DTU Compute
Department of Applied Mathematics and Computer Science

High-Performance Computing

Parallel Programming in OpenMP – part II

Programming OpenMP

Outline

- Data scoping – cont'd
- Orphaning
- Tasking
- OpenMP correctness & Data Races
- Runtime library
- Scheduling
- A real world example

OpenMP Syntax

More on data scoping

Programming OpenMP

OpenMP Syntax

Reminder: the “private” clause –

- declares variables private to each thread:

```
#pragma omp directive private (list)
```

- i.e. a **new** variable is declared once for each thread
- all references are replaced with references to the newly declared variable
- variables declared private are uninitialized for each thread!

OpenMP Syntax

Consequences of private(...):

```
main() {
    ...
    A = 10;

    #pragma omp parallel
    {
    #pragma omp for private(i, A, B) ...
    for(i = 0; i < n; i++) {
      ...
      B = A + i;   // A undefined!
                   // unless declared firstprivate
      ...
    } /* end of omp for */
      ...
    } /* end of omp parallel */

    C = B;         // B undefined!
                   // unless declared lastprivate
}
```


OpenMP Syntax

Solutions:

`#pragma omp ... firstprivate(list)`

- All variables in list are initialized with the value the original object had before entering the parallel construct.

`#pragma omp ... lastprivate(list)`

- The thread that executes the <u>sequentially</u> <u>last</u> iteration updates all variables in list.

OpenMP Syntax

Programming OpenMP

The “threadprivate” and “copyin” clauses:

- threadprivate(list): creates a private copy of global data (e.g. common blocks or global variables in modules in Fortran) for each thread
- copyin(list): copies the values from the master thread into the private copies – like a ‘firstprivate’ for global variables
- subsequent modificications of list affect only the private copies – within one parallel region

OpenMP Syntax

Programming OpenMP

Example 1:

```
int counter = 0;
#pragma omp threadprivate(counter)

int increment_counter()
{
    counter++;
    return(counter);
}
```

```
INTEGER FUNCTION INCREMENT_COUNTER()
   COMMON/A22_COMMON/COUNTER
!$OMP THREADPRIVATE(/A22_COMMON/)
   COUNTER = COUNTER +1
   INCREMENT_COUNTER = COUNTER
   RETURN
END FUNCTION INCREMENT_COUNTER
```

OpenMP Syntax

Programming OpenMP

Example 2:

```
int
increment_counter()
{
     static int counter = 0;
     #pragma omp threadprivate(counter)

     counter++;
     return(counter);
}
```


OpenMP Syntax

Programming OpenMP

The copyprivate(...) clause

- copying a value out of a single region into the private data of other threads

```
#pragma omp single copyprivate(list)
{
     ...
}
```

```
!$OMP SINGLE ....

     ...
!$OMP END SINGLE COPYPRIVATE(LIST)
```

Programming OpenMP

OpenMP Syntax

Example:

```
int x, y;  /* global data */
#pragma omp threadprivate(x, y)

void use_values(int id, int a, int b) {
    printf("  TID %d: a = %d, b = %d, c = %d, d = %d\n",
             id, a, b, x, y);
}

void init(int id, int *a, int *b) {
    int r_a, r_b;

#pragma omp single copyprivate(r_a, r_b, x, y)
{   scanf("%d %d %d %d", &r_a, &r_b, &x, &y); }

    *a = r_a; *b = r_b;
    use_values(id, *a, *b);
}
   ...
```


Programming OpenMP

OpenMP Syntax

Example (cont'd):

```
int main(int argc, char *argv[] ) {

    int tid = 0;
    int a, b;

#pragma omp parallel private(tid,a,b)
{
#ifdef _OPENMP
    tid = omp_get_thread_num();
#endif

    init(tid,&a,&b);
    printf("In main - TID %d: a = %d, b = %d,",
           " x = %d, y = %d\n",
            tid, a, b, x, y);
} /* end of omp parallel */

    return(0);
}
```

OpenMP Syntax

Example output:

```
$ OMP_NUM_THREADS=3 ./copypriv
1 2 3 4
          TID 2: a = 1, b = 2, c = 3, d = 4
          TID 1: a = 1, b = 2, c = 3, d = 4
          TID 0: a = 1, b = 2, c = 3, d = 4

In main - TID 0: a = 1, b = 2, x = 3, y = 4
In main - TID 1: a = 1, b = 2, x = 3, y = 4
In main - TID 2: a
```

without copyprivate on r_a and r_b

```
env OMP_NUM_THREADS=3 ./copypriv
1 2 3 4
          TID 1: a = 0, b = 1, c = 3, d = 4
          TID 0: a = 0, b = 0, c = 3, d = 4
          TID 2: a = 1, b = 2, c = 3, d = 4

In main - TID 2: a = 1, b = 2, x = 3, y = 4
In main - TID 0: a = 0, b = 0, x = 3, y = 4
In main - TID 1: a = 0, b = 1, x = 3, y = 4
```


OpenMP Orphaning

Orphaning in OpenMP

OpenMP Orphaning

The OpenMP standard does not restrict worksharing and synchronization directives to be within the lexical extent of a parallel region. Those directives can be orphaned, i.e. they can appear outside a parallel region:

```
#pragma omp parallel
{
         :
     dowork();
         :

}
```

orphaned worksharing directive

```
void dowork(void)  {
         :
     #pragma omp for
     for(i=0; i<N; i++)  {

     }
         :
}
```


OpenMP Orphaning

- When an orphaned directive is detected <u>within the dynamic extent of a parallel region</u>, its behaviour is similar to the non-orphaned case.
- When an orphaned directive is detected in the sequential part of the program, it will be ignored.

```
   dowork(); // serial for

#pragma omp parallel
{
         :
   dowork(); // parallel for
         :

}
```

```
void dowork(void) {
         :
     #pragma omp for
     for(i=0; i<N; i++)  {

     }
         :
}
```

Programming OpenMP

OpenMP syntax

Tasking (since OpenMP 3.0)

- allows parallelization of work that is generated dynamically
- provides a flexible model for irregular parallelism
- uses a “task pool” concept
- new opportunities:
  - while loops
  - recursive structures

Programming OpenMP

OpenMP syntax

- Syntax C/C++:

```
#pragma omp task [clause]
{
    ...
}
```

- clause can be
  - if (int_expr)
  - default(shared|none)
  - private(list), shared(list)
  - firstprivate(list)
  - untied

Programming OpenMP

OpenMP syntax

- Syntax Fortran:

```
!$OMP task [clause]

   ...
!$OMP end task
```

- where clause can be
  - if (int_expr)
  - default(shared|private|firstprivate|none)
  - private(list), shared(list)
  - firstprivate(list)
  - untied

Programming OpenMP

OpenMP syntax

Tasking example I:

while loop:

```
p = lhead;
while (p != NULL)
{
   do_work(p);
   p = next(p);
}
```

parallel while loop with OpenMP tasks:

```
#pragma omp parallel
{
   #pragma omp single
   {
      p = lhead;
      while (p != NULL){
         #pragma omp task
         {
          do_work(p);
         }
         p = next(p);
      }
   } // end of single
}    // end of parallel
```

OpenMP syntax

What's going on?

```
#pragma omp parallel
{
   #pragma omp single
   {
      p = lhead;
      while (p != NULL){
         #pragma omp task
         {
          do_work(p);
         }
         p = next(p);
      }
   } // end of single

}   // end of parallel
```

start of parallel region

one thread only, please

task generation – tasks are added to the task list

all work is done here!

implicit barrier – all unfinished tasks have to be finished

OpenMP syntax

- Tasks and recursion: calculating Fibonacci numbers
- Recursive scheme to calculate the n^{th} Fibonacci number:
  - fib(n) = fib(n-1) + fib(n-2)
  - stopping critererion: return 1 if n < 2
- Caveat: this method is not very effective, but used here to demonstrate the concept of tasking!

Programming OpenMP

OpenMP syntax

The sequential code:

```
int
main(int argc, char* argv[]) {
   [...]
   fib(input);
   [...]
}
```

```
int
fib(int n) {

   int x, y;

   if (n < 2) return n;

   x = fib(n - 1);
   y = fib(n - 2);

   return(x + y);
}
```


Programming OpenMP

OpenMP syntax

OpenMP version of fib() with tasks:

```
int
fib(int n) {

   int x, y;

   if (n < 2) return n;

   #pragma omp task shared(x)
   x = fib(n - 1);
   #pragma omp task shared(y)
   y = fib(n - 2);

   #pragma omp taskwait
   return(x + y);
}
```

note the special scoping rules!

generate two tasks, calling fib() recursively

task synchronization - to get the right results

Programming OpenMP

OpenMP syntax

Scoping rules with tasks:

- Static and global variables are shared
- Local (aka automatic) variables are private
- Orphaned task variables are firstprivate
- Non-orphaned task variables inherit the shared attribute
- (Local) Task variables are firstprivate, unless declared shared
- Thus, we have to declare x and y as shared

Programming OpenMP

OpenMP syntax

Task synchronization:

- #pragma omp taskwait
- suspends the encountering task, until all child tasks are completed
- direct children only, not descendants
- needed here, to make sure that x and y are still exist when we take the sum.

