High-Performance Computing

DTU Compute

Department of Applied Mathematics and Computer Science



Parallel Programming in OpenMP – part II

Outline

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



More on data scoping



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!



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
```



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.



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



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
```



Example 2:

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

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



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)
```



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 ra, rb;
#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);
```



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);
```



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 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
without copyprivate
                       In main - TID 0: a = 0, b = 0, x = 3, y = 4
                       In main - TID 1: a = 0, b = 1, x = 3, y = 4
  on r_a and r_b
```



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:

region:

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



OpenMP Orphaning

- When an orphaned directive is detected within the dynamic extent of a parallel region, 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
    :
}
```



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



■ Syntax C/C++:

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

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



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



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
```



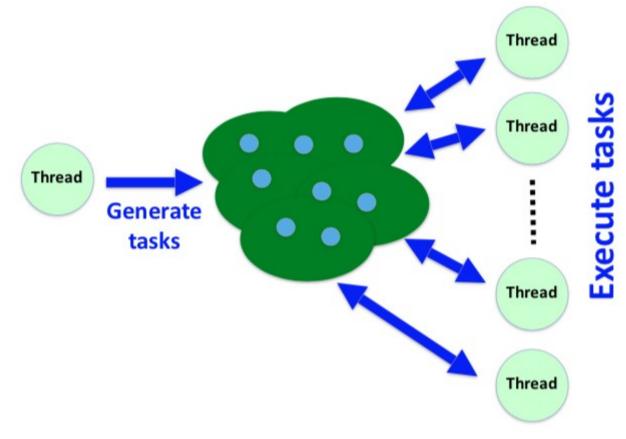
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What's going on?

```
-start of parallel region
#pragma omp parallel
  #pragma omp single
                                       one thread only, please
     p = lhead;
     while (p != NULL) {
        #pragma omp task
                                       task generation – tasks
                                       are added to the task
         do work(p);
                                       list
                                      -all work is done here!
        p = next(p);
                                       implicit barrier – all
  } // end of single
                                       unfinished tasks have
                                       to be finished
    // end of parallel
```



The task pool concept:



courtesy: Ruud van der Pas, Oracle



Tasks and recursion: Fibonacci numbers

- □ Recursive scheme to calculate the nth Fibonacci number:

 - stopping critererion: return 1 if n < 2</p>
- Caveat: this method is not very effective, but used here to demonstrate the concept of tasking!

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 version of fib() with tasks:

```
int
fib(int n) {
   int x, y;
                                         note the special
   if (n < 2) return n;
                                          scoping rules!
   #pragma omp task shared(x)
                                        generate two tasks,
   x = fib(n - 1);
                                       calling fib() recursively
   #pragma omp task shared(y)
   y = fib(n - 2);
                                       task synchronization -
   #pragma omp taskwait
                                       to get the right results
   return (x + y);
```



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



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.



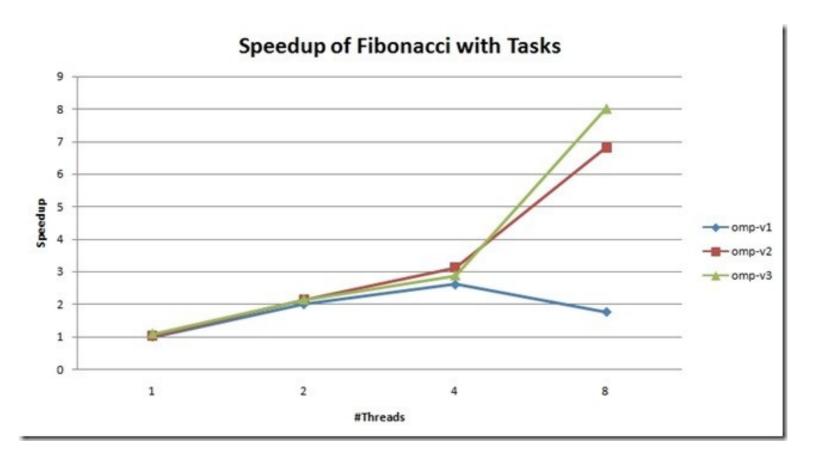
OpenMP version of main() with tasks:

```
int
main(int argc, char* argv[])
   [...]
                                     start of parallel region -
   #pragma omp parallel ◀
                                     team of worker threads
   #pragma omp single
                                     task generation by one
                                          thread, only!
   fib(input);
   } // end of omp parallel
   [...]
```



