Introduction to OpenMP

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Agenda

- What is openMP?

- Starting parallel region
- Data Scopes
- Work sharing
- Dependencies and Reductions
- Synchronization
- Scheduling
- OpenMP tasks

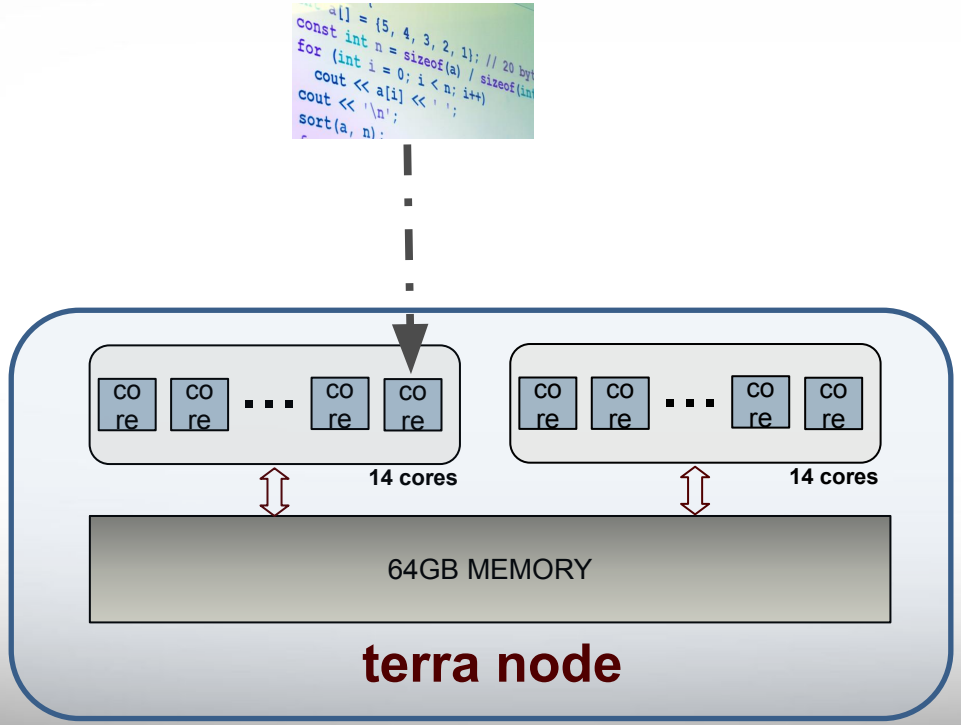
Short course home page:

https://hprc.tamu.edu/training/intro_openmp.html

Setting up OpenMP sample codes:

Type: /scratch/training/OpenMP/setup.sh
(in terra, ada, or curie shell)

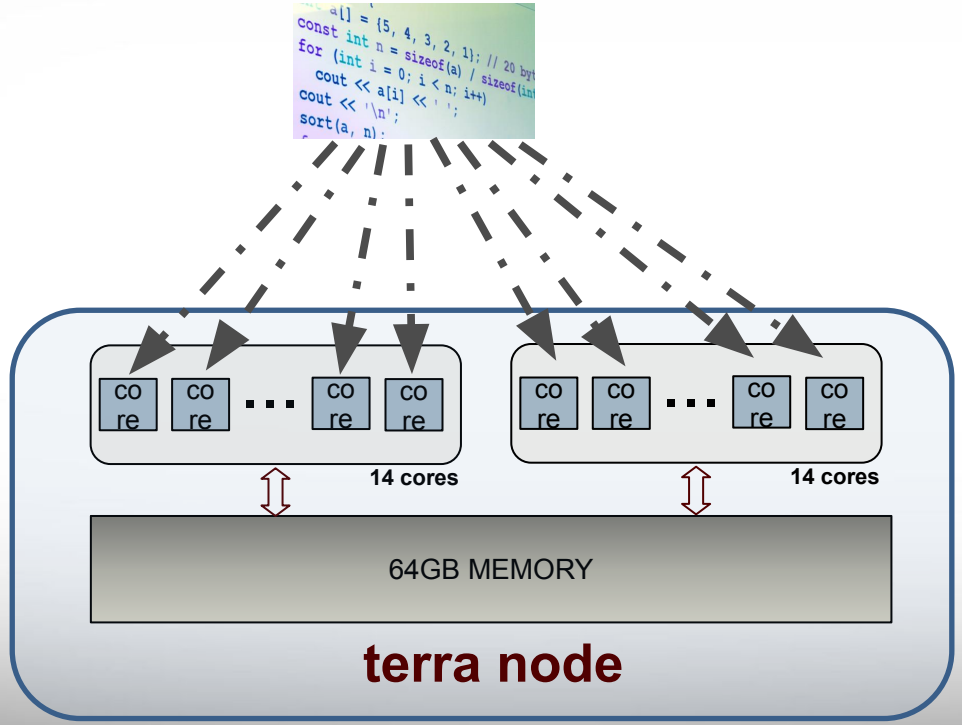
Basic Computer Architecture



All modern computers have multiple processing cores (4 to 8 on average desktop). On terra, each **NODE** has 28 cores (two 14 core cpus) per node and at least 64GB of **SHARED** memory

(NOTE: ada has 20 cores per node and curie has 16)

Basic Computer Architecture



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What is OpenMP?

Defacto standard API for writing ***shared memory*** parallel applications in C, C++, and Fortran

OpenMP API consists of:

- Compiler pragmas/directives
- Runtime subroutines/functions
- Environment variables

In a nutshell: using OpenMP, you can make a serial program run in parallel by annotating parts of the code that you want to run in parallel

C/C++ pragma format:

```
#pragma omp directive [clauses]
{
    :
}
```

New line required

fortran directive format:

```
!$OMP DIRECTIVE   [clauses]
    :
!$OMP END DIRECTIVE
```

Not case sensitive

Starting Parallel Region

```
// some C/C++ code
#pragma omp parallel
{
    // code block, will be
    // executed in parallel
}

// more C/C++ code
```

```
c   some fortran code
!$OMP PARALLEL
c   code block, will be
c   executed in parallel
!$OMP END PARALLEL

c   more fortran code
```

This will start an OpenMP region. The OpenMP runtime will create a team of **threads**. The code inside the parallel block will be executed concurrently by all threads.