OpenMP syntax

Programming OpenMP

OpenMP version of main() with tasks:

```
int
main(int argc, char* argv[]) {
    [...]

    #pragma omp parallel
    {
    #pragma omp single
    {
    fib(input);
    }
    } // end of omp parallel

    [...]
}
```

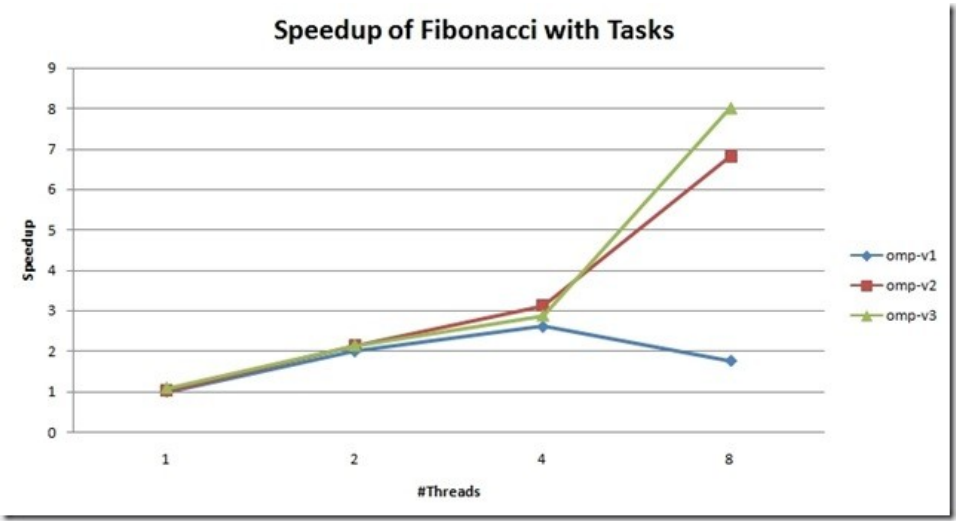
start of parallel region - team of worker threads

task generation by one thread, only!

OpenMP syntax

Programming OpenMP

Results of the Fibonacci program



courtesy: Chr. Terboven, RWTH Aachen

OpenMP syntax

Notes on the Fibonacci speedup results:

- The simple OpenMP version (omp-v1) doesn't scale – as expected – due to the large amount of tasks generated
- Improvement 1 (omp-v2):
  - add an if-clause to the tasks:
    #pragma omp task if(n>=30) shared(...)
  - improves the speed-up, but still not perfect
- Improvement 2 (omp-v3): (see next slide)

OpenMP syntax

version omp-v3 of fib() with tasks:

```
int
fib(int n) {

   int x, y;

   if (n < 2) return n;
   if (n < 30) {
      return(fib(n-1) + fib(n-2));
   }

   #pragma omp task shared(x)
   x = fib(n - 1);
   #pragma omp task shared(y)
   y = fib(n - 2);

   #pragma omp taskwait
   return(x + y);
}
```

OpenMP syntax

Some notes on tasking:

- tasks allow to exploit parallelism with OpenMP, that hasn't been possible before
- the tasking concept has the main focus for future versions of OpenMP, and has been extended in versions 4.x and 5
- this goes beyond our scope in this course

OpenMP: Error detection

Tools to check your OpenMP code

OpenMP compile-time checks

Programming OpenMP

OpenMP checks supported by Oracle Studio compilers:

- -xloopinfo – info on loops
- -xvpara – compile time warnings on ...
  - ... scoping problems
  - ... possible data races

OpenMP run-time checks

Programming OpenMP

OpenMP run-time checks supported by Oracle Studio:

- SUNW_MP_WARN = [true|false]
  - gives you warnings at runtime
  - e.g. dynamic change of threads
  - inconsistencies of barriers
  - ...
- Note: there is a certain performance penalty

Programming OpenMP

OpenMP run-time checks

Example: illegal usage of a barrier

```
 1 #include <omp.h>
 2 #include <stdio.h>
 3
 4 int main(void)
 5 {
 6   #pragma omp parallel num_threads(4)
 7   {
 8       int i = omp_get_thread_num();
 9
10       if (i % 2) {
11           printf("At barrier 1.\n");
12           #pragma omp barrier
13       }
14   }
15   return 0;
16 }
```


Programming OpenMP

OpenMP run-time checks

Example (cont'd): illegal usage of a barrier

```
$ suncc -g -xO3 -xopenmp -xvpara -o bad1 bad1.c
$ ./bad1
At barrier 1.
At barrier 1.
^C
$ SUNW_MP_WARN=true ./bad1
WARNING (libmtsk): Environment variable SUNW_MP_WARN is set
    to TRUE. Runtime error checking will be enabled.
At barrier 1.
At barrier 1.
WARNING (libmtsk): Threads at barrier from different directives.
    Thread at barrier from bad1.c:6.
    Thread at barrier from bad1.c:12.
    Possible Reasons:
    Worksharing constructs not encountered by all threads in
    the team in the same order.
    Incorrect placement of barrier directives.
WARNING (libmtsk): Runtime shutting down while some parallel
    region is still active.
$
```

no compiler warning!!

OpenMP: Data Race Detection

Programming OpenMP

Oracle Studio has a data race detection tool:

- Thread Analyzer (`tha`)
- Quick usage guide:
  - compile and link with `-xinstrument=datarace`
  - run it: `collect -r on a.out`
  - view results (GUI): `tha tha.1.er`
  - or CLI: `er_print -races tha.1.er`

OpenMP: Data Race Detection

Programming OpenMP

Example:

```
int main(int argc, char *argv[]) {

    int i, total = 0, N = 2000000;
    int primes[N];
    #pragma omp parallel for

    for( i = 2; i < N; i++ ) {
        if ( is_prime(i) ) {
            primes[total] = i;
            total++;
        }
    }

    printf("# of prime numbers between 2 and %d: %d\n",
           N, total);
    return(0);
}
```

OpenMP: Data Race Detection

Example (cont'd): compile and run

```
$ suncc -g -fast -o prime prime.c
$ ptime ./prime
# of prime numbers between 2 and 2000000: 148933

real        10.862
user        10.483
sys          0.056


$ suncc -g -fast -xopenmp -xloopinfo -o prime prime.c
$ "prime.c", line 7: PARALLELIZED, user pragma used
$ OMP_NUM_THREADS=4 ptime ./prime
# of prime numbers between 2 and 2000000: 148310

real         3.662    <--- speed-up: 2.9x
user        10.494
sys          0.055
```


OpenMP: Data Race Detection

Example (cont'd): run, run, ... and use collect

```
$ OMP_NUM_THREADS=4 ./prime
# of prime numbers between 2 and 2000000: 148310

$ OMP_NUM_THREADS=4 ./prime
# of prime numbers between 2 and 2000000: 148328


$ suncc -g -fast -xopenmp -xinstrument=datarace \
  -o prime prime.c


$ OMP_NUM_THREADS=4 collect -r on ./prime
Creating experiment database tha.1.er ...
# of prime numbers between 2 and 2000000: 125581

$
```

