Introduction to OpenMP

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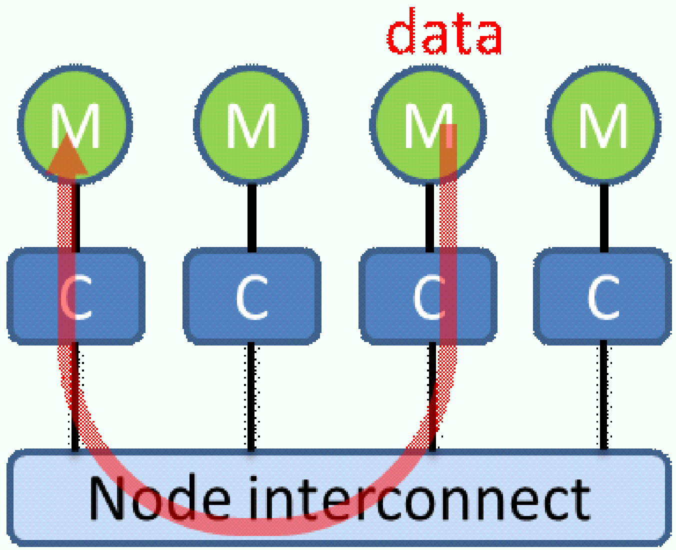
Goals

- Acquaint users with the concept of shared memory parallelism
- Acquaint users with the basics of programming with OpenMP

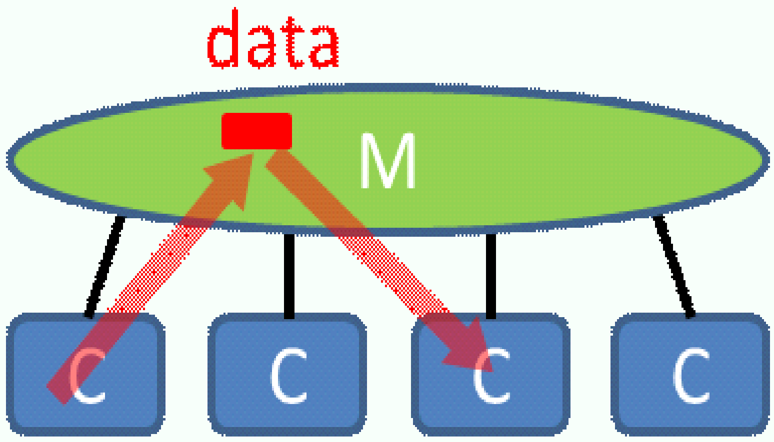
Distributed memory model

- Each process has its own address space
  - Data is local to each process
- Data sharing achieved via explicit message passing
- Example
  - MPI



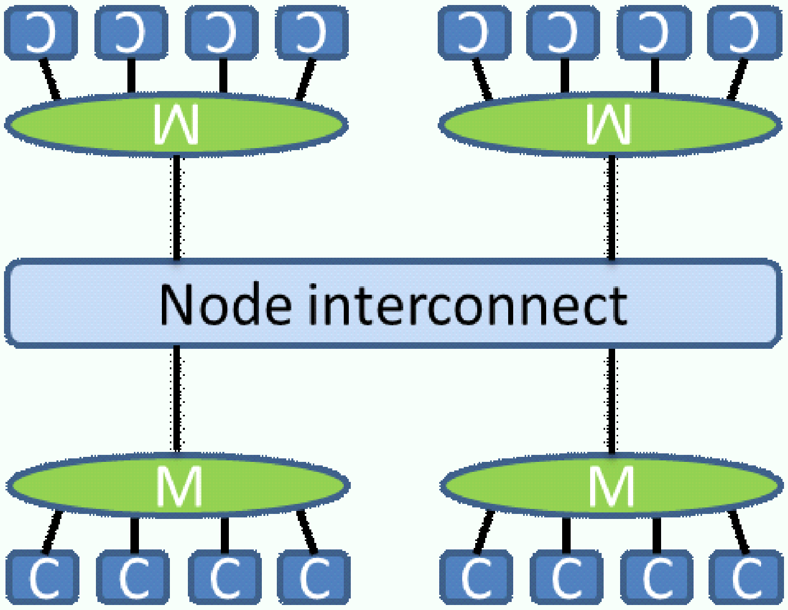
Shared memory model

- All threads can access the global memory space
- Data sharing achieved via writing to/reading from the same memory location
- Example
  - OpenMP
  - Pthreads



Clusters of SMP nodes

- The shared memory model is most commonly represented by Symmetric Multi-Processing (SMP) systems
  - Identical processors
  - Equal access time to memory
- Large shared memory systems are rare, clusters of SMP nodes are popular



Shared vs Distributed

Distributed Memory

- Pros
  - Memory scalable with number of number of processors
  - Easier and cheaper to build
- Cons
  - Difficult load balancing
  - Data sharing is slow

Shared Memory

- Pros
  - Global address space is user-friendly
  - Data sharing is fast
- Cons
  - Lack of scalability
  - Data conflict issues

OpenMP

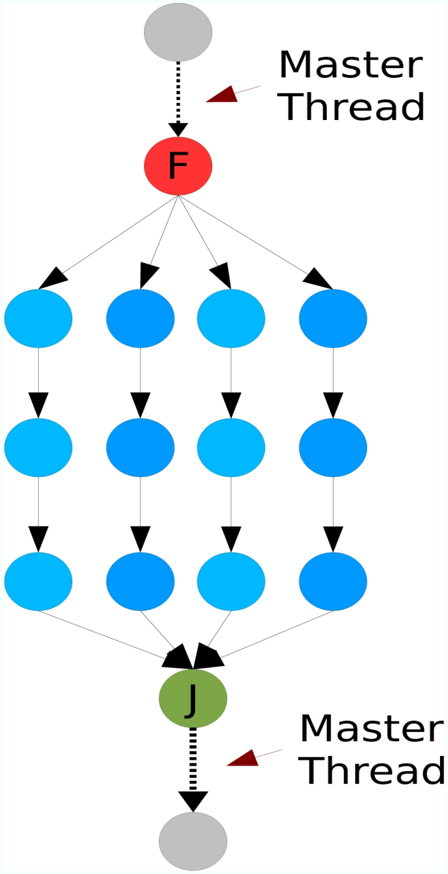
- OpenMP is an Application Program Interface (API) for thread based parallelism; Supports Fortran, C and C++
- Uses a fork-join execution model
- OpenMP structures are built with program directives, runtime libraries and environment variables
- OpenMP has been the industry standard for shared memory programming over the last decade
    - Permanent members of the OpenMP Architecture Review Board: AMD, Cray, Fujutsu, HP, IBM, Intel, Microsoft, NEC, PGI, SGI, Sun
- OpenMP 3.1 was released in September 2011

Advantages of OpenMP

- Portability
  - Standard among many shared memory platforms
  - Implemented in major compiler suites
- Ease to use
  - Serial programs can be parallelized by adding compiler directives
  - Allows for incremental parallelization – a serial program evolves into a parallel program by parallelizing different sections incrementally

Fork-join Execution Model

- Parallelism is achieved by generating multiple threads that run in parallel
  - A fork is when a single thread is made into multiple, concurrently executing threads
  - A join is when the concurrently executing threads synchronize back into a single thread
- OpenMP programs essentially consist of a series of forks and joins.



Building Blocks of OpenMP

- Program directives
  - Syntax
    - C/C++: #pragma omp *<directive> [clause]*
    - Fortran: !$omp *<directive> [clause]*
  - Parallel regions
  - Parallel loops
  - Synchronization
  - Data structure
  - …
- Runtime library routines
- Environment variables

Hello World: C

OpenMP include file

Parallel region starts here

```
#include <omp.h>
#include <stdio.h>
int main() {
#pragma omp parallel
{
printf("Hello from thread %d out of %d
threads\n", omp_get_thread_num(),
omp_get_num_threads());
}
return 0;
}
```

Runtime library functions

Parallel region ends here

Output

```
Hello from thread 0 out of
4 threads
Hello from thread 1 out of
4 threads
Hello from thread 2 out of
4 threads
Hello from thread 3 out of
4 threads
```

Hello World: Fortran

Parallel region starts here

```
program hello
  implicit none
  integer omp_get_thread_num,omp_get_num_threads
  !$omp parallel
  print *,'Hello from thread',omp_get_thread_num(),'out
of',omp_get_num_threads(),'threads'
  !$omp end parallel
end program hello
```

Runtime library functions

Parallel region ends here

Compilation and Execution

- IBM p575 clusters
  - Use the thread-safe compilers (with "_r")
  - Use '-qsmp=omp' option

```
%xlc_r -qsmp=omp test.c && OMP_NUM_THREADS=4 ./a.out
```

- Dell Linux clusters
  - Use '-openmp' option (Intel compiler)

```
%icc -openmp test.c && OMP_NUM_THREADS=4 ./a.out
```

Exercise 1: Hello World

- Write a “hello world” program with OpenMP where
    - If the thread id is odd, then print a message “Hello world from thread x, I'm odd!”
    - If the thread id is even, then print a message “Hello world from thread x, I am even!”

Solution

C/C++

```
#include <omp.h>
#include <stdio.h>
int main() {
  int id;
#pragma omp parallel private(id)
  {
    id = omp_get_thread_num();
    if (id%2==1)
      printf("Hello world from
thread %d, I am odd\n", id);
    else
      printf("Hello world from
thread %d, I am even\n", id);
  }
}
```

Fortran

```
program hello
  implicit none
  integer i,omp_get_thread_num
  !$omp parallel private(i)
  i = omp_get_thread_num()
  if (mod(i,2).eq.1) then
     print *,'Hello world from
thread',i,', I am odd!'
  else
     print *,'Hello world from
thread',i,', I am even!'
  endif
  !$omp end parallel
end program hello
```

Work Sharing: Parallel Loops

- We need to share work among threads to achieve parallelism
- Loops are the most likely targets when parallelizing a serial program
- Syntax
  - Fortran: `!$omp parallel do`
  - C/C++: `#pragma omp parallel for`
- Other working sharing directives available
  - Sections (discussed later)
  - Tasks (new feature in OpenMP 3.0)

Example: Parallel Loops

C/C++

```
#include <omp.h>
int main() {
  int i=0,N=100,a[100];
#pragma omp parallel for
  for (i=0;i<N;i++){
    a[i]=user_function(i);
  }
}
```

Fortran

```
program paralleldo
  implicit none
  integer i,n,a(100)
  i=0
  n=100
  !$omp parallel do
  do i=1,n
     a(i)=user_function(i)
  enddo
end program paralleldo
```

Load Balancing (1)

- OpenMP provides different methods to divide iterations among threads, indicated by the schedule clause
  - Syntax: schedule(<method>,[chunk size])
- Methods include
  - Static: the default schedule; divide iterations into chunks according to size, then distribute chunks to each thread in a round-robin manner;
  - Dynamic: each thread grabs a chunk of iterations, then requests another chunk upon the completion of the current one, until all iterations executed
  - Guided: similar to dynamic; the only difference is that the chunk size starts large and shrinks to size eventually

Load Balancing (2)

4 threads, 100 iterations

Schedule	Iterations mapped onto thread 0	1	2	3
`Static`	1-25	26-50	51-75	76-100
`Static,20`	1-20,81-100	21-40	41-60	61-80
`Dynamic`	1...	2...	3...	4...
`Dynamic,10`	1-10...	11-20...	21-30...	31-40...

Load Balancing (3)

Schedule	When to use
`Static`	Even and predictable workload per iteration; scheduling may be done at compilation time, least work at runtime;
`Dynamic`	Highly variable and unpredictable workload per iteration; most work at runtime
`Guided`	Special case of `dynamic` scheduling; compromise between load balancing and scheduling overhead at runtime

Working Sharing: Sections

- Gives a different block to each thread

C/C++

```
#pragma omp parallel
{
  #pragma omp sections
  {
  #pragma omp section
    some_calculation();
  #pragma omp section
    more_calculation();
  #pragma omp section
    yet_more_calculation();
  }
}
```

Fortran

```
!$omp parallel
  !$omp sections
  !$omp section
    call some_calculation
  !$omp section
    call more_calculation
  !$omp section
    call yet_more_calculation
  !$omp end sections
!$omp end parallel
```

Scope of Variables

- `Shared(list)`
  - Specifies the variables that are shared among all the threads
- `Private(list)`
  - Creates a local copy of the specified variables for each thread
  - the value is uninitialized!
- `Default(shared|private|none)`
  - Defines the default scope of variables
  - **C/C++ API does not have `default(private)`**
- Most variables are shared by default
  - A few exceptions: iteration variables; stack variables in subroutines; automatic variables within a statement block

Private Variables

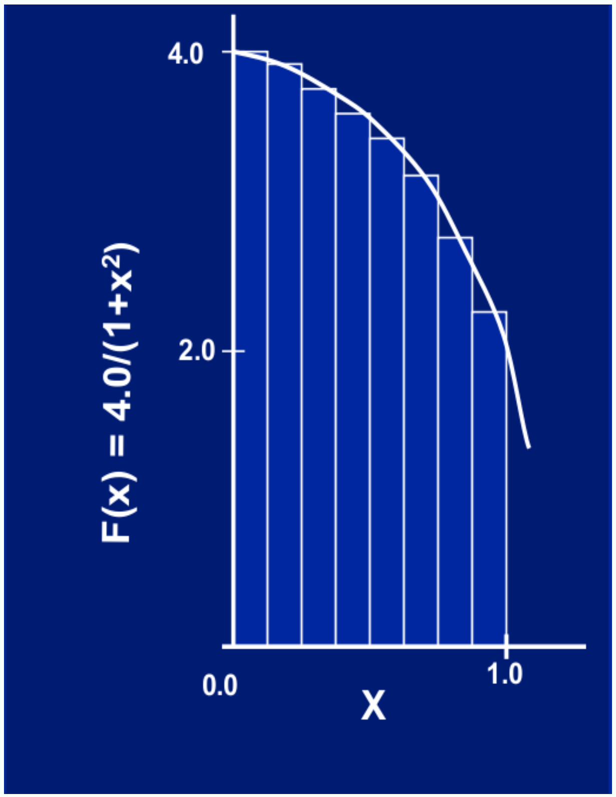
- Not initialized at the beginning of parallel region
- After the parallel region
  - Not defined in OpenMP 2.x
  - 0 in OpenMP 3.x

tmp not initialized here

```
void wrong()
{
  int tmp=0;
#pragma omp for private(tmp)
  for (int j=0; j<100; ++j)
    tmp += j
  printf("%d\n",tmp)
}
```

OpenMP 2.5: tmp undefined
OpenMP 3.0: tmp is 0

Exercise 2: Calculate pi by Numerical Integration



- We know that:

$$\int_0^1 \frac{4.0}{(1+x^2)}\,dx = \pi$$

- So numerically we can approximate pi as the sum of the area of a number of rectangles

$$\sum_{i=0}^{N} F(x_i)\Delta x \approx \pi$$

Source: Meadows et al, A "hands-on" introduction to OpenMP, SC09

Exercise 2: serial version

C/C++

```
double x,deltax,pi,sum=0.0
int i,nstep=<a large number>

deltax=1./(double)nstep

for (i=0; i<nstep; i++)
{
  x=(i+0.5)*deltax
  sum=sum+4./(1.+x*x)
}

pi=deltax*sum
```

Fortran

```
Real*8 :: x,deltax,pi,sum
integer :: i,nstep

nstep=<a large number>
sum=0

deltax=1./float(nstep)

do i=1,nstep
  x=(i+0.5)*deltax
  sum=sum+4./(1.+x*x)
enddo

pi=deltax*sum
```

Exercise 2: OpenMP version

- Create a parallel version of the program with OpenMP

Special Cases of Private

- Firstprivate
  - Initialize each private copy with the corresponding value from the master thread
- Lastprivate
  - Allows the value of a private variable to be passed to the shared variable outside the parallel region

tmp initialized as 0

```
void correct()
{
  int tmp=0;
#pragma omp for firstprivate(tmp) \
  lastprivate(tmp)
  for (int j=0; j<100; ++j)
    tmp += j
  printf("%d\n",tmp)
```

The value of tmp is the value when j=99

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Reduction

- The `reduction` clause allows accumulative operations on the value of variables
- Syntax: `reduction(operator:variable list)`
- A private copy of each variable appears in `reduction` is created as if the `private` clause is specified
- Operators
  - Arithmetic
  - Bitwise
  - Logical

Example: Reduction

C/C++

```
#include <omp.h>
int main() {
  int i,N=100,sum,a[100],b[100];
  for (i=0;i<N;i++){
    a[i]=i;
    b[i]=1;
  }
  sum=0;
#pragma omp parallel for
reduction(+:sum)
  for (i=0;i<N;i++){
    sum=sum+a[i]*b[i];
  }
}
```

Fortran

```
program reduction
  implicit none
  integer i,n,sum,a(100),b(100)
  n=100
  do i=1,n
     a(i)=i
  enddo
  b=1
  sum=0
  !$omp parallel do reduction(+:sum)
  do i=1,n
     sum=sum+a(i)*b(i)
  enddo
end
```

Exercise 3: pi calculation with reduction

- Redo exercise 2 with reduction

Pitfalls (1): False Sharing

- Array elements that are in the same cache line can lead to false sharing
  - The system handles cache coherence on a cache line basis, not on a byte or word basis
  - Each update of a single element could invalidate the entire cache line

```
!$omp parallel
myid=omp_get_thread_num()
nthreads=omp_get_num_threads()
do i=myid+1,n,nthreads
     a(i)=some_function(i)
enddo
```

Pitfalls (2): Race Condition

- Multiple threads try to write to the same memory location at the same time
  - Indeterministic results
- Inappropriate scope of variable can cause indeterministic results too
- When having indeterministic results, set the number of threads to 1 to check
  - If problem persists: scope problem
  - If problem is solved: race condition

```
!$omp parallel do
do i=1,n
    if (a(i).gt.max) then
        max=a(i)
    endif
enddo
```

Synchronization: Barrier

- "Stop sign" where every thread waits until all threads arrive
- Purpose: protect access to shared data
- Syntax
  - Fortran: `!$omp barrier`
  - C/C++: `#pragma omp barrier`
- A barrier is implied at the end of every parallel region
  - Use the `nowait` clause to turn if off
- Synchronizations are costly so their usage should be minimized

Synchronization: Critical and Atomic

- Critical
  - Only one thread at a time can enter a `critical` region

```
double x;
#pragma omp parallel for
for (i=0;i<N;i++)
{
  a = some_calculation(i)
#pragma omp critical
  some_function(a,x);
}
```

- Atomic
  - Only one thread at a time can update a memory location

```
double a;
#pragma omp parallel
{ double b;
  b = some_calculation();
#pragma omp atomic
     a += b;
}
```

Runtime Library Functions

- Modify/query the number of threads
  - omp_set_num_threads(), omp_get_num_threads(), omp_get_thread_num(), omp_get_max_threads()
- Query the number of processes
  - omp_num_procs()
- Query whether or not in an active parallel region
  - omp_in_parallel()
- Control the behavior of dynamic threads
  - omp_set_dynamic(), omp_get_dynamic()

Environment Variables

- OMP_NUM_THREADS: set default number of threads to use
- OMP_SCHEDULE: control how iterations are scheduled for parallel loops

References

- https://docs.loni.org/wiki/Using_OpenMP
- http://en.wikipedia.org/wiki/OpenMP
- http://www.nersc.gov/nusers/help/tutorials/openmp/
- http://www.llnl.gov/computing/tutorials/openMP/

Next week's training

- What: Shell scripting tutorial
- Where: Frey 307
- When: Oct 26, Wednesday, 10am-12pm