Introduction to OpenMP

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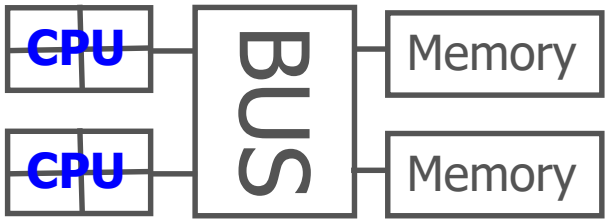
Overview

- Quick introduction.
- Parallel loops.
- Parallel loop directives.
- Parallel sections.
- Some more advanced directives.
- Summary.

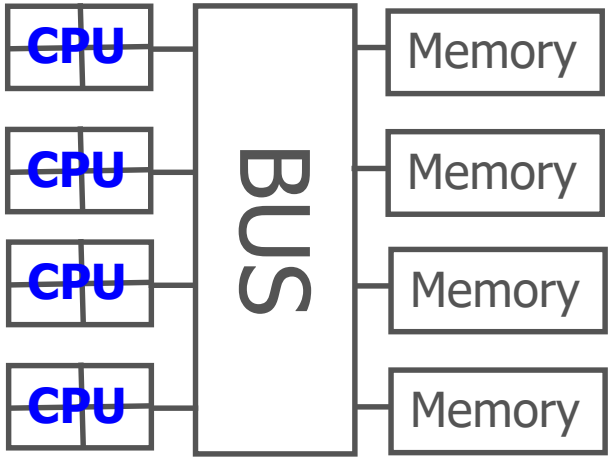
Shared memory

- All processors have access to local memory
- Simpler programming
- Concurrent memory access
- More specialized hardware
- CHPC : Linux clusters 12 - 64 core nodes

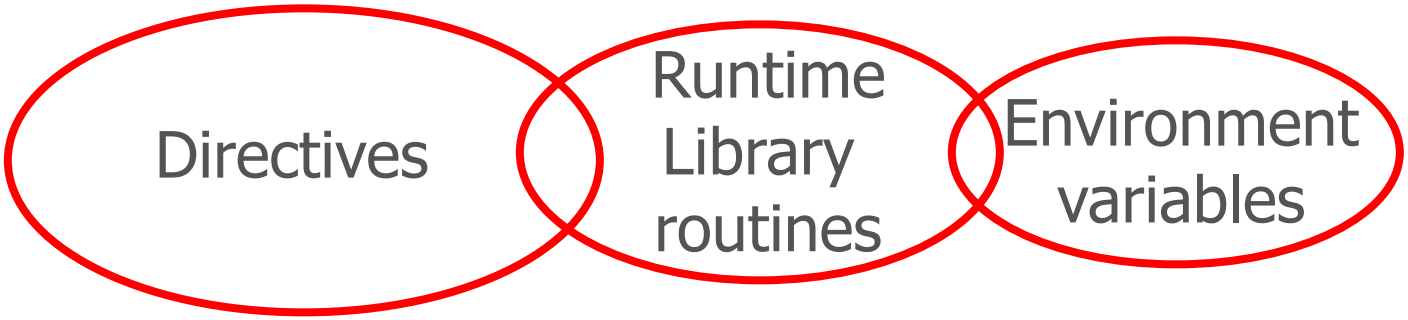
Dual quad-core node



Many-core node (e.g. SGI)



OpenMP basics



- Compiler directives to parallelize
- Fortran – source code comments

```
!$omp parallel/!$omp end parallel
```

