Advanced Topics in Numerical Analysis: High Performance Computing

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March 9, 2020

Slightly adapted from Georg Stadler's lectures.

Today

Last lecture

OpenMP: I

Today

► OpenMP II

Announcements and upcoming

► Homework 2 due Fri, March 14 midnight

Nested parallelism

The parallel directive may also be *nested*:

Usually, this nested mode has to be enabled *explicitly* using either the environment variable OMP_NESTED:

```
> export OMP_NESTED=TRUE # bash
> setenv OMP_NESTED TRUE # tcsh
```

or with the OpenMP function omp_set_nested():

```
omp_set_nested( true );
```

If nested parallelism is not enabled, the nested directives will be handled by only one thread, i.e. sequentially.

Since, by default, the number of threads for a parallel region equals the number of processors, the second parallel region will *not* spawn new threads.

Hence, nested parallel regions should be used together with the num_threads clause:

Here, each of the 4 worker threads will create a new team with 2 threads each, i.e. the inner construct is executed by 8 threads.

Nested parallelism may be used within the whole region of a parallel directive:

This also allows recursive computations to be handled by nested parallel regions:

```
void f () {
    #pragma omp parallel num_threads(2)
    {
       f();
    }
}
```

Here, each call of f() will spawn 2 new threads until all processors are used.

Nested loops

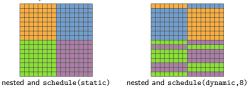
Since parallel directives may be nested, this also applies to nested loops.

In the matrix multiplication algorithm, the two outer loops apply to independent parts of the destination matrix C. Hence, these should be natural candidates for nested parallel loops:

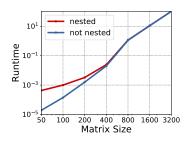
In this example, the rows and the columns will be split in half and 4 threads will handle the corresponding inner dot product computations in parallel.

DEMO: omp08.cpp

Unfortunately, the scheduling of the second loop, e.g. the columns, is applied to each row *individually*:



This may induce a significant scheduling overhead. For the matrix multiplication example, especially for small dimensions, this overhead severly limits the parallel efficiency.



Since the previous loops result in independent computations, both loops form a larger iteration space over rows and columns together.

OpenMP supports such loop collapsing via the collapse clause:

```
#pragma omp for collapse(n)
```

where n specifies the number of nested loops to collapse.

The loops must be perfectly nested and not depend on each other, e.g.

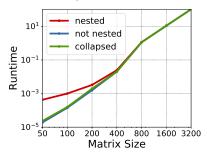
```
#pragma omp for collapse(2)
for ( size_t i = 0; i < n; ++i ) {
    for ( size_t j = 0; j < n; ++j ) {
        ...
    }
    for ( size_t j = 0; j < n; ++j ) {
        // not perfectly nested
        ...
    }
}
or</pre>
```

For the matrix multiplication, the outer loops are perfectly nested and independent, hence, they may be collapsed as an alternative to nested parallelism:

The resulting mapping depends on the specified scheduling and especially the chunk size:



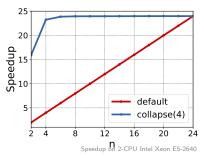
As the scheduling is now applied to all rows and columns simultaneously, the additional overhead of the nested parallelism is eliminated:



Especially for nested loops with *small* loop ranges the collapse clause useful to enlarge the iteration space and thereby, decrease the granularity and increase the number of tasks:

```
 \begin{array}{lll} & \text{for ( size t i = 0; i < n; ++i ) \{ } \\ & \text{for ( size t j = 0; j < n; ++j ) \{ } \\ & \text{for ( size t k = 0; k < n; ++k ) \{ } \\ & \text{for ( size t l = 0; l < n; ++l ) \{ } \\ & \text{compute(i, j, k, l); } \\ & \text{ } \} \end{array} \} \  \, \}
```

A single for directive for the outer most loop would permit at most n threads. With the collapse clause, n^4 threads can be used efficiently:



Reductions

Reduction operations are supported by OpenMP by the reduction clause:

```
#pragma omp for reduction(op: var1, ...)
```

For each variable of a reduction clause, a thread-private copy is created and initialised. The values of all private variables are combined at the end of the loop using the specified operator.

