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Introduction to OpenMP

2021 HPC Workshop: Parallel Programming

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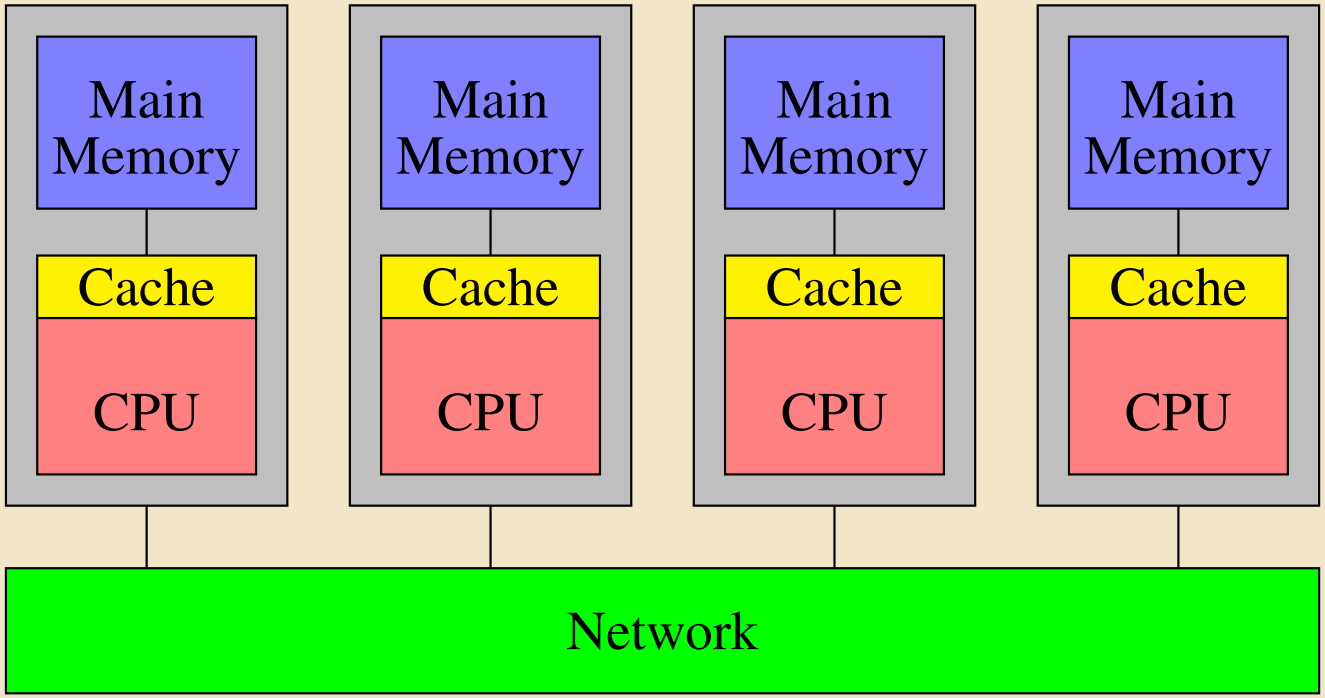
Research Computing