HelloWorld

SOURCE

Exercise:

1) Create OpenMP version of HelloWorld (either C/C++ or Fortran)
   a) Create parallel region
   b) Every thread prints Hello World
   c) Close the parallel region
2) Compile the program (you can use GNU or Intel compiler)
3) Execute the program

HelloWorld

SOURCE

```
#include <iostream>

int main() {
#pragma omp parallel
  {
    std::cout <<  "Hello World\n";
  }
  return 0;
}
```

pragma

directive

```
program HELLO
!$OMP PARALLEL
print *,"Hello World"
!$OMP END PARALLEL
end program HELLO
```

COMPILING

Need to include flag to tell the compiler to process the OpenMP pragmas/directives

intel: icpc -qopenmp -o hi.x hello.cpp
gnu: g++ -fopenmp -o hi.x hello.cpp

intel: ifort -qopenmp -o hi.x hello.f90
gnu: gfortran -fopenmp -o hi.x hello.f90

Compile the program , and run again

HelloWorld

SOURCE

```
#include <iostream>

int main() {
#pragma omp parallel
  {
    std::cout <<  "Hello World\n";
  }
  return 0;
}
```

pragma

```
program HELLO
!$OMP PARALLEL
print *,"Hello World"
!$OMP END PARALLEL
end program HELLO
```

directive

COMPILING

Need to include flag to tell the compiler to process the OpenMP pragmas/directives

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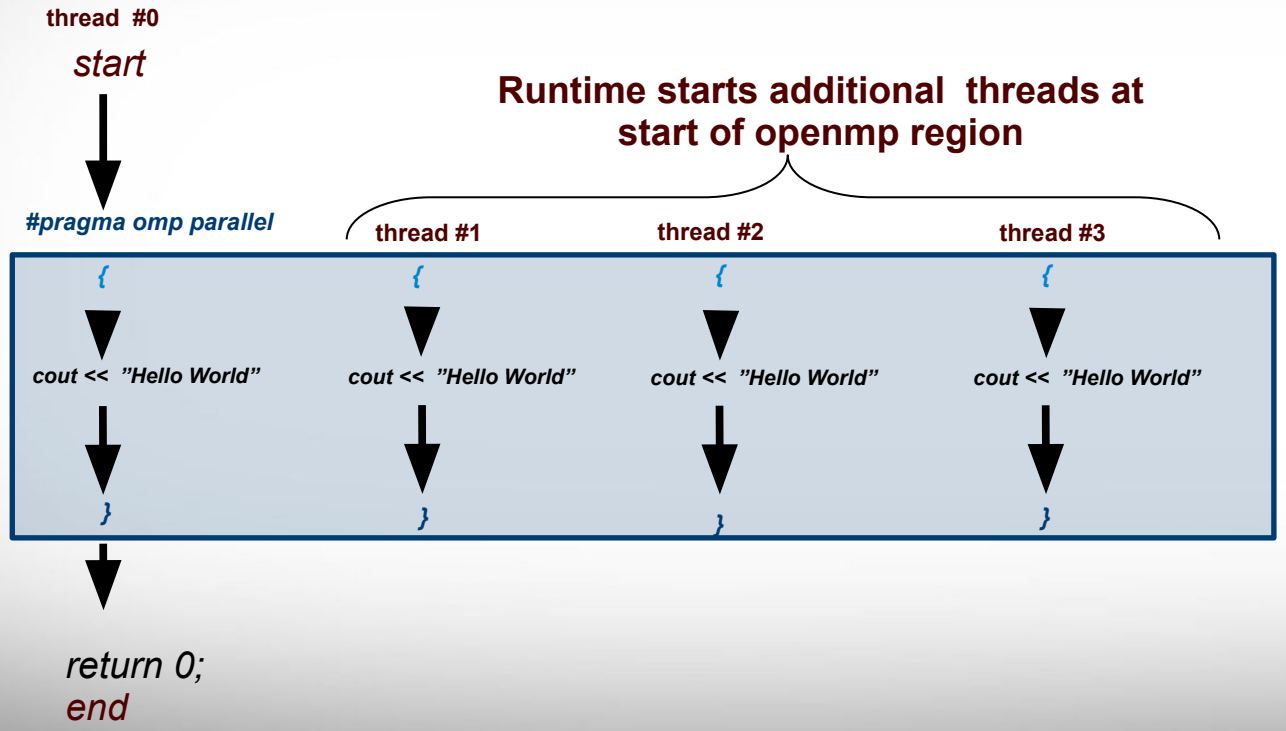
intel: ifort -qopenmp -o hi.x hello.f90
gnu: gfortran -fopenmp -o hi.x hello.f90

RUNNING

export OMP_NUM_THREADS=4
./hi.x

Run the program again
(I promise, it will work now)

Fork/Join




```
#include <iostream>
#include <omp.h>

using std;
int main() {
#pragma omp parallel
  {
    cout << "Hello world\n";
  }
  return 0;
}
```

Threads & Cores

(OpenMP) THREAD: Independent sequence of code, with a single entry and a single exit

CORE: Physical processing unit that receives instructions and performs calculations, or actions, based on those instructions.

- OpenMP threads are mapped onto physical cores
- Possible to map more than 1 thread onto a core
- In practice best to have one-to-one mapping.

Getting Thread info

- Runtime function: **omp_get_thread_num()**

```
id = omp_get_thread_num();   //   0
#pragma omp parallel
{
   id = omp_get_thread_num(); //  <thread id in region>
}
```

- Runtime function: **omp_get_num_threads()**

```
tot = omp_get_num_threads();   //  1
#pragma omp parallel
{
   tot = omp_get_num_threads(); // < total #threads in region>
}
```

Setting the number of Threads

case sensitive

- Environmental variable: **OMP_NUM_THREADS**

```
export OMP_NUM_THREADS=4
./a.out
```

???

- Runtime function: **omp_set_num_threads(n)**

```
omp_set_num_threads(4);
#pragma omp parallel
  :
```

???