DEMO: omp09.cpp

Dot Product

Compute $\sum_i x_i \cdot y_i$ for $x, y \in \mathbb{R}^n$:

```
void dot ( const size_ t n, double const * x, double const * y ) {
    double sum = 0.0;

#pragma omp parallel
#pragma omp for reduction(+: sum)
for ( size_ t i = 0; i < n; ++i )
    sum += x[i] * y[i];  // "sum" is private

return sum;
}</pre>
```

Since each copy of the reduction variable is thread-private, the variable update does not form a critical section.

Supported operators are:

```
+/-/*, min/max, &/|/^, &&/||
```

The order in which the private copies are combined is *not* defined, e.g. different results may be computed in different runs of the program:

```
#pragma omp parallel for reduction(+: sum)
for ( size_t i = 1; i < n; ++i ) {
      sum += std::pow(-1.0,i+1) / double(i);
}</pre>
```

may yield

```
> reduction
6.9319718305994504e-01
> reduction
6.9319718305994582e-01
> reduction
6.9319718305994626e-01
```

Multiple Reductions

More than one reduction clause is supported for a single loop, e.g.

```
#pragma omp parallel for reduction(+: sum) reduction(*: prod) for ( size t i = 0; i < n; ++i ) { sum = sum + ...; prod = prod * ...; }
```

Restrictions

Some restrictions apply to the reduction clause:

- A reduction variable must be shared in the surrounding parallel region.
- ► A reduction variable must not appear in multiple reduction clauses.
- ► A reduction variable must not be declared const.
- Compound types are not supported.

The reduction clause is also available for the parallel directive without a loop, hence the following implementation is equivalent to the previous parallel dot product:

```
void dot ( const size_t n, double const * x, double const * y ) {
    double sum = 0.0; -

#pragma omp parallel reduction(+: sum)
    #pragma omp for
    for ( size t i = 0; i < n; ++i )
        sum += x[i] * y[i];
    return sum;
}</pre>
```

The difference is, that instead of combining the values at the end of the loop, the reduction is performed at the end of the parallel region.

Loop synchronization

By default, threads will synchronise with the end of the loop, e.g. all threads will wait for all others to finish their computations.

Using the nowait clause, this implicit barrier can be eliminated:

```
#pragma omp for nowait
```

A typical application of this clause is several loops with an uneven load per task:

```
#pragma omp parallel
{
    #pragma omp for nowait
    for ( size_t i = 0; i < n; ++i ) {
        ...
}

    #pragma omp for nowait
    for ( size_t j = 0; j < m; ++j ) {
        ...
}

    #pragma omp for nowait
    for ( size_t l = 0; l < k; ++l ) {
        ...
}
</pre>
```

Here, the team threads may proceed to the next loop without waiting for other threads.

Reduction without Barrier

If nowait is used for a loop with a reduction clause, a race condition will occur if the reduction variable is accessed outside the loop:

```
#pragma omp parallel
{
  double sum = 0;
    #pragma omp for nowait reduction(+: sum)
    for ( size_t i = 0; i < n; ++i ) {
        ...
    }
    f( sum );    // race condition
}</pre>
```

Since not all updates to sum may have been applied, the corresponding value is undefined

Loop serialization

Using the ordered clause together with a corresponding block, some part of the loop body may be executed sequentially in the order defined by the loop index:

Since the code within the ordered region is executed in loop order, threads will wait at the entry to the ordered region until the ordered region of all previous iterations have been completed.

Code before the ordered region is not affected by this and may be executed as soon as the corresponding task is mapped to a thread.

Due to this *serialisation*, ordered blocks should contain only fast computations and be used only at the end of a loop.

DEMO: omp10.cpp

Using the ordered clause, *deterministic* behaviour can be enforced:

```
#pragma omp for ordered reduction(+: global_val)
for ( size_t i = 0; i < n; ++i )
{
    const double local_val = compute_value();
    #pragma omp ordered
    global_val += local_val; // sum up in sequential order
}
}</pre>
```

It is also usefull for printing intermediate values, e.g. for debugging:

```
#pragma omp for ordered
for ( size_t i = 0; i < n; ++i )
{
    value = compute_value();
    #pragma omp ordered
    std::cout << value << std::endl;
}</pre>
```

Otherwise, access to the I/O channel induces a race condition which will lead to scrambled output.

