Some more useful commands for HPC clusters

- Software available
  - *module avail (shows the software available on the machine)*
  - *module list (lists the software you have currently loaded in your environment)*
  - *module spider <name> (search for a particular module/software)*
- Interactive session
  - *srun --time=0:02:00 --nodes 1 --account USUCS5030 --pty /bin/bash –l*
- Batch job
  - *sbatch batch_test.sh*

```
#!/bin/bash
#SBATCH --time=00:02:00
#SBATCH --nodes=1
#SBATCH -o slurmjob-%j.out-%N
#SBATCH -e slurmjob-%j.err-%N
#SBATCH --account=usucs5890
#SBATCH --partition=kingspeak

cd /scratch/general/lustre/usucs5890/8-omp

#Run the program with our input
./omp_hello 8
```

SHARED MEMORY PROGRAMMING WITH OPENMP

Dr. Steve Petruzza

UtahStateUniversity

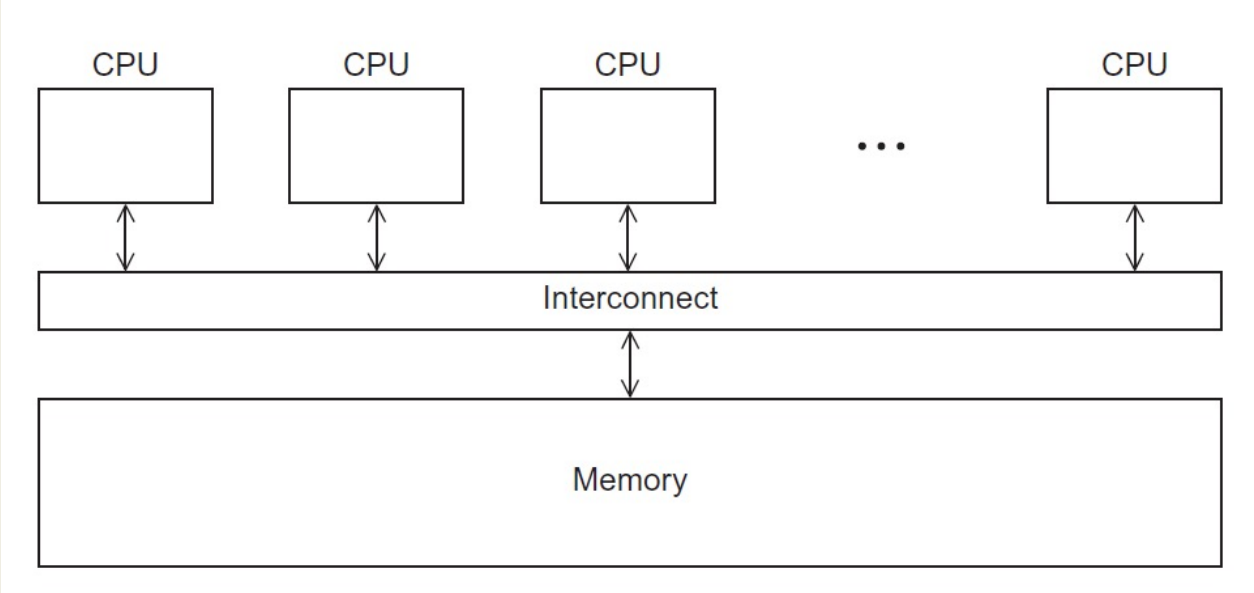
Reference material for part of this presentation :

An Introduction to Parallel Programming by Peter Pacheco

OpenMP

- An API for shared-memory parallel programming.
- MP = multiprocessing
- Designed for systems in which each thread or process can potentially have access to all available memory.
- System is viewed as a collection of cores or CPU's, all of which have access to main memory.

A shared memory system



Pragmas

- Special preprocessor instructions.
- Typically added to a system to allow behaviors that aren’t part of the basic C specification.
- Compilers that don’t support the pragmas ignore them.