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Results of the Fibonacci program





courtesy: Chr. Terboven, RWTH Aachen

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)



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);
```



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

Tools to check your OpenMP code



OpenMP compile-time checks

- Most compiler check for OpenMP syntax
 - area of constant improvement, but quality is very much compiler dependent
- Oracle Studio compilers can do more extensive checks at compile time:
 - -xloopinfo info on loops
 - -xvpara compile time warnings on ...
 - ... scoping problems
 - ... possible data races
 - Problem: limited to OpenMP 4.0, no newer constructs supported – but still nice as a check during code development



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
- Caveat: limited to OpenMP 4.0 and earlier



OpenMP: Data Race Detection

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);
```



Example (cont'd): compile and run

```
$ suncc -g -fast -o prime prime.c
$ ptime ./prime
# of prime numbers between 2 and 2000000:
        10.862
real
         10.483
user
           0.056
SVS
$ 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: 1483
          3.662
                   <--- speed-up: 2.9x
real
           10.494
user
            0.055
SYS
```



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
```



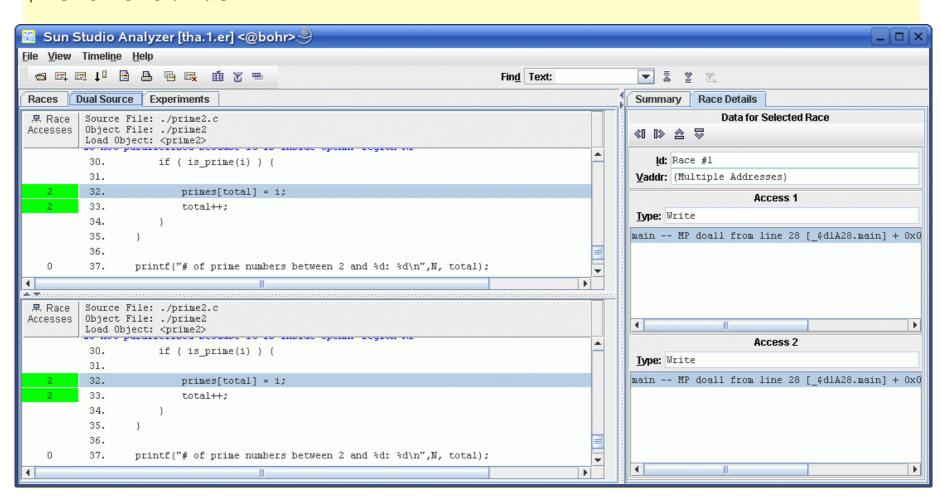
Example (cont'd): analyze the collect data

```
$ 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
```



Example (cont'd): analyze the collect data

\$ tha tha.1.er





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);
```



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
       3.561
real
    10.393
user
         0.051
SYS
```



- 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



Controlling the scheduling of OpenMP threads



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



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.



#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.



#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.



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

Guided schedule:

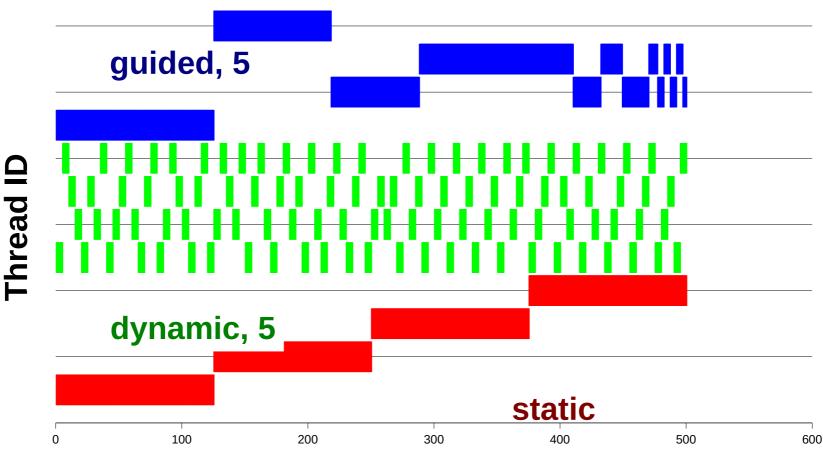
□ The chunk size is exponentially reduced with each chunk that gets dynamically assigned to the threads; chunk defines the minimum number of iterations to assign each time.

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

☐ The default minimum chunk size is 1.











#pragma omp for schedule(runtime)

Runtime schedule:

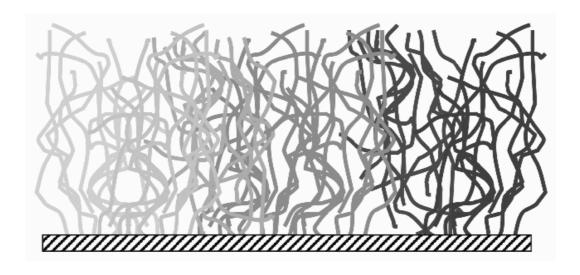
