

# The OpenMP\* Common Core: A hands on exploration

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Notice revision #20110804

## **Preliminaries: Systems for exercises**

- Blue Gene Q ssh <<login\_name>>@vesta.alcf.anl.gov

Use either system or even your laptop if you wish

- X86 cluster ssh <<login\_name>>@cooley.alcf.anl.gov
- The OpenMP compiler

Add the line to ".soft.cooley" and then run the resoft command

+intel-composer-xe icc –qopenmp –O3 << file names>>

Note: the gcc compiler works for OpenMP on Cooley: gcc –fopenmp <<file names>>

- Copy the exercises to your home directory
   \$ cp /projects/ATPESC2018/OMP\_Exercises
- You can just run on the login nodes or use qsub (to get good timing numbers)
- To get a single node for 30 minutes in interactive mode qsub –A ATPESC2018 –n 1 –t 30 -lk

## **Preliminaries: Part 1**

#### Disclosures

- The views expressed in this tutorial are those of the people delivering the tutorial.
  - We are <u>not</u> speaking for our employers.
  - We are not speaking for the OpenMP ARB
- We take these tutorials VERY seriously:
  - Help us improve ... tell us how you would make this tutorial better.

## **Preliminaries: Part 2**

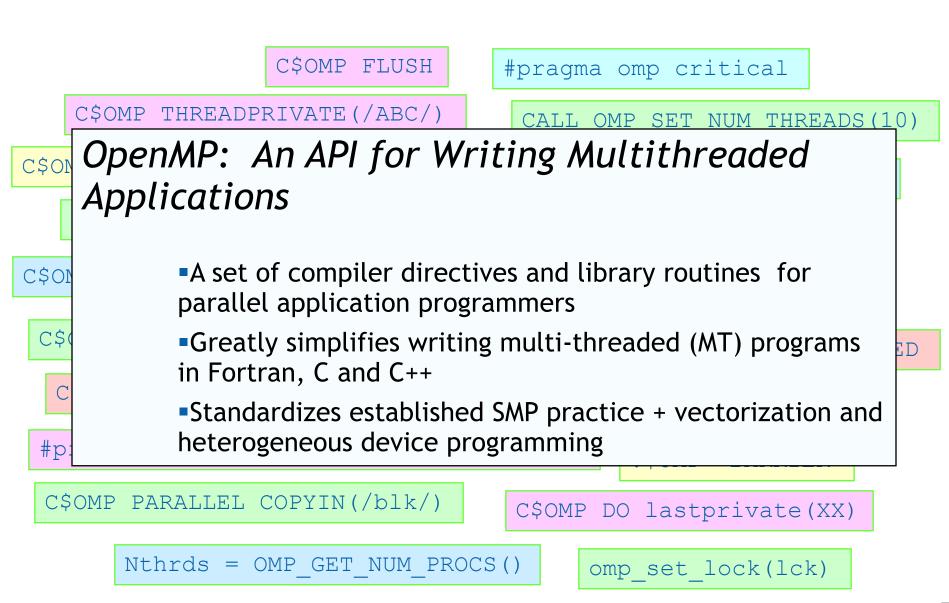
- Our plan for the day .. Active learning!
  - We will mix short lectures with short exercises.
  - You will use your laptop to connect to a multiprocessor server.
- Please follow these simple rules
  - Do the exercises that we assign and then change things around and experiment.
    - Embrace active learning!
  - -Don't cheat: Do Not look at the solutions before you complete an exercise ... even if you get really frustrated.

## **Outline**



- Introduction to OpenMP
  - Creating Threads
  - Synchronization
  - Parallel Loops
  - Data environment
  - Memory model
  - Irregular Parallelism and tasks
  - Recap
  - Beyond the common core:
    - Worksharing revisited
    - Synchronization: More than you ever wanted to know
    - Thread private data

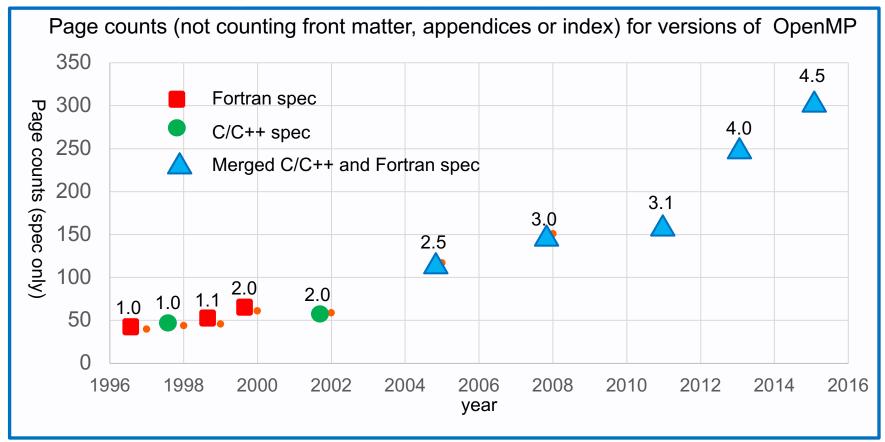
# OpenMP\* overview:



<sup>\*</sup> The name "OpenMP" is the property of the OpenMP Architecture Review Board.

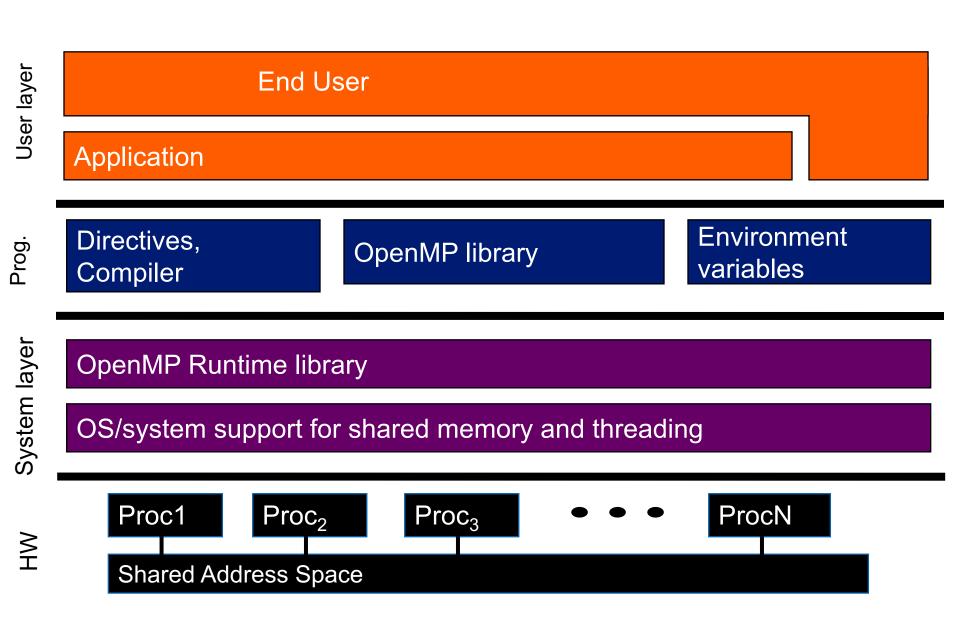
# The growth of complexity in OpenMP

- OpenMP started out in 1997 as a simple interface for application programmers more versed in their area of science than computer science.
- The complexity has grown considerably over the years!



The full spec is overwhelming. Master the 19 constructs OpenMP programmers use all the time (**OpenMP Common Core**), then dive into the rest of the spec. as needed.

## **OpenMP basic definitions:** Basic Solution stack



This is for common-core OpenMP. NUMA and GPU support was added later

# **OpenMP** basic syntax

- Most of the constructs in OpenMP are compiler directives.
   #pragma omp construct [clause [clause]...]
  - Example#pragma omp parallel private(x)
- Function prototypes and types in the file:
   #include <omp.h>

- Most OpenMP\* constructs apply to a "structured block".
  - Structured block: a block of one or more statements with one point of entry at the top and one point of exit at the bottom.
  - It's OK to have an exit() within the structured block.

## **Exercise, Part A: Hello world**

## Verify that your environment works

Write a program that prints "hello world".

```
#include<stdio.h>
int main()
   printf(" hello ");
   printf(" world \n");
```

## **Exercise, Part B: Hello world**

## Verify that your OpenMP environment works

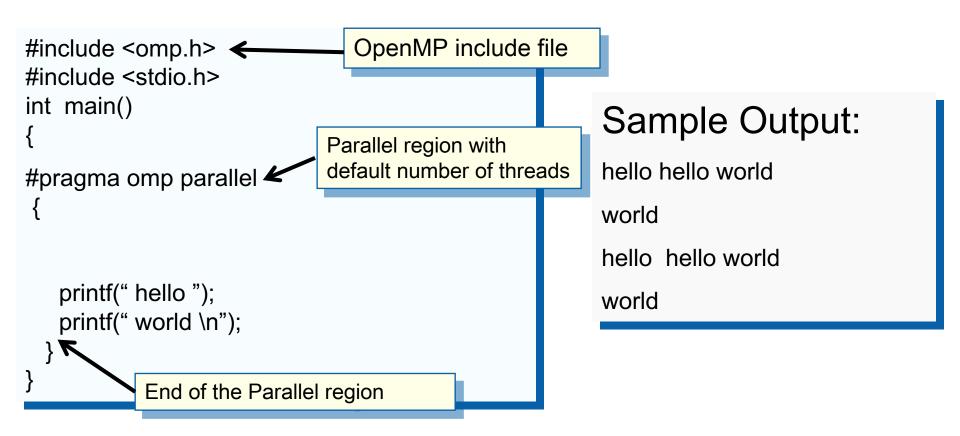
Write a multithreaded program that prints "hello world".

```
Switches for compiling and linking
#include <omp.h>
#include <stdio.h>
                          gcc -fopenmp
                                               Gnu (Linux, OSX)
int main()
                                               PGI (Linux)
                          pgcc -mp pgi
 #pragma omp parallel
                          icl /Qopenmp
                                               Intel (windows)
                                               Intel (Linux, OSX)
                          icc -fopenmp
  printf(" hello ");
  printf(" world \n");
```

## **Solution**

## A multi-threaded "Hello world" program

Write a multithreaded program where each thread prints "hello world".