#pragma

```c
#include <stdio.h>
#include <stdlib.h>
#include <omp.h>

void Hello(void);  /* Thread function */

int main(int argc, char* argv[]) {
   /* Get number of threads from command line */
   int thread_count = strtol(argv[1], NULL, 10);

#  pragma omp parallel num_threads(thread_count)
   Hello();

   return 0;
}  /* main */

void Hello(void) {
   int my_rank = omp_get_thread_num();
   int thread_count = omp_get_num_threads();

   printf("Hello from thread %d of %d\n", my_rank, thread_count);

}  /* Hello */
```

```
gcc -g -Wall -fopenmp -o omp_hello omp_hello.c

./omp_hello 4
```

compiling

running with 4 threads

possible outcomes

Hello from thread 0 of 4
Hello from thread 1 of 4
Hello from thread 2 of 4
Hello from thread 3 of 4

Hello from thread 1 of 4
Hello from thread 2 of 4
Hello from thread 0 of 4
Hello from thread 3 of 4

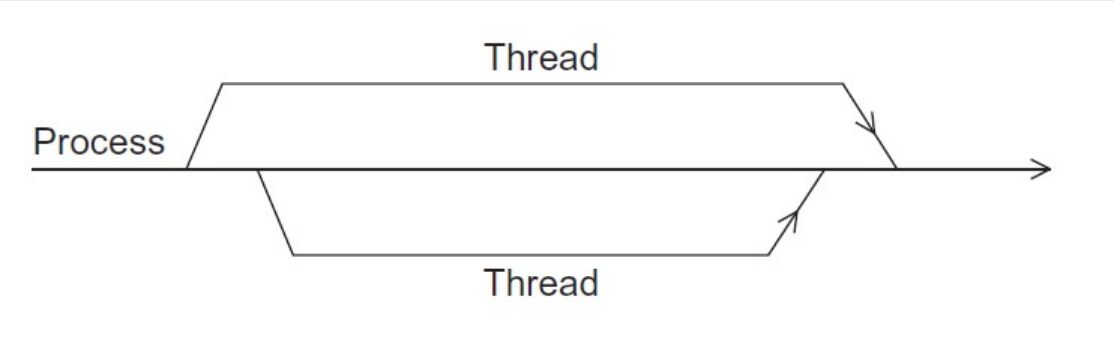
Hello from thread 3 of 4
Hello from thread 1 of 4
Hello from thread 2 of 4
Hello from thread 0 of 4

On MacOSX: clang -Xpreprocessor -fopenmp -lomp omp_hello.c -o omp_hello

OpenMp pragmas

- # pragma omp parallel
  - *Most basic parallel directive.*
  - *The number of threads that run the following structured block of code is determined by the run-time system.*

A process forking and joining two threads



clause

- Text that modifies a directive.
- The num_threads clause can be added to a parallel directive.
- It allows the programmer to specify the number of threads that should execute the following block.

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

Of note…

- There may be system-defined limitations on the number of threads that a program can start.
- The OpenMP standard doesn’t guarantee that this will actually start thread_count threads.
- Most current systems can start hundreds or even thousands of threads.
- Unless we’re trying to start a lot of threads, we will almost always get the desired number of threads.

Some terminology

- In OpenMP parlance the collection of threads executing the parallel block — the original thread and the new threads — is called a team, the original thread is called the master, and the additional threads are called slaves.

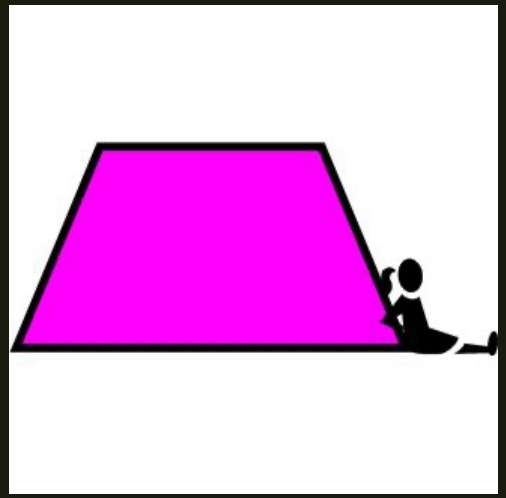
In case the compiler doesn't support OpenMP

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

```
#ifdef _OPENMP
# include <omp.h>
#endif
```