- OMP PARALLEL clause: **num_threads(n)**

```
#pragma omp parallel num_threads(4)
```

Hello Threads

Exercise:

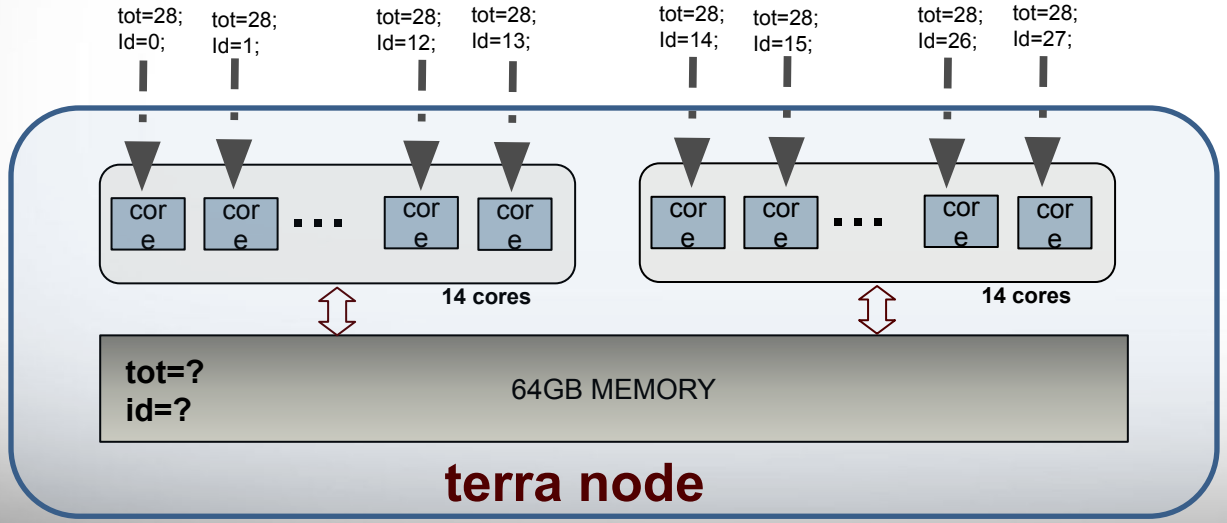
1) Create OpenMP HelloThreads program that does the following:
   a) Create parallel region
   b) Every thread prints its thread id and the total number of threads
   c) Close the parallel region
2) Compile the program (you can use GNU or Intel compiler)
3) Execute the program

HINT: since you will be using OpenMP library functions you include:

C/C++ : *#include "omp.h"*
Fortran : *use omp_lib*

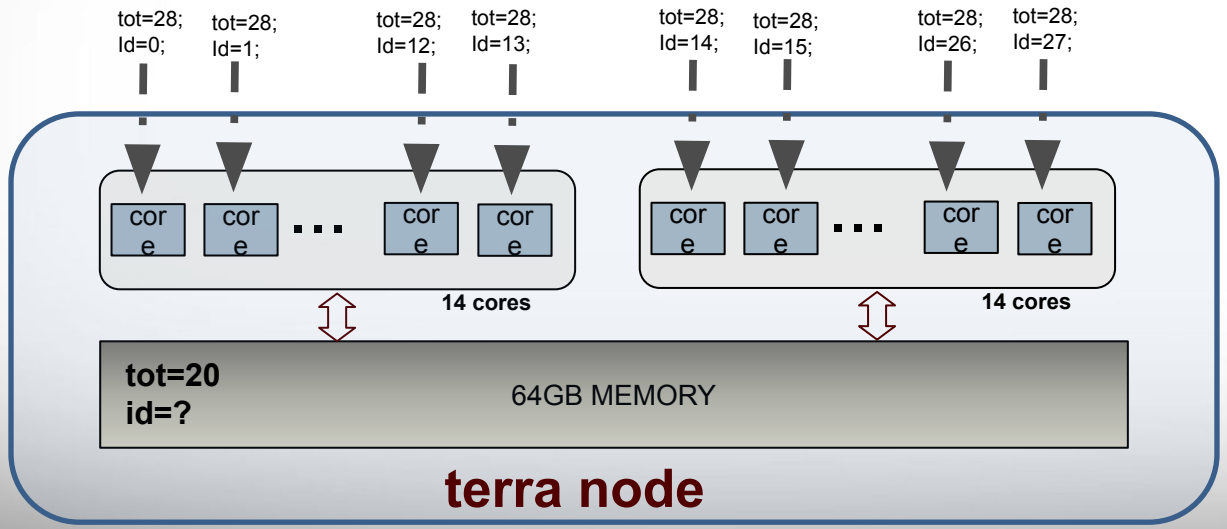
```
#pragma omp parallel
{
  tot = omp_get_num_threads();
  id = omp_get_thread_num();
}
```

Remember: memory is (conceptually) shared by all threads



```
#pragma omp parallel
{
  tot = omp_get_num_threads();
  id = omp_get_thread_num();
}
```

Remember: memory is (conceptually) shared by all threads



All threads try to access the same variable (possibly at the same time). This can lead to a race condition. Different runs of same program might give different results because of these race conditions

Data Scope Clauses

Data scope clauses: **private(list)**

```
#pragma omp parallel private(a,c)
{

}
```

```
!$OMP PARALLEL PRIVATE(a,c)
      :
!$OMP END PARALLEL
```

- Every thread will have it's own **"private"** copy of variables in list
- No other thread has access to this **"private"** copy
- Private variables are NOT initialized with value before region started (use firstprivate instead)
- Private variables are NOT accessible after enclosing region finishes

Index variables (Fortran, C/C++) and variables declared inside parallel region (C/C++) are considered private by default.

Data Scope Clauses

Data scope clauses: **shared(list)**

```
#pragma omp parallel shared(a,c)
{

}
```

```
!$OMP PARALLEL SHARED(a,c)
      :
!$OMP END PARALLEL
```

- All variables in list will be considered shared
- Every OpenMP thread has access to all these variables
- Programmer's responsibility to avoid race conditions

By default most variables in work sharing constructs are considered shared in OpenMP. Exceptions include index variables (Fortran, C/C++) and variables declared inside parallel region (C/C++).

Other Data Scope Clauses

Data scope clauses: **firstprivate(list)**

- Every thread will have it's own **”private”** copy of variables in list.
- No other thread has access to this **”private”** copy.
- firstprivate variables are initialized to value before region started.
- firstprivate variables are NOT accessible after end of enclosing region.

Data scope clause: **default(** *shared* | *private* | *firstprivate* | *lastprivate***)**

- Set default data scoping rule.
- If not set, default depends on the pragma/directive (e.g. Shared for ”for” pragma).

demo datascope

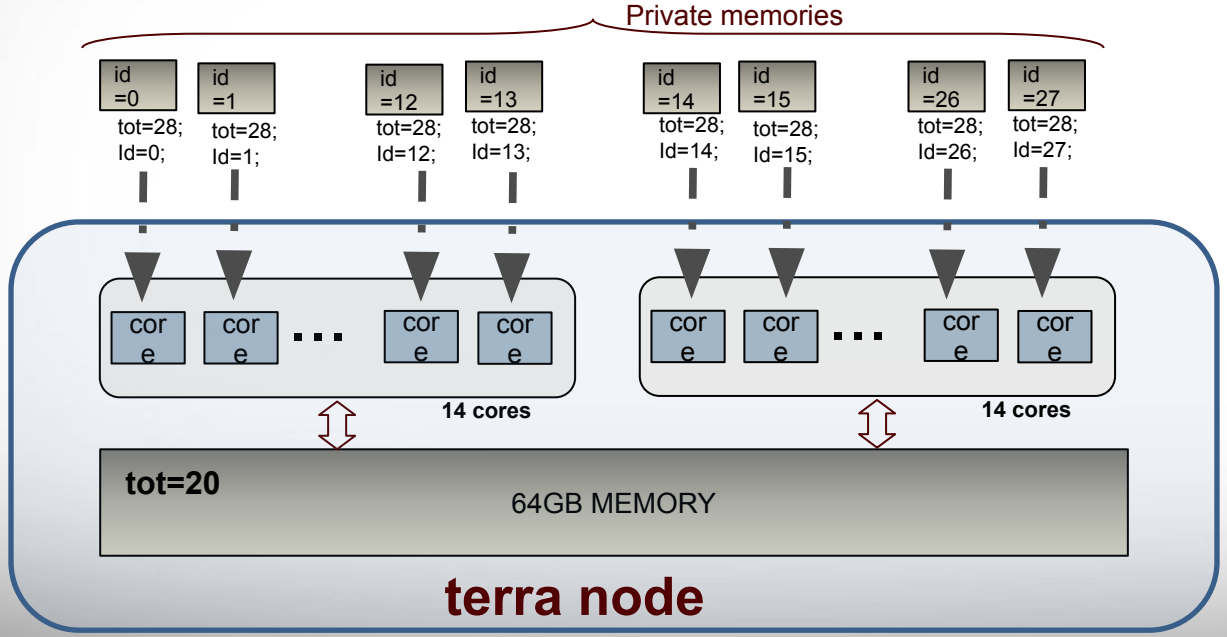
Hello Threads (take 2)

Exercise:

1) Create OpenMP HelloThreads program that does the following:
   a) Create parallel region
   b) Every thread prints **its own** thread id and the **total number of threads**
   c) Close the parallel region
2) Compile the program (you can use GNU or Intel compiler)
3) Execute the program

```
#pragma omp parallel
{
  tot = omp_get_num_threads();
  id = omp_get_thread_num();
}
```

Remember: memory is (conceptually) shared by all threads



TIP: Stack size

- OpenMP creates separate data stack for every worker thread to store private variables (master thread uses regular stack)
- Size of these stacks is not defined by OpenMP standards
- Behavior of program undefined when stack space exceeded
  - ✔ Although most compilers/RT will throw seg fault
- To set stack size use environment var OMP_STACKSIZE:
  - ✔ export OMP_STACKSIZE=512M
  - ✔ export OMP_STACKSIZE=1G
- To make sure master thread has large enough stack space use ulimit -s command (unix/linux).

Let's create a demo program where the threads fill up the stack space

Work Sharing Directives

Work sharing pragma (C/C++): **#pragma omp for** *[clauses]*

```
      :
#pragma omp parallel
#pragma omp for
   for (int i=1;i<N;++i)
     A(i) = A(i) + B;

      :
```

OR

```
      :
#pragma omp parallel for
   for (int i=1;i<N;++i)
     A(i) = A(i) + B;

      :
```

- ***for*** command must immediately follow "***#pragma omp for***"
- Newline required after "***#pragma omp for***"
- Originally iteration variable could only be signed/unsigned integer variable.

Work Sharing Directives

Work sharing directive (Fortran): **!$OMP DO** *[clauses]*

```
!$OMP PARALLEL
!$OMP DO
DO n=1,N
   A(n) = A(n) + B
ENDDO
!$OMP END DO
!$OMP END PARALLEL
```

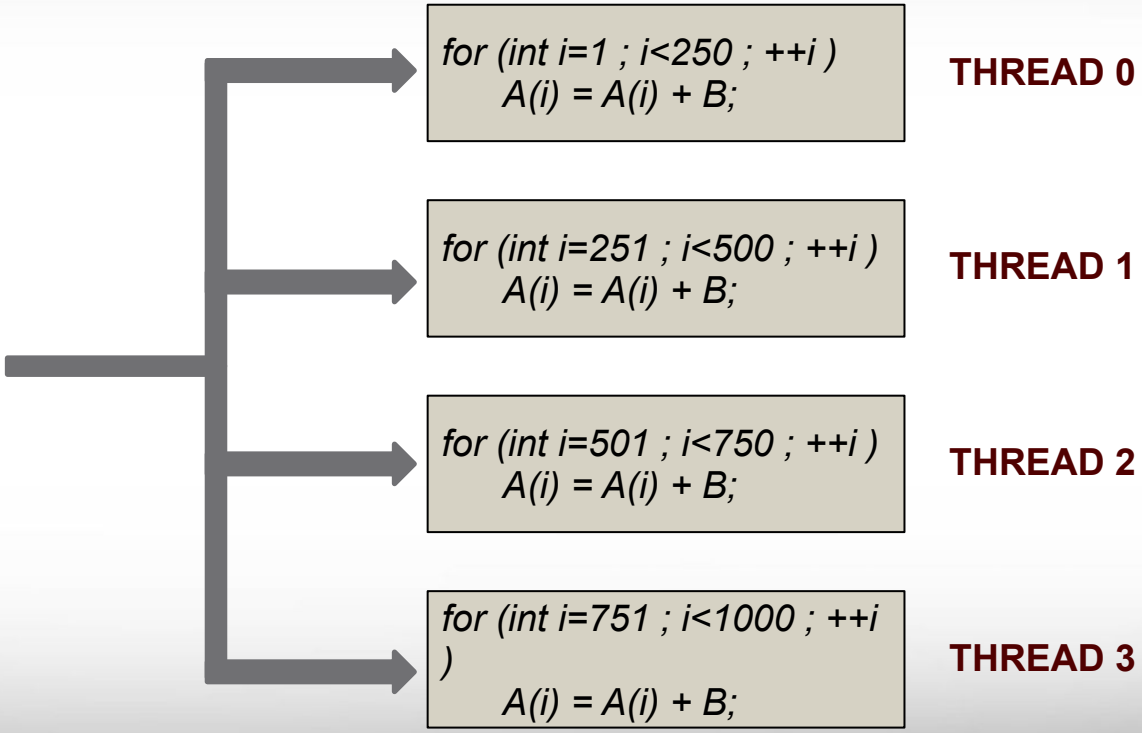
OR

```
!$OMP PARALLEL  DO
DO n=1,N
   A(n) = A(n) + B
ENDDO
!$OMP END PARALLEL DO
```

- DO command must immediately follow “!$OMP DO” directive
- Loop iteration variable is “private” by default
- If “end do” directive omitted it is assumed at end of loop
- Not case sensitive

Work Sharing

```
#pragma omp parallel for
for (int i=1;i<1000;++i)
  A(i) = A(i) + B;
```



Work Sharing Directives

New in OpenMP 3.0

Random access iterators:

```
vector<int> vec(10);
vector<int>::iterator it=
vec.begin();
#pragma omp parallel for
  for ( ; it != vec.end() ; ++it) {
      // do something with *it
  }
```

Pointer type:

```
int N = 1000000;
int arr[N];
#pragma  omp parallel for
  for (int* t=arr;t<arr+N;++t) {
    // do something with *t
}
```

Matrix multiplication

Exercise:

1) Create program that computes simple matrix vector multiplication:
   a) Use the OpenMP work sharing construct
   b) Create as function that takes as arguments matrix and vector
   c) Add timing to see the running time.
2) Compile and run the program
3) Try it with various number of threads
4) Vary the input size and see how it affects run time

Manual Worksharing

Case Study:

Assume the following dummy program:

```
A=int[N]; // set all elements to -1
for (int i=0 ; i<N ; ++i) A[i] = i;
```

We want to run this in parallel. Normally we would use the OpenMP worksharing directive. Let's do it without and partition the loop manually

1) Start a parallel region.
2) Every thread will computes its offsets
3) Every thread will process part of the loop.

TIP: ORPHANED PRAGMAS

An OpenMP pragma that appears independently from another enclosing pragma is called an orphaned pragma. It exists outside of another pragma static extent.

```
int main() {
#pragma omp parallel
   foo()
   return 0;
}
```

```
void foo() {
#pragma omp for
   for (int i=0;i<N;i++) {….}
}
```

Note: OpenMP directives (pragmas) should be in the dynamic extent of a parallel section directive (pragma).

Data Dependencies

Can all loops can be parallelized?

```
for (i=1 ; i<N ; ++i)
  A[i] = A[i-1] + 1
end
```

```
#pragma omp parallel for
for (i=1 ; i<N ; ++i)
  A[i] = A[i-1] + 1
end
```

Is the result guaranteed to be correct if you run this loop in parallel?

Data Dependencies

Can all loops can be parallelized?

```
for (i=1 ; i<N ; ++i)
  A[i] = A[i-1] + 1
end
```

```
#pragma omp parallel for
for (i=1 ; i<N ; ++i)
  A[i] = A[i-1] + 1
end
```

Unroll the loop (partly):

iteration i=1: A[1] = A[0] + 1
iteration i=2: A[2] = A[1] + 1
iteration i=3: A[3] = A[2] + 1

A[1] used here, defined in previous iteration

A[2] used here, defined in previous iteration

Reductions

*A reduction variable is a special variable that is **updated** during every iteration of a loop and there are no other definitions or uses of that variable. Update is always of the form "a = a op b"*

Can we run this in parallel?

```
for (int i=0;i<10;++i)
   sum=sum+a[i];
```

```
#pragma omp parallel for
for (int i=0;i<10;++i)
   sum=sum+a[i];
```

Reductions

*A reduction variable is a special variable that is **updated** during every iteration of a loop and there are no other definitions or uses of that variable. Update is always of the form "a = a op b"*

Data scope clause: **REDUCTION(*op:list*)**

- Only certain kind of operators allowed
  - ✔ +, - , * , max, min,
  - ✔ & , | , ^ , && , || (C/ C++)
  - ✔ .and. , .or. , .eqv. , .neqv. , iand , ior , ieor (Fortran)
- OpenMP 4.0 allows for user defined reductions

Reduction variable has to be shared

```
for (int i=0;i<10;++i)
   sum=sum+a[i];
```

```
#pragma omp parallel for reduction(+:sum)
for (int i=0;i<10;++i)
   sum=sum+a[i];
```

Dot product (take 1)

Exercise:

1) Create program that takes 2 vectors (arrays) and computes:
   a) The dot product of the vectors
   b) the largest element of the two vectors
2) Add timing to compute the run time
3) Compile and run the program
4) Try it with various number of threads

User Defined Reductions

#pragma omp declare reduction (name : type list : combiner) \
initializer(initializer-expression)

!$ omp declare reduction (name : type list : combiner) \
initializer(initializer-expression)

Example: UDR that computes sum (mimics + operator)

```
#pragma omp declare reduction (mysum : int : omp_out = omp_out + omp_in)
initializer(omp_priv = 0)
```

Fixed variable name to represent initializer

Fixed variable names to represent in and out of reduction

User Defined Reductions

Case Study:

suppose we have a vector of random points (with x and y coordinates). We want to find the point with the longest distance (d= sqrt(x^2+y^2))

1) Create a C++ class with
   a) Two members: x and y coordinate
   b) Member function that computes the distance
2) Create User Defined Reduction that takes pair of points and returns one with longest distance
3) Create OpenMP loop with reduction clause that computes the point with longest distance.
4) Compile and run with various number of threads.

Work Sharing Directives

#pragma omp sections (!$OMP SECTIONS)

```
#pragma omp parallel
{
#pragma omp sections
  {
#pragma omp section
    process(A1,A2)
#pragma omp section
    process(B1,B2)
  }
}
```

- In an OpenMP sessions block, all ”sections” will be executed concurrently
- Each section will be processed by a separate thread
- How is this different from **#pragma omp for**

#pragma omp single (!$OMP SINGLE)

```
#pragma omp parallel
{
#pragma omp single
  {
    std::cout << ”thread” <<

omp_get_thread_num() <<
        ” reached here first\n”;
  }
}
```

- One thread (not neccesarily master) executes the block
- Other threads will wait
- Useful for thread-unsafe code
- Useful for I/O operations

NOWAIT Clause

Worksharing constructs have an implicit barrier at the end of their worksharing region. To ommit this barrier:

```
#pragma omp for nowait
    :
```

```
!$OMP DO
    :
!$OMP END DO NOWAIT
```

- At end of work sharing constructs threads will **not** wait
- There is always barrier at end of parallel region

NOTE: In example above the nowait clause is used with a for/do work sharing construct. It also works with the other worksharing construct: sections and single

demo nowait as part of single construct

OpenMP Synchronization

OpenMP programs use shared variables to communicate. Need to make sure these variables are not accessed at the same time by different threads to avoid race conditions.

Synchronization Directive

#pragma omp critical (!$OMP CRITICAL)

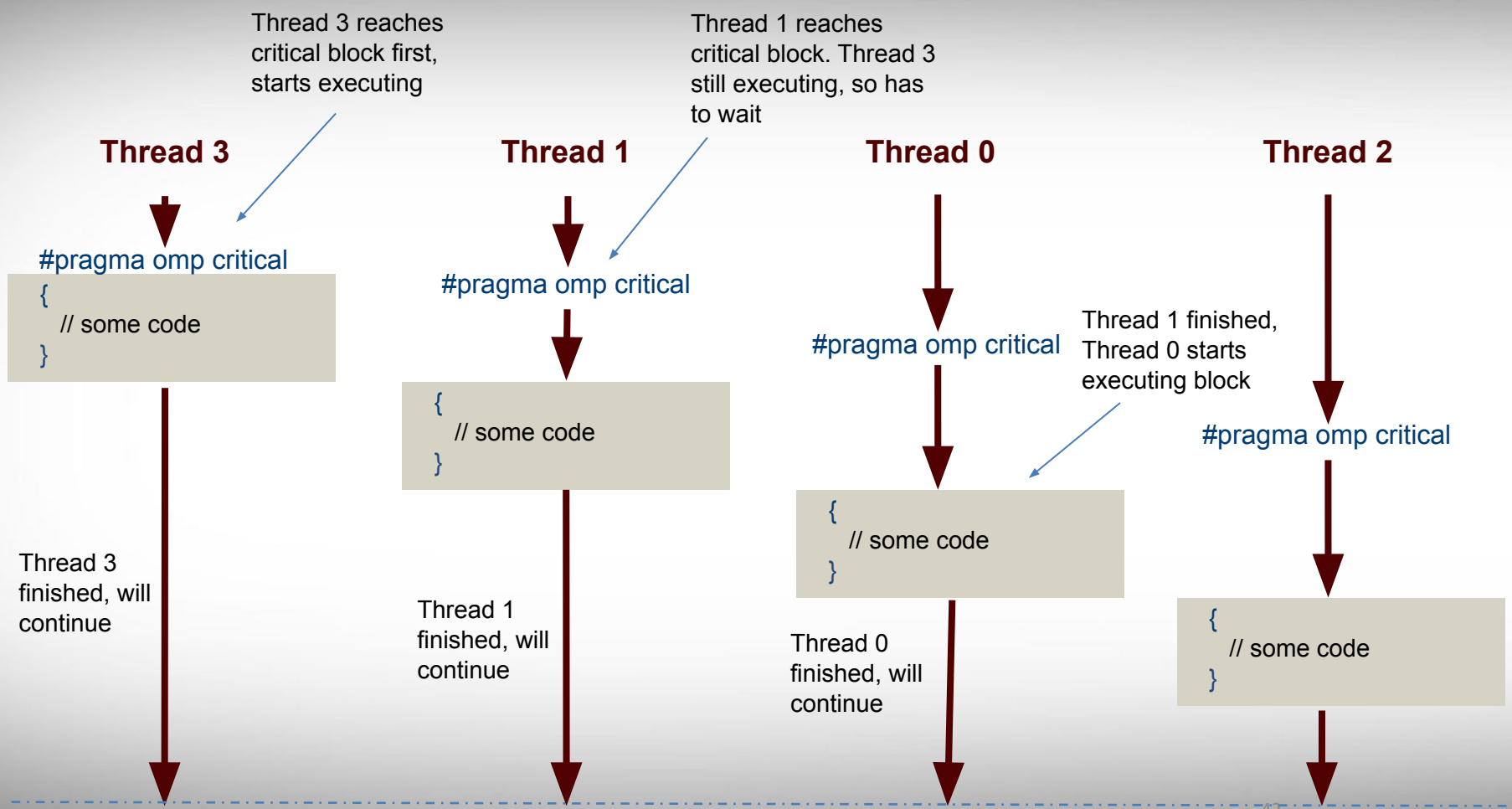
- **ALL** threads will excute the code inside the block
- Execution of the block is serialized, only one thread at a time will execute the block
- Threads will wait at start of block when another thread already inside the block

```
int tot=0; int id=0;
#pragma omp parallel
{
#pragma omp critical
  {
    id = omp_get_thread_num(); tot=tot+id;
    std::cout << "id " << id << ", tot:  " << tot << "\n";
  }
   // do some other stuff
}
```

Only one thread can execute block, other threads will wait

Will threads wait until all other treads have finished?

NOTE: *If block consists of only a single assignment can use* **#pragma omp atomic** instead


Thread 3 reaches critical block first, starts executing
Thread 1 reaches critical block. Thread 3 still executing, so has to wait
Thread 3
Thread 1
Thread 0
Thread 2
#pragma omp critical
{
// some code
}
#pragma omp critical
{
// some code
}
#pragma omp critical
{
// some code
}
Thread 1 finished, Thread 0 starts executing block
#pragma omp critical
{
// some code
}
Thread 3 finished, will continue
Thread 1 finished, will continue
Thread 0 finished, will continue

Dot product (take 2)

Exercise:

1) Create program that takes 2 vectors and computes:
   a) The dot product of the vectors
   b) the largest element of the two vectors
   c) This time use OpenMP atomic blocks
2) Add timing to compute the run time
3) Compile and run the program
4) Try it with various number of threads

Synchronization pragma

#pragma omp master (!$OMP MASTER)

- **ONLY** master threads will excute the code inside the block
- Other threads will skip executing the block
- Other threads will not wait at end of the block

#pragma omp barrier (!$OMP BARRIER)

- **ALL** threads will wait at the barrier.
- Only when all threads have reached the barrier, each thread can continue
- Already seen implicit barriers, e.g. at the end of ”#pragma omp parallel”, ”#pragma omp for”

TIP: IF Clause

OpenMP provides another useful clause to decide at run time if a parallel region should actually be run in parallel (multiple threads) or just by the master thread:

IF (logical expr)

For example:

```
$!OMP PARALLEL IF(n > 100000)          (fortran)
#pragma omp parallel if (n>100000)     (C/C++)
```

This will only run the parallel region when n> 100000

TIP: Printing OMP env vars

OpenMP 4.0 introduces a new environmental variable that instructs the runtime to print version number and all OpenMP environmental variables:

```
OMP_DISPLAY_ENV=VERBOSE
```

To only print the OpenMP version number, you can use:

```
OMP_DISPLAY_ENV=TRUE
```

Scheduling Clauses

SCHEDULE (STATIC,250) **//loop with 1000 iterations, 4 threads**

```
!$OMP PARALLEL DO SCHEDULE (STATIC,250)
DO i=1,1000
   :
ENDDO
!$OMP END PARALLEL DO
```

```
#pragma omp parallel for schedule(static,250)
 for (int i=0;i<1000;++i) {
          :
```

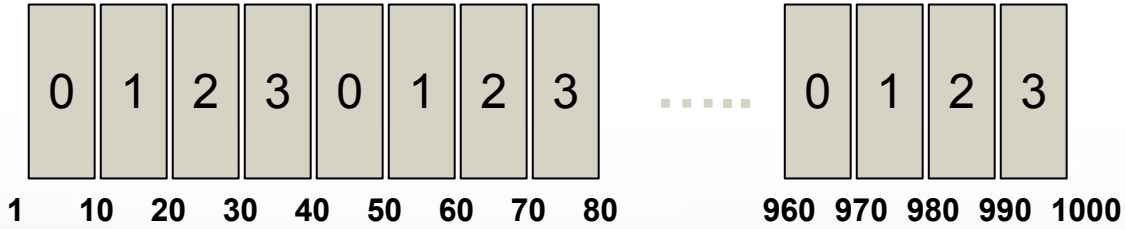
Although the OpenMP standard does not specify how a loop should be partitioned most compilers split the loop in N/p (N #iterations, p #threads) chunks by default.

Scheduling Clauses

SCHEDULE (STATIC,10) **//loop with 1000 iterations, 4 threads**

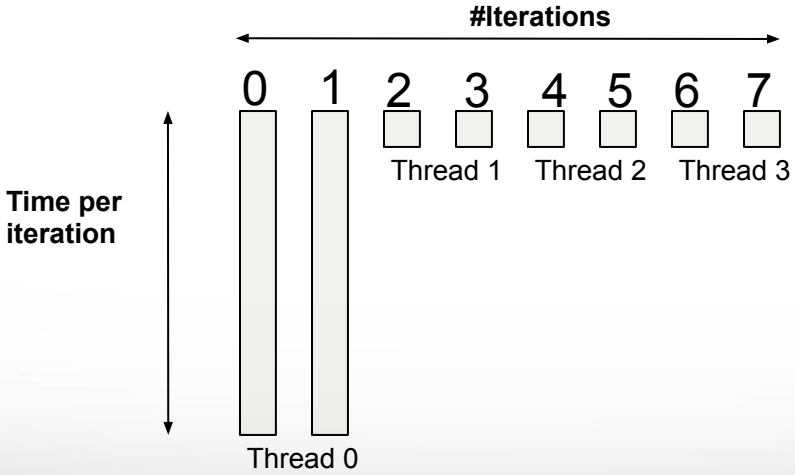
```
!$OMP PARALLEL DO SCHEDULE (STATIC,10)
DO i=1,1000
   :
ENDDO
!$OMP END PARALLEL DO
```

```
#pragma omp parallel for schedule(static,10)
  for (int i=0;i<1000;++i) {
          :
  }
```



Scheduling Clauses

With static scheduling the number of iterations is evenly distributed among all openmp threads. This is not always the best way to partition. Why?



How can this happen?

Scheduling Clauses

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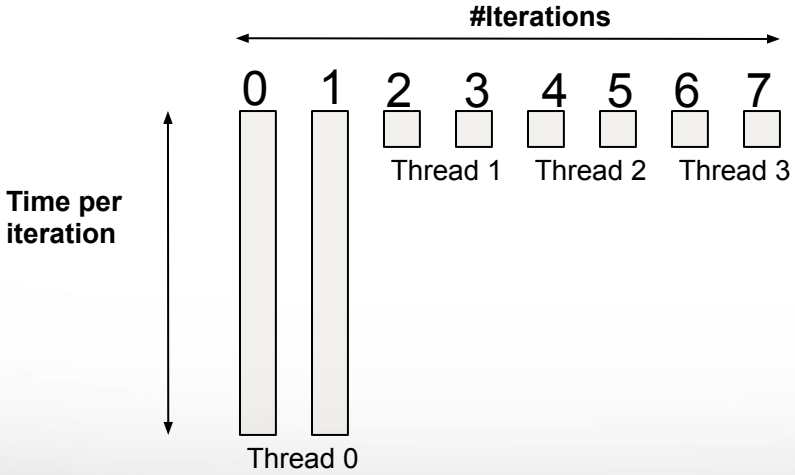


This is called load imbalance. In this case threads 2,3, and 4 will be waiting very long for thread 1 to finish

How can this happen?

Scheduling Clauses

SCHEDULE (DYNAMIC,10) **//loop with 1000 iterations, 4 threads**

```
!$OMP PARALLEL DO SCHEDULE (DYNAMIC,10)
DO i=1,1000
   :
ENDDO
!$OMP END PARALLEL DO
```

```
#pragma omp parallel for schedule(dynamic,10)
for (int i=0;i<1000;++i) {
            :
    }
```

Loop iterations are divided into pieces of size chunk. When a thread finishes one chunk, it is dynamically assigned another.

NOTE: there is a significant overhead involved compared to static scheduling. WHY?

Scheduling Clauses

SCHEDULE (GUIDED,10) **//loop with 1000 iterations, 4 threads**

```
!$OMP PARALLEL DO SCHEDULE (GUIDED,10)
DO i=1,1000
  :
ENDDO
!$OMP END PARALLEL DO
```

```
#pragma omp parallel for schedule(guided,10)
  for (int i=0;i<1000;++i) {
          :
    }
```

Similar to DYNAMIC schedule except that chunk size is relative to number of iterations left.

NOTE: there is a significant overhead involved compared to static scheduling. WHY?

Nested Parallelism

OpenMP allows parallel regions inside other parallel regions

```
#pragma omp parallel for
for (int i=0; i<N;++i) {
        :
        #pragma omp parallel for
        for (j=0;j<M;++j)
}
```

- To enable nested parallelism:
  - ✔ env var: OMP_NESTED=1
  - ✔ lib function: omp_set_nested(1)
- To specify number of threads:
  - ✔ omp_set_ num_threads()
  - ✔ OMP_NUM_THREADS=4,2

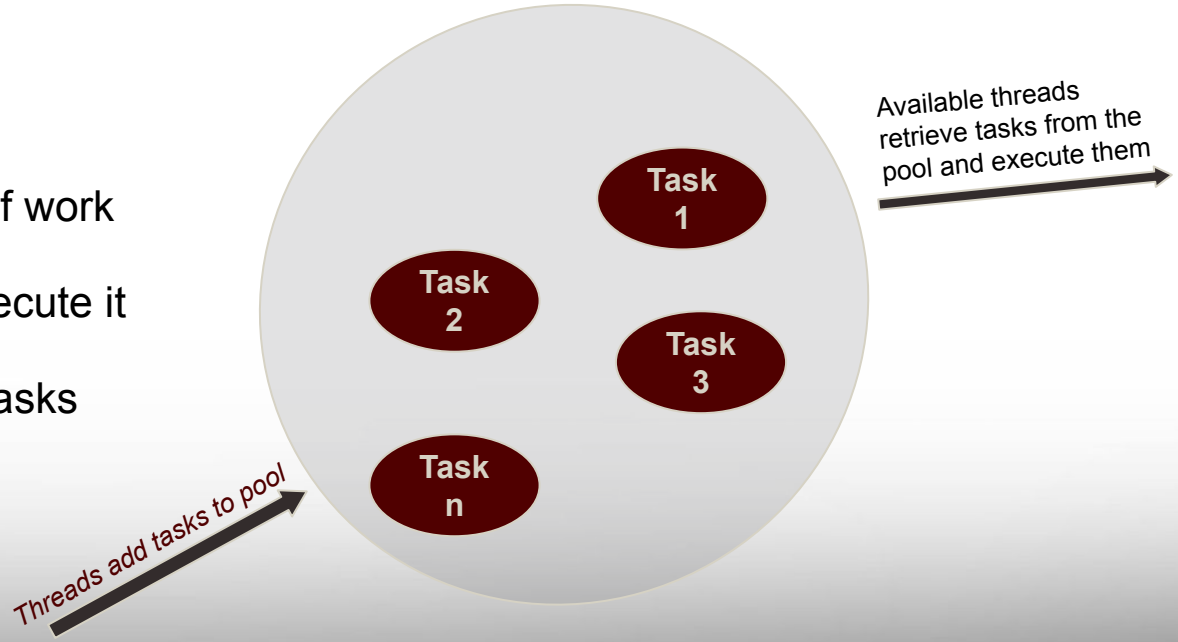
NOTE: using nested parallelism does introduce extra overhead and might over-subscribe of threads

OpenMP Tasks

New in OpenMP 3.0

Especially useful for unbounded loops, Irregular algorithms, Tree/lists, Recursive algorithms, Producer/Consumer type problems.

- Each task is independent unit of work
- When a thread enounter a task construct, thread decides to execute it itself or put in task pool
- Available threads will execute tasks
- Tasks consist of:
  - Code to execute
  - Data environment



OpenMP Tasks

Creating tasks

#pragma omp task

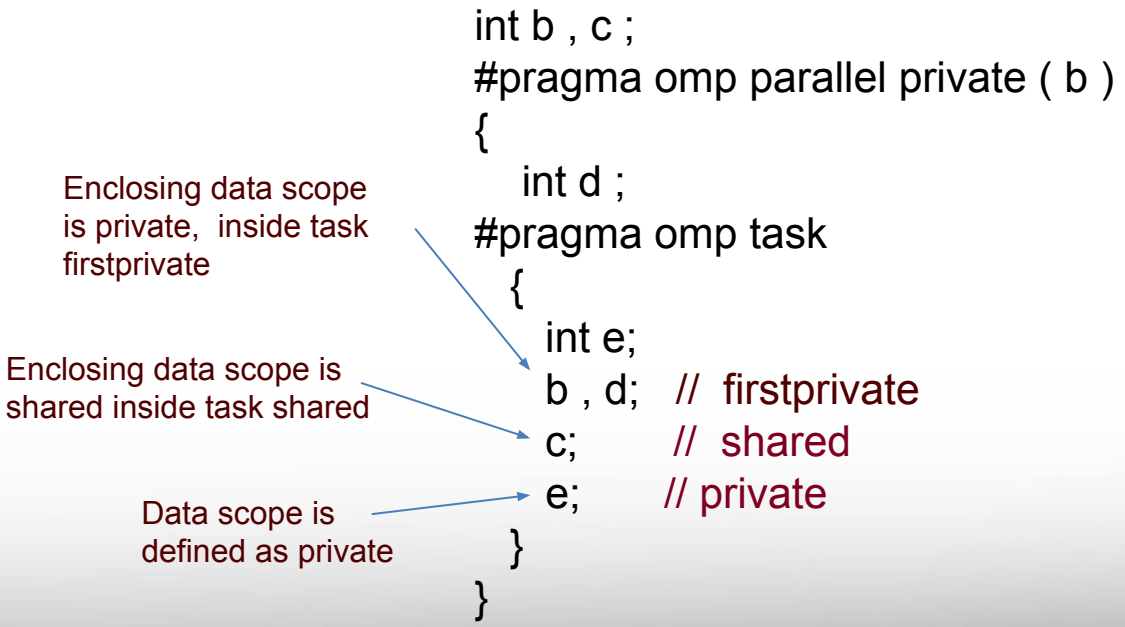
- Defines/creates new task
- Task will be added to task pool
- Idle thread will get tasks from pool and executes it
- Has to be in parallel region

Synchronization

#pragma omp taskwait

- Acts like a barrier
- Thread wait until all child tasks have finished

Default Data Scope Rules



Analysis of OpenMP Tasks

Start a parallel region

Add a single construct (why?)

Add a nowait clause (why?)

Create task

Wait until all child tasks have finished

```
#pragma omp parallel
{
#pragma omp single nowait
  {
#pragma omp task
    cout << “Thread “ << id << “executing task 1\n”;
#pragma omp task
    cout << “Thread “ << id << “executing task 2\n”;
 #pragma omp taskwait
   printf(“Finished with tasks\n”);
  }
  int id = omp_get_thread_num();
  printf(“ Thread %d says hello\n,id);
}
```

What will the code print out, and in what order?

Dot product (take 3)

Exercise:

1) Create program that takes 2 vectors and computes:
   a) The dot product of the vectors
   b) the largest element of the two vectors
   c) This time, use OpenMP tasks
2) Add timing to compute the run time
3) Compile and run the program
4) Try it with various number of threads

MKL

The Intel Math Kernel Library (MKL) has very specialized and optimized versions of many math functions (e.g. blas, lapack). Many of these have been parallelized using OpenMP.

- MKL_NUM_THREADS
- OMP_NUM_THREADS

http://hprc.tamu.edu/wiki/index.php/Ada:MKL

Questions?

You can always reach us at help@hprc.tamu.edu