The statements are interleaved based on how the operating schedules the threads

## **Outline**

Introduction to OpenMP

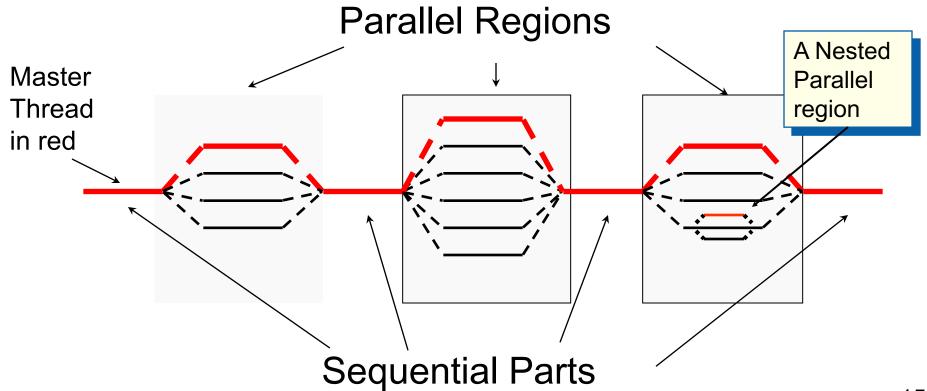


- Creating Threads
  - Synchronization
  - Parallel Loops
  - Data environment
  - Memory model
  - Irregular Parallelism and tasks
  - Recap
  - Beyond the common core:
    - Worksharing revisited
    - Synchronization: More than you ever wanted to know
    - Thread private data

# **OpenMP programming model:**

## Fork-Join Parallelism:

- Master thread spawns a team of threads as needed.
- Parallelism added incrementally until performance goals are met,
   i.e., the sequential program evolves into a parallel program.



# **Thread creation: Parallel regions**

- You create threads in OpenMP\* with the parallel construct.
- For example, To create a 4 thread Parallel region:

Each thread executes a copy of the code within the structured block

```
double A[1000];
omp_set_num_threads(4);
#pragma omp parallel
{
    int ID = omp_get_thread_num();
    pooh(ID,A);
}
Runtime function to request a certain number of threads

Runtime function request a certain number of threads
```

Each thread calls pooh(ID,A) for ID = 0 to 3

# Thread creation: Parallel regions example

 Each thread executes the same code redundantly.

```
double A[1000];

|
omp_set_num_threads(4)
```

```
double A[1000];
omp_set_num_threads(4);
#pragma omp parallel
{
   int ID = omp_get_thread_num();
   pooh(ID, A);
}
printf("all done\n");
```

before proceeding (i.e., a *barrier*)

A single copy of A is shared between all threads.

printf("all done\n"); Threads wait here for all threads to finish

\* The name "OpenMP" is the property of the OpenMP Architecture Review Board

## Thread creation: How many threads did you actually get?

- Request a number of threads with omp\_set\_num\_threads()
- The number requested may not be the number you actually get.
  - An implementation may silently give you fewer threads than you requested.
  - Once a team of threads has launched, it will not be reduced.

Each thread executes a copy of the code within the structured block

```
double A[1000];
omp_set_num_threads(4);
#pragma omp parallel
{
    int ID = omp_get_thread_num();
    int nthrds = omp_get_num_threads();
    pooh(ID,A);
}
Runtime function to request a certain number of threads

**Runtime function to return actual**

Runtime function to return actual

**Runtime function to return actual**

**Runtime function func
```

Each thread calls pooh(ID,A) for ID = 0 to nthrds-1

1

number of threads

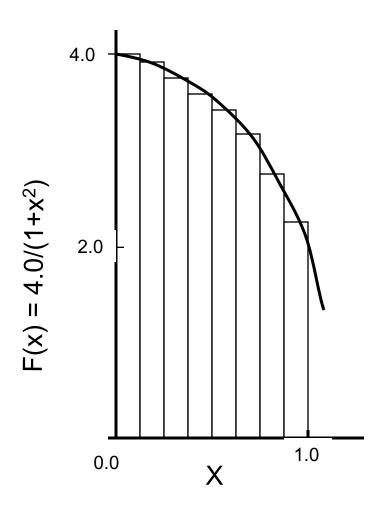
in the team

#### Internal control variables & the number of threads

- There are a few ways to control the number of threads.
  - omp\_set\_num\_threads(4)
- What does omp\_set\_num\_threads() actually do?
  - It <u>resets</u> an "<u>internal control variable</u>" the system queries to select the default number of threads to request on subsequent parallel constructs.
- To change this internal control variable without re-compilation.
  - When an OpenMP program starts up, it queries an environment variable OMP\_NUM\_THREADS and sets the appropriate <u>internal control variable</u> to the value of OMP\_NUM\_THREADS
- For example, to set the initial, default number of threads to request in OpenMP from my apple laptop
  - > export OMP\_NUM\_THREADS=12

# An interesting problem to play with

## **Numerical integration**



Mathematically, we know that:

$$\int_{0}^{1} \frac{4.0}{(1+x^2)} dx = \pi$$

We can approximate the integral as a sum of rectangles:

$$\sum_{i=0}^{N} F(x_i) \Delta x \approx \pi$$

Where each rectangle has width  $\Delta x$  and height  $F(x_i)$  at the middle of interval i.

# Serial PI program

```
static long num steps = 100000;
double step;
int main ()
         int i; double x, pi, sum = 0.0;
         step = 1.0/(double) num steps;
         for (i=0;i < num steps; i++){
                 x = (i+0.5)*step;
                 sum = sum + 4.0/(1.0+x*x);
         pi = step * sum;
```

# Serial PI program

```
#include <omp.h>
static long num steps = 100000;
double step;
int main ()
         int i; double x, pi, sum = 0.0;
         step = 1.0/(double) num steps;
                                               The library routine
         double tdata = omp_get_wtime();
         for (i=0;i < num steps; i++){
                                                get_omp_wtime()
                                                is used to find the
                 x = (i+0.5)*step;
                 sum = sum + 4.0/(1.0+x*x);
                                                  elapsed "wall
                                                time" for blocks of
         pi = step * sum;
                                                      code
         tdata = omp_get_wtime() - tdata;
         printf(" pi = %f in %f secs\n",pi, tdata);
```

## **Exercise: the parallel Pi program**

 Create a parallel version of the pi program using a parallel construct:

#pragma omp parallel.

- Pay close attention to shared versus private variables.
- In addition to a parallel construct, you will need the runtime library routines
  - int omp\_get\_num\_threads();
  - int omp\_get\_thread\_num();–
  - double omp\_get\_wtime();
  - omp\_set\_num\_threads();

Request a number of threads in the team

Number of threads in the team

Thread ID or rank

Time in Seconds since a fixed point in the past

# Hints: the Parallel Pi program

- Use a parallel construct: #pragma omp parallel
- The challenge is to:
  - divide loop iterations between threads (use the thread ID and the number of threads).
  - Create an accumulator for each thread to hold partial sums that you can later combine to generate the global sum.
- In addition to a parallel construct, you will need the runtime library routines
  - int omp\_set\_num\_threads();
  - int omp\_get\_num\_threads();
  - int omp\_get\_thread\_num();
  - double omp\_get\_wtime();

## **Example: A simple SPMD pi program**

```
Promote scalar to an array
#include <omp.h>
                                                                   dimensioned by number of
static long num_steps = 100000;
                                         double step;
                                                                   threads to avoid race
                                                                   condition.
#define NUM_THREADS 2
void main ()
           int i, nthreads; double pi, sum[NUM_THREADS];
           step = 1.0/(double) num_steps;
           omp_set_num_threads(NUM_THREADS);
  #pragma omp parallel
          int i, id,nthrds;
                                                          Only one thread should copy the
         double x;
                                                          number of threads to the global
                                                          value to make sure multiple threads
         id = omp_get_thread_num();
                                                           writing to the same address don't
         nthrds = omp_get_num_threads();
                                                          conflict.
         if (id == 0) nthreads = nthrds;
           for (i=id, sum[id]=0.0;i< num_steps; i=i+nthrds) {
                    x = (i+0.5)*step;
                                                               This is a common trick in
                    sum[id] += 4.0/(1.0+x*x);
                                                               SPMD programs to create a
                                                               cyclic distribution of loop
                                                               iterations
           for(i=0, pi=0.0;i<nthreads;i++)pi += sum[i] * step;
```

# SPMD: Single Program Mulitple Data

- Run the same program on P processing elements where P can be arbitrarily large.
- Use the rank ... an ID ranging from 0 to (P-1) ... to select between a set of tasks and to manage any shared data structures.

This pattern is very general and has been used to support most (if not all) the algorithm strategy patterns.

MPI programs almost always use this pattern ... it is probably the most commonly used pattern in the history of parallel programming.

## Results\*

Original Serial pi program with 100000000 steps ran in 1.83 seconds.