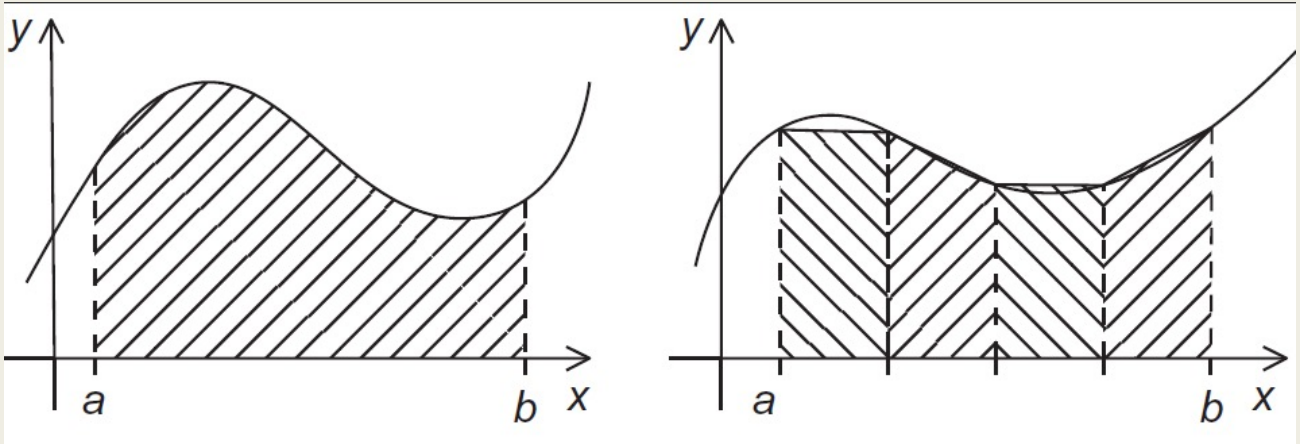
In case the compiler doesn't support OpenMP

```
# ifdef _OPENMP
  int my_rank = omp_get_thread_num ( );
  int thread_count = omp_get_num_threads ( );
# else
  int my_rank = 0;
  int thread_count = 1;
# endif
```



THE TRAPEZOIDAL RULE

The trapezoidal rule



Serial algorithm

```
/* Input:  a, b, n */
h = (b-a)/n;
approx = (f(a) + f(b))/2.0;
for (i = 1; i <= n-1; i++) {
    x_i = a + i*h;
    approx += f(x_i);
}
approx = h*approx;
```

A First OpenMP Version

1) We identified two types of tasks:

   a) computation of the areas of individual trapezoids, and

   b) adding the areas of trapezoids.

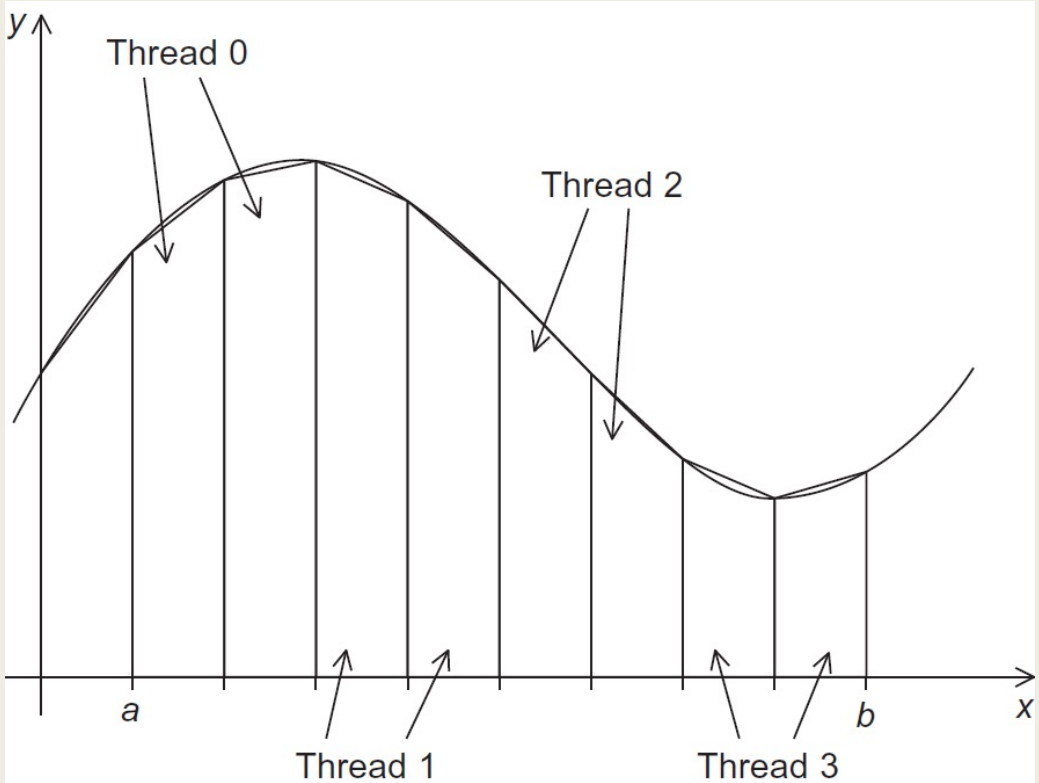
2) There is no communication among the tasks in the first collection, but each task in the first collection communicates with task 1.

