Advanced Research Computing

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Shared-Memory Programming in OpenMP

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Outline

- What is OpenMP?
- How does OpenMP work?
  - Architecture
  - Fork-join model of parallelism
  - Communication
- OpenMP constructs
  - Directives
  - Runtime Library API
  - Environment variables

Overview

What is OpenMP?

- API for parallel programming on shared memory systems
  - Parallel "threads"
- Implemented through the use of:
  - Compiler Directives
  - Runtime Library
  - Environment Variables
- Supported in C, C++, and Fortran
- Maintained by OpenMP Architecture Review Board (http://www.openmp.org/)

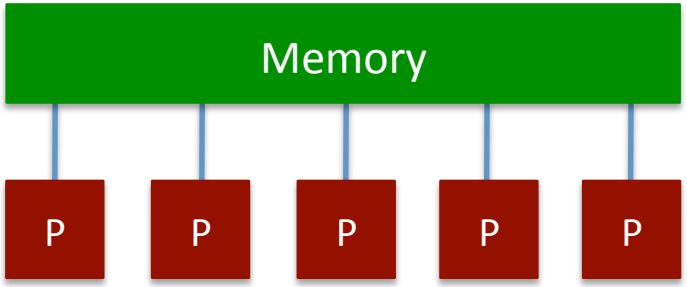
Advantages

- Code looks similar to sequential
  - Relatively easy to learn
  - Adding parallelization can be incremental
- No message passing
- Coarse-grained or fine-grained parallelism
- Widely-supported

Disadvantages

- Scalability limited by memory architecture
  - To a single node (8 to 32 cores) on most machines
- Managing shared memory can be tricky
- Improving performance is not always guaranteed or easy

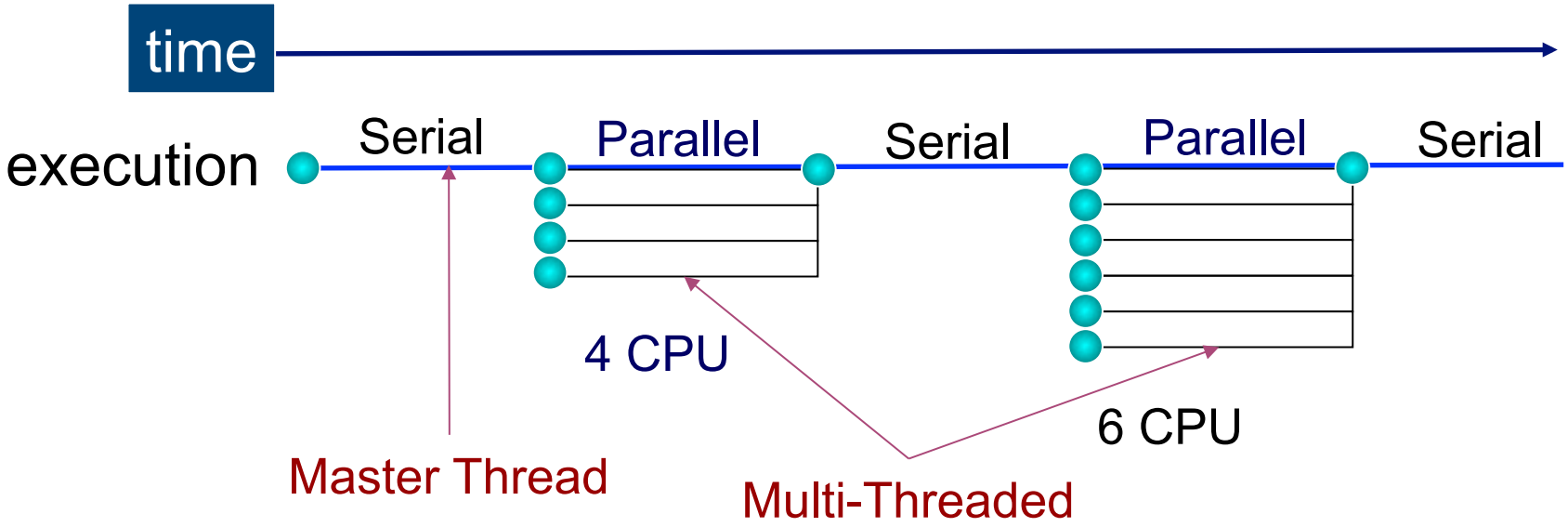
Shared Memory



- Your laptop
- Multicore, multiple memory NUMA system
  - HokieOne (SGI UV)
- One node on a hybrid system

Fork-join Parallelism

- Parallelism by region
- Master Thread: Initiated at run-time & persists throughout execution
  - –Assembles team of parallel threads at parallel regions



How do threads communicate?

- Every thread has access to “global” memory (shared). Each thread has access to a stack memory (private).
- Use shared memory to communicate between threads.
- Simultaneous updates to shared memory can create a *race condition*. Results change with different thread scheduling.
- Use mutual exclusion to avoid data sharing - but don’t use too many because this will serialize performance.

Race Conditions

Example: Two threads ("T1" & "T2") increment x=0

Start: `x=0`

1. T1 reads `x=0`
2. T1 calculates `x=0+1=1`
3. T1 writes `x=1`
4. T2 reads `x=1`
5. T2 calculates `x=1+1=2`
6. T2 writes `x=2`

Result: `x=2`

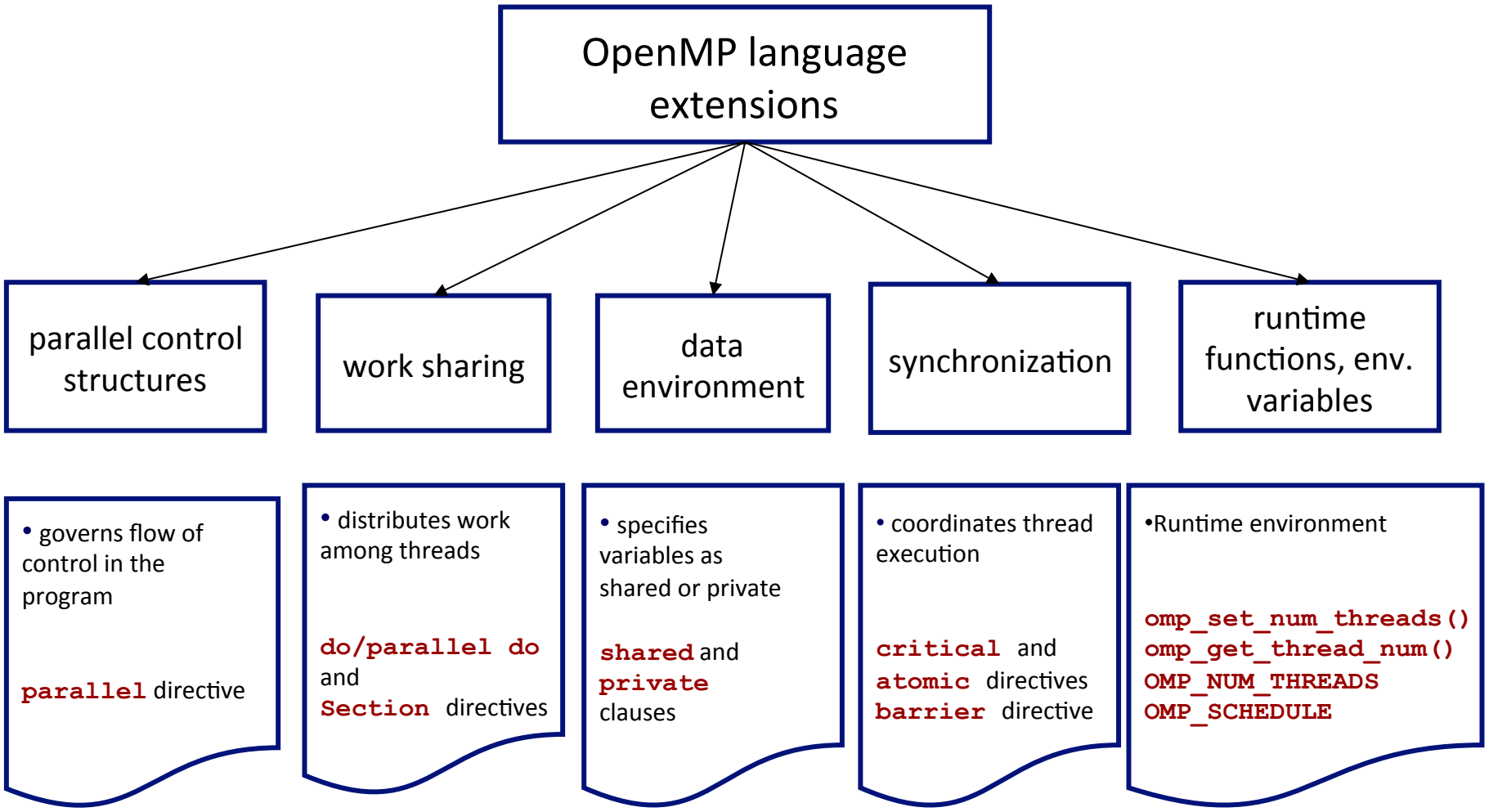
Start: `x=0`

1. T1 reads `x=0`
2. T2 reads `x=0`
3. T1 calculates `x=0+1=1`
4. T2 calculates `x=0+1=1`
5. T1 writes `x=1`
6. T2 writes `x=1`

Result: `x=1`

OpenMP Basics

OpenMP Constructs



OpenMP Directives

OpenMP directives specify parallelism within source code:

- C/C++: directives begin with the **# pragma omp** sentinel.
- FORTRAN: Directives begin with the **!$OMP**, **C$OMP** or ***$OMP** sentinel.
- F90: **!$OMP** free-format

- Parallel regions are marked by enclosing parallel directives
- Work-sharing loops are marked by parallel do/for

Fortran

```
!$OMP parallel
  ...
!$OMP end parallel

!$OMP parallel do
  DO ...
!$OMP end parallel do
```

C/C++

```
# pragma omp parallel
  {...}


# pragma omp parallel for
  for(){...}
```

API: Functions

Function	Description
`omp_get_num_threads()`	Returns number of threads in team
`omp_get_thread_num()`	Returns thread ID (0 to n-1)
`omp_get_num_procs()`	Returns number of machine CPUs
`omp_in_parallel()`	True if in parallel region & multiple threads executing
`omp_set_num_threads(#)`	Changes number of threads for parallel region

Function	Description
`omp_get_dynamic()`	True if dynamic threading is on.
`omp_set_dynamic()`	Set state of dynamic threading (true/false)

API: Environment Variables

- **`OMP_NUM_THREADS`**: Number of Threads
- **`OMP_DYNAMIC`**: TRUE/FALSE for enable/ disable dynamic threading

Parallel Regions

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

- Line 1: Team of threads formed at parallel region
- Lines 2-3:
  - Each thread executes code block and subroutine calls
  - No branching (in or out) in a parallel region
- Line 4: All threads synchronize at end of parallel region (implied barrier).

Example: Hello World

- Update a serial code to run on multiple cores using OpenMP

1. Start from serial "Hello World" example:
   - hello.c, hello.f
2. Create a parallel region
3. Identify individual threads and print out information from each

Hello World in OpenMP

Fortran:

```
!$OMP PARALLEL
      INTEGER tid
      tid = OMP_GET_THREAD_NUM()
      PRINT *, 'Hello from thread = ', tid
!$OMP END PARALLEL
```

C:

```
#pragma omp parallel
{
      int tid;
      tid = omp_get_thread_num();
      printf('Hello from thread =%d\n', tid);
}
```

Compiling with OpenMP

- GNU uses –fopenmp flag

```
gcc program.c -fopenmp -o runme
g++ program.cpp -fopenmp -o runme
gfortran program.f -fopenmp -o runme
```

- Intel uses –openmp flag, e.g.

```
icc program.c -openmp -o runme
ifort program.f -openmp -o runme
```

OpenMP Constructs

Parallel Region/Work Sharing

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

```
Parallel

End Parallel
```

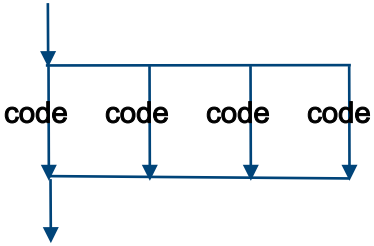
Code block	Each Thread Executes
DO	Work Sharing
SECTIONS	Work Sharing
SINGLE	One Thread
MASTER	Only the master thread
CRITICAL	One Thread at a time

Parallel DO/for
Parallel SECTIONS

Stand-alone
Parallel Constructs

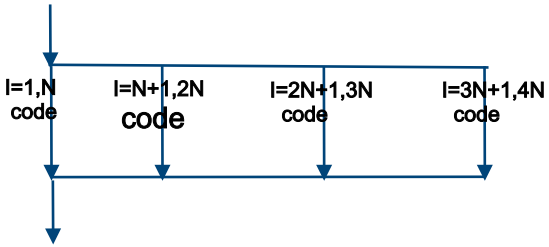
OpenMP parallel constructs

```
PARALLEL
   {code}
END PARALLEL
```



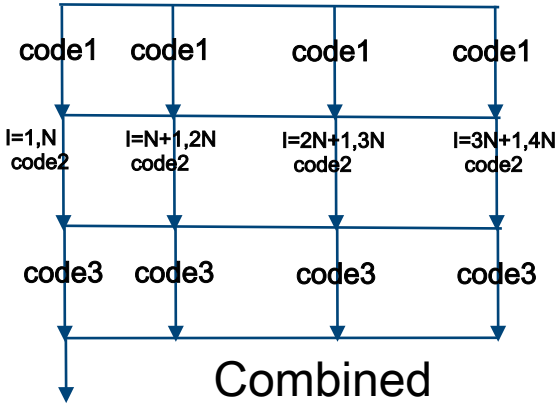
Replicated

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



Work Sharing

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



Combined

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More about OpenMP parallel regions…

There are two OpenMP "modes"

- ***static*** mode
  - Fixed number of threads
- ***dynamic*** mode:
  - Number of threads can change under user control from one parallel region to another (using `OMP_set_num_threads`)
  - Specified by setting an environment variable

```
(csh)   setenv OMP_DYNAMIC true
(bash)  export OMP_DYNAMIC=true
```

Note*: the user can only define the maximum number of threads, compiler can use a smaller number*

Parallel Constructs

- PARALLEL: Create threads, any code is executed by all threads
- DO/FOR: Work sharing of iterations
- SECTIONS: Work sharing by splitting
- SINGLE: Only one thread
- CRITICAL or ATOMIC: One thread at a time
- MASTER: Only the master thread

The DO / for directive

Fortran:

```
!$OMP PARALLEL DO
   do i=0,N
C      do some work
   enddo
!$OMP END PARALLEL DO
```

C:

```
#pragma omp parallel for
{
     for (i=0; i<N; i++)
       // do some work
}
```

The DO / for Directive

```
1   !$OMP PARALLEL DO
2         do i=1,N
3            a(i) = b(i) + c(i)
4         enddo
5   !$OMP END PARALLEL DO
```

Line 1 Team of threads formed (parallel region).

