High-Performance Computing

Parallel Programming in OpenMP

Outline

- OpenMP Overview
- OpenMP
  - Basics
  - Syntax: Directives
  - Syntax: Clauses
  - Example

OpenMP – Overview

What is OpenMP?

OpenMP – Overview

- OpenMP: stands for

  Open Multi Processing

- parallel programming model for shared memory multiprocessors
- 'de-facto' standard, not an industry *standard*
- not a new language, but
  - compiler directives
  - support function library

OpenMP – Overview

- OpenMP development is community driven
- Architecture Review Board (ARB):
  - hardware and software vendors
  - government and academia
- Founded back in 1997
  - unification of different vendor “standards”
- Official OpenMP website:
  - https://www.openmp.org/

OpenMP – Overview

- standard versions:
  - C/C++: version 2.0 (March 2002)
  - Fortran: version 2.0 (November 2000)
  - version 2.5 (Fortran and C/C++ / May 2005)
  - version 3.0 (May 2008)
  - version 3.1 (July 2011)
  - ...

OpenMP – Overview

- 4.0 (Jul 2013)
  - exception handling
- 4.5 – update (Nov 2015)
  - first support for accelerators (“GPU offloading”)
- 5.0 (Nov 2018), 5.2 – update (Nov 2021)
  - is implemented in most compilers now
- 6.0 (Nov 2024)
- The OpenMP standard specifications:
  - http://www.openmp.org/specifications/

OpenMP – Overview

OpenMP Literature:

- “Using OpenMP – The Next Step“ by R. van der Pas, E. Stotzer and C. Terboven, MIT Press (2017) – available via findit.dtu.dk
- “The OpenMP Common Core” by T.G. Mattson, Y. He, and A.E. Koniges, MIT Press (2019)
- “Using OpenMP”, B. Chapman, G. Jost, R. van der Pas, MIT Press (2007)

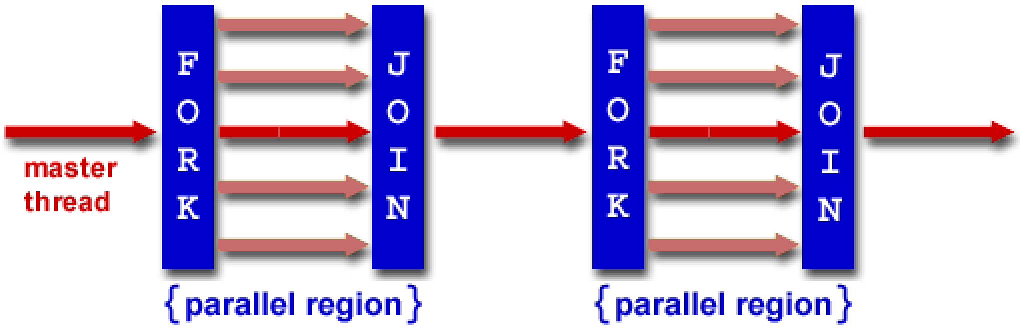
OpenMP Basics

Basic elements of OpenMP

OpenMP Basics

OpenMP uses the "Fork-Join Model":

- All programs begin as a single process: the master thread.
- FORK: the master thread creates a team of parallel threads (parallel region).
- JOIN: synchronization and termination of the worker threads.



OpenMP Basics

OpenMP is mostly based on compiler directives:

- C/C++:

```
#pragma omp directive [clause]
    {...code block...}
```

- Fortran:

```
!$OMP directive [clause]
    ...code block...
!$OMP end directive
```

OpenMP Basics

The OpenMP API has also

- a set of support library functions:
  omp_... ()

  e.g. omp_get_thread_num()

- control via environment variables:

  OMP_...

  e.g. OMP_NUM_THREADS

OpenMP Basics

First OpenMP version of “Hello world”:

```
#include <stdio.h>

int main(int argc, char *argv[]) {
    #pragma omp parallel
    {
    printf("Hello world!\n");
    } /* end parallel */
    return(0);
}
```

OpenMP Basics

Second version of “Hello world”:

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

int main(int argc, char *argv[]) {
    int  t_id = 0;
    #pragma omp parallel private(t_id)
    {
    #ifdef _OPENMP
    t_id = omp_get_thread_num();
    #endif
    printf("Hello world from %d!\n", t_id);
    } /* end parallel */
    return(0);
}
```

OpenMP Basics

```
$ ./hello2
Hello world from 0!

$ OMP_NUM_THREADS=4 ./hello2
Hello world from 0!
Hello world from 3!
Hello world from 1!
Hello world from 2!
```

- Note: The order of execution will be different from run to run!
- The default no. of threads depends on the OpenMP implementation

OpenMP Components

Directives

- Parallel regions
- Worksharing
- Synchronization
- Data scoping
- no. of threads
- Orphaning

Environment variables

- no. of threads
- Scheduling
- Dynamic thread adjustment
- Nested parallelism

Runtime

- no. of threads
- Scheduling
- Dynamic thread adjustment
- Nested parallelism
- API for timers & locking

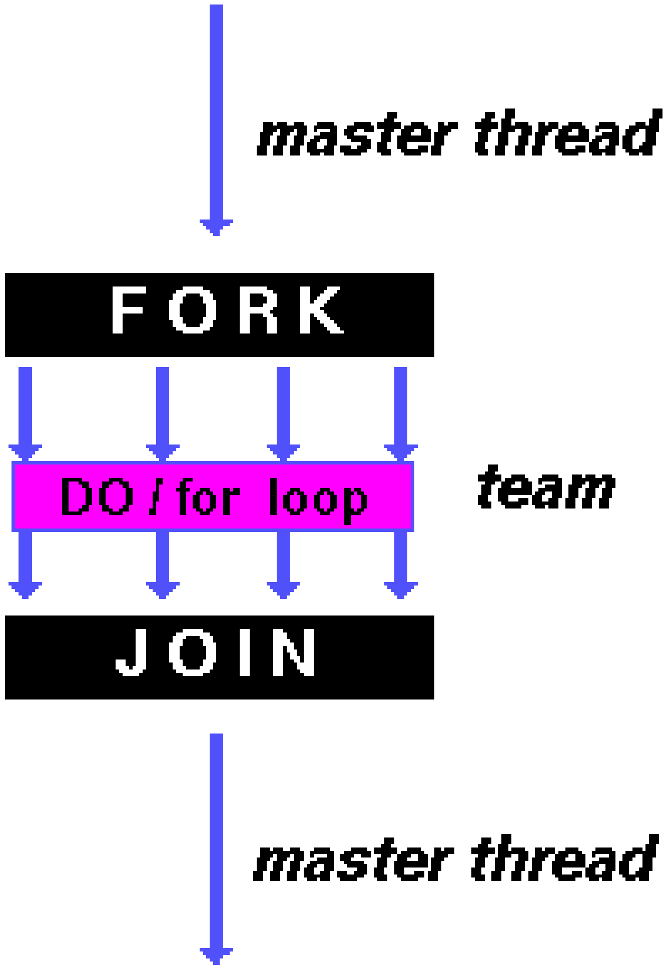
OpenMP Basics

Work-sharing

OpenMP Basics

Work-sharing constructs – 1:

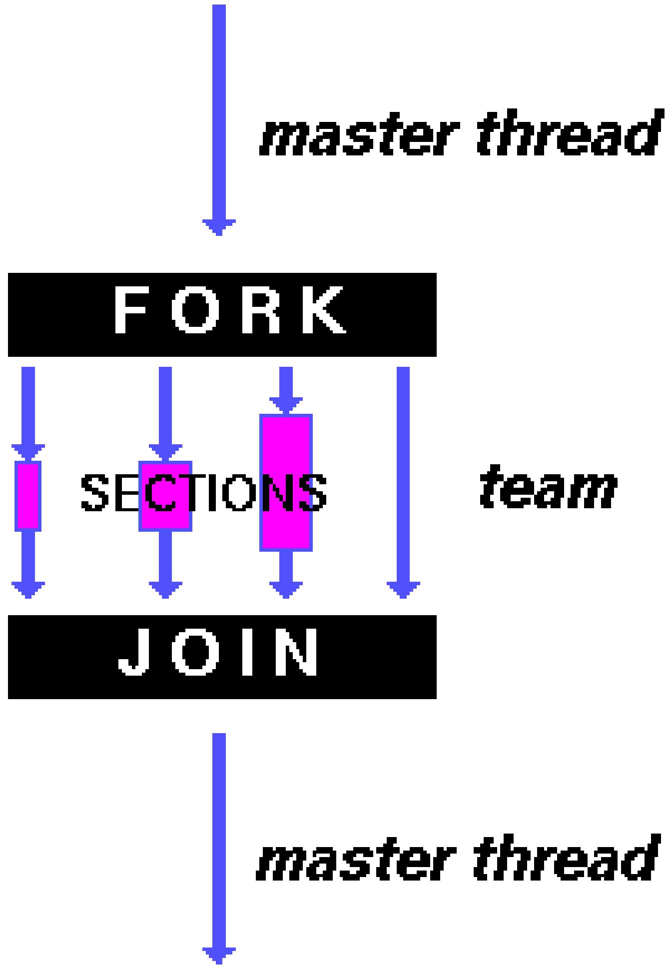
- do/for
- loop parallelism
- most common



OpenMP Basics