A First OpenMP Version

3) We assumed that there would be many more trapezoids than cores.

- So we aggregated tasks by assigning a contiguous block of trapezoids to each thread (and a single thread to each core).

Assignment of trapezoids to threads



Time	Thread 0	Thread 1
0	`global_result = 0` to register	finish `my_result`
1	`my_result = 1` to register	`global_result = 0` to register
2	add `my_result` to `global_result`	`my_result = 2` to register
3	store `global_result = 1`	add `my_result` to `global_result`
4		store `global_result = 2`

Unpredictable results when two (or more) threads attempt to simultaneously execute:

global_result += my_result ;

Mutual exclusion

```
# pragma omp critical
  global_result += my_result ;
```

only one thread can execute
the following structured block at a time

```c
#include <stdio.h>
#include <stdlib.h>
#include <omp.h>

void Trap(double a, double b, int n, double* global_result_p);

int main(int argc, char* argv[]) {
   double  global_result = 0.0;  /* Store result in global_result */
   double  a, b;                 /* Left and right endpoints      */
   int     n;                    /* Total number of trapezoids    */
   int     thread_count;

   thread_count = strtol(argv[1], NULL, 10);
   printf("Enter a, b, and n\n");
   scanf("%lf %lf %d", &a, &b, &n);
#  pragma omp parallel num_threads(thread_count)
   Trap(a, b, n, &global_result);

   printf("With n = %d trapezoids, our estimate\n", n);
   printf("of the integral from %f to %f = %.14e\n",
      a, b, global_result);
   return 0;
}  /* main */
```

```
void Trap(double a, double b, int n, double* global_result_p) {
   double  h, x, my_result;
   double  local_a, local_b;
   int  i, local_n;
   int my_rank = omp_get_thread_num();
   int thread_count = omp_get_num_threads();

   h = (b-a)/n;
   local_n = n/thread_count;
   local_a = a + my_rank*local_n*h;
   local_b = local_a + local_n*h;
   my_result = (f(local_a) + f(local_b))/2.0;
   for (i = 1; i <= local_n-1; i++) {
     x = local_a + i*h;
     my_result += f(x);
   }
   my_result = my_result*h;

#  pragma omp critical
   *global_result_p += my_result;
}  /* Trap */
```

SCOPE OF VARIABLES

Scope

- In serial programming, the scope of a variable consists of those parts of a program in which the variable can be used.

- In OpenMP, the scope of a variable refers to the set of threads that can access the variable in a parallel block.

Scope in OpenMP

- A variable that can be accessed by all the threads in the team has shared scope.
- A variable that can only be accessed by a single thread has private scope.
- The default scope for variables declared before a parallel block is shared.

