High-Performance Computing

– Shared Memory Programming with OpenMP –

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Outline

Basic OpenMP (covered by Pacheco book)

- concepts
- work sharing (loop parallelization)
- variable scoping

More OpenMP (covered in future lecture)

- task parallelism
- SIMD parallelism (vectorization)
- task loops, do across loops

Advanced OpenMP (optionally covered)

- target offloading to GPUs

OpenMP



- MP = multi-processing
- API for explicit multi-threaded, shared-memory parallel programming with three components
 - compiler directives
 - runtime library functions
 - environment variables

Goals of OpenMP

- standardization and portability
 - jointly defined by a group of major hard ware and software vendors
 - widely supported on Unix/Linux and Windows
 - API available for C/C++ and Fortran
- ease of use
 - a very small set of of directives is sufficient to cover many common cases
 - supports incremental parallelization
 - addresses coarse and fine-grained parallelism

OpenMP (2)

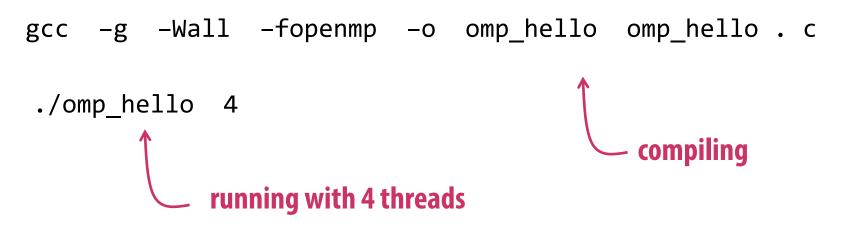
History

- in the early 1990's HPC vendors have developed different OpenMP-like compiler extensions for Fortran
- mid 1990's begin of efforts for a common API for shared memory multi-threading
- OpenMP 1.0 (1997/98) and OpenMP 2.0 (2000/2002) focus on parallelization of highly regular loops
- OpenMP 3.0 (2008) introduces task-level parallelism
- OpenMP 4.0 (2013) adds support target offloading for accelerators, SIMD (vectorization), userdefined reductions, ...
- OpenMP 4.5 (2015) introduces taskloops, do across loops, task priorities and improves target offloading

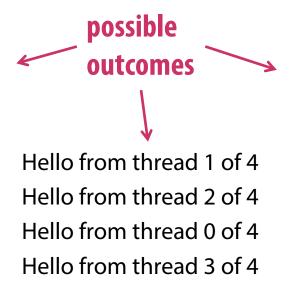
Hello world for OpenMP

```
#include <stdio.h>
 1
2 #include <stdlib.h>
   #include <omp.h>
3
4
 5
   void Hello(void): /* Thread function */
6
    int main(int argc, char* argv[]) {
 7
8
       /* Get number of threads from command line */
9
       int thread_count = strtol(argv[1], NULL, 10);
10
                                                          OpenMP compiler directive
       pragma omp parallel num_threads(thread_count)
11
       Hello():
12
13
       return 0:
14
       /* main */
15
16
17
   void Hello(void) {
                                                          OpenMP runtime library
       int my_rank = omp_get_thread_num();
18
       int thread_count = omp_get_num_threads();
                                                          functions
19
20
       printf("Hello from thread %d of %d\n", my_rank, thread_count);
21
22
23
       /* Hello */
```

Compiling and Executing OpenMP Programs



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

OpenMP Compiler Directives (Pragmas)

OpenMP makes extensive use of compiler directives, e.g.

#pragma omp parallel default(shared) private(a,b)

Compiler directives provide special instructions to the compiler that are not part of the C/C++ standard

- compilers that don't support the directives just ignore them
- All OpenMP directives start with #pragma omp
 - directives can be followed by further clauses to modify and customize the basic operation

Examples for purpose of compiler directives

- spawning a parallel region
- dividing blocks of code among threads
- distributing loop iterations between threads
- serializing sections of code
- synchronization of work among threads

OpenMP Runtime-Library Functions

 Runtime-library functions allow OpenMP programs to query and configure the execution environment (OpenMP runtime system)

#include <omp.h>
int omp_get_num_threads(void)

Examples for purpose of runtime-library functions

- setting and querying the number of threads
- querying a thread's unique identifier (id), a thread's ancestor identifier, team size
- querying if in a parallel region and at what level
- setting and querying nested parallelism
- setting, initializing and terminating locks
- querying wall clock time and resolution

OpenMP Environment Variables

The OpenMP runtime system can be controlled by environment variables

export OMP_NUM_THREADS=8

- The properties affected by the environment variables can also be changed by runtime-library functions
- Examples for purpose of OpenMP environment variables
 - setting the number of threads
 - specifying how loop iterations are divided
 - binding threads to processors and cores
 - enabling/disabling and controlling depth of nested parallelism
 - enabling/disabling dynamic threads
 - setting thread stack size
 - setting threads wait policy

The OpenMP Directive "parallel"

pragma omp parallel

- most basic parallelization directive
- creates a number of threads that run the following structured block of code
- the number of threads that are used is determined by the run-time system

Clauses are used to modify directives

- the num_threads clause can be (optionally) added to a parallel directive
- specifies number of threads that should execute the following block

pragma omp parallel num_threads (thread_count)

Notes

- the OpenMP standard doesn't guarantee that this will actually start thread_count threads
- that number of threads a program can start may be limited by the system
- 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.

The OpenMP Directive "parallel" (2)

• For completeness: the complete specification of parallel directive is

#pragma omp parallel [clause ...] newline
 if (scalar_expression)
 private (list)
 shared (list)
 default (shared | none)
 firstprivate (list)
 reduction (operator: list)
 copyin (list)
 num_threads (integer-expression)

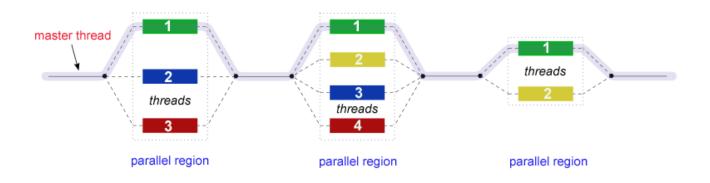
structured_block

Fork-Join Model

The basic parallelization model in OpenMP is fork-join parallelism

When master reaches the parallel directive:

- a collection of threads is created (denoted as team)
- each child thread executes the code of the block that immediately follows the directive
- the end of a parallel region is an implicit barrier, all threads are joined and the master thread continue



Fork-Join Model (2)

The actual number of threads in the team 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 on default or system configuration (typically number of cores)

if clause

- the optional if clause can contain a boolean expression
- a team is only created, if the clause evaluates to a non-zero value, otherwise the region is executed serially by the master thread

Writing Backward-Compatible Code

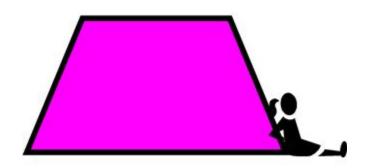
- OpenMP is designed for backward compatibility, i.e. programs can be compiled with a compiler without OpenMP support
 - #pragma omp directives are ignored
 - headers and library functions must be conditionally included

Conditional compilation

compilers with OpenMP support define the symbol _OPENMP that can be used in the preprocessor

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

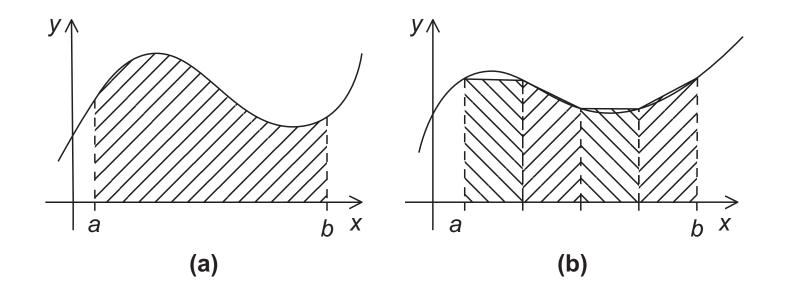
The Trapezoidal Rule



The Trapezoidal Rule



 Reminder: When discussing MPI^bwe looked at numerical integration using the trapezoidal rule



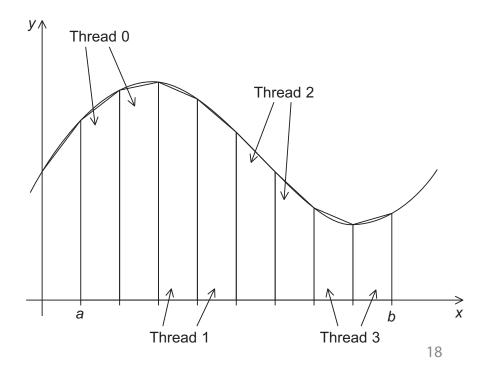
Sum of trapezoid areas $= h[f(x_0)/2 + f(x_1) + f(x_2) + \dots + f(x_{n-1}) + f(x_n)/2].$

Serial Algorithm

A First OpenMP Version

We identify two types of tasks:

- 1. computation of the areas of individual trapezoids, and
- 2. adding the areas of trapezoids
- There is no communication among the tasks computing the areas, but each of those tasks communicates with task to sum the area
 - we assume that there are many more trapezoids than cores
 - hence, we aggregate tasks by assigning a contiguous block of trapezoids to each thread (and a single thread to each core)



A First OpenMP Version (2)

 When summing up the individual areas, we need to protect access to the shared sum variable to prevent a race condition

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

global_result += my_result ;

 OpenMP provides the critical directive for protecting the block following the directive with a mutex

- only one thread may enter the critical section at a time

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

A First OpenMP Version (3)

```
#include <stdio.h>
 1
2 #include <stdlib.h>
3
   #include <omp.h>
4
5
    void Trap(double a, double b, int n, double* global_result_p);
6
    int main(int argc, char* argv[]) {
 7
8
       double global_result = 0.0;
       double a. b:
9
10
       int
              n:
       int
               thread_count;
11
12
13
       thread_count = strtol(argv[1], NULL, 10);
       printf("Enter a, b, and n \in);
14
       scanf("%lf %lf %d", &a, &b, &n);
15
                                                         creates implicit tasks (later we will
       pragma omp parallel num_threads(thread_count)
16
                                                         discuss how to create explicit tasks)
       Trap(a, b, n, &global_result);
17
18
       printf("With n = \% d trapezoids, our estimate\n", n);
19
       printf("of the integral from %f to %f = \%.14e\n",
20
          a. b. global_result);
21
       return 0:
22
23
      /* main */
   }
24
```

A First OpenMP Version (4)

```
void Trap(double a, double b, int n, double* global_result_p) {
25
       double h. x, my_result;
26
       double local_a. local_b:
27
       int i. local_n:
28
       int my_rank = omp_get_thread_num():
29
       int thread_count = omp_get_num_threads();
30
31
       h = (b-a)/n:
32
       local_n = n/thread_count:
33
       local_a = a + my_rank*local_n*h;
34
35
       local_b = local_a + local_n*h:
36
       my_result = (f(local_a) + f(local_b))/2.0:
       for (i = 1; i \leq local_n-1; i++) {
37
38
         x = local_a + i*h:
         my_result += f(x);
39
40
       }
41
       my_result = my_result*h;
                                                  we created a multi-threaded
42
                                                  version with only a couple of
   ‡⊧
43
      pragma omp critical
       *global_result_p += my_result;
44
                                                  directives and minimal code
45
       /* Trap */
                                                  changes
```

Scope of Variables in OpenMP

- OpenMP variable scoping rules define how variables can be assigned by threads in a parallel block
 - 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
 - variables declared
 - before a parallel block have a default scope of shared
 - within the block have default scope of private

• Clauses in the OpenMP parallel directive can modify the scoping for variables

- private: new, uninitialized private variable of same type is created for each thread; the variable is created on the stack, i.e. not available when the thread enters the region the next time
- shared: variable is shared among all treads in the team
- default: allows to specify a default scope for all variables, "none" requires explicit scope decls.
- firstprivate: like private, but with automatic initialization
- lastprivate: like private but copies variable value at last loop iteration or section back to scope of main thread
- copyin: for threadprivate variables (need to be declared before); works like firstprivate but the variable is allocated on the heap, i.e. the value persists between leaving and re-entering the parallel region

The Reduction Clause

- We wanted to avoid the use of global variables in the Trapezoid Rule application
 - hence we need to pass an additional shared pointer (global_result_p) to the Trap function
 - this pointer is used to update the global sum (protected by critical section)

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

A more elegant solution would look like this

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

• ... and would be called like this

global_result = Trap(a, b, n);

Image: section anymore

The Reduction Clause (2)

If we use the following workaround, we force the threads to execute sequentially

```
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 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;
}
```

OpenMP Reductions

- OpenMP reductions solve the problem in a more elegant and expressive way
 - a reduction is a computation that repeatedly applies the same reduction operator to a sequence of operands in order to get a single result
 - the reduction operator is a binary operation (such as addition or multiplication)
 - the result of the reduction is stored in the reduction variable
- To use a reduction, the parallel directive can be augmented with a reduction clause

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

supported operators: +, *, -, &, |, ^, &&, ||

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

- The #pragma omp parallel for directive forks a team of threads to execute the block
 - the block must be a for loop
 - the directive 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;
```

parallel for directive applied to a for loop

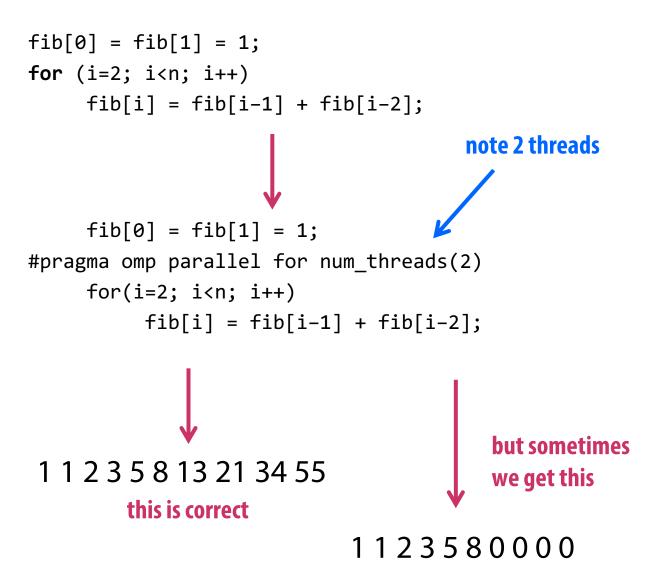
Restrictions for Parallelizable For-Statements

- The "Parallel for" directive works only for loops with simple control structure
 - loop iteration variable must be an integer
 - the expressions start, end, and incr must not change during the loop and must have a compatible type
 - the loop variable index can only be modified by the "increment expression" in the for statement

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

Program correctness must not depend upon which thread executes a particular iteration

Data dependencies



What happened?

- OpenMP compilers don't check for dependences among iterations in a loop that's being parallelized with a parallel for directive
 - dependencies in loops that cause the results of one or more loop iterations depend on other iterations are denoted as loop carried dependencies
 - in general, loops with loop carried dependencies cannot be correctly parallelized by OpenMP

Programmers need check dependencies of loops themselves

Estimating π

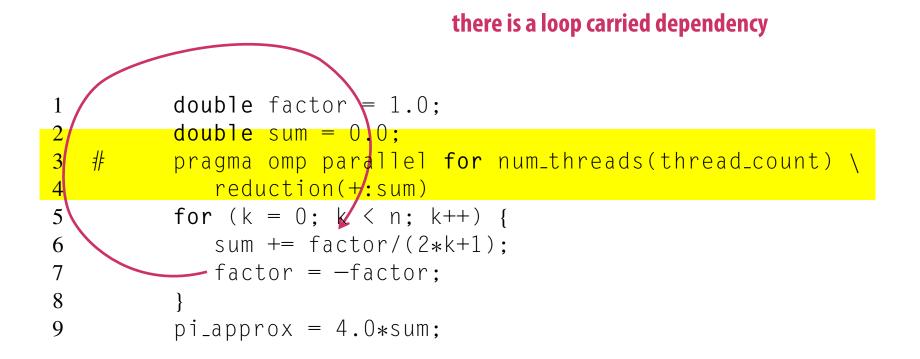
Example from previous lectures

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

Can this loop be parallelized safely?

Or is there a loop carried dependency?

Estimating π: Solution #1



Estimating π: Solution #2

- Remove loop carried dependency for factor
- Compute factor directly in each thread
- Potential for a difficult to find bug
 - by default all variables are shared among threads!
 - hence, the writes to factor in each thread are seen by the other threads in the team, which introduces data races
 - we need to explicitly declare factor as private to prevent this problem

```
double sum = 0.0;
1
   #
2
          pragma omp parallel for num_threads(thread_count) \
             reduction(+:sum) private(factor)
3
          for (k = 0; k < n; k++) {
4
             if (k % 2 == 0)
5
                factor = 1.0:
6
             else
7
                factor = -1.0:
8
                                                        ensures factor has
             sum += factor/(2*k+1);
9
10
          }
                                                        private scope.
```

The default Clause

- Introducing data races by accident is a common problem
- One common technique to prevent this problem is using the OpenMP's default clause with option none

#omp parallel for ... default (none)

- Explicitly choosing a scope of none (instead of relying on the default shared) requires the programmer to explicitly specify the scope of each variable in a block
 - this rule is enforced by the compiler

```
#omp parallel for default (none)
for(i=0; i<1024; i++) {
    a[1] = a[i] + 1;
}
error: no scope declared</pre>
```

```
#omp parallel for default (none)\
    private(i,a)
for(i=0; i<1024; i++) {
    a[i] = a[i] + 1;
}</pre>
```

Estimating π: Solution #3

ŧ

```
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

Reminder: Odd-Even Transposition Sort (discussed in MPI lecture)

```
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]);
```

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

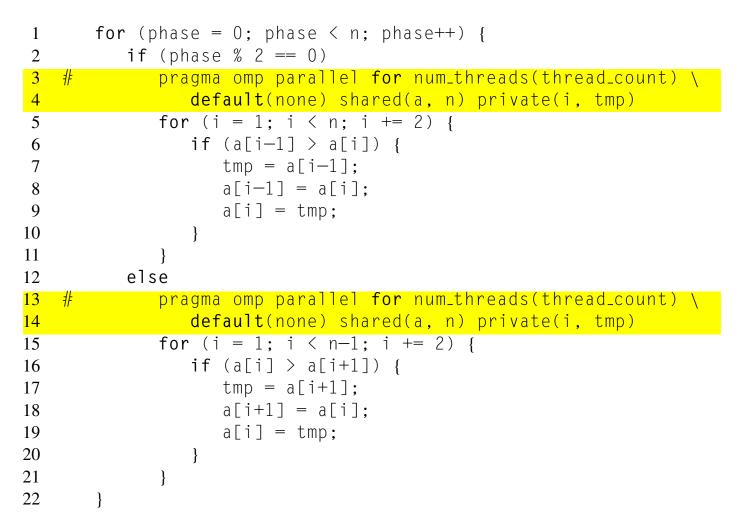
Does this algorithm have loop carried dependencies?

- outer loop has loop carried dependencies, result depends on execution order of iterations
- inner loops does not have loop carried dependencies, all comparison and swaps can be execute in parallel or in arbitrary order → parallel for directive for inner loops should work fine

Potential problems

- all operations in inner loop must complete before next iteration of outer loop is started → guaranteed by implicit barrier after parallel for
- overhead of spawning and joining threads in inner loop over and over again may be too high
 → we can keep the threads spawned, see Solution #2

OpenMP Odd-Even Sort: Solution #1



spawning and joining threads of the inner loop in each phase again

OpenMP Odd-Even Sort: Solution #2

```
spawn threads once
    #
       pragma omp parallel num_threads(thread_count) \
 1
                                                                        with "parallel" directive
           default(none) shared(a, n) private(i, tmp, phase)
 2
3
       for (phase = 0; phase < n; phase++) {</pre>
           if (phase % 2 == 0)
 4
                                                     reuse threads with "for" directive
 5
   -<u></u>]
              pragma omp for
              for (i = 1; i < n; i += 2) {</pre>
6
                                                     instead of "parallel for"
7
                  if (a[i-1] > a[i]) {
8
                     tmp = a[i-1];
9
                     a[i-1] = a[i]:
10
                     a[i] = tmp;
11
                  }
12
13
           else
14 🧍
                                                     reuse threads with "for" directive
              pragma omp for
              for (i = 1; i < n-1; i += 2) {
15
                                                     instead of "parallel for"
16
                  if (a[i] > a[i+1]) {
                     tmp = a[i+1];
17
                     a[i+1] = a[i]:
18
19
                     a[i] = tmp;
20
21
22
        }
```

Odd-Even Sort Performance Evaluation

Compare two solutions

- two "parallel for" directives (spawning and joining threads in each phase)
- two "for" directives (reusing previously spawned threads)

thread_count	1	2	3	4	
Two parallel for directives Two for directives		0.453 0.376			time in

 Reusing threads shows significant performance benefits for this case study

Scheduling Loops

 Assume we want to parallelize the following loop with a (parallel) for directive

 Further assume that the time for evaluating f(i) increases linearly with the size of argument i

```
double f(int i) {
    int j, start = i*(i+1)/2, finish = start + i;
    double return_val = 0.0;
    for (j = start; j <= finish; j++) {
        return_val += sin(j);
    }
    return return_val;
} /* f */</pre>
```

Scheduling Loops (2)

- The performance of the parallelized loop will depend strongly on the assignment
 - block assignment leads to very imbalanced load, because thread 0 gets all the short function evaluations
 - cyclic assignment leads to a much more equally distributed load

thread	iterations (block assignment)	iterations (cyclic assignment)		
0	0, 1, 2, 3, , (n/t)-1	0, n/t, 2n/t,		
1	n/t, (n/t)+1, (n/t)+2,	1, (n/t)+1, (2n/t)+1,		
t-1	(t-1)(n/t), (t-1)(n/t)+1,, n-1	t-1, (n/t)+t, (2n/t)+t,, n-1		

OpenMP Schedule Clause

The OpenMP schedule clause allows the programmer to configure how loop iterations are assigned to threads

schedule(<type> [, <chunksize>])

Type can be:

- static the iterations are assigned to the threads before the loop is executed (default)
- dynamic or guided the iterations are assigned to the threads while the loop is executing
- auto the compiler and/or the run-time system determine the schedule
- runtime the schedule is determined at run-time

The chunksize is a positive integer

- only applicable to static, dynamic and guided

The Static Schedule Type

The static scheduler

- assigns chunks of chunksize iterations to each thread in round robin order
- the assignment of chunks does not consider the actual workload load of the threads at runtime

Example: 12 iterations and 3 threads schedule(static,2) schedule(static,4) schedule(static,1) Thread 0: 0,3,6,9 Thread 0: 0,1,6,7 Thread 0: 0,1,2,3 Thread 1: 1,4,7,10 Thread 1: 2,3,8,9 Thread 1: 4,5,6,7 Thread 2: 2,5,8,11 Thread 2: 4,5,10,11 Thread 2: 8,9,10,11 block distribution block-cyclic distribution cyclic distribution

The Dynamic Schedule Type

- The iterations are also broken up into chunks of chunksize consecutive iterations
 - each thread executes a chunk
 - when a thread finishes a chunk, it requests another one from the run-time system

The chunksize can be omitted

- when it is omitted, a chunksize of 1 is used

The Guided Schedule Type

Like for the dynamic schedule each thread executes a chunk

- when a thread finishes a chunk, it requests another one
- as chunks are completed, the size of the new chunks decreases
- goal: reduce work imbalance between threads

• If no chunksize is specified, the size of the chunks decreases down to 1

- if chunksize is specified, it decreases down to chunksize, with the exception that the very last chunk can be smaller than chunksize

Thread	Chunk	Size of Chunk	Remaining Iterations
0	1–5000	5000	4999
1	5001-7500	2500	2499
1	7501–8750	1250	1249
1	8751–9375	625	624
0	9376–9687	312	312
1	9688–9843	156	156
0	9844–9921	78	78
1	9922–9960	39	39
1	9961–9980	20	19
1	9981–9990	10	9
1	9991–9995	5	4
0	9996–9997	2	2
1	9998–9998	1	1
0	9999–9999	1	0

Assignment of trapezoidal rule iterations 1–9999 using a guided schedule with two threads.

The Runtime Schedule Type

- The system uses the environment variable OMP_SCHEDULE to determine at run-time how to schedule the loop
- The OMP_SCHEDULE environment variable can take on any of the values that can be used for a static, dynamic, or guided schedule

OpenMP "single" and "master" Directives

- The single directive specifies that the enclosed region is executed only by a single thread of the team
 - useful for calling library functions that are not thread-safe (e.g. I/O)

```
#pragma omp single [clause ...] newline
    private (list) firstprivate (list) nowait
#pragma omp single
fprintf(output file, "results");
```

```
The master directive specifies a region that is to be executed only by the master thread
```

- it does not take any clauses

•••

- there is no implicit barrier after a master directive

OpenMP "barrier" Directive

• The barrier directive synchronizes all treads in the team

- when reaching a barrier, a thread will wait at the point until all other threads have reached the same barrier
- then, all threads resume executing the code following the barrier
- useful for calling library functions that are not thread-safe (e.g. I/O)

#pragma omp barrier

Matrix-vector Multiplication

Reminder: Matrix-vector multiplication example from Pthreads chapter

- code is much simpler then Pthreads version
- the problem with false-sharing for the 8 x 8,000,000 matrix still applies

	Matrix Dimension							
	8,000,000 × 8		8000 >	< 8000	8 × 8,000,000			
Threads	Time	Eff.	Time	Eff.	Time	Eff.		
1	0.322	1.000	0.264	1.000	0.333	1.000		
2	0.219	0.735	0.189	0.698	0.300	0.555		
4	0.141	0.571	0.119	0.555	0.303	0.275		

Run-times and efficiencies of matrix-vector multiplication (times are in seconds)

Concluding Remarks

OpenMP is a standard for programming shared-memory systems

- controlled with directives, runtime-library functions and environment variables
- OpenMP programs start multiple threads rather than multiple processes
- Many OpenMP directives can be modified by clauses
- A major problem in the development of shared memory programs is the possibility of race conditions
 - OpenMP provides several mechanisms for insuring mutual exclusion in critical sections
- OpenMP offers a variety of scheduling options.
 - by default most systems use a block-partitioning of the iterations in a parallelized for loop
- In OpenMP the scope of a variable is the collection of threads to which the variable is accessible.
- A reduction is a computation that repeatedly applies the same reduction operator to a sequence of operands in order to get a single result

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OpenMP tutorial published by Lawrence Livermore National Lab

- <u>https://computing.llnl.gov/tutorials/openMP/</u>

Change log

1.1.1 (2017-11-27)

- update for winter term 2017/18
- update outline slide 2
- fix terminology and typos on slide 12, 14, 18, 19, 25, 28

1.1.0 (2017-07-13)

- fix typo on slide 44

1.0.1 (2017-01-30)

- fix typo on slide 30, 48

1.0.0 (2017-01-19)

- initial version of slides