July 13 - 15, 2021

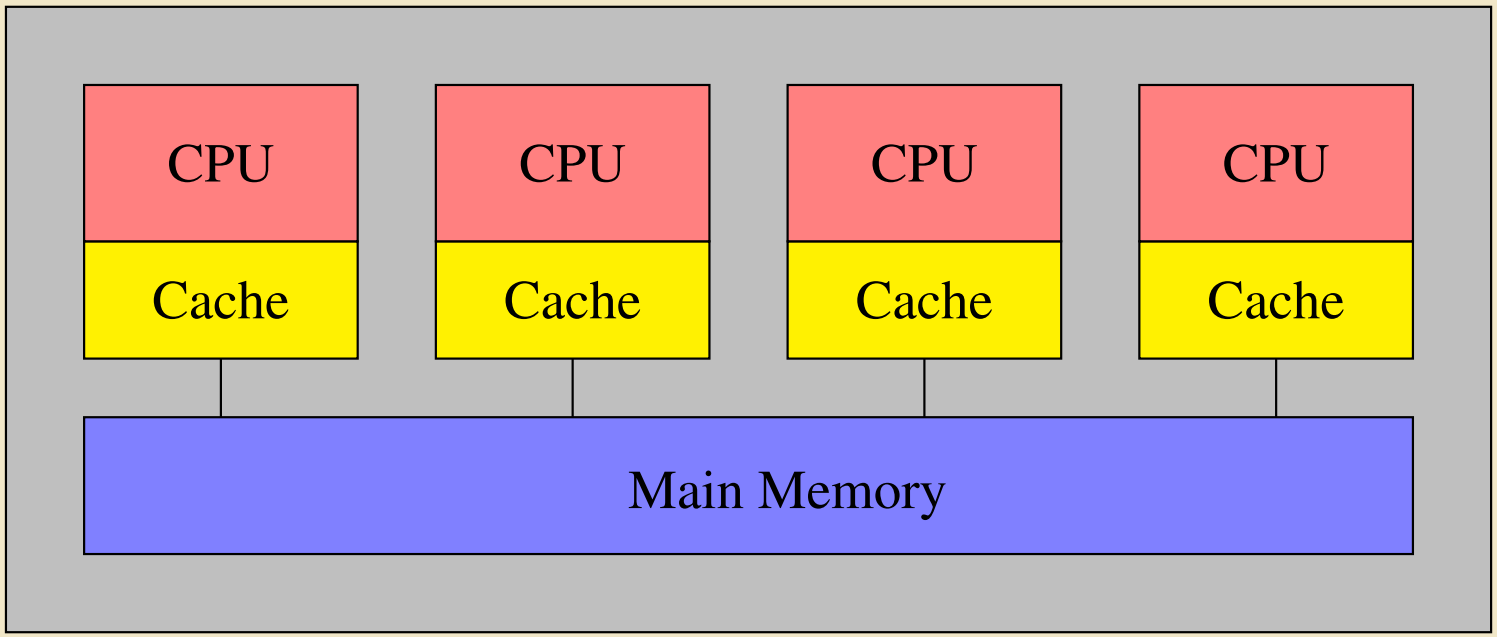
Distributed Memory Model

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



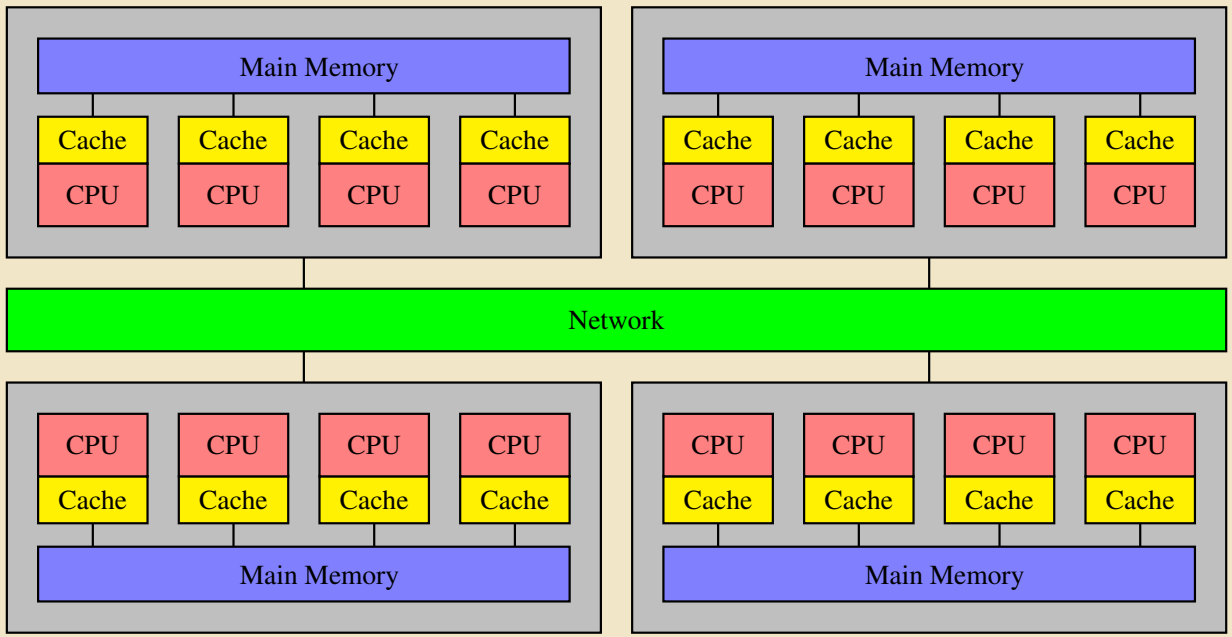
Shared Memory Model

- 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

Shared Memory

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

Distributed Memory

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

Compiler Flags for Automatic Parallelization

GCC	-floop-parallelize-all
Intel	-parallel
XL	-qsmp=auto
PGI	-Mconcur=<flags>

When to consider using OpenMP?

- The compiler may not be able to do the parallelization
  1. A loop is not parallelized
     - The data dependency analysis is not able to determine whether it is safe to parallelize or not
  2. The granularity is not high enough
     - The compiler lacks information to parallelize at the highest possible level

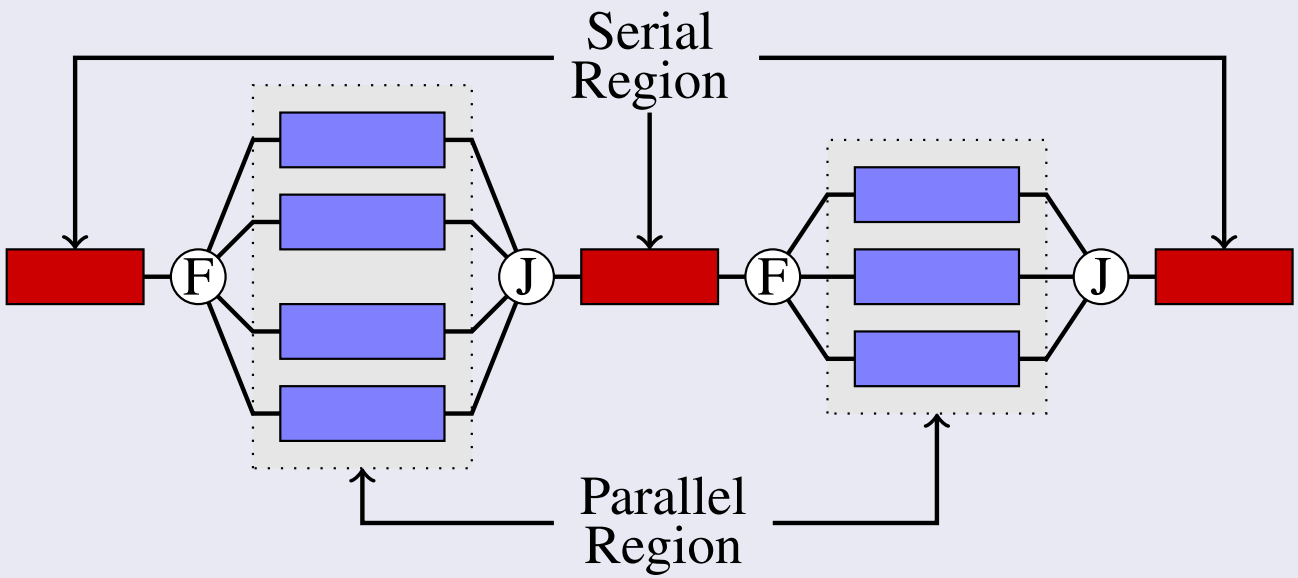
- OpenMP is an Application Program Interface (API) for thread based parallelism; Supports Fortran, C and C++
- Uses a fork-join execution model
- OpenMP structures are built with program directives, runtime libraries and environment variables
- OpenMP has been the industry standard for shared memory 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 4.0 was released in June 2014

Goals of OpenMP

- Standardization
  - Provide a standard among a variety of shared memory architectures/platforms
  - Jointly defined and endorsed by a group of major computer hardware and software vendors
- Lean and Mean
  - Establish a simple and limited set of directives for programming shared memory machines.
  - Significant parallelism can be implemented by using just 3 or 4 directives.
- 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
- Portability
  - Standard among many shared memory platforms
  - Implemented in major compiler suites

Fork-Join Execution Model

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



Building Block 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

OpenMP Basic Syntax

- Fortran: case insensitive
  - Add: use omp_lib or include "omp_lib.h"
  - Usage: Sentinel directive [clauses]
  - Fortran 77
    - Sentinel could be: !$omp, *$omp, c$omp and must begin in first column
  - Fortran 90/95/2003
    - Sentinel: !$omp
  - End of parallel region is signified by the end sentinel statement: !$omp end directive [clauses]
- C/C++: case sensitive
  - Add #include <omp.h>
  - Usage: #pragma omp directive [clauses] newline

Compiler Directives

- Parallel Directive
  - **parallel**
- Worksharing Constructs
  - Fortran: **do**, **workshare**
  - C/C++: **for**
  - Fortran/C/C++: **sections**
- Synchronization
  - **master**, **single**, **ordered**, **flush**, **atomic**

Clauses

- if(scalar_expression)
- private(list), shared(list)
- firstprivate(list), lastprivate(list)
- reduction(operator:list)
- schedule(method[,chunk_size])
- nowait
- num_thread(num)
- threadprivate(list), copyin(list)
- ordered
- more · · ·

Runtime Libraries

- Number of Threads: omp_{set,get}_num_threads
- Thread ID: omp_get_thread_num
- Scheduling: omp_{set,get}_dynamic
- Nested Parallelism: omp_in_parallel
- Locking: omp_{init,set,unset}_lock
- Wallclock Timer: omp_get_wtime
- more · · ·

Environment Variables

- OMP_NUM_THREADS
- OMP_SCHEDULE
- OMP_STACKSIZE
- OMP_DYNAMIC
- OMP_NESTED
- OMP_WAIT_POLICY
- more · · ·

Parallel Directive

- The **parallel** directive forms a team of threads for parallel execution.
- Each thread executes the block of code within the OpenMP Parallel region.

C

```c
#include <stdio.h>

int main() {

#pragma omp parallel
  {
    printf("Hello world\n");
  }

}
```

Fortran

```fortran
program hello

  implicit none

  !$omp parallel
  print *, 'Hello World'
  !$omp end parallel

end program hello
```

Compiling and Running OpenMP programs

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Compiling: `compiler options code`

- The OpenMP compile flag varies based on the compiler

GNU: `-fopenmp`
Intel: `-qopenmp`
NVHPC: `-mp`

```
[alp514.sol](1032): gfortran -fopenmp -o helloc hello.c
[alp514.sol](1033): ifort -qopenmp -o hellof hello.f90
```

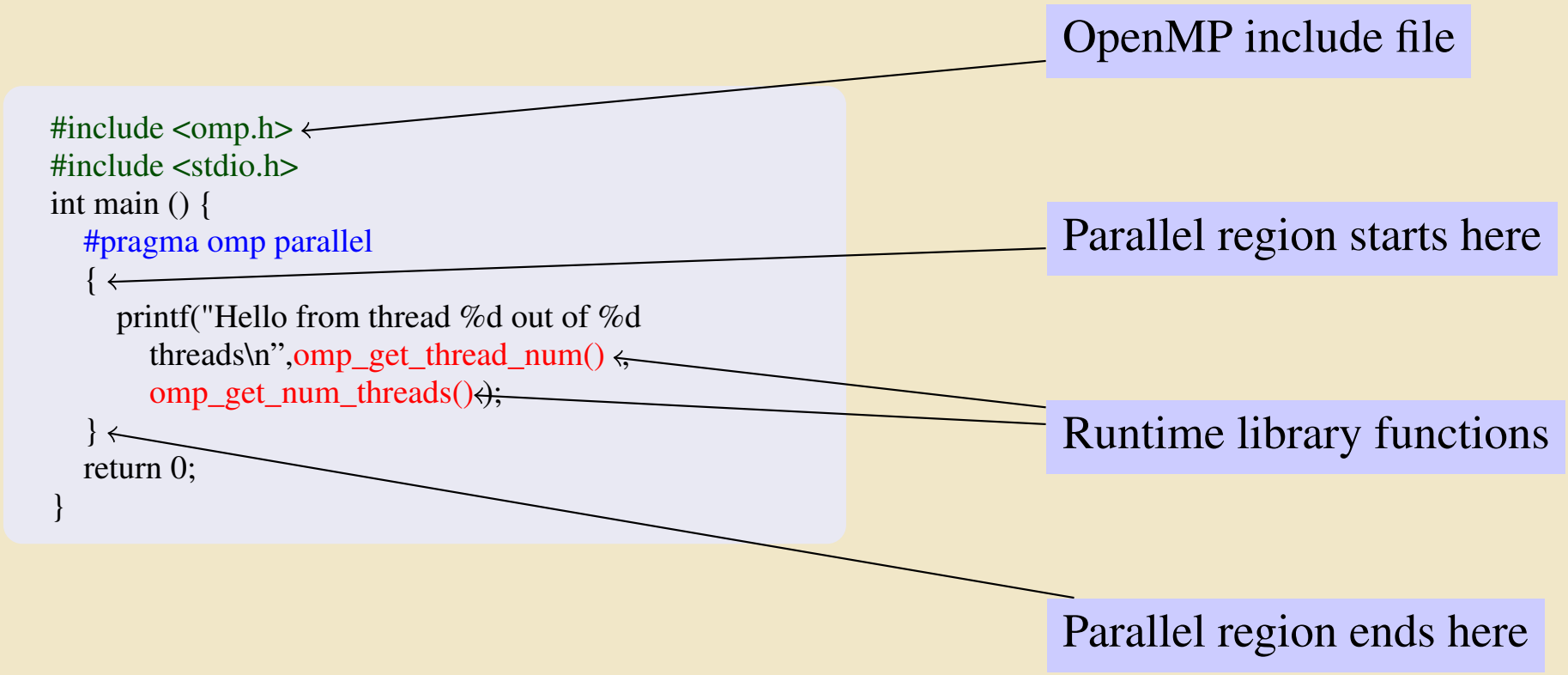
Running : Need to specify number of openmp threads to run code on

```
[alp514.hawk-b624](1001): OMP_NUM_THREADS=4 ./helloc
Hello world
Hello world
Hello world
Hello world
[alp514.hawk-b624](1002): export OMP_NUM_THREADS=2
[alp514.hawk-b624](1003): ./hellof
 Hello World
 Hello World
```

Parallel Directive

- The number of threads in a parallel region is determined by the following factors, in order of precedence:
  - Evaluation of the IF clause
  - Setting of the NUM_THREADS clause
  - Use of the omp_set_num_threads() library function
  - Setting of the OMP_NUM_THREADS environment variable
  - Implementation default
- Threads are numbered from 0 (master thread) to N-1

Hello World: C




```
#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;
}
```

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

Hello World: Fortran

```
program hello

   implicit none
   integer :: omp_get_thread_num, omp_get_num_threads

   !$omp parallel

   print '(a,i3,a,i3,a)', 'Hello from thread',
      omp_get_thread_num() , &
      ' out of ' omp_get_num_threads(),' threads'

   !$omp end parallel
end program hello
```

Parallel region starts here

Runtime library functions

Parallel region ends here

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

Exercise 1: Hello World

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

C

```c
#include <stdio.h>
/* Include omp.h ? */
int main() {
  int id;
  /* Add Opemp pragma */
  {
    id = /* Get Thread ID */
    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

```fortran
program hello
  ! Include/Use omp_lib.h/omp_lib ?
  implicit none
  integer i
  ! Add OMP Directive
  i = ! Get Thread ID
  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
  ! End OMP Directive ?
end program hello
```

Solution

C/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);
  }
}
```

```
[alp514.sol](1898): gcc -fopenmp  -o helloc hello.c
[alp514.sol](1899): export OMP_NUM_THREADS=4
[alp514.sol](1900): srun -p eng -n 1 -c 4 ./helloc
Hello world from thread 0, I am even
Hello world from thread 3, I am odd
Hello world from thread 1, I am odd
Hello world from thread 2, I am even
```

Fortran

```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
```

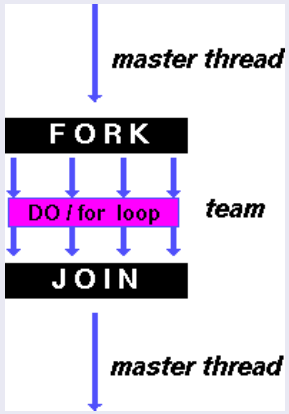
```
[alp514.sol](1906): nvfortran -mp  -o hellof hello.f90
[alp514.sol](1907): interact -p eng -n 1 -c 4
[alp514.sol-b110](893): OMP_NUM_THREADS=4 ./hellof
Hello from thread   0, I am even!
Hello from thread   2, I am even!
Hello from thread   3, I am odd!
Hello from thread   1, I am odd!
```

Work Sharing

- We need to share work among threads to achieve parallelism

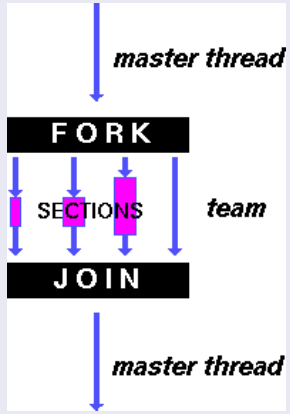
Loops

```
!$omp do
#pragma omp for
```



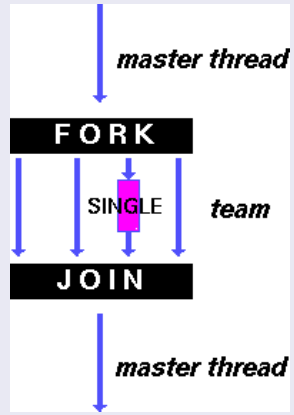
Sections

```
!$omp sections
#pragma sections
```



Single

```
!$omp single
#pragma omp single
```



- The parallel and work sharing directive can be combined as
  - `!$omp parallel do`
  - `#pragma omp parallel sections`

Example: Parallel Loops

C/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] = (i+1) * (i+2) ;
  }
}
```

Fortran

```fortran
program paralleldo

  implicit none
  integer :: i, n, a(100)

  i = 0
  n = 100
  !$omp parallel
  !$omp do
  do i = 1, n
     a(i) = i * (i+1)
  end do
  !$omp end do
  !$omp end parallel
end program paralleldo
```

Load Balancing

- 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 interations 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 completion of the current one, until all iterations are executed.
  - `Guided`: similar to `Dynamic`; the only difference is that the chunk size starts large and shrinks to `size` eventually.

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`	$1, \cdots$	$2, \cdots$	$3, \cdots$	$4, \cdots$
`Dynamic,10`	$1 - 10, \cdots$	$11 - 20, \cdots$	$21 - 30, \cdots$	$31 - 40, \cdots$

Load Balancing

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

Work 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
      some_more_calculation();
#pragma omp section
      yet_some_more_calculation();
    }
  }
```

Fortran

```
!$omp parallel
!$omp sections
!$omp section
call some_calculation
!$omp section
call some_more_calculation
!$omp section
call yet_some_more_calculation
!$omp end sections
!$omp end parallel
```

Scope of variables

- `Shared(list)`
  - Specifies the variables that are shared among all 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.

Exercise: SAXPY

- SAXPY is a common operation in computations with vector processors included as part of the BLAS routines

  $y \leftarrow \alpha x + y$

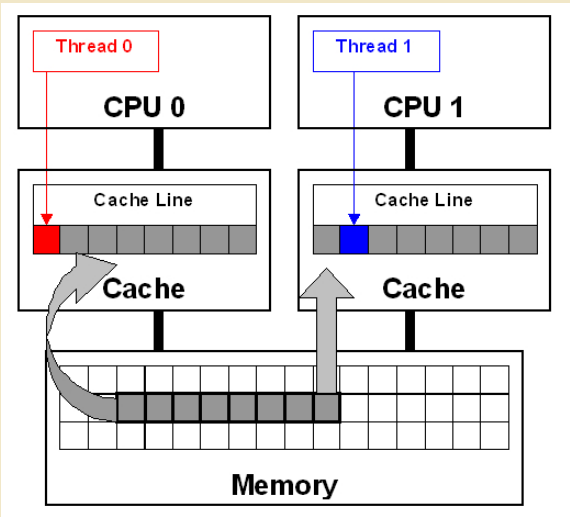
- SAXPY is a combination of scalar multiplication and vector addition
- Parallelize the code in the `exercise/saxpy` folder
- Calculate the speedup with respect to serial code.

SAXPY Timing

Threads	C		Fortran	
	Timing (s)	Speed Up	Timing (s)	Speed Up
1	0.513491	1.00	0.504534	1.00
2	0.264634	1.94	0.300650	1.68
3	0.177902	2.89	0.234661	2.15
4	0.135248	3.80	0.150547	3.35
5	0.109646	4.68	0.120734	4.18
6	0.087660	5.86	0.100535	5.02
12	0.056454	9.10	0.050300	10.03
24	0.048442	10.60	0.026623	18.95
48	0.026348	19.49	0.025263	19.97

Pitfalls: 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.




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

Pitfalls: Race Condition

- Multiple threads try to write to the same memory location at the same time.
  - Indeterministic results
- Inappropriate scope of varibale 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

```
!$omp parallel do
do i = 1, n
   if (a(i) > max) then
      max = a(i)
   end if
end do
!$omp end parallel do
```

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 it off
- Synchronizations are costly so their usage should be minimized.

Synchronization: Crtitical and Atomic

Critical

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

```
!$omp parallel do
do i = 1, n
   b = some_function(i)
   !$omp critical
   call some_routine(b,x)
end do
!$omp end parallel do
```

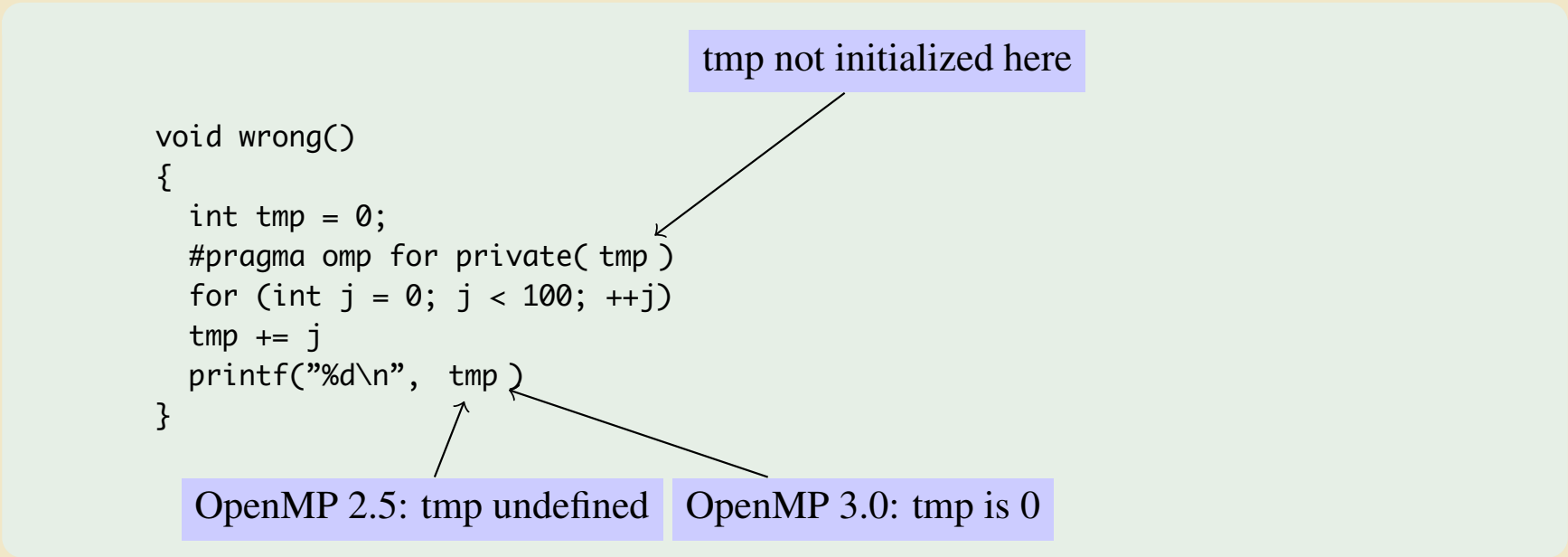
Atomic

Only one thread at a time can update a memory location

```
!$omp parallel do
do i = 1, n
   b = some_function(i)
   !$omp atomic
   x = x + b
end do
!$omp end parallel do
```

Private Variables

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



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 wrong()
{
  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

Exercise: Calculate pi by Numerical Integration

- We know that

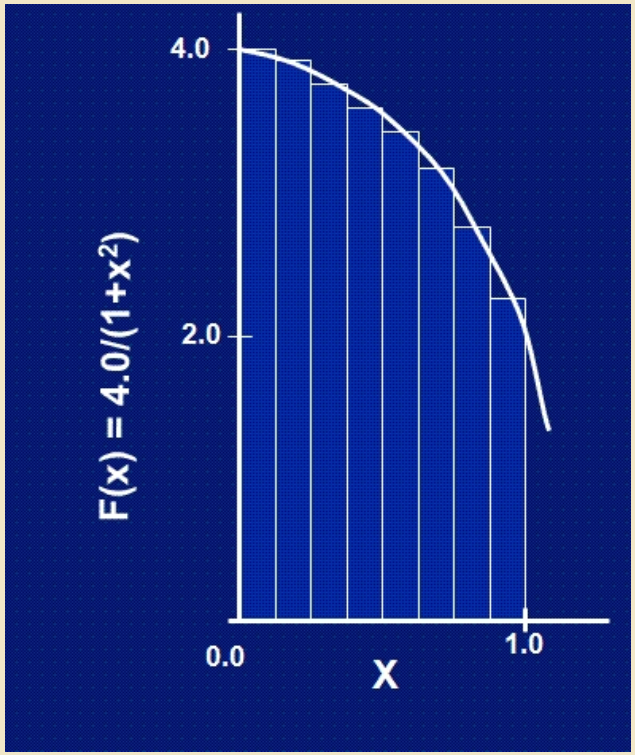
$$\int_0^1 \frac{4.0}{(1+x^2)}\,dx = \pi$$

- So numerically, we can approxiate pi as the sum of a number of rectangles

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

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

- Parallelize the code in the `exercise/calcpi` folder



Reduction

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

Example: Reduction

C/C++

```c
#include <omp.h>
int main() {
  int i, n = 100, sum , a[100], b[10
       0];
  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 += a[i] * b[i];
  }
}
```

Fortran

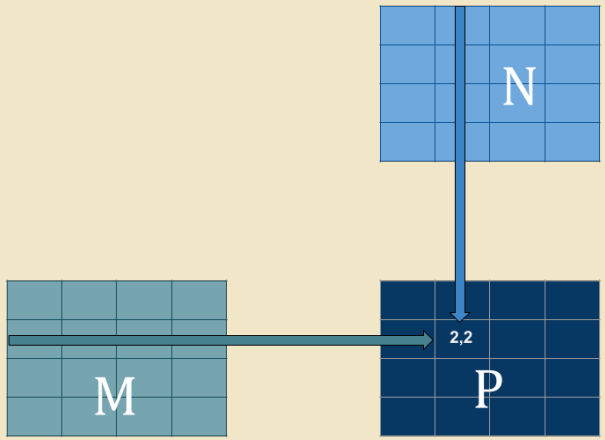
```fortran
program reduction

  implicit none
  integer :: i, n, sum , a(100), b(1
       00)

  n = 100 ; b = 1; sum = 0
  do i = 1 , n
     a(i) = i
  end do
  !$omp parallel do reduction(+:sum)
  do i = 1, n
     sum = sum + a(i) * b(i)
  end do
  !$omp end parallel do

end program reduction
```

Exercise 3: pi calculation with reduction

- Redo exercise 2 with reduction

Exercise: Matrix Multiplication

- Most Computational code involve matrix operations such as matrix multiplication.
- Consider a matrix **C** of two matrices **A** and **B**:
  Element *i,j* of **C** is the dot product of the i^{th} row of **A** and j^{th} column of **B**



- Parallelize the code in the `exercise/matmul` folder
- Calculate the speedup with respect to serial code.

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 processors
  - `omp_num_procs()`
- Query whether or not you are 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

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