THE REDUCTION CLAUSE

We need this more complex version to add each thread's local calculation to get *global_result*.

```
void Trap(double a, double b, int n, double* global_result_p);
```

Although we'd prefer this.

```
double Trap(double a, double b, int n);
```

```
global_result = Trap(a, b, n);
```

If we use this, there's no critical section!

```
double Local_trap(double a, double b, int n);
```

If we fix it like this...

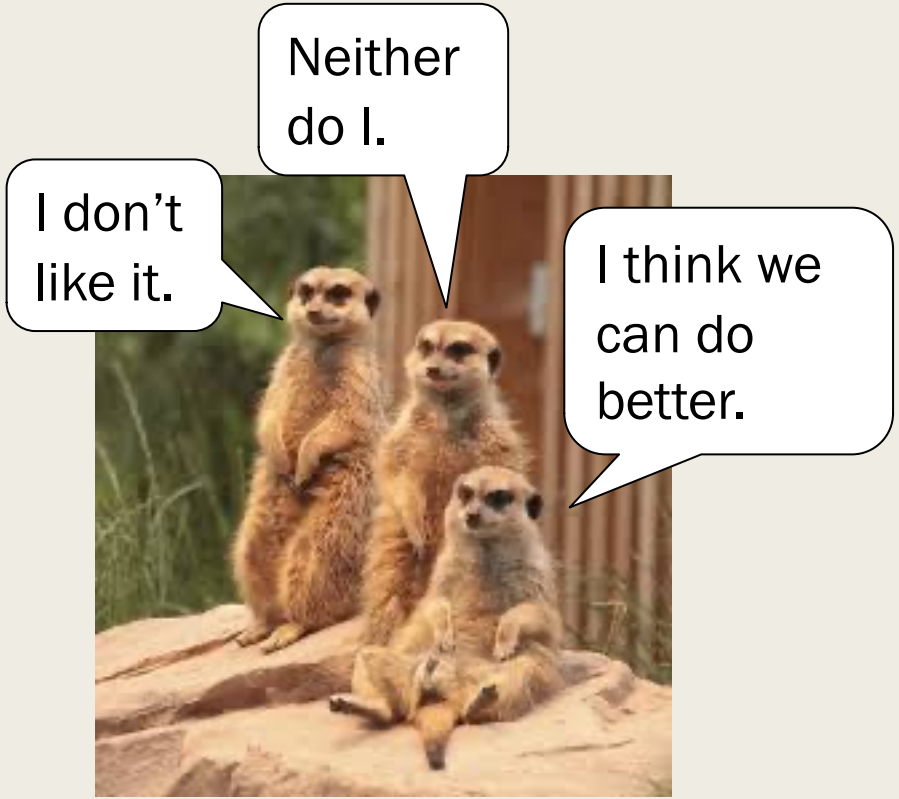
```
   global_result = 0.0;
#  pragma omp parallel num_threads(thread_count)
   {
#     pragma omp critical
      global_result += Local_trap(double a, double b, int n);
   }
```

... we force the threads to execute sequentially.

We can avoid this problem by declaring a private variable inside the parallel block and moving the critical section after the function call.

```
    global_result = 0.0;
#   pragma omp parallel num_threads(thread_count)
    {
        double my_result = 0.0;  /* private */

        my_result += Local_trap(double a, double b, int n);
#       pragma omp critical
        global_result += my_result;
    }
```


Neither do I.
I don’t like it.
I think we can do better.

Reduction operators

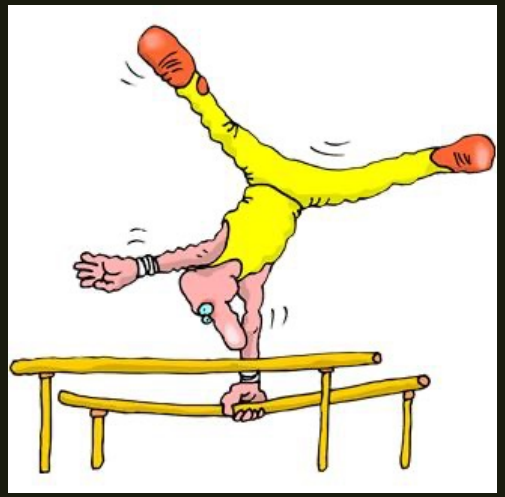
- A reduction operator is a binary operation (such as addition or multiplication).
- A reduction is a computation that repeatedly applies the same reduction operator to a sequence of operands in order to get a single result.
- All of the intermediate results of the operation should be stored in the same variable: the reduction variable.