Line 2-4 Loop iterations are split among threads.

Line 5 (Optional) end of parallel loop (implied barrier at enddo).

Each loop iteration must be independent of other iterations.

The Sections Directive

- Different threads will execute different code
- Any thread may execute a section

```
#pragma omp parallel
{
 #pragma omp sections
 {
   #pragma omp section
    { // do some work }
   #pragma omp section
    { // do some different work }
 } // end of sections
} // end of parallel region
```

Merging Parallel Regions

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

```
!$OMP PARALLEL
  !$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
```

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

OpenMP clauses

Control the behavior of an OpenMP directive:

- Data scoping (Private, Shared, Default)
- Schedule (Guided, Static, Dynamic, etc.)
- Initialization (e.g. COPYIN, FIRSTPRIVATE)
- Whether to parallelize a region or not (if-clause)
- Number of threads used (NUM_THREADS)

Private and Shared Data

- Shared: Variable is shared (seen) by all processors.
- Private: Each thread has a private instance (copy) of the variable.
- Defaults: All DO LOOP indices are private, all other variables are shared.

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

Private data example

- In the following loop, each thread needs its own PRIVATE copy of TEMP.
- If TEMP were shared, the result would be unpredictable since each processor would be writing and reading to/from the same memory location.

```
!$OMP PARALLEL DO SHARED(A,B,C,N) PRIVATE(temp,i)
      do i=1,N
         temp = A(i)/B(i)
         C(i) = temp + cos(temp)
      enddo
!$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)** would copy the global temp value to each stack's temp.

Data Scoping Example (Code)

```
int tid, pr=-1, fp=-1, sh=-1, df=-1;
printf("BEGIN: pr is %d, fp is %d, sh is %d, df is %d.
\n",pr,fp,sh,df);

#pragma omp parallel shared(sh) private(pr,tid) firstprivate(fp)
  {
  tid = omp_get_thread_num();

  printf("Thread %d START : pr is %d, fp is %d, sh is %d, df is %d.
\n",tid,pr,fp,sh,df);

  pr = tid * 4; fp = pr; sh = pr; df = pr;
  printf("Thread %d UPDATE: pr is %d, fp is %d, sh is %d, df is %d.
\n",tid,pr,fp,sh,df);
  }  /* end of parallel section */

printf("END: pr is %d, fp is %d, sh is %d, df is %d.
\n",pr,fp,sh,df);
```

Data Scoping Example (Code)