Work-sharing constructs – 2:

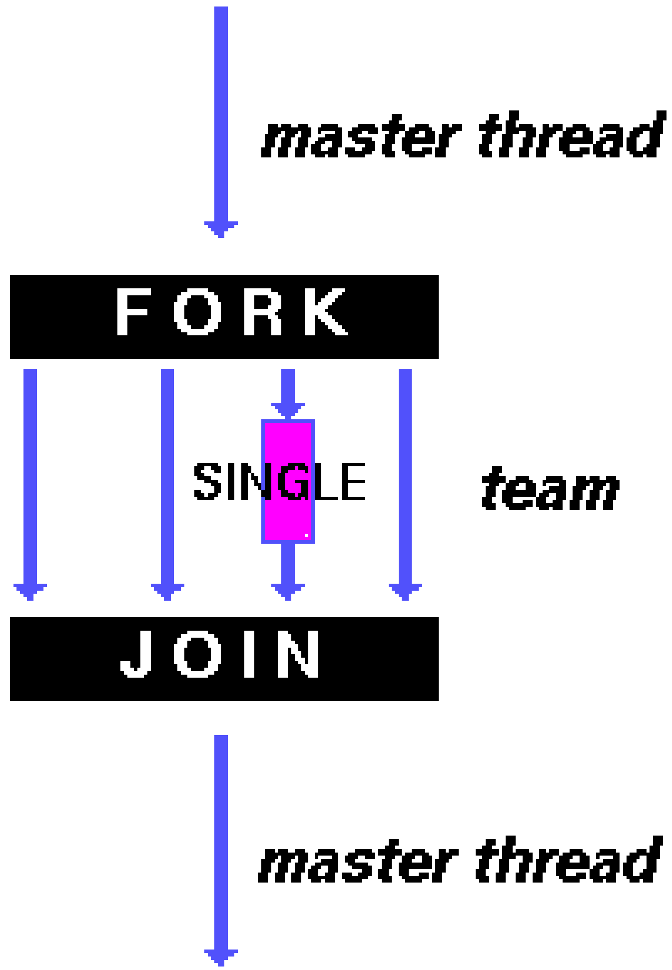
- sections
- functional parallelism
- typically independent calculations



OpenMP Basics

Work-sharing constructs – 3:

- single
- work assigned to one thread only
- typically I/O



OpenMP Basics

Important rules for work-sharing constructs:

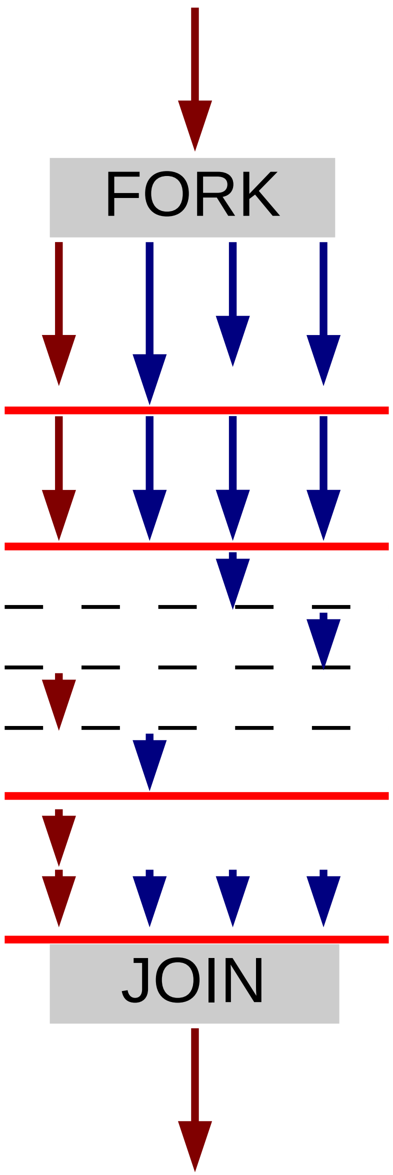
- must be enclosed in a parallel region
- must be encountered by all team members
- must be encountered in the same order

OpenMP Basics

Synchronization

OpenMP Basics

- most synchronization in OpenMP is implicit, but sometimes explicit synchronization is needed:
- barriers
- critical regions
- master only
- explicit locking



OpenMP Syntax

OpenMP programming in C/C++
Part I: Directives

OpenMP Syntax

OpenMP directives – general form:

```
#pragma omp directive [[clause] \
 [clause] ...]
{
  <statements>
} /* end of omp directive */
```

- **Note**: There is **no** “omp end” pragma!
- Best practice: add a comment at the end of the structured block!

OpenMP Syntax

Parallel region:

- Starts a team of parallel threads
- executes code in parallel
- synchronize/terminate threads

```
main() {
    A();
    #pragma omp parallel
    {
    B();   // all threads do B()!
    } /* end omp parallel */
    C();
}
```

OpenMP Syntax

Work-sharing – Loop parallelism:

- OpenMP implements parallel do/for-loops only!

```
int i;
float a[N], b[N], c[N];

for (i=0; i < N; i++)
  a[i] = b[i] = i * 1.0;

#pragma omp parallel shared(a,b,c) private(i)
{
  #pragma omp for
  for (i=0; i < N; i++)
    c[i] = a[i] + b[i];

}  /* end of parallel region */
```

for *has to follow the pragma – no {... }!*

OpenMP Syntax

Work-sharing – Loop parallelism:

- Another version: combined “parallel for”

```
int i;
float a[N], b[N], c[N];

for (i=0; i < N; i++)
  a[i] = b[i] = i * 1.0;

#pragma omp parallel for shared(a,b,c)\
                         private(i)
for (i=0; i < N; i++)
  c[i] = a[i] + b[i];
```

OpenMP Syntax

Work-sharing – Fortran 95 array syntax

- Fortran 95 allows to address parts of or whole arrays – and the compiler will translate this into loops.
- A special Fortran directive:

```
double precision, dimension() :: A, B
double precision, dimension(N,M) :: C

!$ OMP WORKSHARE
   ...
   A(1:M) = A(1:M) + B(1:M)
   C = 0.00
   ...
!$ OMP END WORKSHARE
```

OpenMP Syntax

Work-sharing – Functional parallelism:

- Parallel sections:

```
#pragma omp parallel shared(a,b,c) private(i)
{
  #pragma omp sections
  {
    #pragma omp section
    for (i=0; i < N/2; i++)
      c[i] = a[i] + b[i];

    #pragma omp section
    for (i=N/2; i < N; i++)
      c[i] = a[i] + b[i];
  }  /* end of sections */
} /* end of parallel region */
```

OpenMP Syntax

Work-sharing – Single thread execution:

- Work done by one thread only