- C/C++ - #pragmas

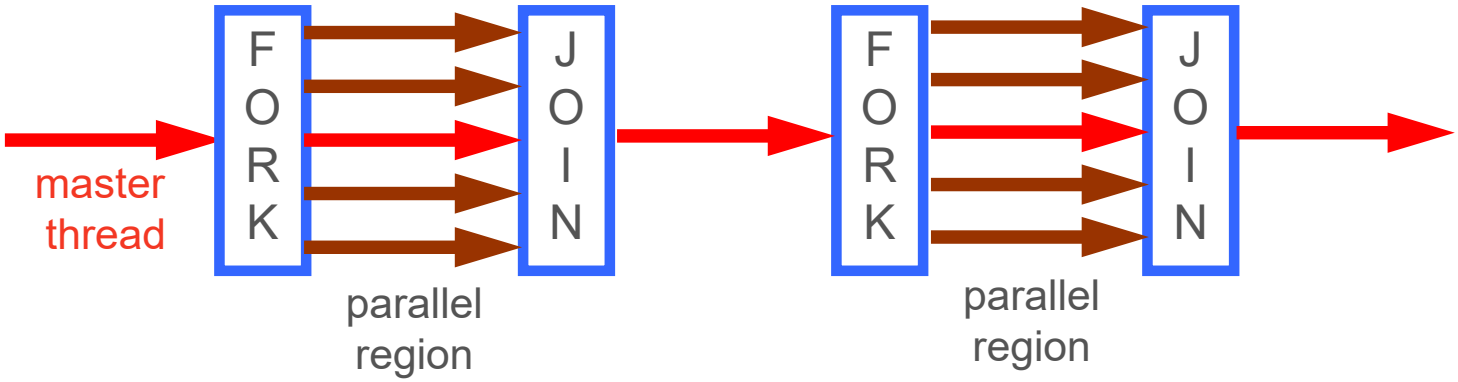
```
#pragma omp parallel
```

- Small set of subroutines, environment variables

```
!$  iam = omp_get_num_threads()
OMP_NUM_THREADS=4
```

Programming model

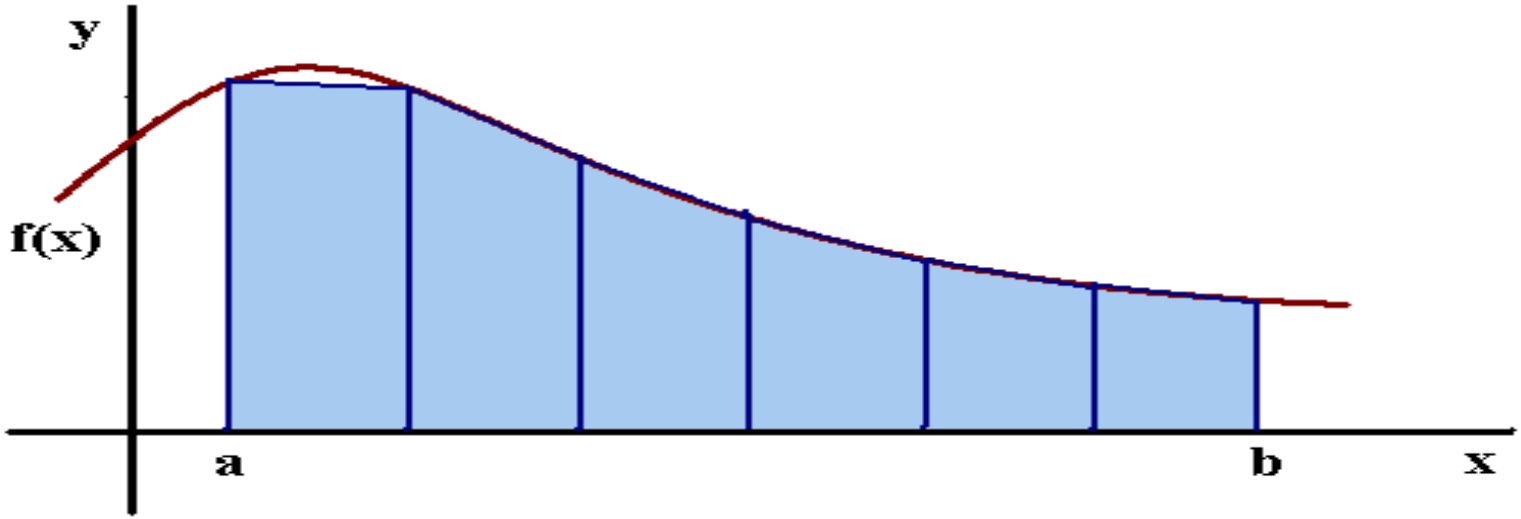
- Shared memory, thread based parallelism
- Explicit parallelism
- Nested parallelism support
- Fork-join model