```
$ icc -openmp omp_scope.c -o omp_scope
$ ./omp_scope
BEGIN: pr is -1, fp is -1, sh is -1, df is -1.
Thread 0 START : pr is 0, fp is -1, sh is -1, df is -1.
Thread 1 START : pr is 0, fp is -1, sh is -1, df is -1.
Thread 1 UPDATE: pr is 4, fp is 4, sh is 4, df is 4.
Thread 2 START : pr is 0, fp is -1, sh is -1, df is -1.
Thread 2 UPDATE: pr is 8, fp is 8, sh is 8, df is 8.
Thread 0 UPDATE: pr is 0, fp is 0, sh is 0, df is 0.
Thread 3 START : pr is 0, fp is -1, sh is 8, df is 8.
Thread 3 UPDATE: pr is 12, fp is 12, sh is 12, df is 12.
END: pr is -1, fp is -1, sh is 12, df is 12.
```

Distribution of work - SCHEDULE Clause

!OMP$ PARALLEL DO SCHEDULE(STATIC)

Each CPU receives one set of contiguous iterations (~total_no_iterations /no_of_cpus).

!OMP$ PARALLEL DO SCHEDULE(STATIC,C)

Iterations are divided round-robin fashion in chunks of size C.

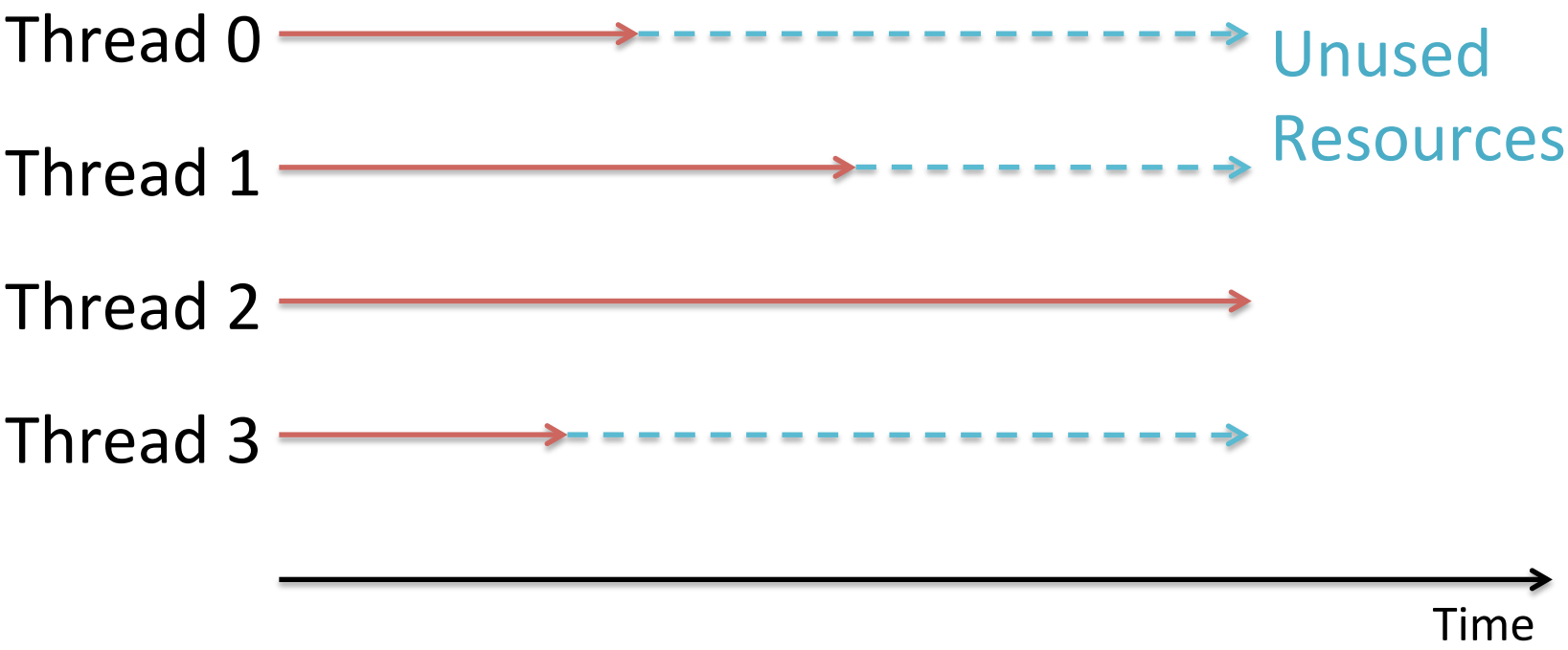
!OMP$ PARALLEL DO SCHEDULE(DYNAMIC,C)

Iterations handed out in chunks of size C as CPUs become available.

!OMP$ PARALLEL DO SCHEDULE(GUIDED,C)

Each of the iterations are handed out in pieces of exponentially decreasing size, with C minimum number of iterations to dispatch each time (Important for load balancing.)

Load Imbalances



Example - SCHEDULE(STATIC,16)

```
!$OMP parallel do schedule(static,16)
      do i=1,128                    !OMP_NUM_THREADS=4
       A(i)=B(i)+C(i)
      enddo
```

thread0:
`do i=1,16`
`  A(i)=B(i)+C(i)`
`enddo`
`do i=65,80`
`  A(i)=B(i)+C(i)`
`enddo`
	thread2:
	`do i=33,48`
	`  A(i)=B(i)+C(i)`
	`enddo`
	`do i = 97,112`
	`  A(i)=B(i)+C(i)`
	`enddo`

thread1:
`do i=17,32`
`  A(i)=B(i)+C(i)`
`enddo`
`do i = 81,96`
`  A(i)=B(i)+C(i)`
`enddo`
	thread3:
	`do i=49,64`
	`  A(i)=B(i)+C(i)`
	`enddo`
	`do i = 113,128`
	`  A(i)=B(i)+C(i)`
	`enddo`

Scheduling Options

Static

PROS

- Low compute overhead
- No synchronization overhead per chunk
- Takes better advantage of data locality

CONS

- Cannot compensate for load imbalance

Dynamic

PROS

- Potential for better load balancing, especially if chunk is low

CONS

- Higher compute overhead
- Synchronization cost associated per chunk of work

Scheduling Options

- When shared array data is reused multiple times, prefer static scheduling to dynamic
- Every invocation of the scaling would divide the iterations among CPUs the same way for static but not so for dynamic scheduling

```
!$OMP parallel private (i,j,iter)
do iter=1,niter
...
!$OMP do
do j=1,n
   do i=1,n
      A(i,j)=A(i,j)*scale
   end do
end do
...
end do
!$OMP end parallel
```

Comparison of scheduling options

name	type	chunk	chunk size	chunk #	static or dynamic	compute overhead
simple static	simple	no	N/P	P	static	lowest
interleaved	simple	yes	C	N/C	static	low
simple dynamic	dynamic	optional	C	N/C	dynamic	medium
guided	guided	optional	decreasing from N/P	fewer than N/C	dynamic	high
runtime	runtime	no	varies	varies	varies	varies

Matrix Multiplication - Serial

```
/*** Initialize matrices ***/
  for (i=0; i<NRA; i++)
    for (j=0; j<NCA; j++)
      a[i][j]= i+j;
[etc…also initialize b and c]

/*** Multiply matrices ***/
  for (i=0; i<NRA; i++)
    for(j=0; j<NCB; j++)
      for (k=0; k<NCA; k++)
        c[i][j] += a[i][k] * b[k][j];
```

Example: Matrix Multiplication

Parallelize matrix multiplication from serial:

C version: mm.c

Fortran version: mm.f

1. Use OpenMP to parallelize loops
2. Determine public / private variables
3. Decide how to schedule loops

Matrix Multiplication - OpenMP

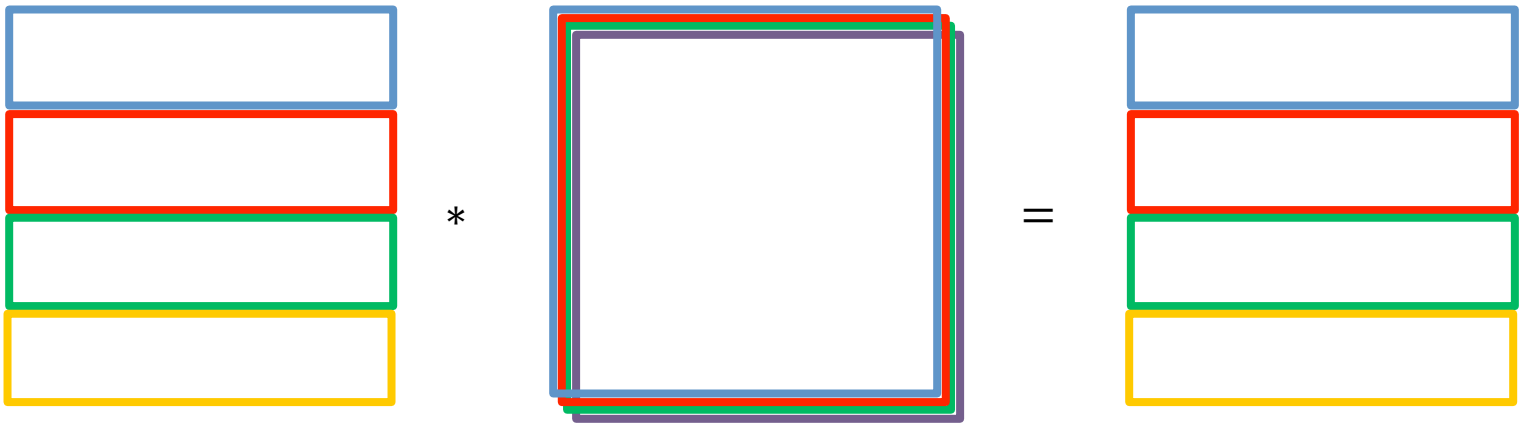
```
/*** Spawn a parallel region explicitly scoping all variables ***/
#pragma omp parallel shared(a,b,c,nthreads,chunk) private(tid,i,j,k)
 {
 tid = omp_get_thread_num();

 /*** Initialize matrices ***/
 #pragma omp for schedule (static, chunk)
 for (i=0; i<NRA; i++)
  for (j=0; j<NCA; j++)
    a[i][j]= i+j;

 #pragma omp for schedule (static, chunk)
 for (i=0; i<NRA; i++)   {
  printf("Thread=%d did row=%d\n",tid,i);
  for(j=0; j<NCB; j++)
    for (k=0; k<NCA; k++)
      c[i][j] += a[i][k] * b[k][j];
  }
}
```

Matrix Multiplication: Work Sharing

- Partition by rows:



Reduction Clause

- Thread-safe way to combine private copies of a variable into a single result
- Variable that accumulates the result is the "reduction variable"
- After loop execution, master thread collects private values of each thread and finishes the (global) reduction
- Reduction operators and variables must be declared

Reduction Example: Vector Norm

```
double n_sqr=0;  //square of the vector norm

#pragma omp parallel shared(vec, dim) private(i) //create threads
{
  //Split up the for loop
  //Use the reduction() clause to have OpenMP
  //sum up all of the private copies of n_sqr
  #pragma omp for reduction(+:n_sqr)
  for(i=0; i<dim; i++) //iterate through the rows of the result
    n_sqr += vec[i]*vec[i];
}

printf("Done.\nVector norm is %.5f.\n\n",sqrt(n_sqr));
```

SYNCHRONIZATION

Nowait Clause

- 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.

```
!$OMP PARALLEL
!$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
!$OMP END DO
!$OMP END PARALLEL
```

Barriers

- Create a barrier to synchronize threads