```
#pragma omp parallel shared(a,b,c) private(i)
{
  #pragma omp single
  { read_array(a); read_array(b); }

  #pragma omp for
  for (i=0; i < N; i++)
    c[i] = a[i] + b[i];

  #pragma omp single
  { write_array(c); }
}  /* end of parallel section */
```

OpenMP Syntax

Work-sharing – conditional parallelism:

- the if(...) clause

```
int i;
float a[N], b[N], c[N];

for (i=0; i < N; i++)
  a[i] = b[i] = i * 1.0;

#pragma omp parallel if (N > 10000) \
        shared(a,b,c) private(i)
{
  #pragma omp for
  for (i=0; i < N; i++)
    c[i] = a[i] + b[i];
}
```

OpenMP Syntax

The num_threads(...) clause:

```
#pragma omp parallel ... num_threads(int_expr)
{
     ...
}
```

- only one num_threads clause per parallel directive
- int_expr is evaluated at runtime, before the parallel region is entered

Programming OpenMP

OpenMP syntax

The collapse(n) clause

- a way to parallelize loop nests

```
subroutine sub()

!$omp do collapse(2) private(i,j,k)
  do k = kl, ku, ks
    do j = jl, ju, js
      do i = il, iu, is
        call bar(a,i,j,k)
      enddo
    enddo
  enddo
!$omp end do
end subroutine
```

collapse the two outer loops over k and j

OpenMP Syntax

Synchronization – Critical region:

- specifies a region of code that must be executed by only **one** thread at a time!
- can be named

```
#pragma omp parallel private(loc_sum)
{
  ...
  #pragma omp for
  for(int i = 0; i < n; i++)
     loc_sum += x[i];

  #pragma omp critical (cr_sum)
  sum += loc_sum;
}  /* end of parallel section */
```

OpenMP Syntax

Synchronization – Atomic construct:

- specifies a single operation(!) that must be executed by only **one** thread at a time!
- restricted syntax (see OpenMP standard)

```
int x = 0;

#pragma omp parallel shared(x)
{
  ...
  #pragma omp atomic
  x = x + 1;
  ...
}  /* end of parallel section */
```

OpenMP Syntax

Synchronization – Master region:

- specifies a region of code that is executed by the master thread only!
- ignored by others – no implicit barriers!

```
#pragma omp parallel
{
  ...
  #pragma omp master
  {
     printf("Hello\n");
  }
  ...
}  /* end of parallel section */
```

OpenMP Syntax

Synchronization – Ordered:

- executes code block in the sequential order
- everything outside can run in parallel
- only within a parallel do/for loop

```
#pragma omp parallel for \
        private(i,myf) ordered
for(i = 0; i < n; i++) {
   myf = i+1;
   #pragma omp ordered
   {
     sum = sum + myf;
   }
}  /* end of parallel for */
```

```
#pragma omp parallel for \
        private(i,myf)
for(i = 0; i < n; i++) {
   myf = i+1;
   #pragma omp critical
   {
     sum = sum + myf;
   }
} /*end of parallel for*/
```

OpenMP Syntax

Output:

non-ordered vs. ordered

non-ordered	ordered
`sum[  1] =      1`	`sum[  1] =      1`
`sum[  6] =      7`	`sum[  2] =      3`
`sum[  2] =      9`	`sum[  3] =      6`
`sum[  7] =     16`	`sum[  4] =     10`
`sum[  3] =     19`	`sum[  5] =     15`
`sum[  8] =     27`	`sum[  6] =     21`
`sum[  4] =     31`	`sum[  7] =     28`
`sum[  9] =     40`	`sum[  8] =     36`
`sum[ 10] =     50`	`sum[  9] =     45`
`sum[  5] =     55`	`sum[ 10] =     55`
`Result: 55`	`Result: 55`

OpenMP Syntax

Ordered with dependences (OpenMP 4.5)

- new clause depend(...) enhances ordered by adding dependences
  - #pragma omp ordered depend(sink: vec)
    - start the ordered region with the dependences given in vec
  - #pragma omp ordered depend(source)
    - ends the ordered execution defined by sink above
- this new feature allows to parallelize e.g. loops with dependences (see next slide)

OpenMP Syntax

doacross loops:

- loops with dependencies

# of dependences

dependence vector