Example 1 – numerical integration

$$\int_a^b f(x) \approx \sum_{i=1}^{n} \frac{1}{2} h\left[f(x_{i-1}) + f(x_i)\right] =$$

$$\frac{1}{2} h\left[f(x_0) + f(x_n)\right] + \sum_{i=1}^{n-1} h\left[f(x_i)\right]$$



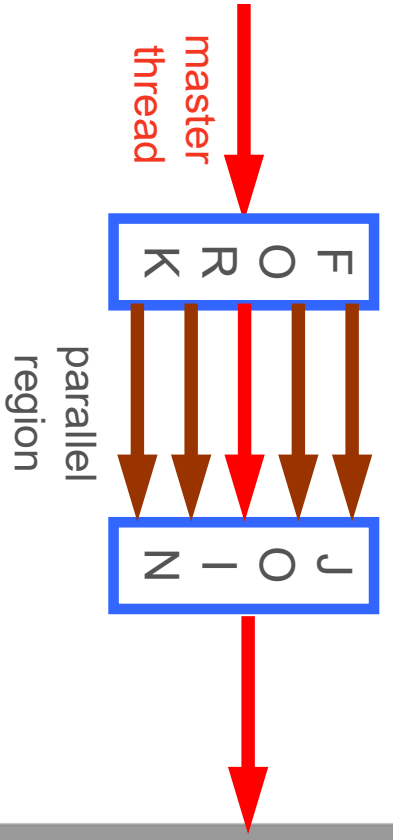
Program code

```
      program trapezoid
       integer n, i
       double precision a, b, h, x, integ, f
```

1.
```
       print*,"Input integ. interval, no. of trap:"
       read(*,*)a, b, n
       h = (b-a)/n
       integ = 0.
```

2.
```
!$omp parallel do reduction(+:integ) private(x)
       do i=1,n-1
          x = a+i*h
          integ = integ + f(x)
       enddo
```

3.
```
       integ = integ + (f(a)+f(b))/2.
       integ = integ*h
       print*,"Total integral = ",integ
       end
```



Program output

```
lp001:>%module load gcc
lp001:>%gfortran -fopenmp trap.f -o
  trap
lp001:>%setenv OMP_NUM_THREADS 12
lp001:>%trap
Input integ. interval, no. of trap:
0 10 100
 Total integral =    333.350000000001
```

Parallel do directive

- Fortran

```
!$omp parallel do [clause [, clause]]
[!$omp end parallel do]
```

- C/C++

```
#pragma omp parallel for [clause [clause]]
```

- Loops must have precisely determined *trip count*
  - no do-while loops
  - no change to loop indices, bounds inside loop (C)
  - no jumps out of the loop (Fortran – exit, goto; C – break, goto)
  - cycle (Fortran), continue (C) are allowed
  - stop (Fortran), exit (C) are allowed

Clauses

- Control execution of parallel loop

- scope `(shared, private)`
  sharing of variables among the threads
- `if`
  whether to run in parallel or in serial
- `schedule`
  distribution of work across the threads
- `collapse(n)`
  combine nested loops into a single loop for more parallelism
- `ordered`
  perform loop in certain order
- `copyin`
  initialize private variables in the loop

Data sharing

- `private` – each thread creates a private instance
- not initialized upon entry to parallel region
  undefined upon exit from parallel region
- default for loop indices, variables declared inside parallel loop
- `shared` – all threads share one copy
- update modifies data for all other threads
- default everything else
- Changing default behavior
- `default (shared | private | none)`

Data reduction

- Threads distribute work
- Need to collect work at the end
  - sum up total
  - find minimum or maximum
- Reduction clause – global operation on a variable

```
!$omp parallel do reduction(+:var)
#pragma omp parallel for reduction(+:var)
```

- Allowed operations - commutative
  - +, *, max, min, logical

Data dependence

- Data in one loop iteration often depend on data written in another loop iteration
- Anti-dependence

```
x = a(i)
b(i) = c + x
```

  race between statement S_1 writing and S_2 reading
  - removal: privatization
- Output dependence

  values from the last iteration used outside the loop
  - removal: `lastprivate` clause
- Flow dependence

```
a(i) = a(i+1) + x
```

  data at one iteration depend on data from another iteration
  - removal: reduction, rearrangement, often impossible

Removing data dependencies

- Serial trapezoidal rule

```
integ = 0.
do i=1,n-1
   x = a+i*h
   integ = integ + f(x)
enddo
```

x – anti-dependence – privatization
integ – flow dependence - reduction

Thread 1	Thread 2
x=a+i*h	x=a+i*h
integ=integ+f(x)	integ=integ+f(x)

- Parallel solution

```
integ = 0.
!$omp parallel do private(x) reduction (+:integ)
   do i=1,n-1
      x = a+i*h
      integ = integ + f(x)
   enddo
```

Variable initialization and finalization

- `firstprivate/lastprivate` clause
  - initialization of a private variable

```
!$omp parallel do firstprivate(x)
```

  - finalization of a private variable

```
!$omp parallel do lastprivate(x)
```

Parallel overhead

- Parallelization costs CPU time
- Nested loops

  parallelize the outermost loop
- `if` clause

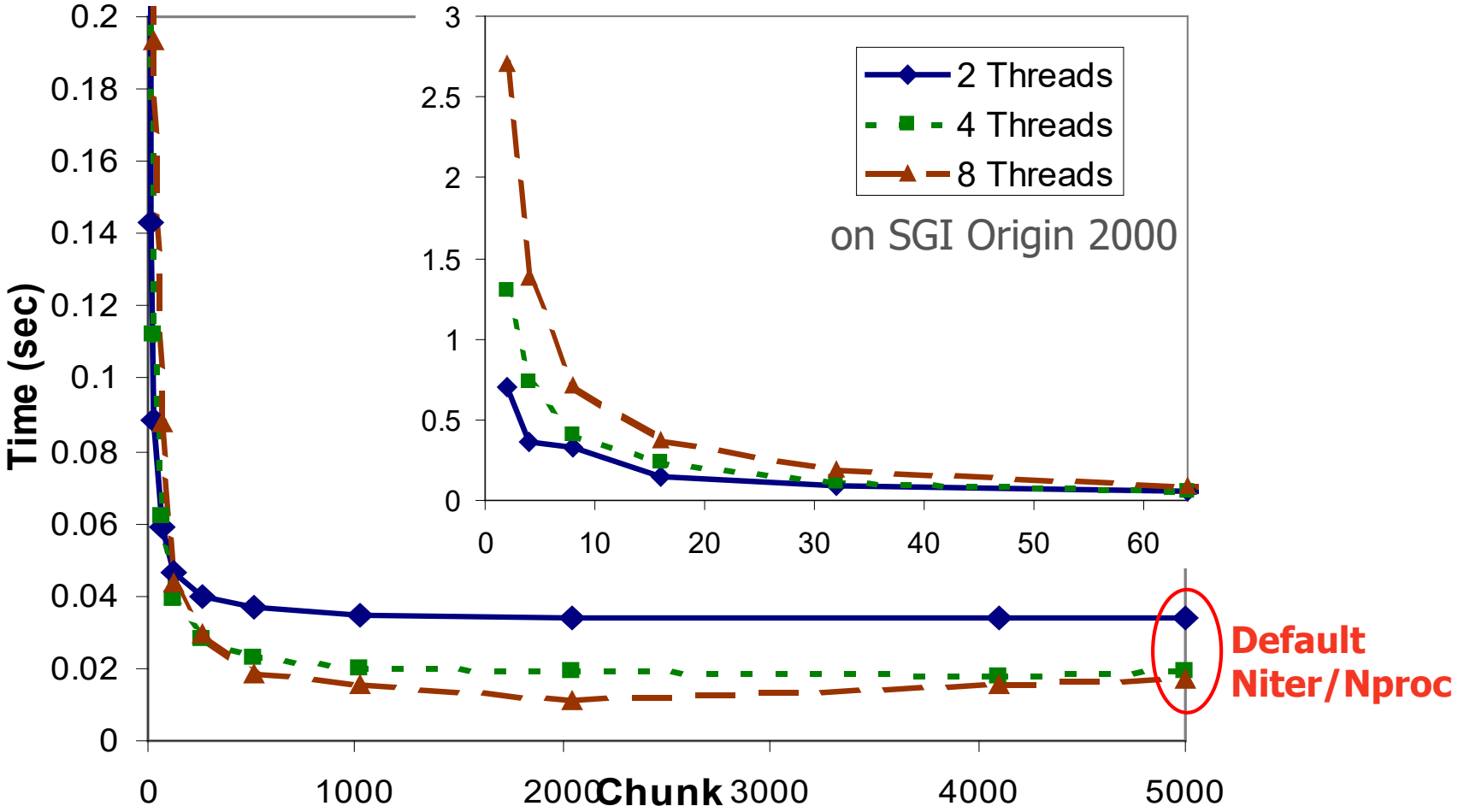
  parallelize only when it is worth it – above certain number of iterations:

```
!$omp parallel do if (n .ge. 800)
  do i = 1, n
     ...
  enddo
```

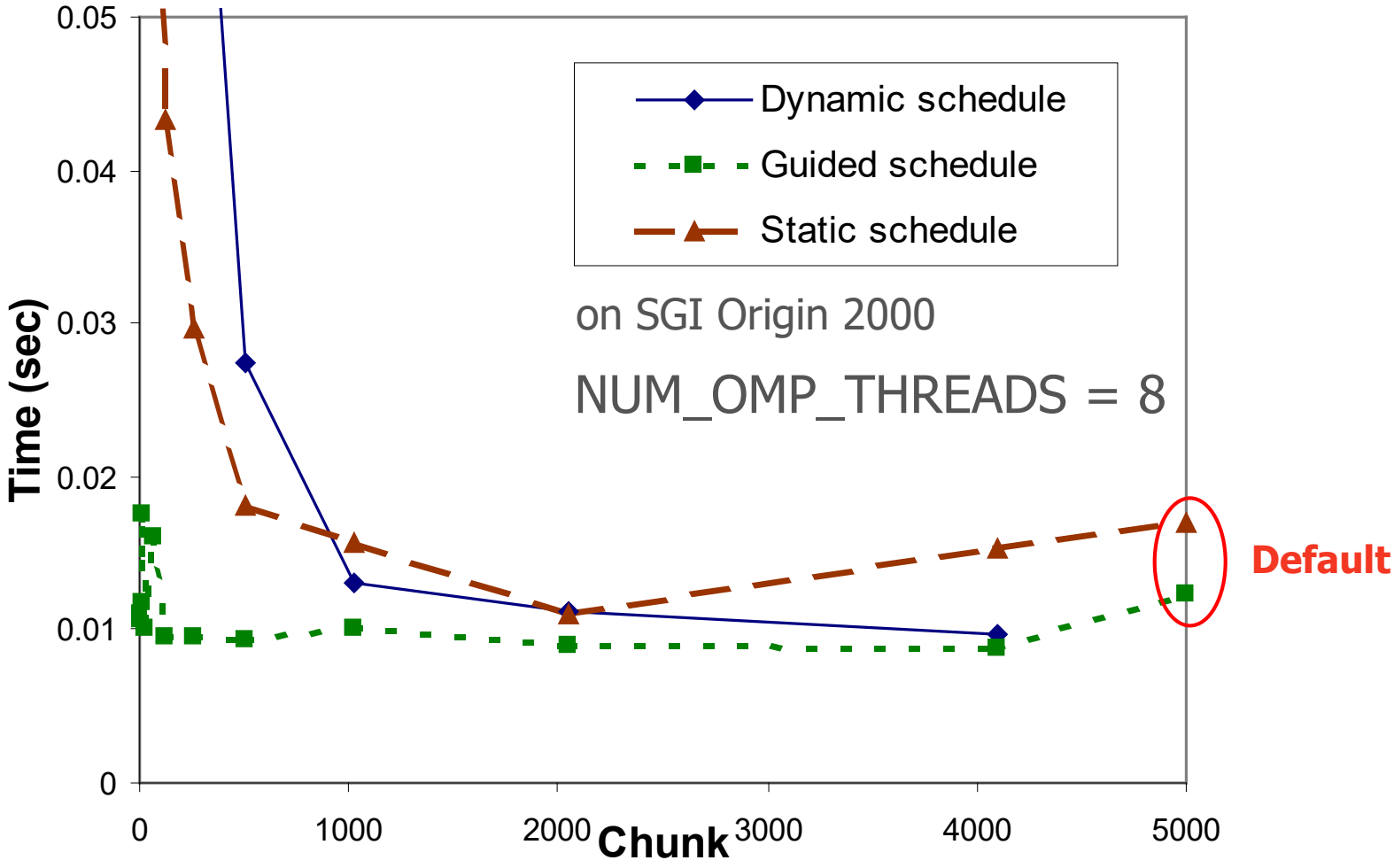
Load balancing – scheduling

- user-defined work distribution
  `schedule (type[, chunk])`
- `chunk` – number of iterations contiguously assigned to threads
- `type`
  - `static` – each thread gets a constant chunk
  - `dynamic` – work distribution to threads varies
  - `guided` – chunk size exponentially decreases
  - `runtime` – schedule decided at the run time

Static schedule timings



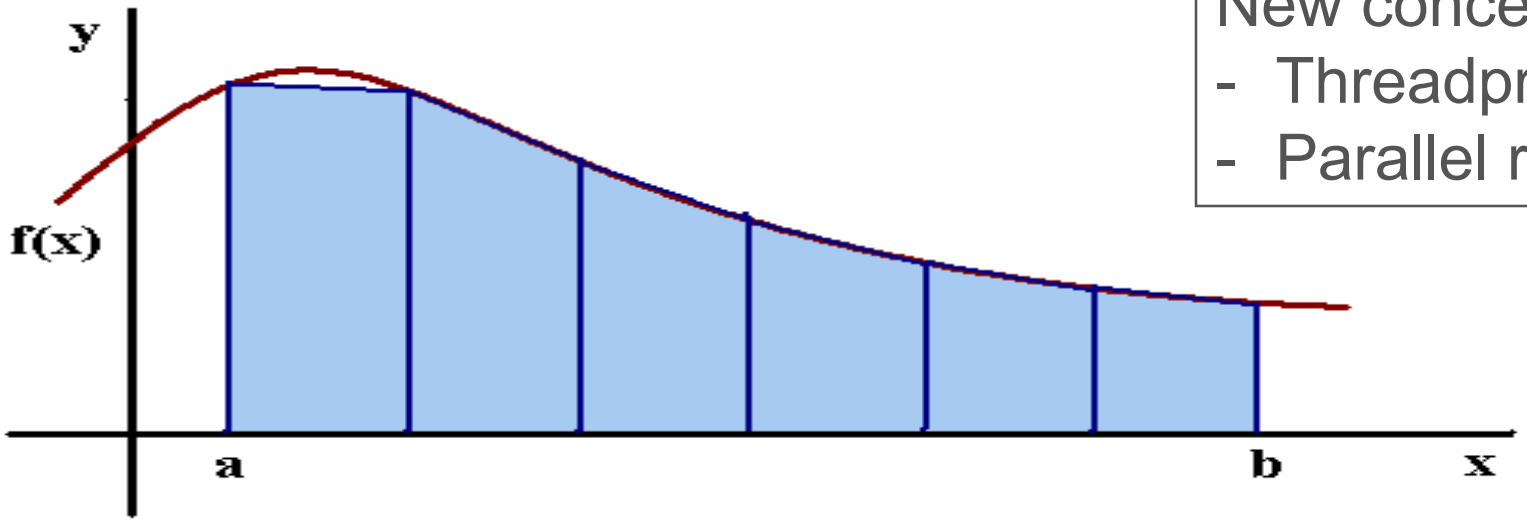
Different schedule timings



Example 2 numerical integration

$$\int_a^b f(x) \approx \sum_{i=1}^{n} \frac{1}{2} h\left[f(x_{i-1}) + f(x_i)\right] =$$

$$\frac{1}{2} h\left[f(x_0) + f(x_n)\right] + \sum_{i=1}^{n-1} h\left[f(x_i)\right]$$



New concepts:
- Threadprivate
- Parallel regions

Example 2
MPI-like parallelization

```
#include <stdio.h>
#include "omp.h"
#define min(a,b) ((a) < (b) ? (a) : (b))

int istart,iend;
#pragma omp threadprivate(istart,iend)

int main (int argc, char* argv[]){
int n,nthreads,iam,chunk; float a, b;
double h, integ, p_integ;
double f(double x);
double get_integ(double a, double h);

printf("Input integ. interval, no. of trap:\n");
scanf("%f %f %d",&a,&b,&n);
h = (b-a)/n;
integ = 0.;
```

1. istart, iend – global variables

f, get_integ – local functions

2.

Example 2, cont.

```
3.  #pragma omp parallel shared(integ)
    private(p_integ,nthreads,iam,chunk){
    nthreads = omp_get_num_threads();
    iam = omp_get_thread_num();
    chunk = (n + nthreads -1)/nthreads;
    istart = iam * chunk + 1;
    iend = min((iam+1)*chunk+1,n);

4.  p_integ = get_integ(a,h);

5.  #pragma omp atomic
       integ += p_integ;
    }
6.  integ += (f(a)+f(b))/2.;
    integ *= h;
    printf("Total integral = %f\n",integ);
    return 0;}
```

parallel section, explicit computation distribution

istart, iend – threadprivate global variables

function call with global variables inside

explicit reduction via mutual exclusion (atomic is faster but only works on one operation)

Example 2, cont.

```
double get_integ(double a, double h)
{
int i;
double sum,x;

sum = 0;
for (i=istart;i<iend;i++)
{
   x = a+i*h;
   sum += f(x);
}
return sum;
}
```

istart, iend – threadprivate global variables

Parallel regions

- Fortran

```
!$omp parallel … !$omp end parallel
```

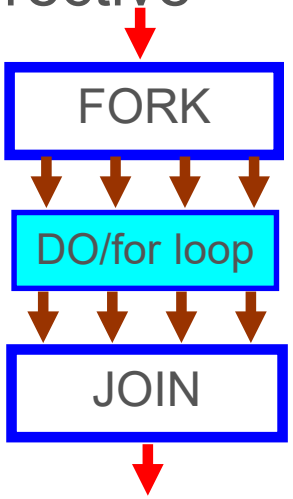
- C/C++

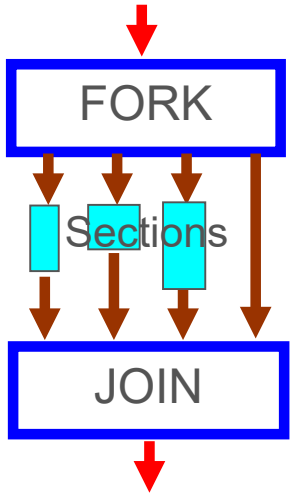
```
#pragma omp parallel
```

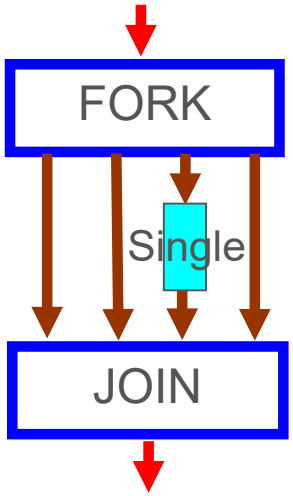
- SPMD parallelism – replicated execution
- must be a self-contained block of code – 1 entry, 1 exit
- implicit barrier at the end of parallel region
- can use the same clauses as in `parallel do/for`

Work-sharing constructs

- DO/for loop – distributes loop - `do` directive
- Sections – breaks work into separate, discrete sections - `section` directive
- Workshare – parallel execution of separate units of work - `workshare` directive
- Single/master – serialized section of code - `single` directive







Work-sharing cont.

