scheduling!)

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>omp_set_dynamic()</td>
<td>Set state of dynamic threading (true/false)</td>
</tr>
<tr>
<td>omp_get_dynamic()</td>
<td>True if dynamic threading is on</td>
</tr>
</tbody>
</table>

- To control the OpenMP runtime environment

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>OMP_NUM_THREADS</td>
<td>Set to permitted number of threads</td>
</tr>
<tr>
<td>OMP_DYNAMIC</td>
<td>TRUE/FALSE for enable/disable dynamic threading</td>
</tr>
</tbody>
</table>
OpenMP 2.0/2.5: what’s new?

- Wallclock timers
- Workshare directive (Fortran 90/95)
- Reduction on array variables
- NUM_THREAD clause
OpenMP wallclock timers

Real*8 :: omp_get_wtime, omp_get_wtick() (Fortran)
double omp_get_wtime(), omp_get_wtick(); (C)

double t0, t1, dt, res;
...
t0=omp_get_wtime();
<work>
t1=omp_get_wtime();
dt=t1-t0; res=1.0/omp_get_wtick();
printf("Elapsed time = %lf\n",dt);
printf("clock resolution = %lf\n",res);
References

• Current standard
  – http://www.openmp.org/

• Books
  – *Parallel Programming in OpenMP*, by Chandra, Dagum, Kohr, Maydan, McDonald, Menon
  – *Using OpenMP*, by Chapman, Jost, Van der Pas (OpenMP 2.5)

• Training website