```
#pragma omp parallel
{
    #pragma omp for ordered(1)
    for (int i=1; i<n; i++) {

        #pragma omp ordered depend(sink:i-1)
        a[i] = a[i-1] + b[i];
        #pragma omp ordered depend(source)

        c[i] = 2*a[i];
    } // End of for-loop
} // End of parallel region
```

OpenMP Syntax

ordered depend(...) and doacross loops:

- provides logic in the OpenMP runtime, that else would have to be done manually
- helps to “resolve” static dependences and allows part of the code to run in parallel
- useful, if the parallel part of the loop(s) is more computational intensive than the ordered part
- might need a different loop scheduling (depends on compiler/runtime)

OpenMP Syntax

Synchronization – Barrier:

- synchronizes all threads in a team

```
#pragma omp parallel
{
   ...

   #pragma omp barrier


   ...
}  /* end of parallel section */
```

OpenMP Syntax

Synchronization – Implied barriers:

- exit from parallel region
- exit from `omp for/omp do/omp workshare`
- exit from sections
- exit from single

No *implied* barrier on the master construct, neither on entry nor on exit!

OpenMP Syntax

OpenMP programming in C/C++
Part II: Clauses

OpenMP Syntax

Data scoping clauses:

- Understanding and the use of data scoping is really essential.
- Most problems/errors are due to wrong data scoping.
- Most variables are shared by default (shared memory programming model).
- Private variables: loop indices, stack of subroutines.

OpenMP Syntax

OpenMP Data scope attribute clauses:

- private
- shared
- default
- reduction
- firstprivate
- lastprivate
- copyin

OpenMP Syntax

The “private” clause:

- declares variables private to each thread:

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

- 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

The “shared” clause:

- declares variables to be shared among all threads:

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

- a shared variable exists in only one memory location and all threads have read/write access to that address
- proper access to the variable is left to the programmer – that's YOU!

OpenMP Syntax

The “default” clause:

- allows the programmer to specify the default scope for all variables:

```
#pragma omp dir default(shared|none)
```

- C/C++ knows only those two types
- only one default clause per parallel region
- Best practice: use default(none) and scope all your variables explicitly

OpenMP Example

Two examples

Programming OpenMP

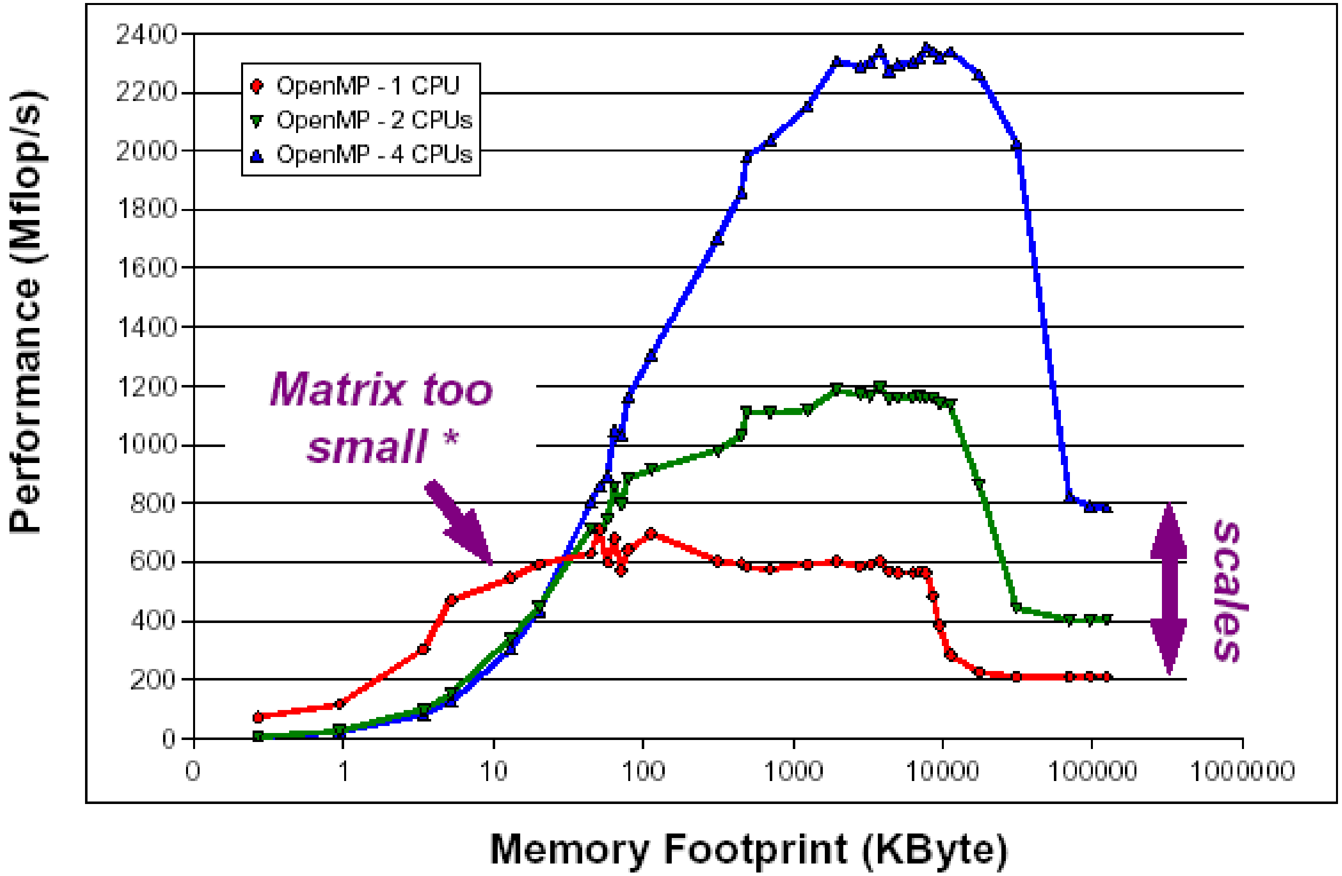
OpenMP Example

Matrix times vector

```
void
mxv(int m, int n, double *a, double *b, double *c)
{
  int i, j;
  double sum;

  #pragma omp parallel for default(none) \
              shared(m,n,a,b,c) private(i,j,sum)
  for (i=0; i<m; i++) {
    sum = 0.0;
    for (j=0; j<n; j++)
      sum += b[i*n+j] * c[j];
    a[i] = sum;
  }
}
```

OpenMP Example



SunFire 6800
UltraSPARC III Cu @ 900 MHz
8 MB L2-cache

*) *With the IF-clause in OpenMP this performance degradation can be avoided*

OpenMP Example

Matrix times vector (using C99 standard)

```
void
mxv(int m, int n, double *a, double *b, double *c)
{
  double sum;

  #pragma omp parallel for default(none) \
              shared(m,n,a,b,c) private(sum)
  for (int i=0; i<m; i++) {
    sum = 0.0;
    for (int j=0; j<n; j++)
      sum += b[i*n+j] * c[j];
    a[i] = sum;
  }
}
```

variables declared inside a parallel region are already private!

OpenMP Example

Example: numerical integration of f(x)

```
int i, n;
double h, x, sum;

h = 1.0 / (double)n;
sum = 0.0;
#pragma omp parallel for default(none) \
        shared(n,h,sum) private(i,x)

for(i=1; i<=n; i++) {
   x = h * ((double)i + 0.5);
   #pragma omp critical
   sum += f(x);
}
```

sequential code!

~~**Race condition!**~~

OpenMP Example

Example: numerical integration of f(x)

- Improvement 1

```
int i, n;
double h, x, fx, sum;

h = 1.0 / (double)n;
sum = 0.0;

#pragma omp parallel for default(none) \
        shared(n,h,sum) private(i,x,fx)
for(i=1; i<=n; i++) {
   x = h * ((double)i + 0.5);
   fx = f(x);
#pragma omp critical
   sum += fx;
}
```

function evalution in parallel

OpenMP Example

Example: numerical integration of f(x)

- Improvement 2

```
int i, n; double h, x, t_sum, sum;

h = 1.0 / (double)n; sum = 0.0;
#pragma omp parallel default(none) \
        shared(n,h,sum) private(i,x,t_sum)    {
  t_sum = 0.0;
  #pragma omp for
  for(i=1; i<=n; i++) {
     x = h * ((double)i + 0.5);
     t_sum += f(x);
  }
  #pragma omp critical
  sum += t_sum;
} // end omp parallel
```

OpenMP Syntax

The “reduction” clause:

- performs a reduction on the variables that appear on the list:

```
#pragma omp dir reduction(op: list)
```

- a private copy for each thread of all variables on the list is created
- at the end, the reduction operation is carried out and the result(s) written to the global variable(s)

OpenMP Example

Example: numerical integration of f(x)

- smart OpenMP solution

```
int i, n;
double h, x, sum;

h = 1.0 / (double)n;
sum = 0.0;

#pragma omp parallel for default(none) \
        shared(n,h) private(i,x) \
        reduction(+: sum)
for(i=1; i<=n; i++) {
    x = h * ((double)i + 0.5);
    sum += f(x);
}
```

OpenMP Excercises – I

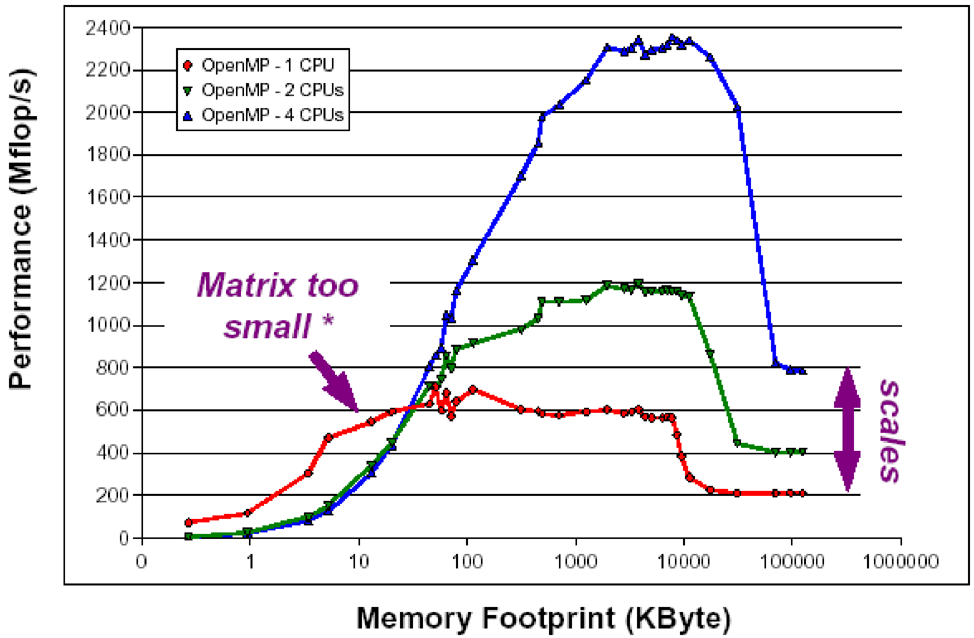
- Write an OpenMP code to calculate π, using

$$\pi = \int_0^1 \frac{4}{\left(1+x^2\right)} dx \approx \frac{1}{N} \sum_{i=1}^{N} \frac{4}{1+\left(\frac{i-0.5}{N}\right)^2}$$

  - implement the integrand as a function
  - write your own reduction code
  - use the OpenMP reduction clause
  - compare the run-times

OpenMP Excercises – II

- Improve the matrix times vector example by adding an if-clause to the omp pragma – experiment with the threshold value!



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