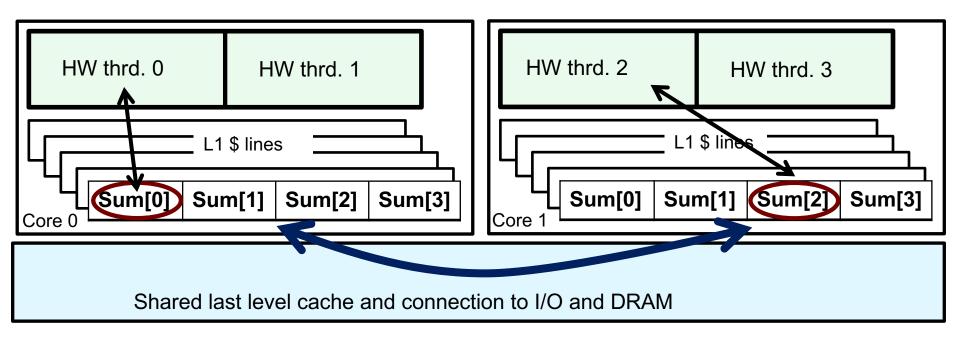
```
Example: A simple Parallel pi program
#include <omp.h>
static long num_steps = 100000;
                                 double step:
#define NUM_THREADS 2
void main ()
                                                                            1st
                                                           threads
         int i, nthreads; double pi, sum[NUM_THREADS];
         step = 1.0/(double) num_steps;
                                                                        SPMD*
         omp_set_num_threads(NUM_THREADS);
  #pragma omp parallel
                                                                          1.86
        int i, id,nthrds;
                                                                          1.03
        double x:
        id = omp get thread num();
                                                               3
                                                                          1.08
        nthrds = omp get num threads();
        if (id == 0) nthreads = nthrds;
                                                               4
                                                                          0.97
         for (i=id, sum[id]=0.0;i< num_steps; i=i+nthrds) {
                 x = (i+0.5)*step;
                 sum[id] += 4.0/(1.0+x*x);
         for(i=0, pi=0.0;i<nthreads;i++)pi += sum[i] * step;
```

\*SPMD: Single Program Multiple Data

<sup>\*</sup>Intel compiler (icpc) with no optimization on Apple OS X 10.7.3 with a dual core (four HW thread) Intel® Core™ i5 processor at 1.7 Ghz and 4 Gbyte DDR3 memory at 1.333 Ghz.

# Why such poor scaling? False sharing

• If independent data elements happen to sit on the same cache line, each update will cause the cache lines to "slosh back and forth" between threads ... This is called "false sharing".



- If you promote scalars to an array to support creation of an SPMD program, the array elements are contiguous in memory and hence share cache lines ... Results in poor scalability.
- Solution: Pad arrays so elements you use are on distinct cache lines.

## **Example:** Eliminate false sharing by padding the sum array

```
#include <omp.h>
static long num_steps = 100000; double step;
#define PAD 8 // assume 64 byte L1 cache line size
#define NUM_THREADS 2
void main ()
         int i, nthreads; double pi, sum[NUM_THREADS][PAD];
         step = 1.0/(double) num_steps;
         omp_set_num_threads(NUM_THREADS);
  #pragma omp parallel
                                                     Pad the array so
        int i, id,nthrds;
                                                     each sum value is
        double x;
                                                       in a different
        id = omp_get_thread_num();
                                                        cache line
        nthrds = omp_get_num_threads();
        if (id == 0) nthreads = nthrds;
         for (i=id, sum[id]=0.0;i< num_steps; i=i+nthrds) {
                x = (i+0.5)*step;
                sum[id][0] += 4.0/(1.0+x*x);
         for(i=0, pi=0.0; i < nthreads; i++)pi += sum[i][0] * step;
```

## Results\*: pi program padded accumulator

Original Serial pi program with 100000000 steps ran in 1.83 seconds.

```
Example: eliminate False sharing by padding the sum array
#include <omp.h>
static long num_steps = 100000;
                                 double step;
#define PAD 8
                        // assume 64 byte L1 cache line size
#define NUM THREADS 2
void main ()
                                                                                1st
         int i, nthreads; double pi, sum[NUM_THREADS][PAD];
                                                                threads
                                                                                             1st
         step = 1.0/(double) num_steps;
                                                                             SPMD
                                                                                          SPMD
         omp set num threads(NUM THREADS);
                                                                                          padded
  #pragma omp parallel
                                                                               1.86
                                                                                            1.86
        int i, id.nthrds;
       double x:
                                                                               1.03
                                                                                            1.01
        id = omp_get_thread_num();
       nthrds = omp_get_num_threads();
                                                                    3
                                                                               1.08
                                                                                            0.69
       if (id == 0) nthreads = nthrds;
         for (i=id, sum[id]=0.0;i< num_steps; i=i+nthrds) {
                                                                              0.97
                                                                                            0.53
                 x = (i+0.5)*step;
                 sum[id][0] += 4.0/(1.0+x*x);
         for(i=0, pi=0.0;i<nthreads;i++)pi += sum[i][0] * step;
```

<sup>\*</sup>Intel compiler (icpc) with no optimization on Apple OS X 10.7.3 with a dual core (four HW thread) Intel® Core™ i5 processor at 1.7 Ghz and 4 Gbyte DDR3 memory at 1.333 Ghz.

## **Outline**

- Introduction to OpenMP
- Creating Threads
- Quantifying Performance and Amdahl's law



- Synchronization
  - Parallel Loops
  - Data environment
  - Memory model
  - Irregular Parallelism and tasks
  - Recap
  - Beyond the common core:
    - Worksharing revisited
    - Synchronization: More than you ever wanted to know
    - Threadprivate data

# **Synchronization**

- High level synchronization included in the common core (the full OpenMP specification has MANY more):
  - -critical
  - -barrier

Synchronization is used to impose order constraints and to protect access to shared data

# Synchronization: critical

 Mutual exclusion: Only one thread at a time can enter a critical region.

Threads wait their turn – only one at a time calls consume()

```
float res;
#pragma omp parallel
   float B; int i, id, nthrds;
   id = omp_get_thread_num();
    nthrds = omp_get_num_threads();
    for(i=id;i<niters;i+=nthrds){</pre>
        B = big job(i);
#pragma omp critical
        res += consume (B);
```

# Synchronization: barrier

- Barrier: a point in a program all threads much reach before any threads are allowed to proceed.
- It is a "stand alone" pragma meaning it is not associated with user code ... it is an executable statement.

```
double Arr[8], Brr[8];
                            int numthrds;
omp_set_num_threads(8)
#pragma omp parallel
  int id, nthrds;
   id = omp get thread num();
   nthrds = omp get num threads();
   if (id==0) numthrds = nthrds;
   Arr[id] = big ugly calc(id, nthrds);
#pragma omp barrier
   Brr[id] = really_big_and_ugly(id, nthrds, A);
```

Threads wait until all threads hit the barrier. Then they can go on.

## **Exercise**

- In your first Pi program, you probably used an array to create space for each thread to store its partial sum.
- If array elements happen to share a cache line, this leads to false sharing.
  - Non-shared data in the same cache line so each update invalidates the cache line ... in essence "sloshing independent data" back and forth between threads.
- Modify your "pi program" to avoid false sharing due to the partial sum array.

```
int omp_get_num_threads();
int omp_get_thread_num();
double omp_get_wtime();
omp_set_num_threads();
#pragma parallel
#pragma critical
```

# Pi program with false sharing\*

Original Serial pi program with 100000000 steps ran in 1.83 seconds.

## Example: A simple Parallel pi program

```
#include < omp.h>
static long num_steps = 100000;
                                    double step;
#define NUM_THREADS 2
void main ()
         int i, nthreads; double pi, sum[NUM_THREADS];
         step = 1.0/(double) num_steps;
          omp_set_num_threads(NUM_THREADS);
   #pragma omp parallel
         int i, id,nthrds;
        double x;
        id = omp get thread num();
        nthrds = omp get num threads();
        if (id == 0) nthreads = nthrds;
         for (i=id, sum[id]=0.0;i< num_steps; i=i+nthrds) {
                  x = (i+0.5)*step;
                  sum[id] += 4.0/(1.0+x*x);
         for(i=0, pi=0.0;i<nthreads;i++)pi += sum[i] * step;
```

Recall that promoting sum to an array made the coding easy, but led to false sharing and poor performance.

threads	<b>1</b> st
	SPMD
1	1.86
2	1.03
3	1.08
4	0.97

<sup>\*</sup>Intel compiler (icpc) with no optimization on Apple OS X 10.7.3 with a dual core (four HW thread) Intel® Core<sup>TM</sup> i5 processor at 1.7 Ghz and 4 Gbyte DDR3 memory at 1.333 Ghz.