OpenMP: Data Race Detection

Example (cont'd): analyze the collect data

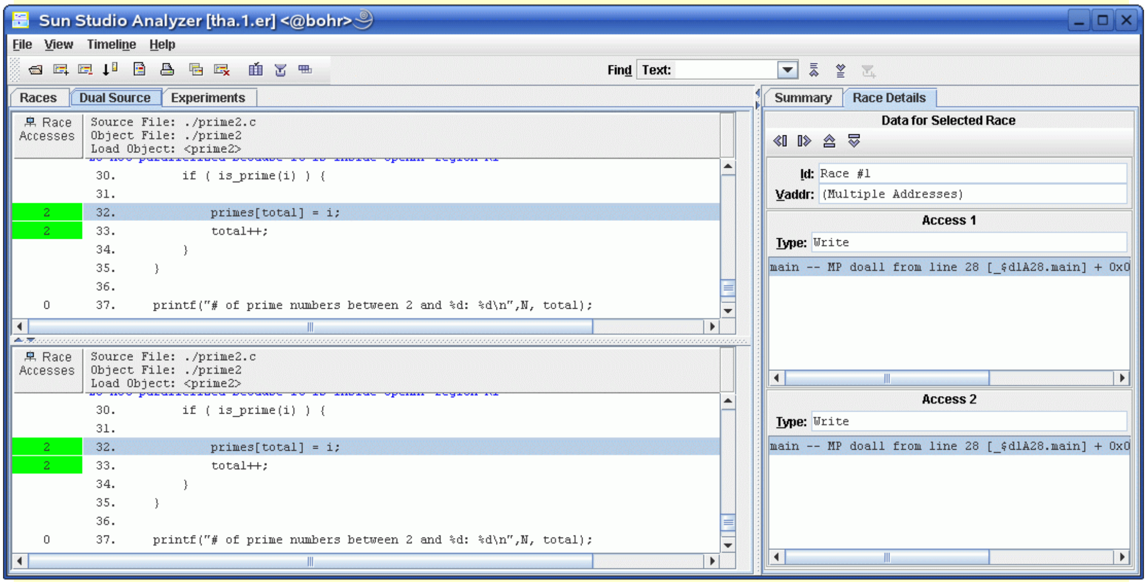
```
$ er_print -races tha.1.er
Total Races:  2 Experiment:  tha.1.er

Race #1, Vaddr: (Multiple Addresses)
      Access 1: Write, main -- MP doall from line 6 ...
                       line 10 in "prime.c"
      Access 2: Write, main -- MP doall from line 6 ...
                       line 10 in "prime.c"
  Total Traces: 1

Race #2, Vaddr: 0xffbfecb4
      Access 1: Write, main -- MP doall from line 6 ...
                       line 11 in "prime.c"
      Access 2: Write, main -- MP doall from line 6 ...
                       line 11 in "prime.c"
  Total Traces: 1
```


Programming OpenMP

OpenMP: Data Race Detection

Example (cont'd): analyze the collect data

```
$ tha tha.1.er
```



OpenMP: Data Race Detection

Example (cont'd): fix the bug

```
int main(int argc, char *argv[]) {

    int i, total = 0, N = 2000000;
    int primes[N];
    #pragma omp parallel for

    for( i = 2; i < N; i++ ) {
        if ( is_prime(i) ) {
            #pragma omp critical
            { primes[total] = i;
              total++;
            }
        }
    }
    printf("# of prime numbers between 2 and %d: %d\n",
           N, total);
    return(0);
}
```


OpenMP: Data Race Detection

Programming OpenMP

Example (cont'd): check – and recompile

```
$ suncc -g -fast -xopenmp -xinstrument=datarace \
  -o prime prime.c

$ OMP_NUM_THREADS=4 collect -r on ./prime
Creating experiment database tha.2.er ...
# of prime numbers between 2 and 2000000: 148933

$ er_print -races tha.2.er
Total Races:  0 Experiment:  tha.2.er

$ cc -g -fast -xopenmp -o prime prime.c
$ OMP_NUM_THREADS=4 ptime ./prime
# of prime numbers between 2 and 2000000: 148933

real        3.561
user       10.393
sys         0.051
```

OpenMP: Data Race Detection

- Some notes:
  - Oracle Studio does only support OpenMP up to version 4.0
  - most of the features we use here are supported, but not all
  - thus, using this tool will not work for everything

OpenMP Scheduling

Controlling the scheduling
of OpenMP threads

Programming OpenMP

OpenMP Scheduling

Load balancing:

- Important aspect of performance
- Especially for less regular workloads, e.g.
  - transposing a matrix
  - multiplications of triangular matrices
  - parallel searches in a linked list
- The schedule clause provides different iteration scheduling algorithms for loops

Programming OpenMP

OpenMP Scheduling

The “schedule” clause:

```
#pragma omp for schedule(static[,chunk])
#pragma omp for schedule(dynamic[,chunk])
#pragma omp for schedule(guided[,chunk])
#pragma omp for schedule(auto) – new in 3.0
#pragma omp for schedule(runtime)
```

- If there is no schedule clause, the default is static.

OpenMP Scheduling

Programming OpenMP

```
#pragma omp for schedule(static[,chunk])
```

Static schedule:

- Iterations are divided into pieces of size chunk and then **statically** assigned to the threads.
- If chunk is not defined, the work (N) is equally divided among the number of threads (P), i.e. chunk = N/P.

OpenMP Scheduling

Programming OpenMP

```
#pragma omp for schedule(dynamic[,chunk])
```

Dynamic schedule:

- Iterations are divided into pieces of size chunk and then **dynamically** assigned to the threads – i.e. when a thread has finished one chunk, it is assigned a new one.
- The default chunk size is 1.

Programming OpenMP

OpenMP Scheduling

```
#pragma omp for schedule(guided[,chunk])
```

Guided schedule:

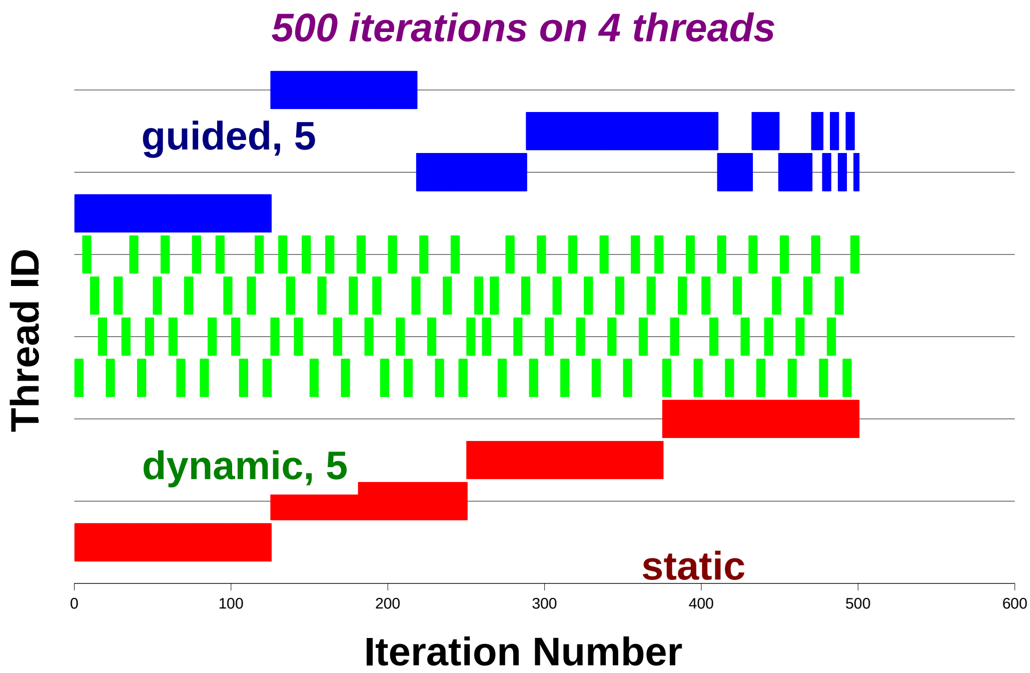
- The chunk size is exponentially reduced with each chunk that gets **dynamically** assigned to the threads; chunk defines the minimum number of iterations to assign each time.

```
chunk = unass_iter/(weight * n_thr)
```

- The default minimum chunk size is 1.

Programming OpenMP

OpenMP Scheduling



OpenMP Scheduling

```
#pragma omp for schedule(runtime)
```

Runtime schedule:

- The schedule is detected at runtime from the setting of the OMP_SCHEDULE environment variable.
- Syntax: OMP_SCHEDULE=type,chunk

OpenMP Scheduling

```
#pragma omp for schedule(auto)
```

Automatic schedule (new in OpenMP 3.0):

- When schedule(auto) is specified, the decision regarding scheduling is delegated to the compiler and/or runtime system. The programmer gives the implementation the freedom to choose any possible mapping of iterations to threads in the team.

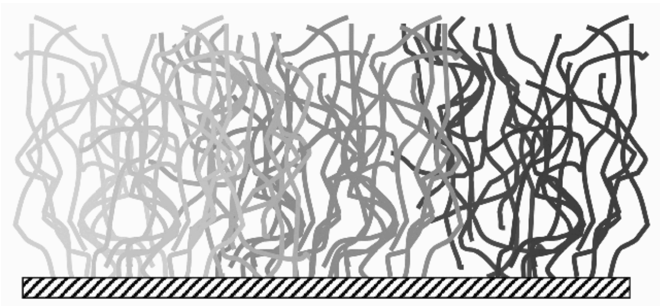
Programming OpenMP

A real world example:
Molecular Dynamics simulation

Programming OpenMP

Example: MD simulation

- Molecular Dynamics simulation of long carbon molecules on a surface:

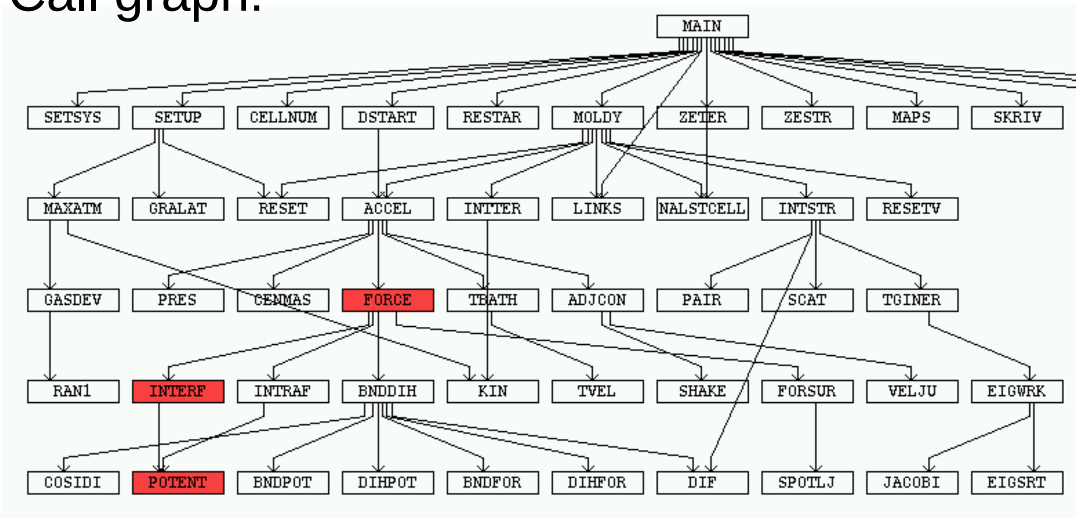


- 7200+ lines of Fortran 77 code
- GOTOs, COMMON blocks, ...
- one source file

Programming OpenMP

Example: MD simulation

Call graph:



more than 80% of the runtime are spent in the red part of the call graph

Programming OpenMP

Example: MD simulation

- The loop to be parallelized contains a call to another subroutine.
- Data is passed the old Fortran style via COMMON blocks
- First try: Inserted one PARALLEL DO pragma in the code, using autoscoping, i.e. a feature of the Oracle Studio compiler
- The compiler generated a parallel version!

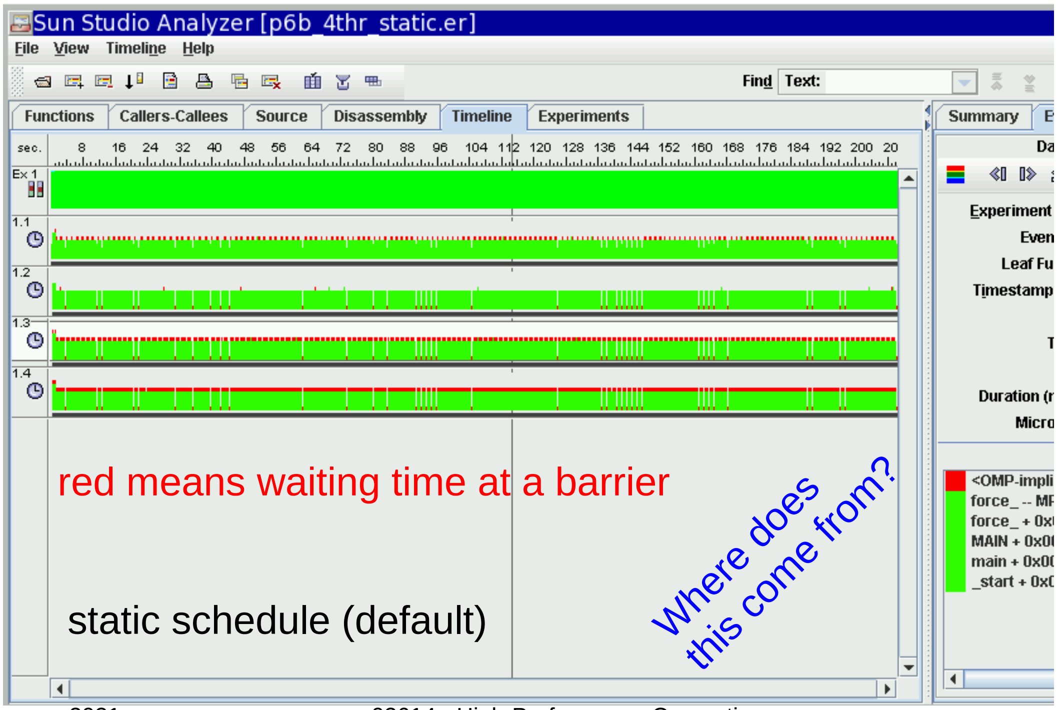
This took us by surprise!

Example: MD simulation

- First test runs:
  - It didn't scale ...
  - The results were dependent on the number of threads ...
- Thread analyzer revealed data races in two variables inside the called subroutine.
- Fix: Added additional scoping for those variables in the OpenMP pragma!
- This solved the data race problem.

Example: MD simulation

Analysis of the scaling problem:

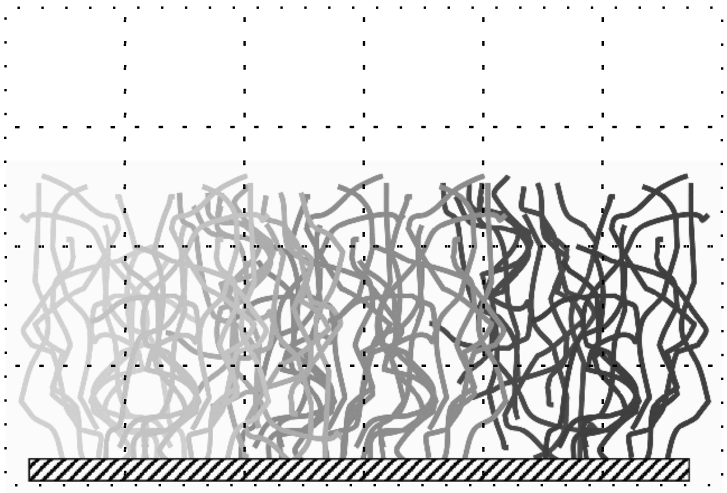


Programming OpenMP

Example: MD simulation

The simulation box:

seen from the side



← thread 4

← thread 3

← thread 2

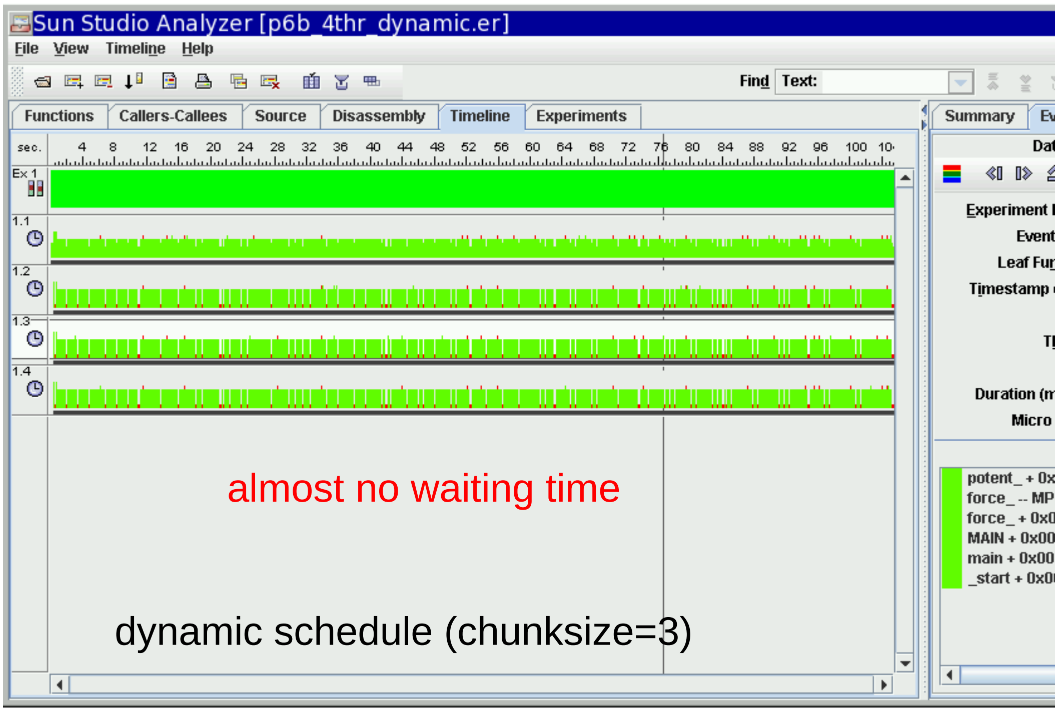
← thread 1

subdivision into smaller cells

Programming OpenMP

Example: MD simulation

Adapted the schedule:



almost no waiting time

dynamic schedule (chunksize=3)

Example: MD simulation

Speed-up results: