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

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

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

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

Example 2:

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

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

OpenMP Syntax

The copyprivate(...) clause

- copying a value out of a single region into the private data of other threads ("broadcast")

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

```
!$OMP SINGLE ....

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

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);
}
   ...
```

OpenMP Syntax

Programming OpenMP

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();
        :

}
```

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

    }
        :
}
```

orphaned worksharing directive

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++) {

    }
       :
}
```

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

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

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

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

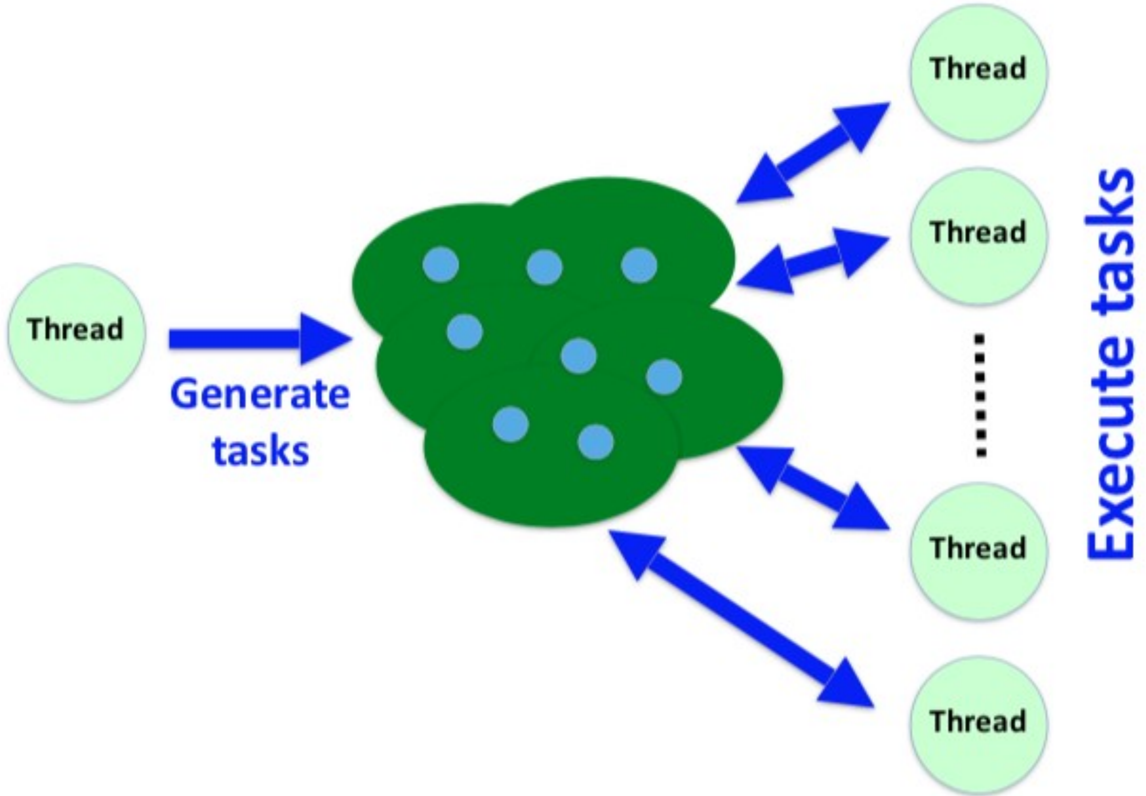
task generation – tasks are added to the task list

all work is done here!

implicit barrier – all unfinished tasks have to be finished

OpenMP syntax

The task pool concept:



courtesy: Ruud van der Pas, Oracle

OpenMP syntax

Tasks and recursion: Fibonacci numbers

- Recursive scheme to calculate the nth 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!

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);
}
```

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

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

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

OpenMP version of main() with tasks:

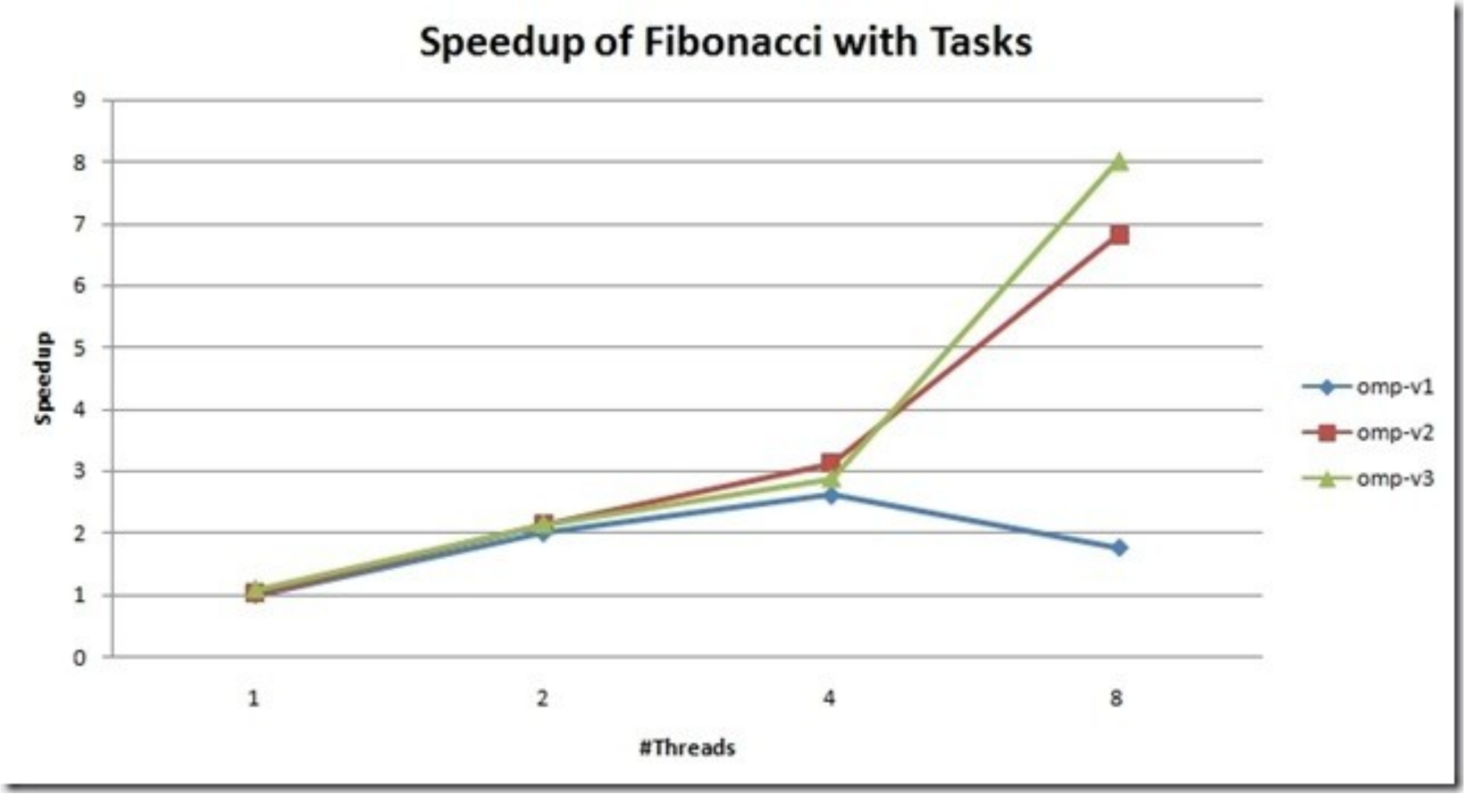
```
int
main(int argc, char* argv[]) {
    [...]

    #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

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

Programming OpenMP

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
- this makes OpenMP a more powerful parallel programming API
    - goes beyond the scope in this course
- a nice intro about tasking in OpenMP: https://www.openmp.org/events/webinar-how-to-get-openmp-tasks-to-do-your-work/

OpenMP: Error detection

Programming OpenMP

Tools to check your OpenMP code

OpenMP compile-time checks

OpenMP checks supported by Oracle Studio compilers:

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

OpenMP: Data Race Detection

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

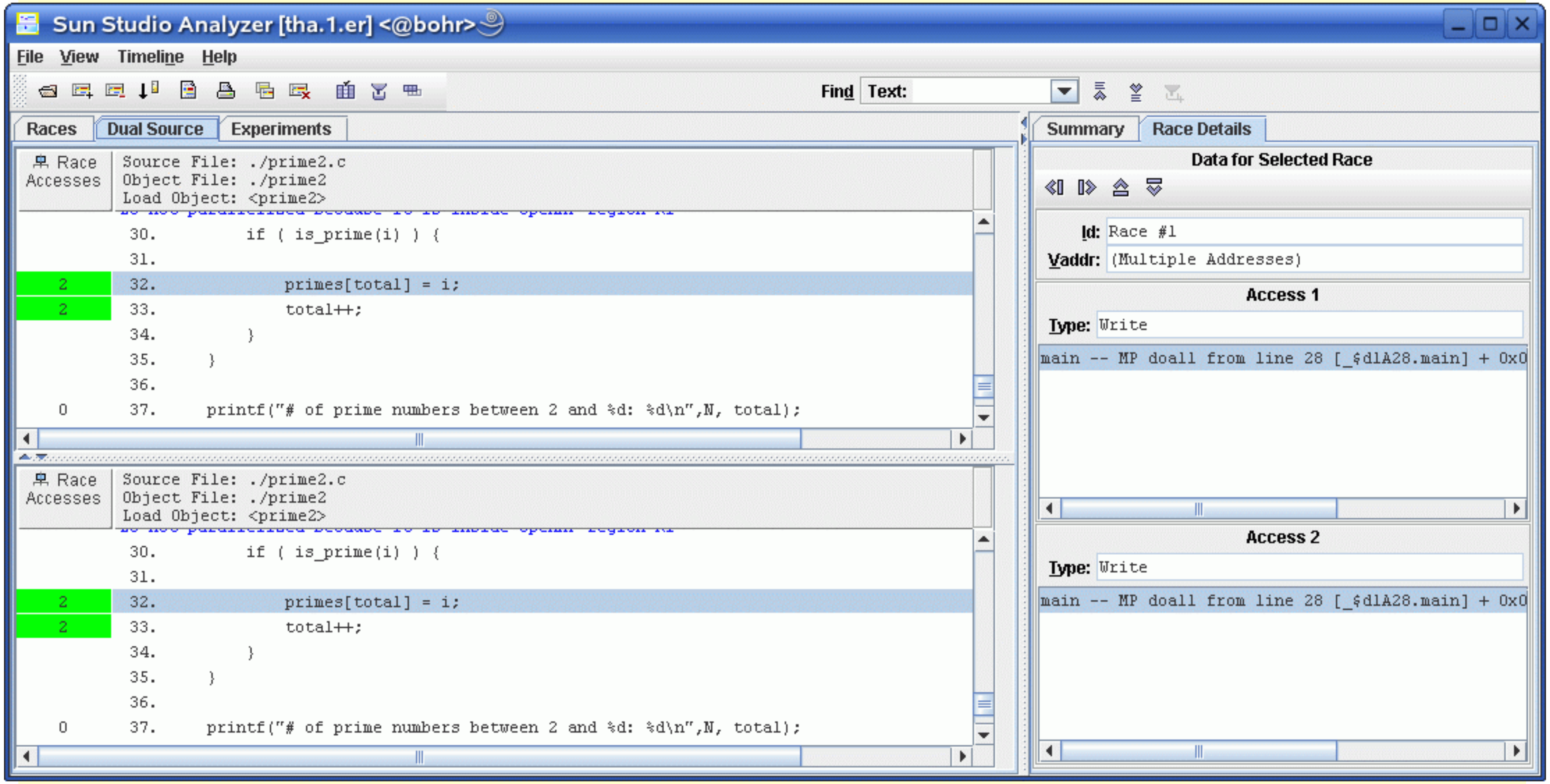
Example (cont'd): analyze the collect data

```
$ 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
```

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

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
    - e.g. “doacross” loops

OpenMP Scheduling

Controlling the scheduling
of OpenMP threads

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

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

```
#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.

Programming OpenMP

OpenMP Scheduling

```
#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.

OpenMP Scheduling

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

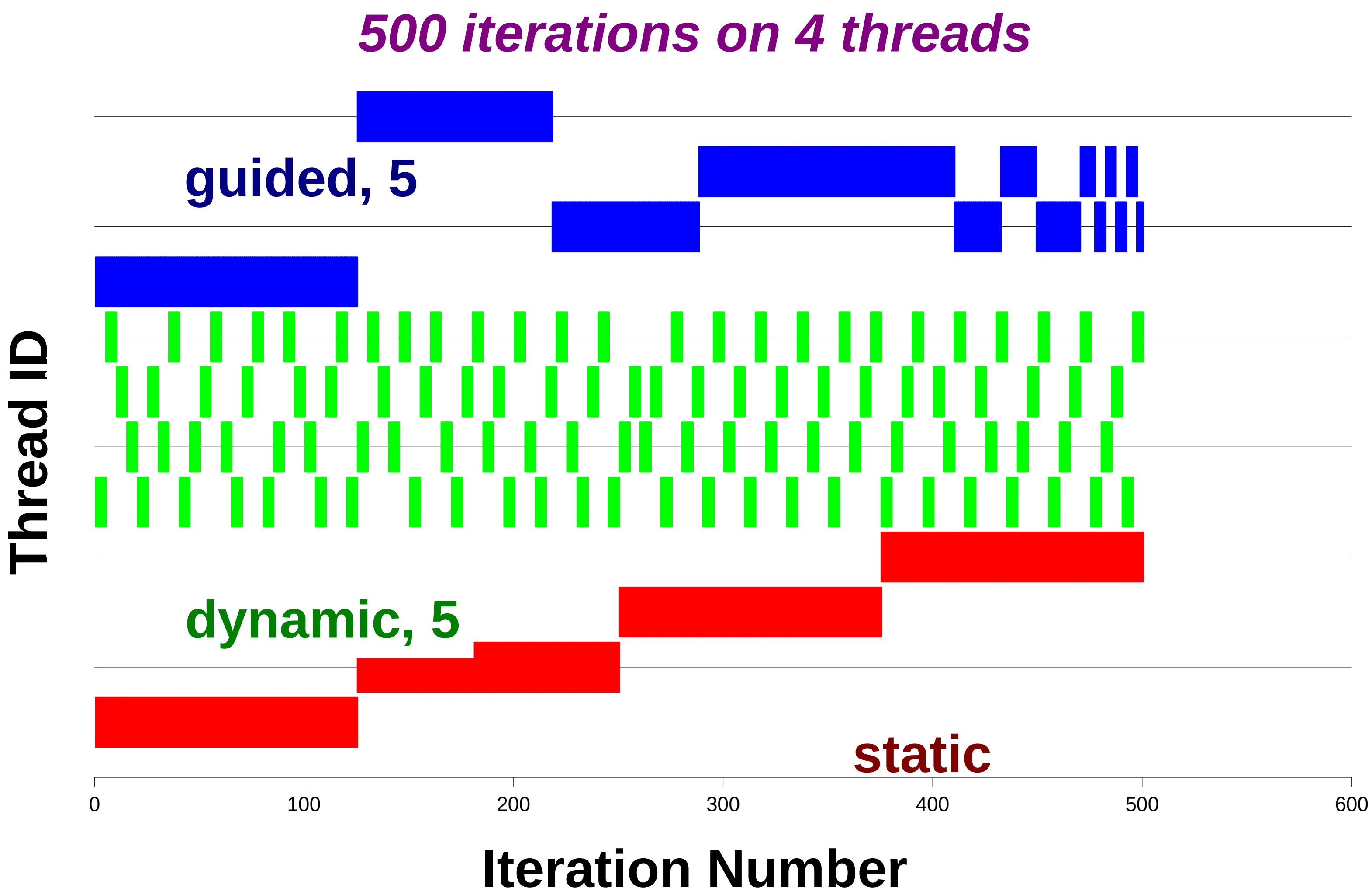
Guided schedule:

- 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.

OpenMP Scheduling



OpenMP Scheduling

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

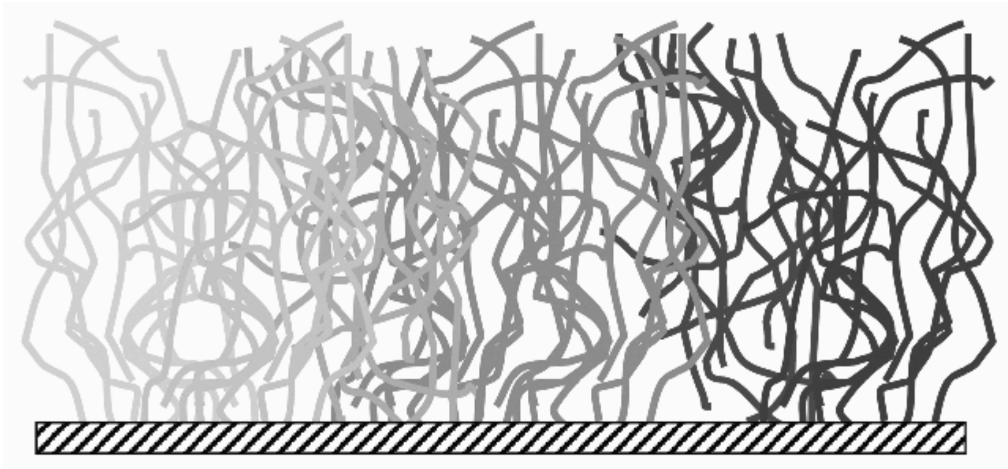
Runtime schedule:

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

A real world example: Molecular Dynamics simulation

Example: MD simulation

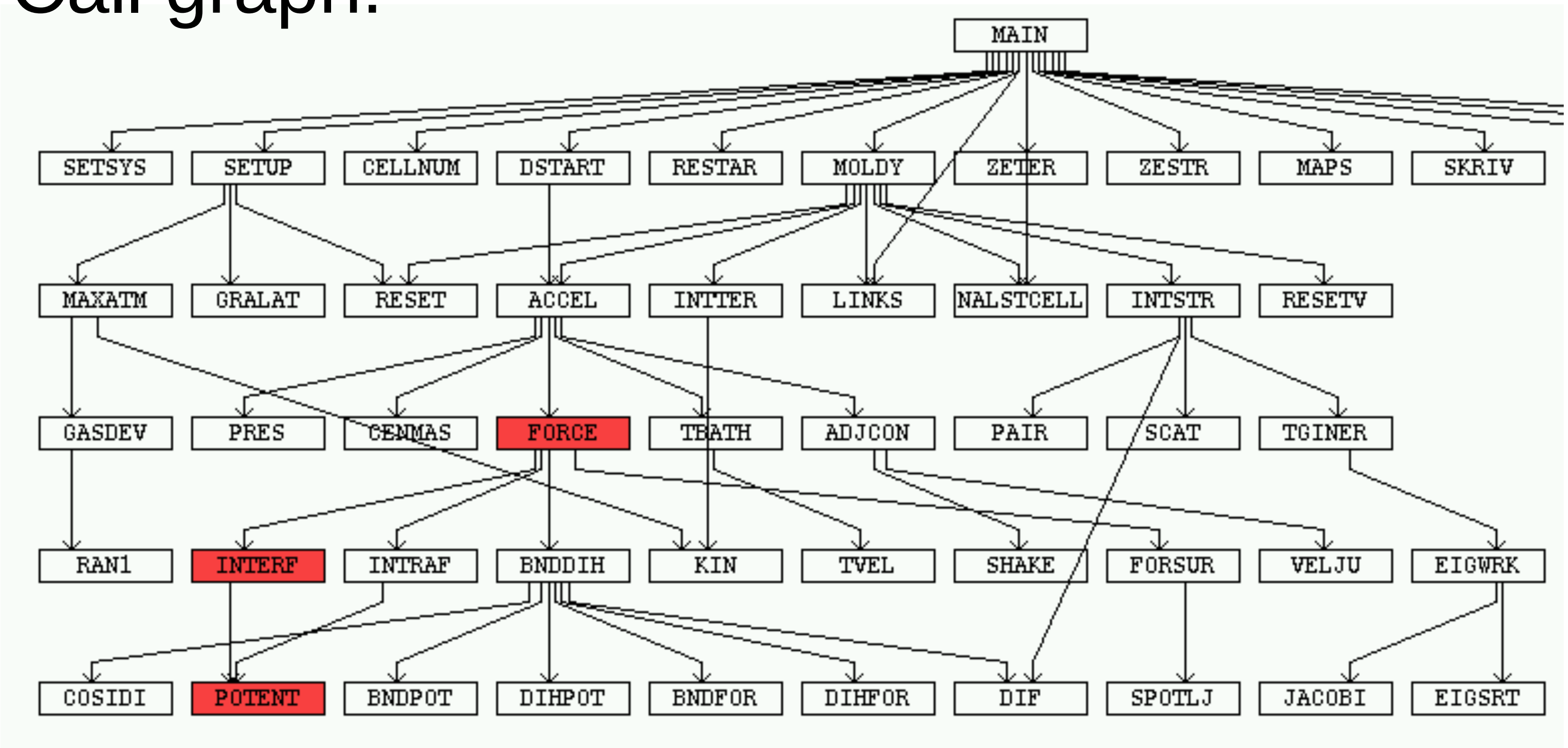
- Molecular Dynamics simulation of long carbon molecules on a surface:



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

Example: MD simulation

Call graph:



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

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!

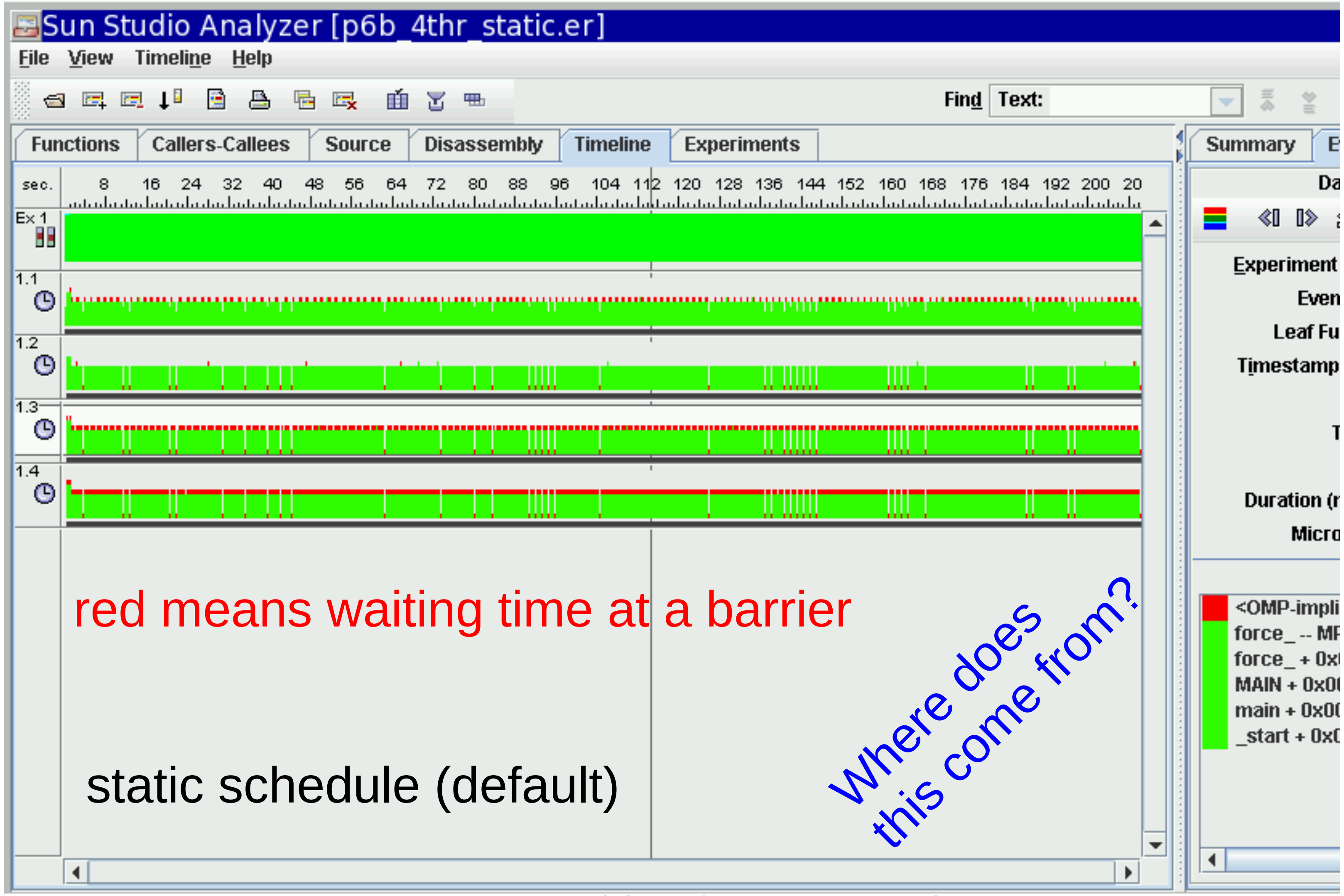
Programming OpenMP