A reduction clause can be added to a parallel directive.

```
reduction(<operator>: <variable list>)
```

+, *, -, &, |, ^, &&, ||

```
   global_result = 0.0;
#  pragma omp parallel num_threads(thread_count) \
      reduction(+: global_result)
   global_result += Local_trap(double a, double b, int n);
```

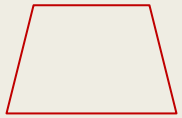


THE “PARALLEL FOR” DIRECTIVE

Parallel for

- Forks a team of threads to execute the following structured block.
- However, the structured block following the parallel for directive must be a for loop.
- Furthermore, with the parallel for directive the system parallelizes the for loop by dividing the iterations of the loop among the threads.

```
h = (b-a)/n;
approx = (f(a) + f(b))/2.0;
for (i = 1; i <= n-1; i++)
   approx += f(a + i*h);
approx = h*approx;
```



```
   h = (b-a)/n;
   approx = (f(a) + f(b))/2.0;
#  pragma omp parallel for num_threads(thread_count) \
      reduction(+: approx)
   for (i = 1; i <= n-1; i++)
      approx += f(a + i*h);
   approx = h*approx;
```

Legal forms for parallelizable for statements

```
                                          index++
                                          ++index
                        index < end       index--
                        index <= end      --index
for  index = start  ;   index >= end  ;   index += incr
                        index > end       index -= incr
                                          index = index + incr
                                          index = incr + index
                                          index = index - incr
```

Caveats

- The variable index must have integer or pointer type (e.g., it can’t be a float).
- The expressions start, end, and incr must have a compatible type. For example, if index is a pointer, then incr must have integer type.

Caveats

- The expressions start, end, and incr must not change during execution of the loop.
- During execution of the loop, the variable index can only be modified by the "increment expression" in the for statement.

DATA DEPENDENCY

Fibonacci series example

Data dependencies

```
fibo[ 0 ] = fibo[ 1 ] = 1;
for (i = 2; i < n; i++)
    fibo[ i ] = fibo[ i – 1 ] + fibo[ i – 2 ];
```

note 2 threads

```
fibo[ 0 ] = fibo[ 1 ] = 1;
# pragma omp parallel for num_threads(2)
for (i = 2; i < n; i++)
    fibo[ i ] = fibo[ i – 1 ] + fibo[ i – 2 ];
```

1 1 2 3 5 8 13 21 34 55

this is correct

but sometimes
we get this

1 1 2 3 5 8 0 0 0 0

What happened?

1. OpenMP compilers don’t check for dependences among iterations in a loop that’s being parallelized with a parallel for directive.
2. A loop in which the results of one or more iterations depend on other iterations cannot, in general, be correctly parallelized by OpenMP.

Estimating π

$$\pi = 4\left[1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \cdots\right] = 4\sum_{k=0}^{\infty}\frac{(-1)^k}{2k+1}$$

```
double factor = 1.0;
double sum = 0.0;
for (k = 0; k < n; k++) {
    sum += factor/(2*k+1);
    factor = -factor;
}
pi_approx = 4.0*sum;
```

OpenMP solution #1

loop dependency

```
        double factor = 1.0;
        double sum = 0.0;
#       pragma omp parallel for num_threads(thread_count) \
            reduction(+:sum)
        for (k = 0; k < n; k++) {
            sum += factor/(2*k+1);
            factor = -factor;
        }
        pi_approx = 4.0*sum;
```

OpenMP solution #2

```
        double sum = 0.0;
#       pragma omp parallel for num_threads(thread_count) \
           reduction(+:sum) private(factor)
        for (k = 0; k < n; k++) {
           if (k % 2 == 0)
              factor = 1.0;
           else
              factor = -1.0;
           sum += factor/(2*k+1);
        }
```

Insures factor has private scope.