- □ The schedule is detected at runtime from the setting of the OMP_SCHEDULE environment variable.
- Syntax: OMP_SCHEDULE=type,chunk



A real world example: Molecular Dynamics simulation



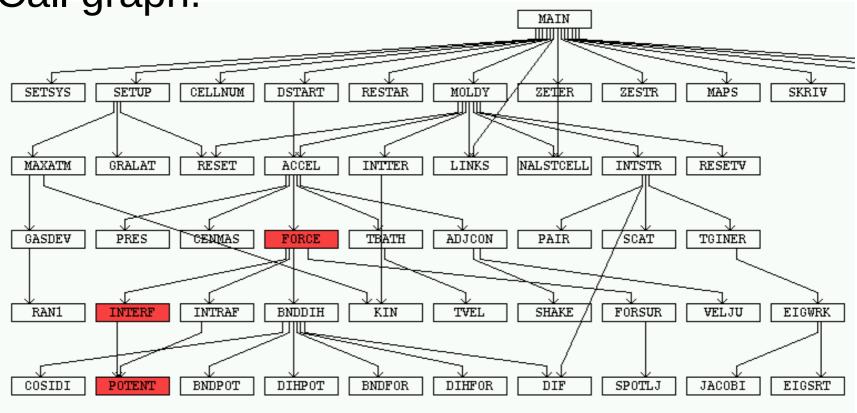
Molecular Dynamics simulation of long carbon molecules on a surface:



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



Call graph:



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



- 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!

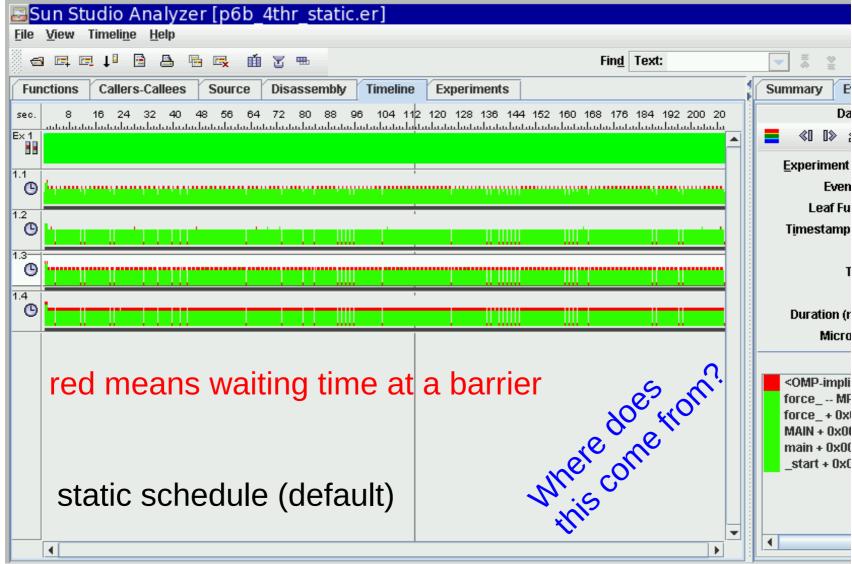
This took us by surprise!



- 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.



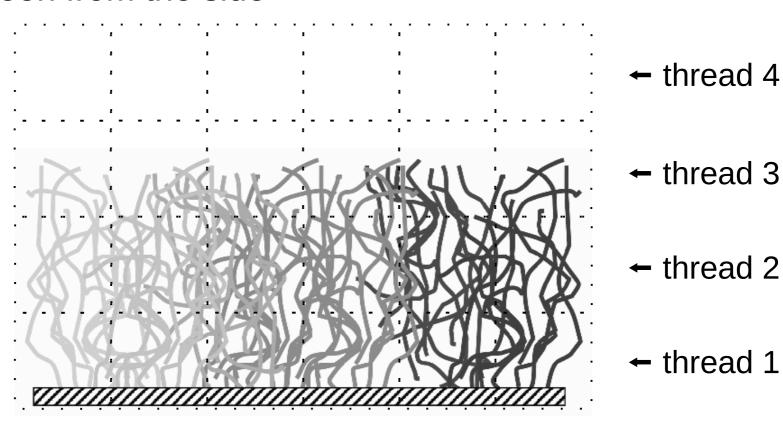
Analysis of the scaling problem:





The simulation box:

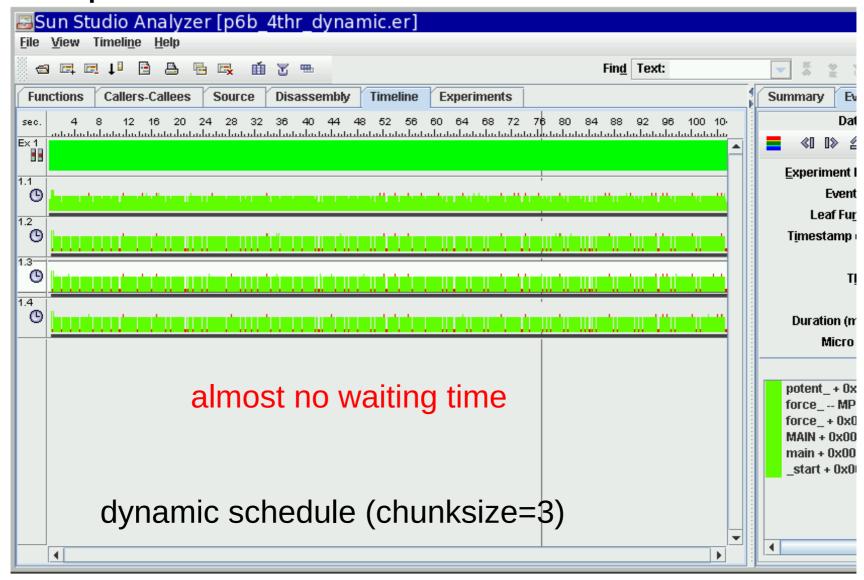
seen from the side



subdivision into smaller cells

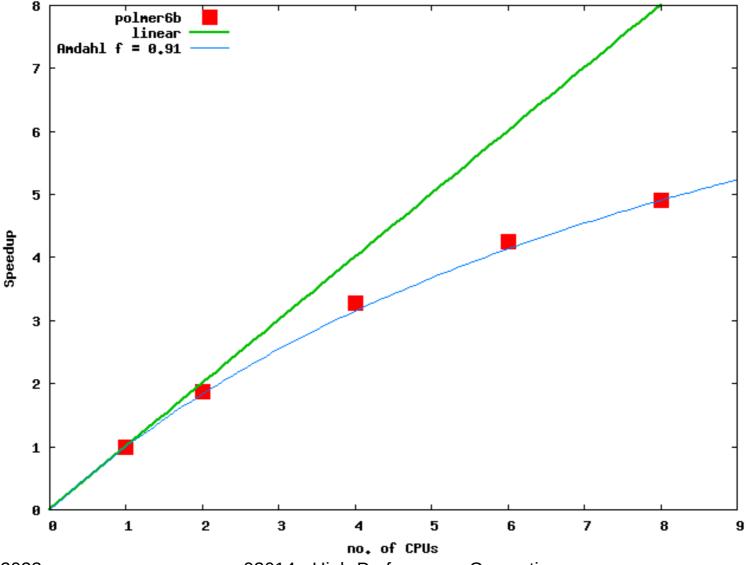


Adapted the schedule:





Speed-up results:





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