

# Tutorial on OpenMP programming

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# Justification

OpenMP is a flexible tool for incrementally parallelizing a shared memory-based code. This course introduces the main concepts through lecturing and exercises.

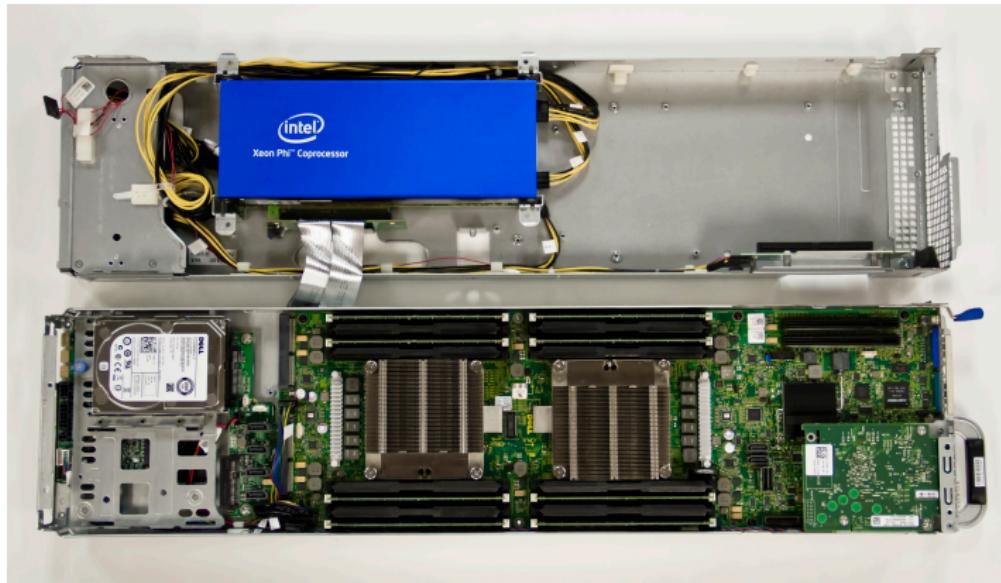
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# Part I

## The Fork-Join model

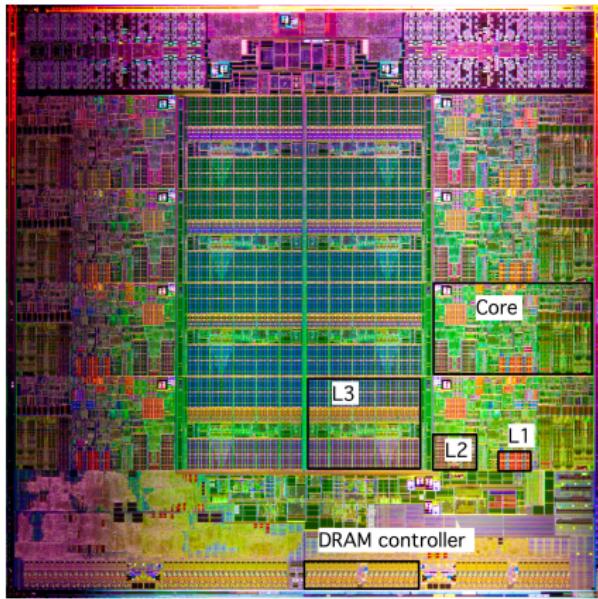
# Computer architecture terminology

One cluster node:



A node will have 1 or 2 or (sometimes) 4 'sockets': processor chips.  
There may be a co-processor attached.

# Structure of a socket

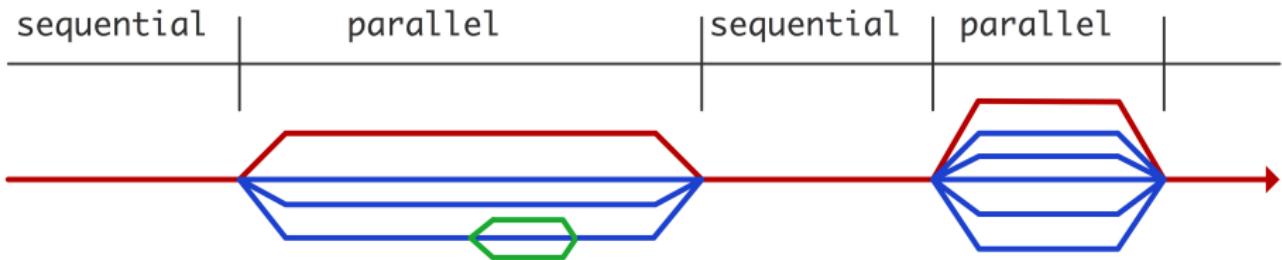


Eight cores per socket, making 16 per node.  
They all access the same data.

# Threads

Process: stream of instructions

Thread: process can duplicate itself, same code, access to same data



The OS will place threads on different cores: parallel performance.

Note: threads are software. More threads than cores or fewer is allowed.

## To write an OpenMP program

```
#include "omp.h"
```

in C, and

```
use omp_lib
```

or

```
#include "omp_lib.h"
```

for Fortran.

# To compile an OpenMP program

```
# gcc  
gcc -o foo foo.c -fopenmp  
# Intel compiler  
icc -o foo foo.c -openmp
```

# To run an OpenMP program

```
export OMP_NUM_THREADS=8  
./my_omp_program
```

Stampede has 16 cores; more than 16 threads does not make sense.

Quick experiment:

```
for t in 1 2 4 8 12 16; do  
    OMP_NUM_THREADS=$t ./my_omp_program  
done
```

## Exercise 1 (parallel)

Take the hello world program of exercise ?? and insert the above functions, before, in, and after the parallel region. What are your observations?

# What happens if I press that button?

Who of you has tried setting the number of threads (much) larger than the number of cores? What happened?

## Threads and threads

- Threads are software, cores are hardware.
- The OS can move threads between cores: not a good idea for performance.
- Set: `export OMP_PROC_BIND=true` and you'll be good in most of the cases.
- Look up 'affinity' in the OMP standard for all the details.

## Exercise 2

Extend the program from exercise 1. Make a complete program based on the lines:

**Code:**

```
1 // reduct.c
2     int tsum=0;
3 #pragma omp parallel
4     {
5         tsum += // expression
6     }
7     printf("Sum is %d\n",tsum);
```

**Output:**

Missing      output  
sumthread

Compile and run again. (In fact, run your program a number of times.) Do you see something unexpected? Can you think of an explanation?

# Shared memory problems

Race condition: simultaneous update of shared data:

process 1:  $I = I + 2$

process 2:  $I = I + 3$

Results can be indeterminate:

scenario 1.	scenario 2.	scenario 3.
	$I = 0$	
read $I = 0$ compute $I = 2$ write $I = 2$	read $I = 0$ compute $I = 3$  write $I = 3$	read $I = 0$ compute $I = 2$ write $I = 3$
$I = 3$	$I = 2$	read $I = 2$ compute $I = 5$ write $I = 5$  $I = 5$

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## Part II

### Loop parallelism

# Loop parallelism

Much of parallelism in scientific computing is in loops:

- Vector updates and inner products
- Matrix-vector and matrix-matrix operations
- Finite Element meshes
- Multigrid

## Work distribution

- Suppose loop iterations are independent:
- Distribute them over the threads:
- Use `omp_get_thread_num` to determine disjoint subsets.
- How would you do this specifically?

## Workshare constructs

Here's the two-step parallelization in OpenMP:

- You use the `parallel` directive to create a team of threads;
- then you use a 'workshare' construct to distribute the work over the team;
- For loops that is the `for` (or `do`) construct.

# Workshare construct for loops

C: directive followed by statement or block:

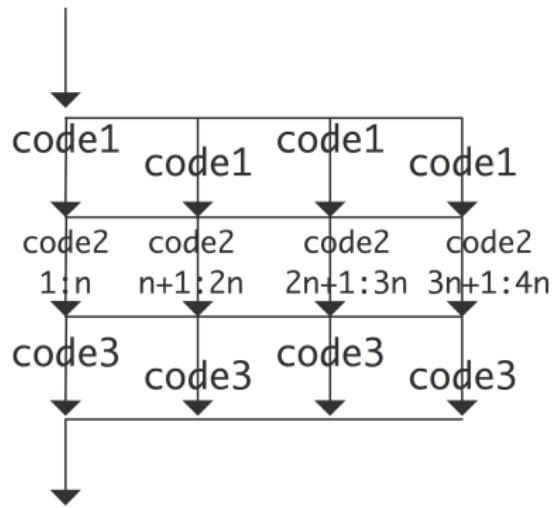
```
#pragma omp parallel
{
#pragma omp for
    for (i=0; i<N; i++)
        ... something with i ...
}
```

Fortran: matching end directive

```
!$omp parallel
 !$omp do
    do i=1,n
        ... something with i ...
    end do
 !$omp end do
 !$omp end parallel
```

# Stuff inside a parallel region

```
#pragma omp parallel
{
    code1();
#pragma omp for
    for (i=1; i<=4*N; i++) {
        code2();
    }
    code3();
}
```



## Exercise 3 (pi)

Compute  $\pi$  by *numerical integration*. We use the fact that  $\pi$  is the area of the unit circle, and approximate this by computing the area of a quarter circle using *Riemann sums*.

- Let  $f(x) = \sqrt{1 - x^2}$  be the function that describes the quarter circle for  $x = 0 \dots 1$ ;
- Then we compute

$$\pi/4 \approx \sum_{i=0}^{N-1} \Delta x f(x_i) \quad \text{where } x_i = i\Delta x \text{ and } \Delta x = 1/N$$

Write a program for this, and parallelize it using OpenMP parallel for directives.

- Put a `parallel` directive around your loop. Does it still compute the right result? Does execution time go down with the number of threads? (The answers should be no and no.)
- Change the `parallel` to `parallel for` (or `parallel do`). Now is the result correct? Is execution speed up? (The answers should now be no and yes.)
- Put a `critical` directive in front of the update. (Yes and very much no.)
- Remove the `critical` and add a clause `reduction(+:quarterpi)` to the `for` directive. Now it should be correct and efficient.

Use different numbers of cores and compute the speedup you attain over the sequential computation. Is there a performance difference between the OpenMP code with 1 thread and

# Loop schedules

- Default: static scheduling of iterations.

Very efficient. Good if all iterations take the same amount of time.

`schedule(static)`

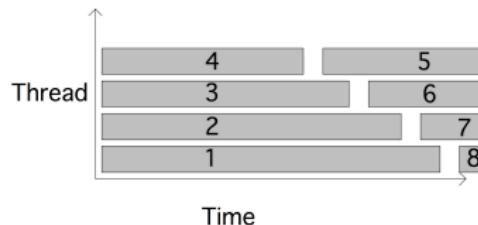
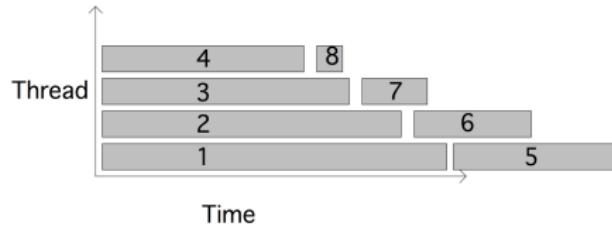
- Other possibility: dynamic.

Runtime overhead; better if iterations do not take the same amount of time.

`schedule(dynamic)`

Four threads, 8 tasks of decreasing size

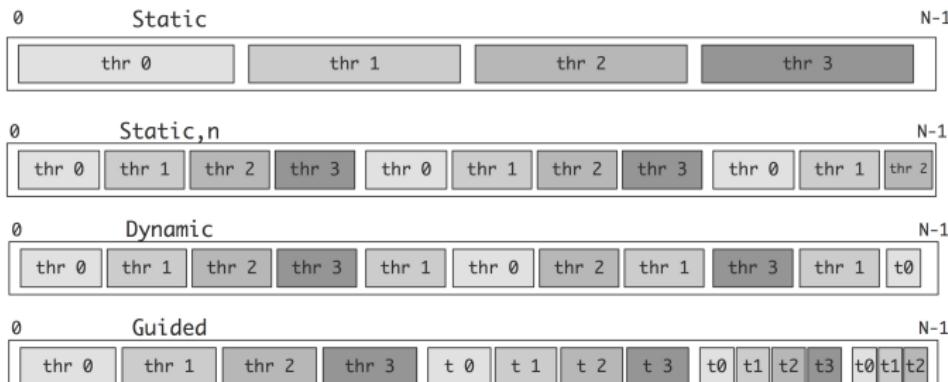
dynamic schedule is better:



# Chunk size

With  $N$  iterations and  $t$  threads:

- Static: each thread gets  $N/t$  iterations.  
explicit chunk size: `schedule(static,123)`
- Dynamic: each thread gets 1 iteration at a time  
explicit chunk size: `schedule(dynamic,45)`
- Help from OpenMP:  
guided schedule uses decreasing chunk size (with optional minimum chunk):  
`schedule(guided,6)`



# Reductions

- Inner product loop:

```
s = 0.;  
for (i=0; i<N; i++)  
    s += x[i]*y[i];
```

- Use the reduction(+:s) clause.
- All the usual operations are available; you can also make your own.

## Exercise 4 (piadapt)

We continue with exercise 3. We add 'adaptive integration': where needed, the program reduces the step size<sup>1</sup>. This means that the iterations no longer take a predictable amount of time.

```
1  for (int i=0; i<nsteps; i++) {           ↪is++) {
2      double                         11          double
3          x = i*h, x2 = (i+1)*h,       12          hs = h/samples,
4          y = sqrt(1-x*x),           13          xs = x+ is*hs,
5          y2 = sqrt(1-x2*x2),         14          ys = sqrt(1-xs*xs);
6          slope = (y-y2)/h;          15          quarterpi += hs*ys;
7          if (slope>15) slope = 15;   16          nsamples++;
8      int                           17      }
9      samples = 1+(int)slope, is;    18  }
10     for (int is=0; is<samples;      19  pi = 4*quarterpi;
```

- 1 Use the `omp parallel for` construct to parallelize the loop. As in the previous lab, you may at first see an incorrect result. Use the `reduction` clause to fix this.
- 2 Your code should now see a decent speedup, but possibly not for all cores. It is possible to get completely linear speedup by adjusting the schedule.

Start by using `schedule(static,n)`. Experiment with values for `n`. When can you get better speedup? Explain this.

## same exercise

- ① Use the `omp parallel for` construct to parallelize the loop. As in the previous lab, you may at first see an incorrect result. Use the `reduction` clause to fix this.
- ② Your code should now see a decent speedup, using up to 8 cores. However, it is possible to get completely linear speedup. For this you need to adjust the schedule. Start by using `schedule(static,$n$)`. Experiment with values for  $n$ . What can you get a better speedup? Explain this.
- ③ Since this code is somewhat dynamic, try `schedule(dynamic)`. This will actually give a fairly bad result. Why? Use `schedule(dynamic,$n$)` instead, and experiment with values for  $n$ .
- ④ Finally, use `schedule(guided)`, where OpenMP uses a heuristic. What results does that give?
- ⑤ `schedule(auto)` : leave it up to the system.
- ⑥ `schedule(runtime)` : leave it up to environment variables; good for experimenting.

## More loop topics

- Multiple loops can be collapsed: `collapse(2)`. Improves performance.
- Ordered iterations: normally OpenMP can execute iterations in any sequence. You can force ordering if you absolutely have to. Bad for performance!
- There is a barrier at the end of a `for`: use `nowait` to let threads continue

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## Part III

### Workshare constructs

# What is worksharing again?

- The `omp parallel` creates a team of threads.
- Now you need to distributed work among them.
- Already seen: `for`, `do`
- Similar: `sections`
- Not obvious: `single`
- Fortran only: `workshare` (works with array notation, but compiler support seems mediocre)
- Story in itself: `task`

# Sections

Independent separate calculations:

```
double fx = f(x), gx = g(x), hx = h(x);  
..... fx ... gx ... hx .....
```

```
#pragma omp sections  
{  
    #pragma omp section  
    fx = f(x)  
    #pragma omp section  
    gx = g(x)  
    #pragma omp section  
    hx = h(x)  
}
```

Adding them together:

```
s = f(x)+g(x)+h(x);
```

Use reduction.  
*Victor Eijkhout*

## Single

```
int a;  
#pragma omp parallel  
{  
    #pragma omp single  
        a = f(); // some computation  
    #pragma omp sections  
        // various different computations using `a'  
}
```

- Is executed by a single thread.
- Has implicit barrier, so the result is available to everyone after.
- **master** is similar, does not have barrier.

## Exercise 5

What is the difference between this approach and how the same computation would be parallelized in MPI?

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## Part IV

### Thread data

# Shared and private data

You have already seen some of the basics:

- Data declared outside a parallel region is shared.
- Data declared in the parallel region is private.  
(Fortran does not have this block scope mechanism)

```
int i;  
#pragma omp parallel  
{ double i; .... }
```

- You can change all this with clauses:

```
int i;  
#pragma omp parallel private(i)
```

# Variables in loops

```
int i; double t;  
#pragma omp parallel for  
for (i=0; i<N; i++) {  
    t = sin(i*pi*h);  
    x[i] = t*t;  
}
```

- The loop variable is automatically private.
- The temporary  $t$  is shared, but conceptually private to each iteration: needs to be declared private.  
(What happens if you don't?)

# Copying to/from private data

- Private data is uninitialized

```
int i = 3;  
#pragma omp parallel private(i)  
    printf("%d\n",i); // undefined!
```

- To import a value:

```
int i = 3;  
#pragma omp parallel firstprivate(i)  
    printf("%d\n",i); // undefined!
```

- lastprivate to preserve value of last iteration.

## Default behaviour

- `default(shared)` or `default(private)`
- useful for debugging: `default(none)`  
because you have to specify everything as shared/private

## Persistent thread data

- Private data disappears after the parallel region.  
What if you want data to persist?

- Directive `threadprivate`

```
double seed;  
#pragma omp threadprivate(seed)
```

- Standard application: random number generation.
- Tricky: has to be global or static.

# Arrays

- Statically allocated arrays can be made private.
- Dynamically allocated ones can not: the pointer becomes private.

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## Part V

### Synchronization

## Need for synchronization

- The loop and sections directives do not specify an ordering, sometimes you want to force an ordering.
- Barriers: global synchronization.
- Critical sections: only one process can execute a statement this prevents race conditions.
- Locks: protect data items from being accessed.

# Barriers

- Every workshare construct has an implicit barrier:

```
#pragma omp parallel
{
    #pragma omp for
    for ( .. i .. )
        x[i] = ...
    #pragma omp for
    for ( .. i .. )
        y[i] = ... x[i] ... x[i+1] ... x[i-1] ...
}
```

First loop is completely finished before second.

- Explicit barrier:

```
#pragma omp parallel
{
    x = f();
    #pragma omp barrier
    .... x ...
```

## Critical sections

- Critical section: One update at a time.

```
#pragma omp parallel
{
    double x = f();
#pragma omp critical
    global_update(x);
}
```

- atomic : special case for simple operations, possible hardware support

```
#pragma omp atomic
t += x;
```

# Warning

- Critical sections are not cheap! The operating system takes thousands of cycles to coordinate the threads.
- Use only if minor amount of work.
- Do not use if a reduction suffices.
- Name your critical sections.
- Explore locks if there may not be a data conflict.

# Locks

- Critical sections are coarse:  
they dictate exclusive access to a *statement*
- Suppose you update a big table  
updates to non-conflicting locations should be allowed
- Locks protect a single data item.

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## Part VI

### Tasks

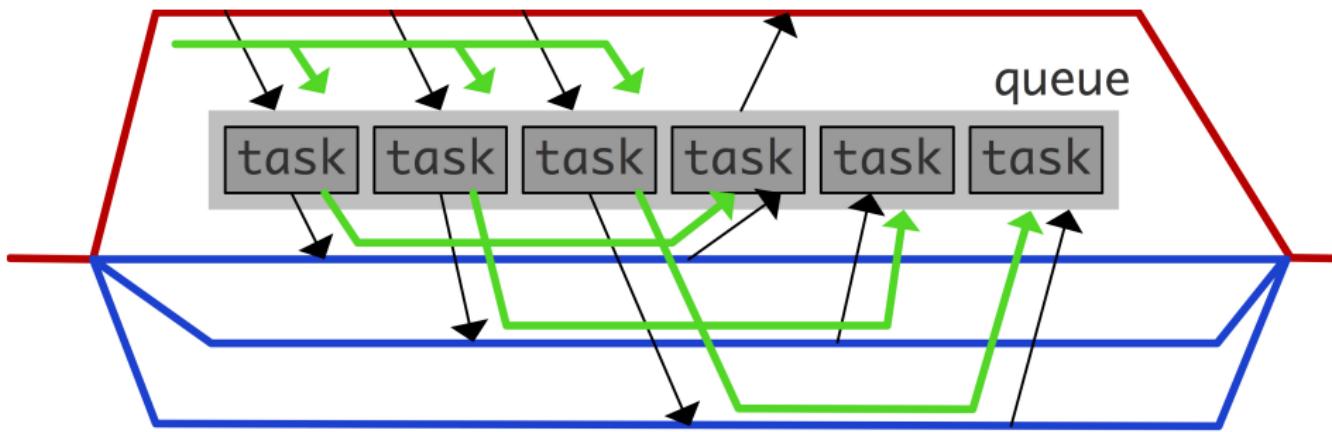
## More flexibility

- You have seen loops and sections.
- How about linked lists or trees?
- Tasks are very flexible:  
you create work, it goes on a queue, gets executed later

```
p = head_of_list();
while (!end_of_list(p)) {
#pragma omp task
    process( p );
    p = next_element(p);
}
```

# Threads, tasks, queues

- There is one queue (per team), not visible to the programmer.
- One thread starts generating tasks.
- Tasks can recursively generate tasks.
- You never know who executes what.



## Exercise 6 (taskfactor)

Use tasks to find the smallest factor of a large number (using  $2999 \cdot 3001$  as case): generate a task for each trial factor. Start with this code:

```
1     int factor=0;
2     #pragma omp parallel
3     #pragma omp single
4     for (int f=2; f<4000; f++) {
5         { // see if `f' is a factor
6             if (N%f==0) { // found factor!
7                 factor = f;
8             }
9         }
10        if (factor>0)
11            break;
12    }
13    if (factor>0)
14        printf("Found a factor: %d\n",factor);
```

- Turn the factor finding block into a task.
- Run your program a number of times:

Victor Eijkhout for i in `seq 1 1000` ; do ./taskfactor ; done | grep -v 2

# Task synchronization

Mechanisms for task synchronization:

- `taskwait`: wait for all previous tasks (not nested)
- `taskgroup`: wait for all tasks, including nested
- `depend`: synchronize on data items.

## Example: tree traversal

```
int process( node n ) {  
    if (n.is_leaf)  
        return n.value;  
    for ( c : n.children) {  
#pragma omp task  
        process(c);  
#pragma omp taskwait  
        return sum_of_children();  
    }  
}
```

## Example: Fibonacci

```
long fib(int n) {  
    if (n<2) return n;  
    else { long f1,f2;  
#pragma omp task  
        f1 = fib(n-1);  
#pragma omp task  
        f2 = fib(n-2);  
#pragma omp taskwait  
        return f1+f2;  
    }  
  
#pragma omp parallel  
#pragma omp single  
    printf("Fib(50)=%ld",fib(50));
```

(what is conceptually wrong with this example?)

## Fibonacci once more

```
long fibs[100];
void fib(n) {
    if (n>=2) {
        #pragma omp task \
            depend( in:fibs[n-2],in:fibs[n-1] ) \
            depend( out:fibs[n] )
        fibs[n] = fibs[n-2]+fibs[n-1];
    };
}

#pragma omp parallel
#pragma omp single
for (i<50)
    fib(i);
```

---

## Part VII

Remaining topics

# Affinity

How do you place threads on cores?

- Two socket design NUMA
- Intel KNL has quadrants and hardware multi-threading
- `OMP_PROC_BIND` and `OMP_PLACES`

# Accelerators

OpenMP 4 has mechanisms for offloading.

# SIMD

Processors have 4 or 8-wide SIMD.  
convert OpenMP loop to SIMD vector instructions.