```
#pragma omp parallel
{
    // all threads do some work
#pragma omp barrier
    // all threads do more work
}
```

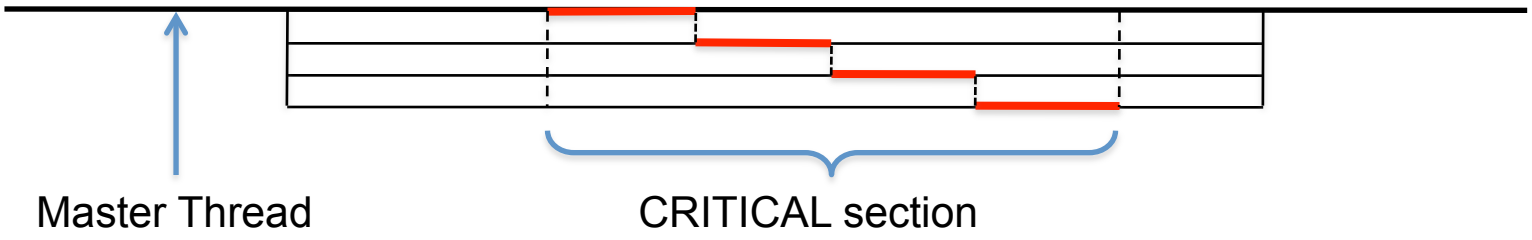
- Barrier is implied at the end of a parallel region

Mutual Exclusion: Critical/Atomic Directives

- ATOMIC For a single command (e.g. incrementing a variable)
- CRITICAL Directive: Longer sections of code

```
!$OMP PARALLEL SHARED(X,Y)
 ...
!$OMP ATOMIC
      sum=sum+1
...
!$OMP END PARALLEL
```

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



Mutual exclusion: lock routines

When each thread must execute a section of code serially, locks provide a more flexible way of ensuring serial access than **CRITICAL** and **ATOMIC** directives

```
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)
```

Performance Optimization

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);
```

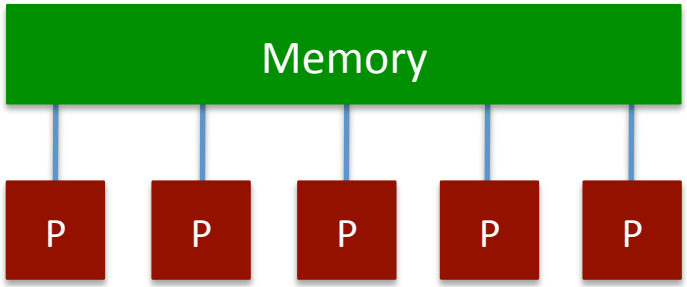
Timer Comparison

```
#Case 1:
Normal C Timer: 0.230 seconds
OpenMP Timer: 0.105319 seconds

#Case 2 (more efficient
threading):
Normal C Timer: 0.200 seconds
OpenMP Timer: 0.012919 seconds
```

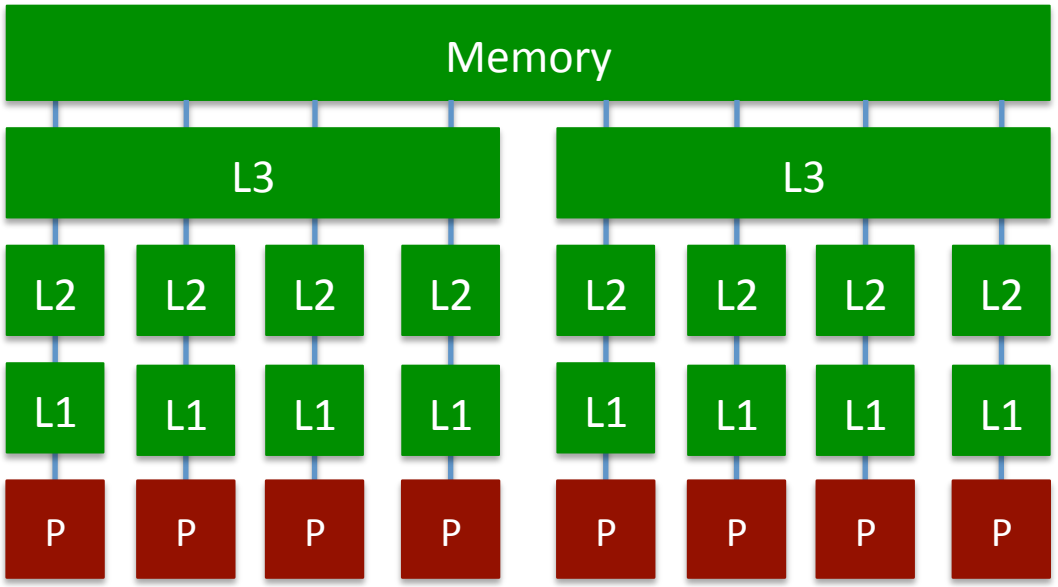
Shared memory to OpenMP

- All processors connected to same memory and all memory is identical



Reality is More Complicated

- Ithaca node (8 cores, 24 GB memory):
  - 2 sockets with 4 cores each
  - 32 KB L1 cache, 256KB L2 cache, 8MB L3 cache



likwid-topology

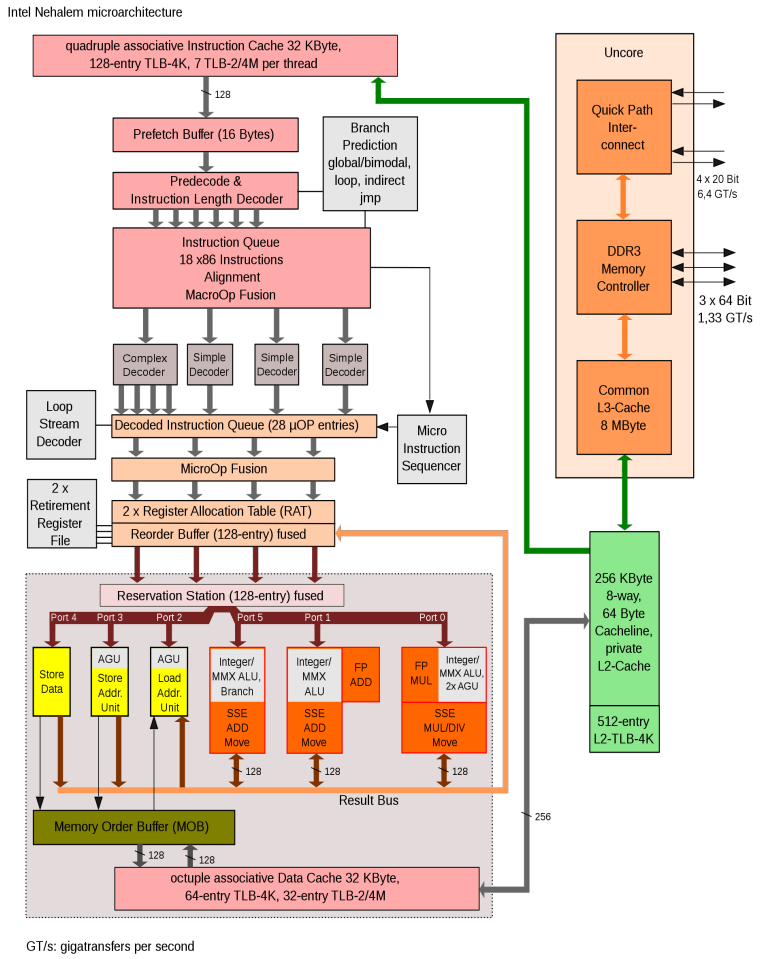
```
********************************************************************************
Cache Topology
********************************************************************************
Level:  1
Size:   32 kB
Cache groups:   ( 0 ) ( 1 ) ( 2 ) ( 3 ) ( 4 ) ( 5 ) ( 6 ) ( 7 )
--------------------------------------------------------------------------------
Level:  2
Size:   256 kB
Cache groups:   ( 0 ) ( 1 ) ( 2 ) ( 3 ) ( 4 ) ( 5 ) ( 6 ) ( 7 )
--------------------------------------------------------------------------------
Level:  3
Size:   8 MB
Cache groups:   ( 0 1 2 3 ) ( 4 5 6 7 )
--------------------------------------------------------------------------------
```

likwid-topology

```
********************************************************************************
NUMA Topology
********************************************************************************
NUMA domains: 2
--------------------------------------------------------------------------------
Domain 0:
Processors:  0 1 2 3
Relative distance to nodes:  10 21
Memory: 10444.7 MB free of total 12277.5 MB
--------------------------------------------------------------------------------
Domain 1:
Processors:  4 5 6 7
Relative distance to nodes:  21 10
Memory: 11551.6 MB free of total 12288 MB
--------------------------------------------------------------------------------
```

OpenMP and cc-NUMA

- cc-NUMA = cache coherent non-uniform memory access
- Modern CPU's utilize multiple levels of cache to reduce the time to get data to the ALU



OpenMP and cc-NUMA

- Setup is advantageous because it allows individual CPU cores to get data more quickly from memory
- Maintaining cache coherence is expensive
- Result: you want to associate specific memory to specific CPU cores

OpenMP and cc-NUMA

1. Bind specific threads to specific cores:

   Intel: export KMP_AFFINITY="proclist=[$CPUSET]"

   GCC: export GOMP_CPU_AFFINITY="$CPUSET"

2. Associate memory with a specific thread:
   - First-touch policy: use parallel initialization so that values are initialized by the thread that will modify the value

SAXPY Example (Code)

```
//serial initialization:
//OS will allocate all data close to initial thread
for (i=0;i<N;i++) a[i]=b[i]=c[i]=0.0;
//saxpying with poor memory placement
#pragma omp parallel for
for(i=0;i<N;i++) a[i]=b[i]+scalar*c[i];

//parallel initialization: data allocated where
used
# pragma omp parallel for
for (i=0;i<N;i++) a[i]=b[i]=c[i]=0.0;
//saxpying with optimal memory placement
#pragma omp parallel for
for(i=0;i<N;i++) a[i]=b[i]+scalar*c[i];
```

SAXPY Example (Output)

```
$ icc -openmp omp_saxpy.c -o saxpy
$ ./saxpy
SAXPY with Serial Initialization:
Elapsed time = 0.105552

SAXPY with Parallel
Initialization:
Elapsed time = 0.012795
```

Online Content

- ARC OpenMP page: http://www.arc.vt.edu/openmp
- OpenMP Application Programming Interface: http://www.openmp.org/mp-documents/OpenMP4.0.0.pdf
- LLNL Examples: https://computing.llnl.gov/tutorials/openMP/exercise.html

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Thank You!