- Restrictions:
  - continuous block; no nesting
  - all threads must reach the same construct
  - constructs can be outside lexical scope of the parallel construct (e.g. subroutine)

threadprivate variables

- global/common block variables are private only in lexical scope of the parallel region
- possible solutions
  - pass private variables as function arguments
  - use `threadprivate` – identifies common block/global variable as private
  - `!$omp threadprivate (/cb/ [,/cb/] …)`

    `#pragma omp threadprivate (list)`
  - use `copyin` clause to initialize the `threadprivate` variable

e.g. `!$omp parallel copyin(istart,iend)`

Mutual exclusion

- `critical` section
  - limit access to the part of the code to one thread at the time

```
!$omp critical [name]
...
!$omp end critical [name]
```

- `atomic` section
  - atomically updating single memory location

```
sum += x
```

- also available via runtime library functions

`task` construct

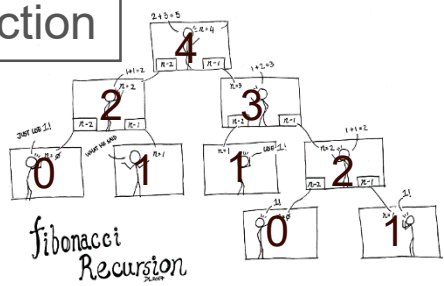
- Used to parallelize irregular, recursive algorithms
- All tasks run independent of each other in parallel, on up to OMP_NUM_THREADS
- Use `taskwait` to wait for all tasks to finish
- Each task has its own data space – use `mergeable` for shared variables to reduce storage needs
- Use `depend` to specify data dependencies
- Often started from `serial` section

task example

- Calculate Fibonacci number using recursion

```
int fib(int n) {
int i, j;
if (n<2) return n;
else {
  #pragma omp task shared(i)
    i=fib(n-1);
  #pragma omp task shared(j)
    j=fib(n-2);
  #pragma omp taskwait
return i+j;
}
#pragma omp parallel {
  #pragma omp single {
  fibn = fib(n); }}
```

recursive function



independent task #1

independent task #2

wait till completion of both tasks

main program – need to start parallel section in which the tasks will run

Event synchronization

- barrier - `!$omp barrier`
  - synchronizes all threads at that point
- ordered - `!$omp ordered`
  - imposes order across iterations of a parallel loop
- master - `!$omp master`
  - sets block of code to be executed only on the master thread
- flush - `!$omp flush`
  - synchronizes memory and cache on all threads

Library functions, environmental variables

- thread set/inquiry

```
omp_set_num_threads(integer)
OMP_NUM_THREADS
integer omp_get_num_threads()
integer omp_get_max_threads()
integer omp_get_thread_num()
```

- set/query dynamic thread adjustment

```
omp_set_dynamic(logical)
OMP_DYNAMIC
logical omp_get_dynamic()
```

Library functions, environmental variables

- lock/unlock functions

```
omp_init_lock()
omp_set_lock()
omp_unset_lock()
logical omp_test_lock()
omp_destroy_lock()
```

- other

```
integer omp_get_num_procs()
logical omp_in_parallel()

OMP_SCHEDULE
```

Advanced OpenMP

- nested parallel loops
- accelerator support (4.0)
- user defined reduction (4.0)
- thread affinity (4.0)
- SIMD (=vectorization) (4.0)

Summary

- parallel do/for loops
- variable scope, reduction
- parallel overhead, loop scheduling
- parallel regions
- mutual exclusion
- work sharing, tasking
- synchronization

`http://www.chpc.utah.edu/short_courses/intro_openmp`

References

- Spec

http://www.openmp.org/

- Books

Chapman, Jost, van der Pas – Using OpenMP

Pacheco – Introduction to Parallel Computing

- Wednesday 11/3, 9am-3pm - XSEDE Monthly Workshop – OpenMP
- XSEDE online training https://www.xsede.org/web/xup/online-training