The default clause

- Lets the programmer specify the scope of each variable in a block.

```
default(none)
```

- With this clause the compiler will require that we specify the scope of each variable we use in the block and that has been declared outside the block.

The default clause

```
        double sum = 0.0;
#       pragma omp parallel for num_threads(thread_count) \
           default(none) reduction(+:sum) private(k, factor) \
           shared(n)
        for (k = 0; k < n; k++) {
           if (k % 2 == 0)
              factor = 1.0;
           else
              factor = -1.0;
           sum += factor/(2*k+1);
        }
```

MORE ABOUT LOOPS IN OPENMP: SORTING

Bubble Sort

```
for (list_length = n; list_length >= 2; list_length--)
   for (i = 0; i < list_length-1; i++)
      if (a[i] > a[i+1]) {
         tmp = a[i];
         a[i] = a[i+1];
         a[i+1] = tmp;
      }
```

Serial Odd-Even Transposition Sort

```
for (phase = 0; phase < n; phase++)
   if (phase % 2 == 0)
      for (i = 1; i < n; i += 2)
         if (a[i-1] > a[i]) Swap(&a[i-1],&a[i]);
   else
      for (i = 1; i < n-1; i += 2)
         if (a[i] > a[i+1]) Swap(&a[i], &a[i+1]);
```

Unsorted array: 2, 1, 4, 9, 5, 3, 6, 10

Step 1(odd):	2	1	4	9	5	3	6	10
Step 2(even):	1	2	4	9	3	5	6	10
Step 3(odd):	1	2	4	3	9	5	6	10
Step 4(even):	1	2	3	4	5	9	6	10
Step 5(odd):	1	2	3	4	5	6	9	10
Step 6(even):	1	2	3	4	5	6	9	10
Step 7(odd):	1	2	3	4	5	6	9	10
Step 8(even):	1	2	3	4	5	6	9	10

Sorted array: 1, 2, 3, 4, 5, 6, 9, 10

Serial Odd-Even Transposition Sort

Phase	Subscript in Array 0		1		2		3
0	9	↔	7		8	↔	6
	7		9		6		8
1	7		9	↔	6		8
	7		6		9		8
2	7	↔	6		9	↔	8
	6		7		8		9
3	6		7	↔	8		9
	6		7		8		9

First OpenMP Odd-Even Sort

```
   for (phase = 0; phase < n; phase++) {
      if (phase % 2 == 0)
#        pragma omp parallel for num_threads(thread_count) \
            default(none) shared(a, n) private(i, tmp)
         for (i = 1; i < n; i += 2) {
            if (a[i-1] > a[i]) {
               tmp = a[i-1];
               a[i-1] = a[i];
               a[i] = tmp;
            }
         }
      else
#        pragma omp parallel for num_threads(thread_count) \
            default(none) shared(a, n) private(i, tmp)
         for (i = 1; i < n-1; i += 2) {
            if (a[i] > a[i+1]) {
               tmp = a[i+1];
               a[i+1] = a[i];
               a[i] = tmp;
            }
         }
   }
```

Second OpenMP Odd-Even Sort

```
#  pragma omp parallel num_threads(thread_count) \
      default(none) shared(a, n) private(i, tmp, phase)
   for (phase = 0; phase < n; phase++) {
      if (phase % 2 == 0)
#        pragma omp for
         for (i = 1; i < n; i += 2) {
            if (a[i-1] > a[i]) {
               tmp = a[i-1];
               a[i-1] = a[i];
               a[i] = tmp;
            }
         }
      else
#        pragma omp for
         for (i = 1; i < n-1; i += 2) {
            if (a[i] > a[i+1]) {
               tmp = a[i+1];
               a[i+1] = a[i];
               a[i] = tmp;
            }
         }
   }
```

Odd-even sort with two parallel for directives and two for directives.
(Times are in seconds.)

thread_count	1	2	3	4
Two parallel **for** directives	0.770	0.453	0.358	0.305
Two **for** directives	0.732	0.376	0.294	0.239

- Why this difference in performance?
  - *Parallel for has a implicit barrier at the end of the loop*
  - *The **for** directive does not fork new threads but instead uses the one already available*