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:

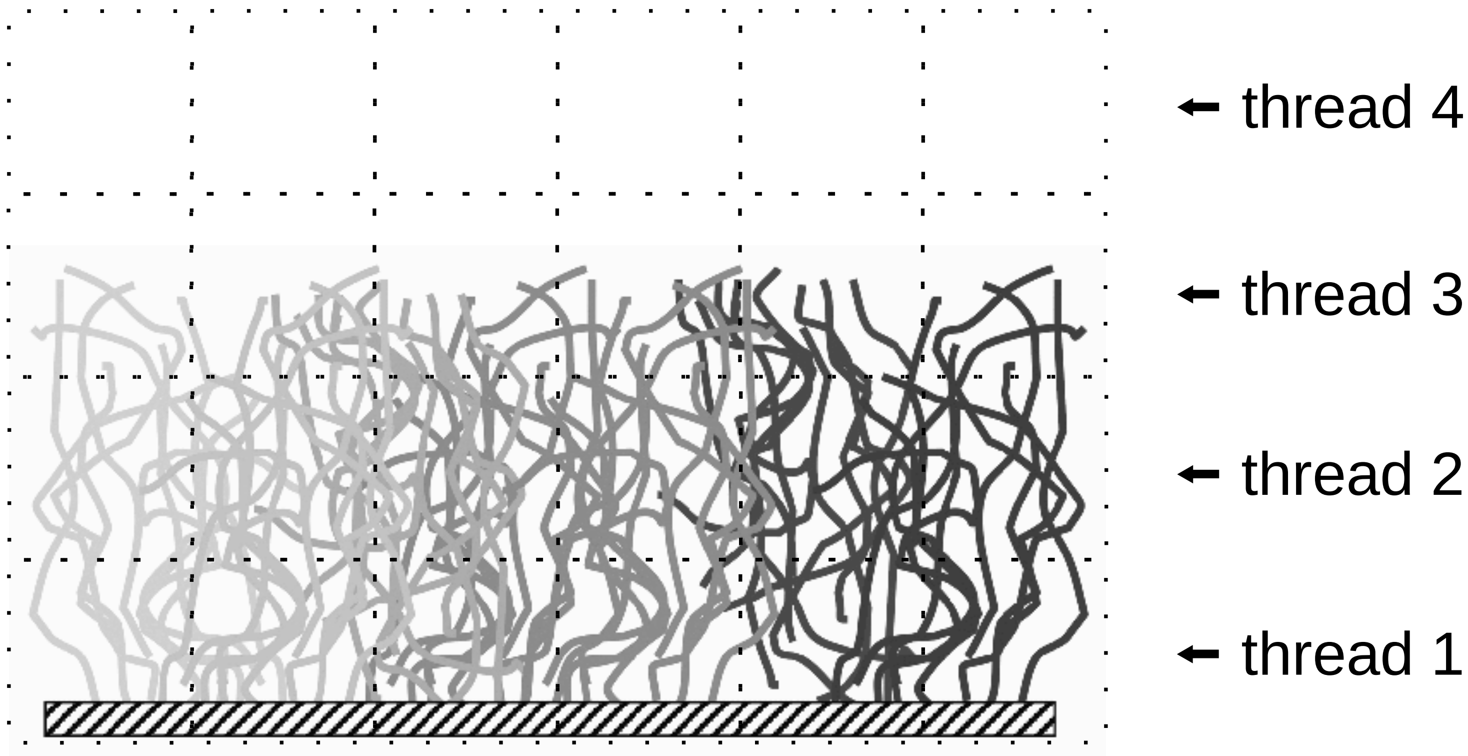


Example: MD simulation

Programming OpenMP

The simulation box:

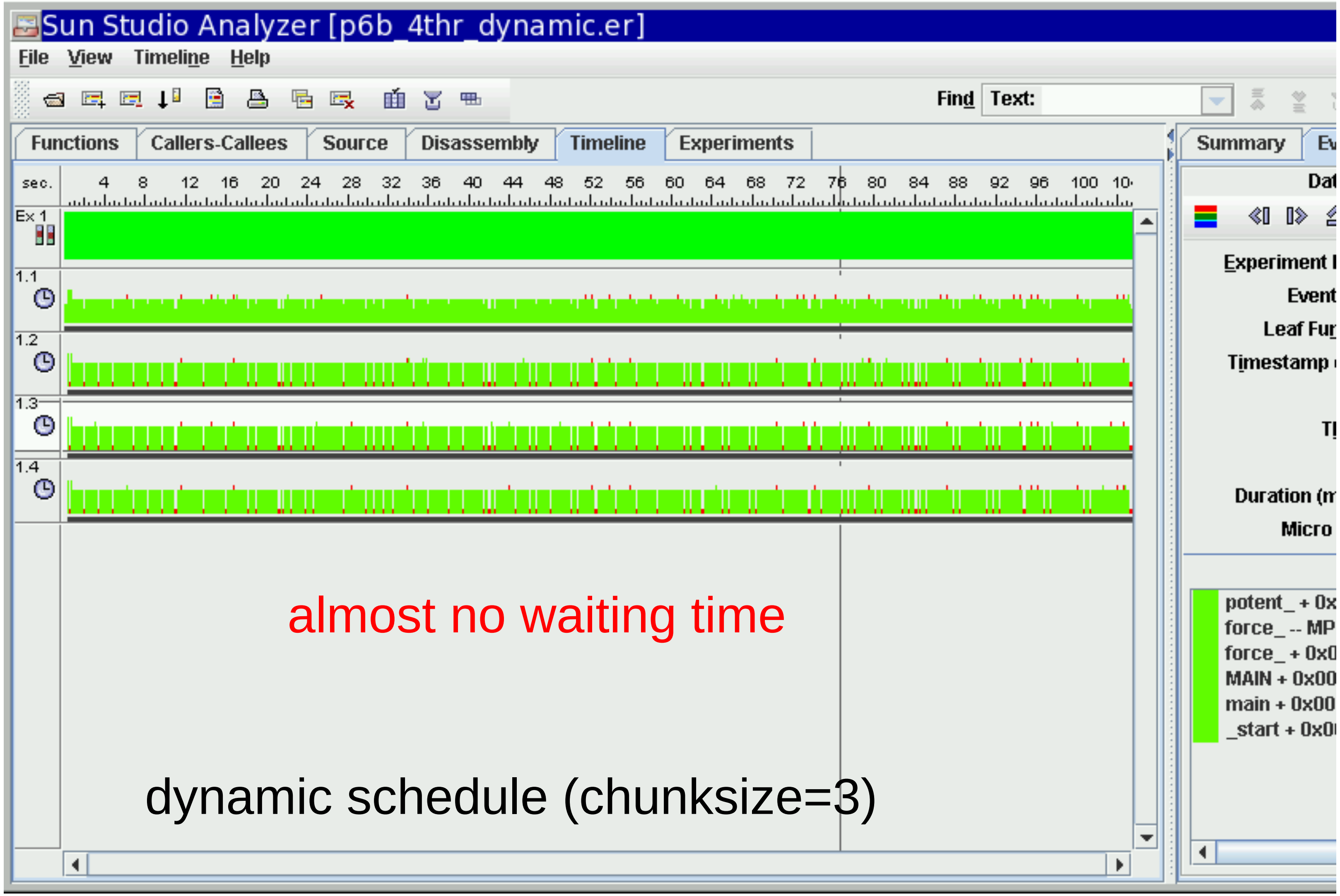
seen from the side



subdivision into smaller cells

Example: MD simulation

Adapted the schedule:



Example: MD simulation

Speed-up results: