Introduction to OpenMP

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Outline

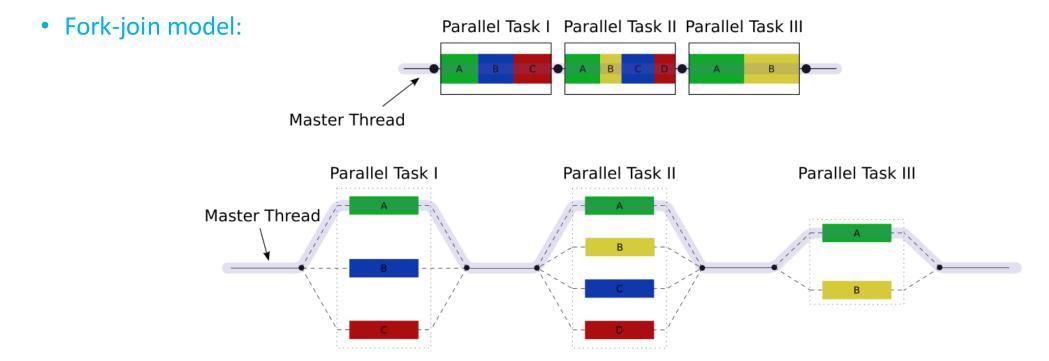
- A brief overview of OpenMP
- Constructs and clauses
- Parallel loops
- Data race
- OpenMP in Numpy

OpenMP

- ☐ OpenMP (Open Multi-Processing) is an API (application programming interface) that supports multi-platform shared memory multiprocessing programming.
- ☐ Supporting languages: C, C++, and Fortran.
- ☐ Consists of a set of compiler directives, library routines, and environment variables that influence run-time behavior.
- ☐ OpenMP supports accelerators.

Parallelism of OpenMP

• Multithreading: a master thread forks a specified number of slave threads and the system divides a task among them. The threads then run concurrently, with the runtime environment allocating threads to different processors (or cores).



Reference: http://en.wikipedia.org/wiki/OpenMP

The first OpenMP program: Hello world!

Hello world in C

```
#include <omp.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);
```

Hello world in Fortran

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

OpenMP directive syntax

• In C/C++ programs

```
#pragma omp directive-name [clause[[,] clause]. . . ]
```

• In Fortran programs

```
!$omp directive-name [clause[[,] clause]. . . ]
```

- Directive-name is a specific keyword, for example *parallel*, that defines and controls the action(s) taken.
- Clauses, for example private, can be used to further specify the behavior.

Compile and run OpenMP programs

Compile C/Fortran codes

```
gcc -fopenmp name.c -o name
gfortran -fopenmp name.f90 -o name
```

Run OpenMP programs

```
export OMP_NUM_THREADS=8 # set number of threads
./name
time ./name # run and measure the time.
```

OpenMP programming

- Parallel Construct
- Work-Sharing Constructs
- Clauses
- Data race: atomic, reduction

Construct: An OpenMP executable directive and the associated statement, loop, or structured block, not including the code in any called routines.

Parallel construct

Syntax in C/C++ programs

```
#pragma omp parallel [clause[[,] clause]. . . ] ..... code block .....
```

• Syntax in Fortran programs

```
!$omp parallel [clause[[,] clause]. . . ]
..... code block .....
!$omp end parallel
```

- Parallel construct is used to specify the computations that should be executed in parallel.
- A team of threads is created to execute the associated parallel region.
- The work of the region is replicated for every thread.
- At the end of a parallel region, there is an implied barrier that forces all threads to wait until the computation inside the region has been completed.

Work-sharing constructs

Functionality	Syntax in C/C++	Syntax in Fortran
Distribute iterations	#pragma omp for	!\$omp do
Distribute independent works	#pragma omp sections	!\$omp sections
Use only one thread	#pragma omp single	!\$omp single
Parallelize array syntax	N/A	!\$omp workshare

• Many applications can be parallelized by using just a parallel region and one or more of work-sharing constructs, possibly with clauses.

- The parallel and work-sharing (except single) constructs can be combined.
- Following is the syntax for combined parallel and work-sharing constructs,

Combine parallel construct with	Syntax in C/C++	Syntax in Fortran
Loop construct	#pragma omp parallel for	!\$omp parallel do
Sections construct	#pragma omp parallel sections	!\$omp parallel sections
Workshare construct	N/A	!\$omp parallel workshare

Loop construct

• The loop construct causes the iterations of the loop immediately following it to be executed in parallel.

Syntax in C/C++ programs

```
#pragma omp for [clause[[,] clause]. . . ]
..... for loop .....
```

Syntax in Fortran programs

```
!$omp do [clause[[,] clause]. . . ]
..... do loop .....
[!$omp end do]
```

• The terminating !\$omp end do directive in Fortran is optional but recommended.

Distribute iterations in a parallel region

```
#pragma omp parallel for shared(n,a) private(i)
for (i=0; i<n; i++)
    a[i] = i + n;</pre>
```

- shared clause: All threads can read from and write to a shared variable.
- private clause: Each thread has a local copy of a private variable.
- The maximum iteration number n is shared, while the iteration number i is private.
- Each thread executes a subset of the total iteration space i = 0, . . . , n − 1
- The mapping between iterations and threads can be controlled by the schedule clause.

• Two work-sharing loops in one parallel region

```
#pragma omp parallel shared(n,a,b) private(i)
  #pragma omp for
  for (i=0; i< n; i++) a[i] = i+1;
  // there is an implied barrier
  #pragma omp for
  for (i=0; i< n; i++) b[i] = 2 * a[i];
   /*-- End of parallel region --*/
```

- The distribution of iterations to threads could be different for the two loops.
- The implied barrier at the end of the first loop ensures that all the values of a[i] are updated before they are used in the second loop.

Exercise 1

SAXPY in OpenMP:

The SAXPY program is to add a scalar multiple of a real vector to another real vector: s = a*x + y.

- 1. Provided a serial SAXPY code, parallelize it using OpenMP directives.
- 2. Compare the performance between serial and OpenMP codes.

Sections construct

Syntax in C/C++ programs

```
#pragma omp sections [clause[[,] clause]. . . ]
[#pragma omp section]
..... code block 1 .....
[#pragma omp section
..... code block 2 ......
```

Syntax in Fortran programs

```
!$omp sections [clause[[,] clause]...]
[!$omp section]
..... code block 1 .....
[!$omp section
..... code block 2 .....]
....
!$omp end sections
```

- The work in each section must be independent.
- Each section is distributed to one thread.

Example of parallel sections

```
#pragma omp parallel sections
{
    #pragma omp section
    funcA();
    #pragma omp section
    funcB();
} /*-- End of parallel region --*/
```

- The most common use of the sections construct is probably to execute function or subroutine calls in parallel.
- There is a load-balancing problem, if the amount of work in different sections are not equal.

Single construct

• Syntax in C/C++ programs

```
#pragma omp single [clause[[,] clause]. .
..... code block ......
```

• Syntax in Fortran programs

```
!$omp single [clause[[,] clause]...]
..... code block .....
!$omp end single
```

- The code block following the single construct is executed by one thread only.
- The executing thread could be any thread (not necessary the master one).
- The other threads wait at a barrier until the executing thread has completed.

An example of the single construct

```
#pragma omp parallel shared(a,b) private(i)
 #pragma omp single
    a = 10;
 /* A barrier is automatically inserted here */
 #pragma omp for
 for (i=0; i<n; i++)
    b[i] = a;
  /*-- End of parallel region --*/
```

- Only one thread initializes the shared variable a.
- If the single construct is omitted here, multiple threads could assign the value to a at the same time, potentially resulting in a memory problem.
- The implicit barrier at the end of the single construct ensures that the correct value is assigned to the variable a before it is used by all threads.

Data race

- A data race condition arises when multithreads read or write the same shared data simultaneously.
- Example: two threads each increases the value of a shared integer variable by one.

Correct sequence

Thread 1	Thread 2		value
			0
read value		←	0
Increase value			0
write back		\rightarrow	1
	read value	←	1
	increase value		1
	write back	\rightarrow	2

Incorrect sequence

Thread 1	Thread 2		value
			0
read value		←	0
	read value	←	0
increase value			0
	increase value		0
write back		\rightarrow	1
	write back	\rightarrow	1

Example of data race: sums up elements of a vector

Different threads read and write the shared data sum simultaneously.

A data race condition arises!

The final result of *sum* could be incorrect!

```
sum = 0;
#pragma omp parallel for shared(sum,a,n) private(i)
for (i=0; i<n; i++)
{
    sum = sum + a[i];
} /*-- End of parallel for --*/
printf("Value of sum after parallel region: %f\n",sum);</pre>
```

Atomic construct

- The atomic construct allows multiple threads to safely update a shared variable.
- The memory update (such as write) in the next instruction will be performed atomically. It does not make the entire statement atomic. Only the memory update is atomic.
- It is applied only to the (single) assignment statement that immediately follows it.

C/C++ programs

• Syntax

#pragma omp atomic

..... a single statement

Supported operators

+, *, -, /, &, ^, |, <<, >>.

Fortran programs

!\$omp atomic

..... a single statement

!\$omp end atomic

+, *, -, /, .AND., .OR., .EQV., .NEQV. .

- The first try to solve the data-race problem: use atomic (correct but slow)
- The atomic construct avoids the data racing condition. Therefore, the result is correct.
- But all elements are added sequentially, and there is performance penalty for using atomic, because the system coordinates all threads.
- This code is even slower than a serial code!

```
sum = 0;
#pragma omp parallel for shared(n,a,sum) private(i) // Optimization: use reduction instead
of atomic
for (i=0; i<n; i++)
   #pragma omp atomic
    sum += a[i];
  /*-- End of parallel for --*/
printf("Value of sum after parallel region: %d\n",sum);
```

• A partially parallel scheme to avoid data race

Step 1: Calculate local sums in parallel

Thread 1	Thread 2	•••••	Thread m
a_0	a_{m}		a _{n-m-1}
+	+		+
a_1	a _{m+1}	•••••	a _{n-m}
+	+		+
•	:		:
+	+		+
a _{m-1}	a _{2m-1}	•••••	a_n
II	II		H
LS ₁	LS ₂	•••••	LS _m

m: number of

threads

n: array length

LS: local sum

Step 2: Update total sum sequentially

Thread 1	Thread 2	•••••	Thread m
Read initial S			
$S = S + LS_1$			
Write S			
	Read S		
	$S = S + LS_2$		
	Write S		
		•••••	
			Read S
			$S = S + LS_m$
			Write S

m: number of

threads

LS: local sum

S: total sum

- The second try to solve the data-race problem: use *atomic* (correct and fast)
- Each thread adds up its local sum.
- The atomic is only applied for adding up local sums to obtain the total sum.

```
sum = 0;
#pragma omp parallel shared(n,a,sum) private(sumLocal)
  sumLocal = 0;
  #pragma omp for
  for (i=0; i<n; i++) sumLocal += a[i];
  #pragma omp atomic
  sum += sumLocal;
  /*-- End of parallel region --*/
printf("Value of sum after parallel region: %d\n",sum);
```

Reduction clause

• The third try to solve the data-race problem: use *reduction* (correct, fast and simple)

```
#pragma omp parallel for default(none) shared(n,a) private(i) reduction(+:sum)
for (i=0; i<n; i++)
    sum += a[i];
/*-- End of parallel reduction --*/</pre>
```

- The reduction variable is protected to avoid data race.
- The partially parallel scheme is applied behind the scene.
- The reduction variable is shared by default and it is unnecessary to specify it explicitly.

• Operators and statements supported by the reduction clause

	C/C++	Fortran
Typical statements	<pre>x = x op expr x binop = expr x = expr op x (except for subtraction) x++ ++x x</pre>	<pre>x = x op expr x = expr op x (except for subtraction) x = intrinsic (x, expr_list) x = intrinsic (expr_list, x)</pre>
op could be	+, *, -, &, ^, , &&, or	+, *, -, .and., .or., .eqv., or .neqv.
binop could be	+, *, -, &, ^, or	N/A
<i>Intrinsic</i> function could be	N/A	max, min, iand, ior, ieor

Exercise 2

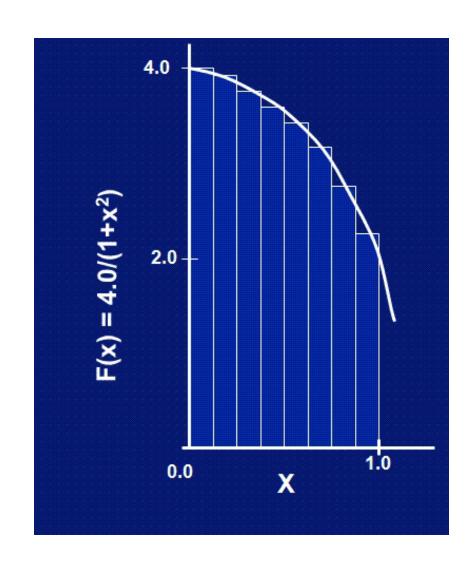
Compute the value of pi:

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

The integration can be numerically approximated as the sum of a number of rectangles.

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

- 1. Provided the serial code for computing the value of pi, parallelize it using OpenMP directives.
- 2. Compare the performance between seral and OpenMP codes.



Using OpenMP in Numpy

- OpenMP-enabled Libraries
- OpenBLAS: BLAS = Basic Linear Algebra Subprograms
- MKL: Linear algebra libraries optimized for intel CPUs.
- Numpy
- Install Numpy with precompiled OpenBLAS or MKL
- Numpy calls OpenMP-enabled routines under the hood.

Run a python program with multiple threads

pip install numpy

import numpy as np

n = 10000

a = np.random.rand(n,n)

b = np.random.rand(n,n)

c = np.matmul(a, b)

export OMP_NUM_THREADS=8 pyton name.py

Appendix A: OpenMP built-in functions

• Enable the usage of OpenMP functions:

C/C++ program: include omp.h.

Fortran program: include omp_lib.h or use omp_lib module.

• List of OpenMP functions:

```
omp_set_num_threads(integer) : set the number of threads
omp_get_num_threads(): returns the number of threads
omp_get_thread_num(): returns the number of the calling thread.
omp_set_dynamic(integer|logical): dynamically adjust the number of threads
omp_get_num_procs(): returns the total number of available processors when it is called.
omp_in_parallel(): returns true if it is called within an active parallel region. False otherwise.
```

Appendix B: OpenMP runtime variables

```
OMP_NUM_THREADS: the number of threads (=integer)

OMP_SCHEDULE: the schedule type (=kind,chunk . Kind could be static, dynamic or guided)

OMP_DYNAMIC: dynamically adjust the number of threads (=true | =false).

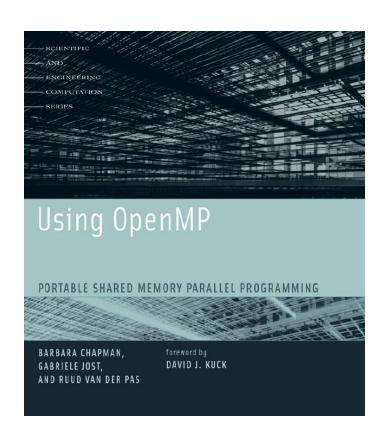
KMP_AFFINITY: only for intel compiler, to bind OpenMP threads to physical processing units.

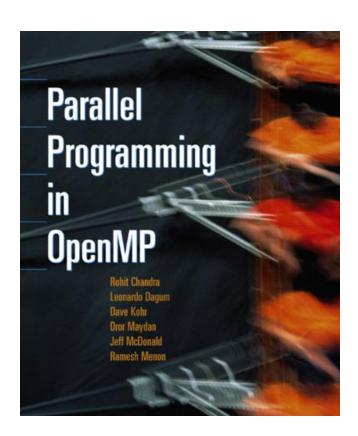
(=compact | =scatter | =balanced).

Example usage: export KMP_AFFINITY= compact,granularity=fine,verbose .
```

Further information

References





☐ OpenMP official website: http://openmp.org/wp/