Restriction

During the iteration of a loop, each thread must executed at most *one* ordered block, i.e. the following code is not allowed:

```
#pragma omp for ordered
for ( ... )
{
    #pragma omp ordered
    { ... }
    #pragma omp ordered // error
    { ... }
}
```

However,

```
#pragma omp for ordered
for ( ... )
{
   if ( condition ) {
        #pragma omp ordered
        { ... }
   } else {
        #pragma omp ordered
        { ... }
}
```

is legal code, since only one ordered block is executed.

Any problem swith the following code?

```
#pragma omp for schedule(static) ordered
for ( size_t i = 0; i < 16; ++i )
{
    double    x = f();
    #pragma omp ordered
    std::cout << x << std::endl;
}</pre>
```

Loop Scheduling and ordered

Using the default static scheduling together with ordered blocks will often *prevent* parallel execution, since neighboured indices are executed by the same thread *in order*.

For example, the following loop is executed almost sequentially while using 4 threads:

With dynamic scheduling (or "static,1") all threads run in parallel:

N-body problem

N-body problem: DEMO: omp11.cpp

Adapted from slides by Roland Kriemann

N-body problem

N-body problem: DEMO: omp11.cpp

Jacobi iterations: DEMO: omp14.cpp

If the computation consists of independent but *non-iterative* parts, the sections directive can be used to distributed the work to several threads:

Each section block inside the construct of the sections directive will be executed *once* by *one* team thread.

By default, all team threads will synchronise at the end of the sections block.

The sections directive must be placed inside a parallel region, otherwise it is executed sequentially.

The sections directive must be placed inside a parallel region, otherwise it is executed sequentially.

The construct of a sections directive may contain *only* section blocks, e.g. the following will lead to an error:

```
#pragma omp sections
{
#pragma omp section
{ ... }
#pragma omp section
{ ... }

f(); // error
}
```

The sections directive must be placed inside a parallel region, otherwise it is executed sequentially.

The construct of a sections directive may contain *only* section blocks, e.g. the following will lead to an error:

```
#pragma omp sections
{
#pragma omp section
{
...}
#pragma omp section
{
...}
f();
// error
}
```

The optional clauses of the sections directive include:

private: create unintialised thread-private variables,

firstprivate: create copy-initialised thread-private variables,

lastprivate: enclosing context's version of the variable is set equal to the private version of whichever thread executes the final iteration (for-loop construct) or last section

reduction: combine thread-private copies at end of sections construct,

nowait: remove implicit barrier at end of sections construct.

For all clauses, the standard restrictions apply.

Single execution

With the single directive

```
#pragma omp single
```

the corresponding block is executed by only *one* thread of the current team.

All other threads will wait at the end of the single block until the executing thread finishes.

In the example:

f() will be executed in parallel, followed by a single thread printing the message. Only then will g() be executed again in parallel.

Copyprivate clause

A special clause is available for the single directive:

```
#pragma omp single copyprivate(var1,var2,...)
```

The value of any variable in the list of the copyprivate clause will be copied to all other threads at the end of the single clause:

All variables in the copyprivate clause have to be *private* in the surrounding parallel region.

Remark

The copy operation is performed using standard copy assignment for elemental types, entry-wise copy for arrays or using the copy operator for classes.

A similar effect has a shared variable. But this may lead to a race condition before the single block since the barrier is only at it's end:

The copyprivate clause provides a safe alternative since the update of all copies takes place at the barrier:

Since the single directive has an implicit barrier, *all* team threads must encounter the directive during their execution or none at all:

```
#pragma omp parallel
{
  if ( do_loop() ) { // conditional execution
      #pragma omp single
      for ( ... ) {
      }
    }
}
```

Removing the barrier by the nowait clause will usually work, but the resulting program is non-conforming.

Master directive

A single block may be executed by any thread of the team. Using the master directive:

```
#pragma omp master
```

the corresponding construct will be executed only by the master thread of the team, i.e. the thread with thread id 0.

In contrast to the single directive, no implicit barrier exists at the end of the master block. Also no clauses are available for the master directive.

Thread synchronization

Beside thread creation and scheduling, thread synchronisation is equally important due to the shared address space and the potential for race conditions.

OpenMP provides a wide variety of synchronisation methods, namely

- Mutexes, directive and type/function based,
- Barriers,
- ► Atomic Operations and
- Memory Flushes

Another form of synchronisation for loops is the ordered clause, which enables loop serialisation (see above).

Critical

A critical section in a program can be guarded using the critical directive:

```
#pragma omp critical [(name)]
```

In contrast to other OpenMP directives, the critical directive applies to *all* running threads and not just to the threads in the current team:

Even though f is called from different thread teams, the critical section may only be entered by a single thread at a time.

Without a name, *all* critical sections are considered to have the *same* name, i.e. all anonymous critical sections form a single critical section:

Without a name, *all* critical sections are considered to have the *same* name, i.e. all anonymous critical sections form a single critical section:

With the optional name, this program global mutual exclusion can be limited to critical sections with an equal name:

DEMO: omp12.cpp

DEMO: omp12.cpp

Remark

Recursive function calls within critical sections may lead to deadlocks:

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Dot Product The previous dot product compution can also be implemented using critical:

```
double dot ( const std::vector< double > & x, const std::vector< double > & y ) {
    double sum = 0.0;
    #pragma omp parallel
    {
        double s = 0.0;
        #pragma omp for
        for ( size t i = 0; i < x.size(); ++i )
            s += x[i] * y[i];
        #pragma omp critical
        sum += s;
    }
    return sum;
}</pre>
```

Mutexes

As an alternative, OpenMP provides mutex types and corresponding functions. The data type for an OpenMP mutex is:

```
omp_lock_t
```

Functions for locking and unlocking mutexes are:

```
void omp_set_lock ( omp_lock_t * mutex );  // lock mutex
void omp_unset_lock ( omp_lock_t * mutex );  // unlock mutex
```

Both are imported via the OpenMP header file omp.h.

Before using an OpenMP mutex, it has to be initialised with:

```
void omp_init_lock ( omp_lock_t * mutex );
```

After initialisation, the mutex is unlocked.

Remark

No other OpenMP lock function must be called with an uninitialised mutex!

Finally, if the mutex is no longer used, it should be destroyed using

```
\label{eq:cond_cond} \begin{tabular}{ll} void & omp\_lock\_t * mutex \end{tabular} ); \\ \end{tabular}
```

Before calling omp_destroy_lock, the mutex has to be *unlocked*.

Furthermore, a test function is provided, which either locks an unlocked mutex or immediately returns:

```
int omp_test_lock ( omp_lock_t * mutex );
```

If the mutex could successfully be locked, the function returns a non-zero value, i.e. true. Otherwise, 0 is returned, i.e. false.

Dot Product

The previous dot product computation implemented using omp_lock_t:

```
double dot (const std::vector< double > & x, const std::vector< double > & y) {
 double
             sum = 0.0:
 omp lock t mutex;
 omp init lock( & mutex );
 #pragma omp parallel
   double s = 0.0;
   #pragma omp for
   for ( size t i = 0; i < x.size(); ++i )
     s + x[i] * y[i];
   omp set lock( & mutex );
   sum == s:
   omp unset lock( & mutex );
 omp destroy lock( & mutex );
  return sum;
```

Mutex overhead

Locking, unlocking or testing OpenMP mutexes involve read/write operations with respect to the the main memory, which induces some overhead.

Furthermore, the different mutex types will perform different operations, and hence, may have different overhead.

The following table contains timings for some typical mutex operations on an Intel Xeon E5-2640:

| Operation (20000000x) | Intel Compiler | GNU Compiler |
|-------------------------------------|----------------|--------------|
| omp_lock_t | | |
| locking/unlocking | 0.687s | 0.313s |
| testing locked mutex | 0.446s | 0.202s |
| omp_nest_lock_t | | |
| locking/unlocking | 0.747s | 0.466s |
| n 	imeslocking $/n 	imes$ unlocking | 0.433s | 0.174s |
| testing locked mutex | 0.402s | 0.063s |

Barrier

Most OpenMP directives will have an implicit barrier at the end of their construct, which enforces a synchronisation between all threads of the current team.

With the barrier directive, an explicit barrier can be defined in the program:

```
#pragma omp barrier
```

The barrier directive has no associated construct.

All threads of the current team have to finish execution of all tasks *before* the barrier directive, e.g. all threads will wait until all other threads have reached the barrier:

Atomic

Atomic operations are supported in OpenMP in the form of the atomic directive:

```
#pragma omp atomic [read — write — update — capture]
```

The atomic directive applies to the immediately following statement. Depending on the atomic operation, this statement is restricted to one of the following forms:

```
read: y = x;

write: x = expression;

update: x + +; x -; + +x; -x;
x \cdot op = expression;

capture: y = x + +; y = x -;
y = x \cdot op = expression;
```

Here, x and y are both scalar types, e.g. char, int or double, and expression is a scalar expression. Furthermore, op is a standard arithmetic or bit operator, e.g. +, -, *, /, ^, &, |, << or >>.

Remark

The arithmetic and bit operators must not be overloaded.

Examples for atomic operations are:

```
double pi = 355.0/113.0, x, y;

#pragma omp atomic read // atomically read "pi"
x = pi;

#pragma omp atomic write // atomically write "y"
y = 2.0 * pi;

#pragma omp atomic update // atomically update "y"
y = y+1;

#pragma omp atomic capture // atomically update "x" and write y
y = x++;
```

Atomic operations are performed with respect to memory addresses. All atomic operations affecting the *same* memory address will enforce a mutually exclusive access for *all* threads in the program.

```
double x = 0:
int main () {
 #pragma omp parallel sections
   #pragma omp section
     #pragma omp parallel // team 1
      f();
    #pragma omp section
     #pragma omp parallel // team 2
      g(2.0);
                                          void g (double v) {
void f () {
 #pragma omp atomic update
                                           #pragma omp atomic write
 x += 1;
                                            x = y;
```

Since x is referenced in both atomic operations, both teams will be affected and the write and update operation will be performed only in *one* thread of the *whole* program at a time.

Atomic vs critical

Which ones would you prefer? Why? \rightarrow DEMO omp15.cpp

```
#pragma omp parallel for
for ( size_t i = 0; i < n; ++i )
{
    #pragma omp critical
    x[index[i]] = f( i );
}</pre>
```

When working with arrays, each array element has a different memory address and hence, will induce a different atomic operation:

```
#pragma omp parallel for
for ( size_t i = 0; i < n; ++i )
{
    #pragma omp atomic write
    x[index[i]] = f( i );
}</pre>
```

Here, write operations to different index positions form different atomic operations and may therefore be executed in parallel.

In such cases, atomic is a better alternative to critical:

```
#pragma omp parallel for
for ( size_t i = 0; i < n; ++i )
{
    #pragma omp critical
    x[index[i]] = f( i );
}</pre>
```

which would enforce sequential execution.

Dot Product

Implementing the dot product using atomic:

```
double dot ( const std::vector< double > & x, const std::vector< double > & y ) {
    double sum = 0.0;
    #pragma omp parallel
    {
        double s = 0.0;
        #pragma omp for
        for ( size t i = 0; i < x.size(); ++i )
            s += x[i] * y[i];
        #pragma atomic update
        sum += s;
    }
    return sum;
}</pre>
```

Limits of atomic

During an atomic update of a variable x, only reading and writing the corresponding memory position will be atomic, *not* the evaluation of the expression.

Due to this, the expression must *not* contain references to x, e.g.

```
#pragma omp atomic update x \leftarrow y + x + 3; // race condition
```

- 1. Evaluate expression y*x+3 (potential interrupts during evaluation of expression)
- 2. Atomic: Read-x, add value of expression, write-x

Similarly, for an atomic capture, e.g.

```
#pragma omp atomic capture y = x++;
```

only reading and writing corresponding to x is performed atomic. Not the evaluation of an expression or writing y.