#### **Example:** Using a critical section to remove impact of false sharing

```
#include <omp.h>
static long num_steps = 100000;
                                    double step;
#define NUM THREADS 2
void main ()
         int nthreads; double pi=0.0;
                                            step = 1.0/(double) num_steps;
         omp_set_num_threads(NUM_THREADS);
#pragma omp parallel
                                                      Create a scalar local
                                                      to each thread to
        int i, id, nthrds; double x, sum,
                                                      accumulate partial
        id = omp_get_thread_num();
                                                      sums.
        nthrds = omp_get_num_threads();
        if (id == 0) nthreads = nthrds;
                                                               No array, so
         for (i=id, sum=0.0;i< num_steps; i=i+nthrds) {
                                                               no false
                  x = (i+0.5)*step;
                                                               sharing.
                  sum += 4.0/(1.0+x*x);
       #pragma omp critical
                                   Sum goes "out of scope" beyond the parallel
              pi += sum * step; region ... so you must sum it in here. Must
                                   protect summation into pi in a critical region so
                                   updates don't conflict
```

### Results\*: pi program critical section

Original Serial pi program with 100000000 steps ran in 1.83 seconds.

```
Example: Using a critical section to remove impact of false sharing
#include <omp.h>
                                   double step:
static long num_steps = 100000;
#define NUM_THREADS 2
void main ()
         int nthreads; double pi=0.0; step = 1.0/(double) num_steps;
         omp_set_num_threads(NUM_THREADS);
#pragma omp parallel
        int i, id, nthrds; double x, sum;
        id = omp_get_thread_num();
        nthrds = omp_get_num_threads();
        if (id == 0) nthreads = nthrds;
          for (i=id, sum=0.0;i< num_steps; i=i+nthrds) {
                  x = (i+0.5)*step;
                  sum += 4.0/(1.0+x*x);
        #pragma omp critical
              pi += sum * step;
```

threads	1 <sup>st</sup>	1 <sup>st</sup>	SPMD
	SPMD	SPMD	critical
		padded	
1	1.86	1.86	1.87
2	1.03	1.01	1.00
3	1.08	0.69	0.68
4	0.97	0.53	0.53

<sup>\*</sup>Intel compiler (icpc) with no optimization on Apple OS X 10.7.3 with a dual core (four HW thread) Intel® Core™ i5 processor at 1.7 Ghz and 4 Gbyte DDR3 memory at 1.333 Ghz.

#### **Example:** Using a critical section to remove impact of false sharing

```
#include <omp.h>
static long num_steps = 100000;
                                    double step;
#define NUM THREADS 2
void main ()
         int nthreads; double pi=0.0; step = 1.0/(double) num_steps;
         omp_set_num_threads(NUM_THREADS);
#pragma omp parallel
                                                        Be careful where
                                                        you put a critical
        int i, id,nthrds; double x;
                                                        section
        id = omp_get_thread_num();
        nthrds = omp_get_num_threads();
        if (id == 0) nthreads = nthrds;
         for (i=id, sum=0.0;i< num_steps; i=i+nthreads){
                                                         What would happen if
                  x = (i+0.5)*step;
                                                         you put the critical
                  #pragma omp critical
                                                         section inside the
                      pi += 4.0/(1.0+x*x);
                                                         loop?
  *= step;
```

#### **Outline**

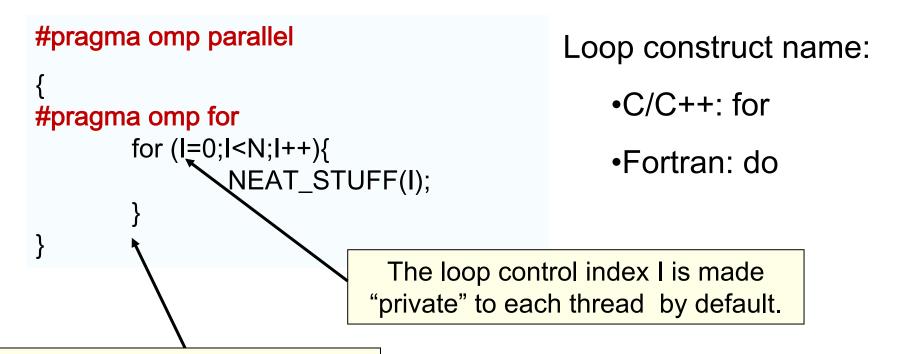
- Introduction to OpenMP
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- Synchronization



- Parallel Loops
  - Data environment
  - Memory model
  - Irregular Parallelism and tasks
  - Recap
  - Beyond the common core:
    - Worksharing revisited
    - Synchronization: More than you ever wanted to know
    - Threadprivate data

#### The loop worksharing constructs

 The loop worksharing construct splits up loop iterations among the threads in a team



Threads wait here until all threads are finished with the parallel loop before any proceed past the end of the loop

# Loop worksharing constructs

#### A motivating example

Sequential code

```
for(i=0;i<N;i++) { a[i] = a[i] + b[i];}
```

OpenMP parallel region

```
#pragma omp parallel
{
    int id, i, Nthrds, istart, iend;
    id = omp_get_thread_num();
    Nthrds = omp_get_num_threads();
    istart = id * N / Nthrds;
    iend = (id+1) * N / Nthrds;
    if (id == Nthrds-1)iend = N;
    for(i=istart;i<iend;i++) { a[i] = a[i] + b[i];}
}</pre>
```

OpenMP parallel region and a worksharing for construct

```
#pragma omp parallel
#pragma omp for
for(i=0;i<N;i++) { a[i] = a[i] + b[i];}</pre>
```

# Loop worksharing constructs: The schedule clause

- The schedule clause affects how loop iterations are mapped onto threads
  - schedule(static [,chunk])
    - Deal-out blocks of iterations of size "chunk" to each thread.
  - schedule(dynamic[,chunk])
    - Each thread grabs "chunk" iterations off a queue until all iterations have been handled.
  - #pragma omp for schedule(dynamic, CHUNK)

Schedule Clause	When To Use	
STATIC	Pre-determined and predictable by the programmer	
DYNAMIC	Unpredictable, highly variable work per iteration	

Least work at runtime: scheduling done at compile-time

Most work at runtime: complex scheduling logic used at run-time

## Combined parallel/worksharing construct

 OpenMP shortcut: Put the "parallel" and the worksharing directive on the same line

```
double res[MAX]; int i;
#pragma omp parallel
{
    #pragma omp for
    for (i=0;i< MAX; i++) {
        res[i] = huge();
    }
}</pre>
```

```
double res[MAX]; int i;
#pragma omp parallel for
  for (i=0;i< MAX; i++) {
    res[i] = huge();
  }</pre>
```

## Working with loops

- Basic approach
  - Find compute intensive loops
  - Make the loop iterations independent ... So they can safely execute in any order without loop-carried dependencies
  - Place the appropriate OpenMP directive and test

```
Note: loop index
                           "i" is private by
                                                 int i, A[MAX];
int i, j, A[MAX];
                           default
                                                  #pragma omp parallel for
i = 5;
                                                  for (i=0;i< MAX; i++) {
for (i=0;i< MAX; i++) {
                                                     int j = 5 + 2*(i+1);
   j +=2;
                                                     A[i] = big(i);
   A[i] = big(j);
                              Remove loop
                              carried
                              dependence
```

#### Reduction

How do we handle this case?

```
double ave=0.0, A[MAX]; int i;
for (i=0;i< MAX; i++) {
    ave + = A[i];
}
ave = ave/MAX;</pre>
```

- We are combining values into a single accumulation variable (ave) ...
  there is a true dependence between loop iterations that can't be trivially
  removed
- This is a very common situation ... it is called a "reduction".
- Support for reduction operations is included in most parallel programming environments.

#### Reduction

OpenMP reduction clause:

```
reduction (op: list)
```

- Inside a parallel or a work-sharing construct:
  - A local copy of each list variable is made and initialized depending on the "op" (e.g. 0 for "+").
  - Updates occur on the local copy.
  - Local copies are reduced into a single value and combined with the original global value.
- The variables in "list" must be shared in the enclosing parallel region.

```
double ave=0.0, A[MAX]; int i;
#pragma omp parallel for reduction (+:ave)
for (i=0;i< MAX; i++) {
    ave + = A[i];
}
ave = ave/MAX;</pre>
```

### **OpenMP: Reduction operands/initial-values**

- Many different associative operands can be used with reduction:
- Initial values are the ones that make sense mathematically.

Operator	Initial value	
+	0	
*	1	
-	0	
min	Largest pos. number	
max	Most neg. number	

C/C++ only		
Operator	Initial value	
&	~0	
	0	
۸	0	
&&	1	
	0	

Fortran Only		
Operator	Initial value	
.AND.	.true.	
.OR.	.false.	
.NEQV.	.false.	
.IEOR.	0	
.IOR.	0	
.IAND.	All bits on	
.EQV.	.true.	

## **Exercise: Pi with loops**

- Go back to the serial pi program and parallelize it with a loop construct
- Your goal is to minimize the number of changes made to the serial program.

```
#pragma omp parallel
#pragma omp for
#pragma omp parallel for
#pragma omp for reduction(op:list)
#pragma omp critical
int omp_get_num_threads();
int omp_get_thread_num();
double omp_get_wtime();
```

## Example: Pi with a loop and a reduction

```
#include <omp.h>
static long num steps = 100000;
                                               double step;
void main ()
    int i;
                  double x, pi, sum = 0.0;
                                                 Create a team of threads ...
    step = 1.0/(double) num steps;
                                                 without a parallel construct, you'll
                                                 never have more than one thread
    #pragma omp parallel
                                        Create a scalar local to each thread to hold
        double x;
                                        value of x at the center of each interval
       #pragma omp for reduction(+:sum)
           for (i=0;i < num steps; i++){
                  x = (i+0.5)*step;
                                                       Break up loop iterations
                  sum = sum + 4.0/(1.0+x*x)
                                                       and assign them to
                                                       threads ... setting up a
                                                       reduction into sum.
                                                       Note ... the loop index is
                                                       local to a thread by default.
          pi = step * sum;
```

## Results\*: pi with a loop and a reduction

Original Serial pi program with 100000000 steps ran in 1.83 seconds.

```
Example: Pi with a
                            threads
                                         1st
                                                    1 st
                                                             SPMD
                                                                        PI Loop
                                       SPMD
                                                  SPMD
                                                             critical
#include <omp.h>
                                                 padded
static long num steps = 1000
                                        1.86
                                                   1.86
                                                              1.87
                                                                          1.91
void main ()
                               2
                                        1.03
                                                   1.01
                                                              1.00
                                                                          1.02
  int i:
             double x, pi, su
   step = 1.0/(double) num_s
                               3
                                        1.08
                                                   0.69
                                                              0.68
                                                                         0.80
   #pragma omp parallel
                               4
                                        0.97
                                                   0.53
                                                              0.53
                                                                         0.68
      double x:
     #pragma omp for reduction(+:sum)
        for (i=0;i < num steps; i++){
             x = (i+0.5)*step;
             sum = sum + 4.0/(1.0+x*x);
       pi = step * sum;
```

<sup>\*</sup>Intel compiler (icpc) with no optimization on Apple OS X 10.7.3 with a dual core (four HW thread) Intel® Core<sup>TM</sup> i5 processor at 1.7 Ghz and 4 Gbyte DDR3 memory at 1.333 Ghz.

#### The nowait clause

 Barriers are really expensive. You need to understand when they are implied and how to skip them when its safe to do so.

```
double A[big], B[big], C[big];
#pragma omp parallel
       int id=omp_get_thread num();
       A[id] = big calc1(id);
                                    implicit barrier at the end of a for
#pragma omp barrier
                                    worksharing construct
#pragma omp for
       for(i=0;i<N;i++)\{C[i]=big\ calc3(i,A);\}
#pragma omp for nowait
       for(i=0;i<N;i++){ B[i]=big_calc2(C, i); }
       A[id] = big calc4(id);
                                                no implicit barrier
            implicit barrier at the end
                                                due to nowait
            of a parallel region
```

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- Introduction to OpenMP
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# Data environment: Default storage attributes

- Shared memory programming model:
  - Most variables are shared by default
- Global variables are SHARED among threads
  - Fortran: COMMON blocks, SAVE variables, MODULE variables
  - C: File scope variables, static
  - Both: dynamically allocated memory (ALLOCATE, malloc, new)
- But not everything is shared...
  - Stack variables in subprograms(Fortran) or functions(C) called from parallel regions are PRIVATE
  - Automatic variables within a statement block are PRIVATE.

### Data sharing: Examples

```
double A[10];
int main() {
 int index[10];
 #pragma omp parallel
    work(index);
 printf("%d\n", index[0]);
}
```

A, index and count are shared by all threads.

temp is local to each thread

```
extern double A[10];
              void work(int *index) {
               double temp[10];
               static int count;
A, index, count
       temp
                    temp
                                temp
  index, count
```

## Data sharing: Changing storage attributes

- One can selectively change storage attributes for constructs using the following clauses\* (note: list is a comma-separated list of variables)
  - -shared(list)
  - private(list)
  - -firstprivate(list)
- These can be used on parallel and for constructs ... other than shared which can only be used on a parallel construct
- Force the programmer to explicitly define storage attributes
  - -default (none)

default() can only be used on parallel constructs

### Data sharing: Private clause

- private(var) creates a new local copy of var for each thread.
  - The value of the private copies is uninitialized
  - The value of the original variable is unchanged after the region

When you need to reference the variable tmp that exists prior to the construct, we call it the original variable.

## Data sharing: Private and the original variable

- The original variable's value is unspecified if it is referenced outside of the construct
  - Implementations may reference the original variable or a copy ..... a dangerous programming practice!
  - For example, consider what would happen if the compiler inlined work()?

```
int tmp;
void danger() {
    tmp = 0;
#pragma omp parallel private(tmp)
    work();
    printf("%d\n", tmp);
}

tmp has unspecified value
```

```
extern int tmp;
void work() {
    tmp = 5;
}

unspecified which
copy of tmp
```

## Firstprivate clause

- Variables initialized from a shared variable
- C++ objects are copy-constructed

```
incr = 0;
#pragma omp parallel for firstprivate(incr)
for (i = 0; i <= MAX; i++) {
    if ((i%2)==0) incr++;
        A[i] = incr;
}</pre>
```

Each thread gets its own copy of incr with an initial value of 0

### **Data sharing:**

#### A data environment test

Consider this example of PRIVATE and FIRSTPRIVATE

```
variables: A = 1,B = 1, C = 1
#pragma omp parallel private(B) firstprivate(C)
```

- Are A,B,C private to each thread or shared inside the parallel region?
- What are their initial values inside and values after the parallel region?

#### Inside this parallel region ...

- "A" is shared by all threads; equals 1
- "B" and "C" are private to each thread.
  - B's initial value is undefined
  - C's initial value equals 1

#### Following the parallel region ...

- B and C revert to their original values of 1
- A is either 1 or the value it was set to inside the parallel region

## Data sharing: Default clause

- default(none): Forces you to define the storage attributes for variables that appear inside the static extent of the construct ... if you fail the compiler will complain. Good programming practice!
- You can put the default clause on parallel and parallel + workshare constructs.

```
#include <omp.h>
                   int main()
                      int i, j=5; double x=1.0, y=42.0;
   The static
                      #pragma omp parallel for default(none) reduction(*:x)
 extent is the
                      for (i=0;i<N;i++)
  code in the
                         for(i=0; i<3; i++)
compilation unit -
                                                                The compiler would
 that contains
                             x+= foobar(i, j, y);
                                                              complain about i and y,
                                                              which is important since
the construct.
                                                               you don't want j to be
                       printf(" x is %f\n",(float)x);
                                                                     shared
```

The full OpenMP specification has other versions of the default clause, but they are not used very often so we skip them in the common core

#### **Exercise: Mandelbrot set area**

- The supplied program (mandel.c) computes the area of a Mandelbrot set.
- The program has been parallelized with OpenMP, but we were lazy and didn't do it right.
- Find and fix the errors (hint ... the problem is with the data environment).
- Once you have a working version, try to optimize the program.
  - Try different schedules on the parallel loop.
  - Try different mechanisms to support mutual exclusion … do the efficiencies change?

### The Mandelbrot area program

```
#include <omp.h>
# define NPOINTS 1000
# define MXITR 1000
struct d complex{
 double r; double i;
void testpoint(struct d_complex);
struct d complex c;
int numoutside = 0;
int main(){
 int i, j;
 double area, error, eps = 1.0e-5;
#pragma omp parallel for private(c, j) firstpriivate(eps)
  for (i=0; i<NPOINTS; i++) {
   for (j=0; j<NPOINTS; j++) {
    c.r = -2.0 + 2.5*(double)(i)/(double)(NPOINTS)+eps;
    c.i = 1.125*(double)(j)/(double)(NPOINTS)+eps;
    testpoint(c);
area=2.0*2.5*1.125*(double)(NPOINTS*NPOINTS-
numoutside)/(double)(NPOINTS*NPOINTS);
 error=area/(double)NPOINTS;
```

```
void testpoint(struct d_complex c){
struct d complex z;
    int iter:
    double temp;
    z=c;
    for (iter=0; iter<MXITR; iter++){
     temp = (z.r*z.r)-(z.i*z.i)+c.r;
     z.i = z.r*z.i*2+c.i:
     z.r = temp;
     if ((z.r*z.r+z.i*z.i)>4.0) {
     #pragma omp critical
       numoutside++;
       break;
```

- eps was not initialized
- Protect updates of numoutside
- Which value of c does testpoint() see? Global or private?

#### **Outline**

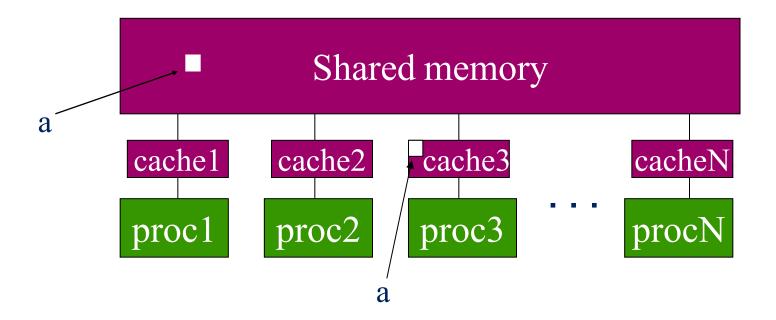
- Introduction to OpenMP
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- Data environment



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## **OpenMP memory model**

- OpenMP supports a shared memory model
- All threads share an address space, but it can get complicated:



Multiple copies of data may be present in various levels of cache, or in registers

# OpenMP and relaxed consistency

- OpenMP supports a relaxed-consistency shared memory model
  - Threads can maintain a temporary view of shared memory that is not consistent with that of other threads
  - These temporary views are made consistent only at certain points in the program
  - The operation that enforces consistency is called the **flush operation**

## Flush operation

- Defines a sequence point at which a thread is guaranteed to see a consistent view of memory
  - All previous read/writes by this thread have completed and are visible to other threads
  - No subsequent read/writes by this thread have occurred
- A flush operation is analogous to a fence in other shared memory APIs

## Flush and synchronization

- A flush is implied where it makes sense:
  - at entry/exit of parallel regions
  - at implicit and explicit barriers
  - at entry/exit of critical regions

. . . .

(but not at entry to worksharing regions)

This means if you are mixing reads and writes of a variable across multiple threads, you cannot assume the reading threads see the results of the writes unless:

- the writing threads follow the writes with a construct that implies a flush.
- the reading threads proceed the reads with a construct that implies a flush.

If you use the common core of OpenMP ... this isn't an issue. You should avoid writing code that depends on ordering reads/writes around flushes.

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## Irregular parallelism

- Let's call a problem "irregular" when one or both of the following hold:
  - Data Structures are sparse
  - Control structures are not basic for-loops

Example: Traversing Linked lists:

```
p = listhead ;
while (p) {
   process(p);
   p=p->next;
}
```

 Using what we've learned so far, traversing a linked list in parallel using OpenMP is difficult.

## **Exercise: traversing linked lists**

- Consider the program linked.c
  - Traverses a linked list computing a sequence of Fibonacci numbers at each node.
- Parallelize this program selecting from the following list of constructs:

```
#pragma omp parallel
#pragma omp for
#pragma omp parallel for
#pragma omp for reduction(op:list)
#pragma omp critical
int omp_get_num_threads();
int omp_get_thread_num();
double omp_get_wtime();
schedule(static[,chunk]) or schedule(dynamic[,chunk])
private(), firstprivate(), default(none)
```

 Hint: Just worry about the contents of main(). You don't need to make any changes to the "list functions"

# Linked lists with OpenMP pre 3.0

See the file solutions/Linked\_notasks.c

```
while (p != NULL) {
   p = p-next;
    count++;
p = head:
for(i=0; i<count; i++) {
    parr[i] = p;
    p = p-next;
#pragma omp parallel
   #pragma omp for schedule(static,1)
   for(i=0; i<count; i++)
     processwork(parr[i]);
```

Count number of items in the linked list

Copy pointer to each node into an array

Process nodes in parallel with a for loop

	Default schedule	Static,1
One Thread	48 seconds	45 seconds
Two Threads	39 seconds	28 seconds

## Linked lists with OpenMP pre 3.0

See the file solutions/Linked\_notasks.c

```
while (p != NULL) {
   p = p-next;
    count++:
p = head:
for(i=0; i<count; i++) {
    parr[i] = p;
    p = p-next;
#pragma omp parallel
   #pragma omp for schedule(static,1)
   for(i=0; i<count; i++)
     processwork(parr[i]);
```

Count number of items in the linked list

With so much code to add and three passes through the data, this is really ugly.

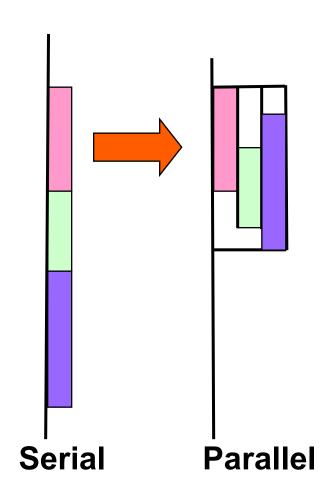
There has got to be a better way to do this

Process nodes in parallel with a for loop

	Default schedule	Static,1
One Thread	48 seconds	45 seconds
Two Threads	39 seconds	28 seconds

#### What are tasks?

- Tasks are independent units of work
- Tasks are composed of:
  - code to execute
  - data to compute with
- Threads are assigned to perform the work of each task.
  - The thread that encounters the task construct may execute the task immediately.
  - The threads may defer execution until later

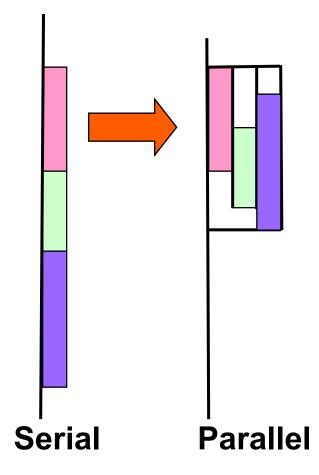


#### What are tasks?

The task construct includes a structured block of code

 Inside a parallel region, a thread encountering a task construct will package up the code block and its data for execution

 Tasks can be nested: i.e. a task may itself generate tasks.



A common Pattern is to have one thread create the tasks while the other threads wait at a barrier and execute the tasks

## **Single worksharing Construct**

- The single construct denotes a block of code that is executed by only one thread (not necessarily the master thread).
- A barrier is implied at the end of the single block (can remove the barrier with a nowait clause).

#### **Task Directive**

```
#pragma omp task [clauses]
    structured-block
```

```
#pragma omp parallel ____
                                  Create some threads
  #pragma omp single _
                                       One Thread
                                       packages tasks
      #pragma omp task
         fred();
      #pragma omp task
                                      Tasks executed by
         daisy();
                                       some thread in some
      #pragma omp task
                                       order
         billy();
```

All tasks complete before this barrier is released

## **Exercise: Simple tasks**

- Write a program using tasks that will "randomly" generate one of two strings:
  - I think race cars are fun
  - I think car races are fun
- Hint: use tasks to print the indeterminate part of the output (i.e. the "race" or "car" parts).
- This is called a "Race Condition". It occurs when the result of a program depends on how the OS schedules the threads.
- NOTE: A "data race" is when threads "race to update a shared variable".
   They produce race conditions. Programs containing data races are undefined (in OpenMP but also ANSI standards C++'11 and beyond).

```
#pragma omp parallel
#pragma omp task
#pragma omp single
```

## Racey cars: solution

```
#include <stdio.h>
#include <omp.h>
int main()
{ printf("I think");
 #pragma omp parallel
   #pragma omp single
     #pragma omp task
       printf(" car");
     #pragma omp task
       printf(" race");
  printf("s");
  printf(" are fun!\n");
```

## Data scoping with tasks

- Variables can be shared, private or firstprivate with respect to task
- These concepts are a little bit different compared with threads:
  - If a variable is shared on a task construct, the references to it inside the construct are to the storage with that name at the point where the task was encountered
  - If a variable is private on a task construct, the references to it inside the construct are to new uninitialized storage that is created when the task is executed
  - If a variable is firstprivate on a construct, the references to it inside the construct are to new storage that is created and initialized with the value of the existing storage of that name when the task is encountered

## Data scoping defaults

- The behavior you want for tasks is usually firstprivate, because the task may not be executed until later (and variables may have gone out of scope)
  - Variables that are private when the task construct is encountered are firstprivate by default
- Variables that are shared in all constructs starting from the innermost enclosing parallel construct are shared by default

```
#pragma omp parallel shared(A) private(B)
{
    ...

#pragma omp task
    A is shared
    B is firstprivate
    int C;
    compute(A, B, C);
}
```

## **Exercise: traversing linked lists**

- Consider the program linked.c
  - Traverses a linked list computing a sequence of Fibonacci numbers at each node.
- Parallelize this program selecting from the following list of constructs:

```
#pragma omp parallel
#pragma omp single
#pragma omp task
int omp_get_num_threads();
int omp_get_thread_num();
double omp_get_wtime();
private(), firstprivate()
```

 Hint: Just worry about the contents of main(). You don't need to make any changes to the "list functions"

#### Parallel linked list traversal

```
Only one thread
                                        packages tasks
#pragma omp parallel
  #pragma omp single*
    p = listhead ;
    while (p) {
        #pragma omp task firstprivate(p)
                 process (p);
        p=next (p) ;
                                      makes a copy of p
                                      when the task is
                                      packaged
```

## When/where are tasks complete?

- At thread barriers (explicit or implicit)
  - applies to all tasks generated in the current parallel region up to the barrier
- At taskwait directive
  - i.e. Wait until all tasks defined in the current task have completed.
     #pragma omp taskwait
  - Note: applies only to tasks generated in the current task, not to "descendants".

## **Example**

```
#pragma omp parallel
  #pragma omp single
     #pragma omp task
         fred();
     #pragma omp task
                                   fred() and daisy()
         daisy();
                                   must complete before
     #pragma taskwait 🚄
                                   billy() starts
     #pragma omp task
         billy();
```

## **Example: Fibonacci numbers**

```
int fib (int n)
  int x,y;
  if (n < 2) return n;
  x = fib(n-1);
  y = fib (n-2);
  return (x+y);
Int main()
  int NW = 5000;
  fib(NW);
```

- $F_n = F_{n-1} + F_{n-2}$
- Inefficient O(n²) recursive implementation!

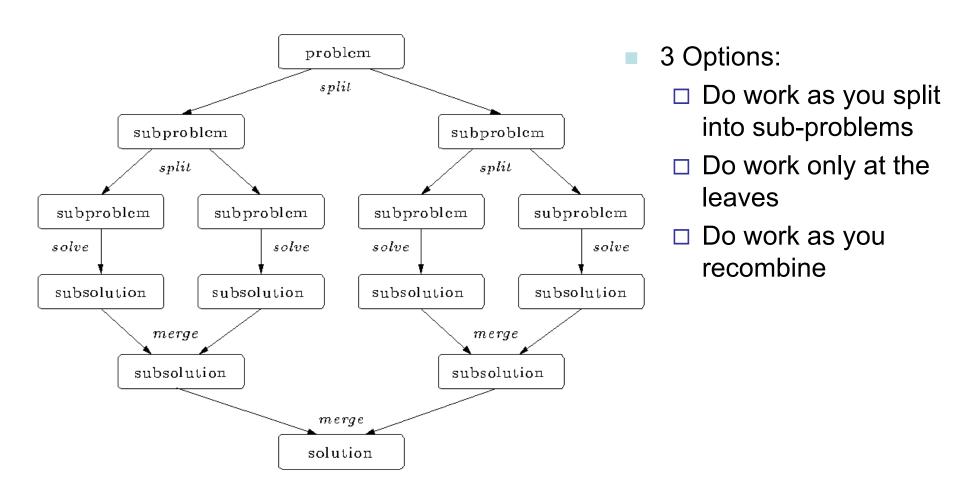
#### **Parallel Fibonacci**

```
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);
Int main()
 int NW = 5000;
 #pragma omp parallel
    #pragma omp single
        fib(NW);
```

- Binary tree of tasks
- Traversed using a recursive function
- A task cannot complete until all tasks below it in the tree are complete (enforced with taskwait)
- x,y are local, and so by default they are private to current task
  - must be shared on child tasks so they don't create their own firstprivate copies at this level!

## Divide and conquer

 Split the problem into smaller sub-problems; continue until the sub-problems can be solve directly



#### **Exercise: Pi with tasks**

- Go back to the original pi.c program
  - Parallelize this program using OpenMP tasks

```
#pragma omp parallel
#pragma omp task
#pragma omp taskwait
#pragma omp single
double omp_get_wtime()
int omp_get_thread_num();
int omp_get_num_threads();
```

 Hint: first create a recursive pi program and verify that it works. Think about the computation you want to do at the leaves.

#### **Program: OpenMP tasks**

```
include <omp.h>
                                                      int main ()
static long num steps = 100000000;
#define MIN BLK 10000000
                                                       int i;
double pi comp(int Nstart,int Nfinish,double step)
                                                       double step, pi, sum;
  int i,iblk;
                                                        step = 1.0/(double) num steps;
 double x, sum = 0.0,sum1, sum2;
                                                        #pragma omp parallel
 if (Nfinish-Nstart < MIN BLK){
   for (i=Nstart;i< Nfinish; i++){
                                                          #pragma omp single
     x = (i+0.5)*step:
                                                             sum =
     sum = sum + 4.0/(1.0+x*x);
                                                               pi_comp(0,num_steps,step);
 else{
                                                         pi = step * sum;
   iblk = Nfinish-Nstart;
   #pragma omp task shared(sum1)
      sum1 = pi comp(Nstart,
                                  Nfinish-iblk/2,step);
   #pragma omp task shared(sum2)
       sum2 = pi_comp(Nfinish-iblk/2, Nfinish,
                                                 step);
   #pragma omp taskwait
     sum = sum1 + sum2;
 }return sum;
```

## Results\*: pi with tasks

threads	1 <sup>st</sup> SPMD	SPMD critical	PI Loop	Pi tasks
1	1.86	1.87	1.91	1.87
2	1.03	1.00	1.02	1.00
3	1.08	0.68	0.80	0.76
4	0.97	0.53	0.68	0.52

<sup>\*</sup>Intel compiler (icpc) with no optimization on Apple OS X 10.7.3 with a dual core (four HW thread) Intel® Core™ i5 processor at 1.7 Ghz and 4 Gbyte DDR3 memory at 1.333 Ghz.

## **Using tasks**

- Don't use tasks for things already well supported by OpenMP
  - e.g. standard do/for loops
  - the overhead of using tasks is greater

- Don't expect miracles from the runtime
  - best results usually obtained where the user controls the number and granularity of tasks

#### **Outline**

- Introduction to OpenMP
- Creating Threads
- Quantifying Performance and Amdahl's law
- Synchronization
- Parallel Loops
- Data environment
- Memory model
- Irregular Parallelism and tasks



- Recap
- Beyond the common core:
  - Worksharing revisited
  - Synchronization: More than you ever wanted to know
  - Thread private data

#### The OpenMP Common Core: Most OpenMP programs only use these 19 items

OpenMP pragma, function, or clause	Concepts
#pragma omp parallel	Parallel region, teams of threads, structured block, interleaved execution across threads
<pre>int omp_get_thread_num() int omp_get_num_threads()</pre>	Create threads with a parallel region and split up the work using the number of threads and thread ID
double omp_get_wtime()	Speedup and Amdahl's law. False Sharing and other performance issues
setenv OMP_NUM_THREADS N	Internal control variables. Setting the default number of threads with an environment variable
#pragma omp barrier #pragma omp critical	Synchronization and race conditions. Revisit interleaved execution.
#pragma omp for #pragma omp parallel for	Worksharing, parallel loops, loop carried dependencies
reduction(op:list)	Reductions of values across a team of threads
schedule(dynamic [,chunk]) schedule (static [,chunk])	Loop schedules, loop overheads and load balance
private(list), firstprivate(list), shared(list)	Data environment
nowait	Disabling implied barriers on workshare constructs, the high cost of barriers, and the flush concept (but not the flush directive)
#pragma omp single	Workshare with a single thread
#pragma omp task #pragma omp taskwait	Tasks including the data environment for tasks.  94

# There is much more to OpenMP than the Common Core.

- Synchronization mechanisms
  - locks, flush and several forms of atomic
- Data environment
  - lastprivate, threadprivate, default(private|shared)
- Fine grained task control
  - dependencies, tied vs. untied tasks, task groups, task loops ...
- Vectorization constructs
  - simd, uniform, simdlen, inbranch vs. nobranch, ....
- Map work onto an attached device
  - target, teams distribute parallel for, target data ...
- ... and much more. The OpenMP 4.5 specification is over 350 pages!!!

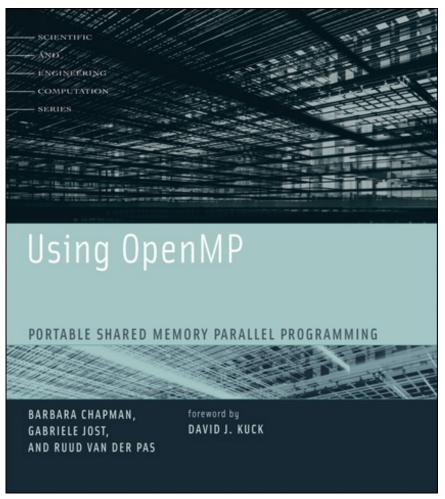
Don't become overwhelmed. Master the common core and move on to other constructs when you encounter problems that require them.

## **OpenMP organizations**

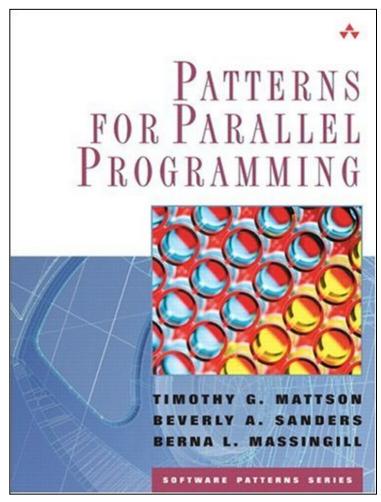
- OpenMP architecture review board URL, the "owner" of the OpenMP specification: www.openmp.org
- OpenMP User's Group (cOMPunity) URL: www.compunity.org

Get involved, join the ARB and cOMPunity and help define the future of OpenMP

## **Books about OpenMP**



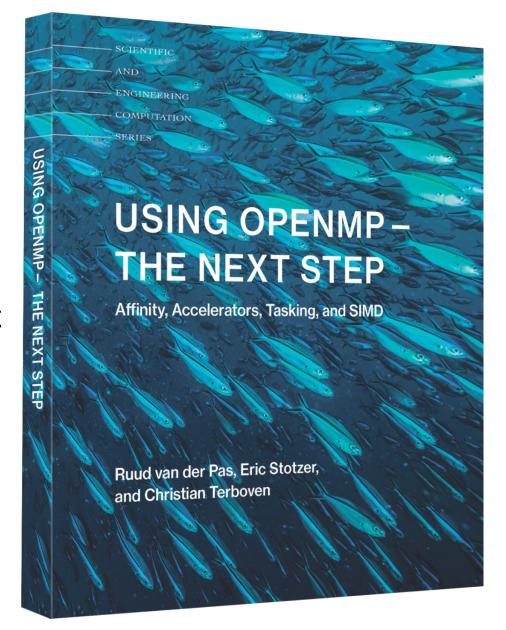
 A book about OpenMP by a team of authors at the forefront of OpenMP's evolution.



 A book about how to "think parallel" with examples in OpenMP, MPI and java

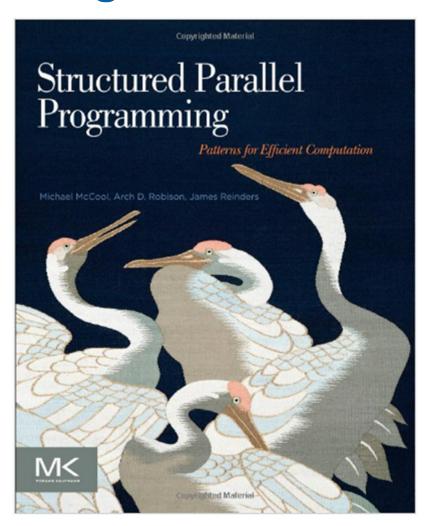
#### Resources:

A great new book that covers OpenMP features beyond OpenMP 2.5

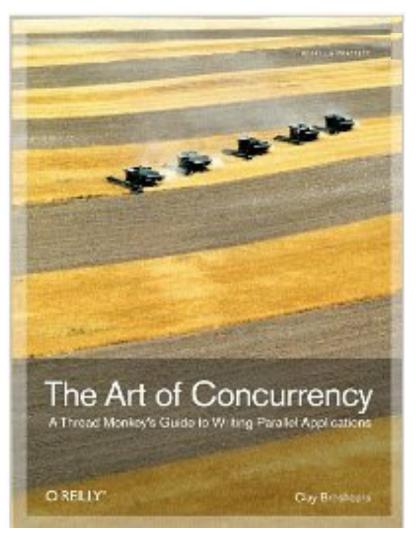


Visit the OpenMP booth and enter a drawing for a chance to win a copy of the book. Drawing Tues and Wed @ 4:30, Thurs @ 2:00. You must be present to win.

## **Background references**



A great book that explores key patterns with Cilk, TBB, OpenCL, and OpenMP (by McCool, Robison, and Reinders)



An excellent introduction and overview of multithreaded programming in general (by Clay Breshears)

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## The loop worksharing constructs

 The loop worksharing construct splits up loop iterations among the threads in a team

The variable I is made "private" to each thread by default. You could do this explicitly with a "private(I)" clause

## Loop worksharing constructs: The schedule clause

- The schedule clause affects how loop iterations are mapped onto threads
  - schedule(static [,chunk])
    - Deal-out blocks of iterations of size "chunk" to each thread.
  - schedule(dynamic[,chunk])
    - Each thread grabs "chunk" iterations off a queue until all iterations have been handled.
  - schedule(guided[,chunk])
    - Threads dynamically grab blocks of iterations. The size of the block starts large and shrinks down to size "chunk" as the calculation proceeds.
  - schedule(runtime)
    - Schedule and chunk size taken from the OMP\_SCHEDULE environment variable (or the runtime library).
  - schedule(auto)
    - Schedule is left up to the runtime to choose (does not have to be any of the above).

### loop work-sharing constructs:

#### The schedule clause

Schedule Clause	When To Use
STATIC	Pre-determined and predictable by the programmer
DYNAMIC	Unpredictable, highly variable work per iteration
GUIDED	Special case of dynamic to reduce scheduling overhead
AUTO	When the runtime can "learn" from previous executions of the same loop

Least work at runtime: scheduling done at compile-time

Most work at runtime: complex scheduling logic used at run-time

## **Nested loops**

 For perfectly nested rectangular loops we can parallelize multiple loops in the nest with the collapse clause:

```
#pragma omp parallel for collapse(2)
for (int i=0; i<N; i++) {
  for (int j=0; j<M; j++) {
    .....
}
</pre>
Number of loops
to be
parallelized,
counting from
the outside
```

- Will form a single loop of length NxM and then parallelize that.
- Useful if N is O(no. of threads) so parallelizing the outer loop makes balancing the load difficult.

## **Sections worksharing Construct**

• The Sections worksharing construct gives a different structured block to each thread.

```
#pragma omp parallel
 #pragma omp sections
 #pragma omp section
       X calculation();
 #pragma omp section
       y calculation();
 #pragma omp section
       z calculation();
```

By default, there is a barrier at the end of the "omp sections". Use the "nowait" clause to turn off the barrier.

## **Array sections with reduce**

return 0;

```
#include <stdio.h>
                                       Works the same as the other reductions:
                                          A private array is formed for each
#define N 100
                                          thread.
void init(int n, float (*b)[N]);
                                          Initialized according to the identify for
                                          the operator

    element wise combination across

int main(){
                                          threads at end of the construct.
int i,j; float a[N], b[N][N]; init(N,b);
                                          elementwise combination with original
for(i=0; i<N; i++) a[i]=0.0e0;
                                          array at the end of the construct.
#pragma omp parallel for reduction(+:a[0:N]) private(j)
for(i=0; i<N; i++){
  for(j=0; j<N; j++){
      a[j] += b[i][j];
printf(" a[0] a[N-1]: %f %f\n", a[0], a[N-1]);
```

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## **Synchronization**

High level synchronization:

-critical -barrier Covered earlier

- -atomic
- -ordered
- Low level synchronization
  - -flush
  - locks (both simple and nested)

Synchronization is used to impose order constraints and to protect access to shared data

## Synchronization: atomic

 Atomic provides mutual exclusion but only applies to the update of a memory location (the update of X in the following example)

```
#pragma omp parallel
    double B;
    B = DOIT();
#pragma omp atomic
       X += big_ugly(B);
```

## Synchronization: atomic

 Atomic provides mutual exclusion but only applies to the update of a memory location (the update of X in the following example)

```
#pragma omp parallel
{
    double B, tmp;
    B = DOIT();
    tmp = big_ugly(B);

#pragma omp atomic
    X += tmp;
}
Atomic only protects the read/update of X
```

### **Exercise**

- In your first Pi program, you probably used an array to create space for each thread to store its partial sum.
- You fixed this by using a critical section instead of updating the array (remember .. the array you created by promoting the scalar "sum" to an array).
- Use and atomic instead. Does the performance improve?

## Parallel loop with ordered region

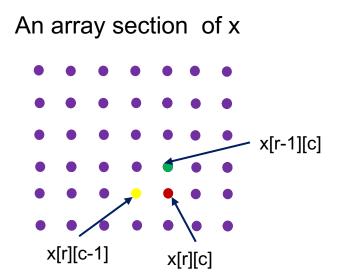
- An ordered clause on a loop worksharing construct
  - indicates that the loop contains an ordered region
- The ordered construct defines an ordered region
  - The Statements in ordered region execute in iteration order

```
#pragma omp for ordered
  for (i=0; i<N; i++) {
    float res = work(i);
    #pragma omp ordered
    {
       printf("result for %d was %f\n", i, res);
       fflush(stdout);
    }
  }</pre>
```

## Parallelizing nested loops

Will these nested parallel loops execute correctly?

```
#pragma omp parallel for collapse(2)
for (r=1; r<N; r++) {
   for (c=1; c<N; c++) {
     x[r][c] += fn(x[r-1][c], x[r][c-1]);
   }
}</pre>
```



- Pattern of dependencies between elements of x prevent straightforward parallelization
- is there a way to manage the synchronization so we can parallelize this loop?

#### Ordered stand-alone directive

Specifies cross-iteration dependencies in a doacross loop nest
 i.e. loop level parallelism over nested loops with a regular pattern of synchronization to manage dependencies.

#pragma omp ordered depend(sink : vec)
#pragma omp ordered depend(source)

vec is a comma separated list of dependencies ... one per loop involved in the dependencies

- Depend clauses specify the order the threads execute ordered regions.
  - The **sink** dependence-type
    - specifies a cross-iteration dependence, where the iteration vector vec indicates the iteration that satisfies the dependence.
  - The **source** dependence-type
    - specifies the cross-iteration dependences that arise from the current iteration.

## Parallelizing DOACROSS loops

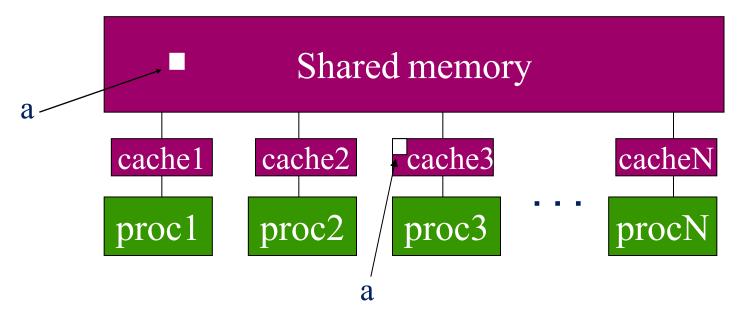
```
2 loops contribute to the pattern
of dependencies ... so the
dependency relations for each
depend(sink) is of length 2
```

Threads wait here until x[r-1][c] and x[r][c-1] have been released

x[r][c] is complete and released for use by other threads

## **OpenMP memory model**

- OpenMP supports a shared memory model
- All threads share an address space, where variable can be stored or retrieved:



Threads maintain their own temporary view of memory as well ... the
details of which are not defined in OpenMP but this temporary view
typically resides in caches, registers, write-buffers, etc.

## Flush operation

- Defines a sequence point at which a thread enforces a consistent view of memory.
- For variables visible to other threads and associated with the flush operation (the flush-set)
  - The compiler can't move loads/stores of the flush-set around a flush:
    - All previous read/writes of the flush-set by this thread have completed
    - No subsequent read/writes of the flush-set by this thread have occurred
  - Variables in the flush set are moved from temporary storage to shared memory.
  - Reads of variables in the flush set following the flush are loaded from shared memory.

IMPORTANT POINT: The flush makes the calling threads temporary view match the view in shared memory. Flush by itself does not force synchronization.

## Memory consistency: flush example

 Flush forces data to be updated in memory so other threads see the most recent value

Flush without a list: flush set is all

```
thread visible variables

A = compute();

#pragma omp flush(A)

// flush to memory to make sure other
// threads can pick up the right value
```

Note: OpenMP's flush is analogous to a fence in other shared memory APIs

## Flush and synchronization

- A flush operation is implied by OpenMP synchronizations, e.g.,
  - at entry/exit of parallel regions
  - at implicit and explicit barriers
  - at entry/exit of critical regions
  - whenever a lock is set or unset

. . . .

(but not at entry to worksharing regions or entry/exit of master regions)

## **Example:** prod\_cons.c

- Parallelize a producer/consumer program
  - One thread produces values that another thread consumes.

```
int main()
 double *A, sum, runtime; int flag = 0;
 A = (double *) malloc(N*sizeof(double));
 runtime = omp get wtime();
 fill_rand(N, A); // Producer: fill an array of data
 sum = Sum_array(N, A); // Consumer: sum the array
 runtime = omp get wtime() - runtime;
 printf(" In %lf secs, The sum is %lf \n",runtime,sum);
```

- Often used with a stream of produced values to implement "pipeline parallelism"
- The key is to implement pairwise synchronization between threads

## Pairwise synchronization in OpenMP

- OpenMP lacks synchronization constructs that work between pairs of threads.
- When needed, you have to build it yourself.
- Pairwise synchronization
  - Use a shared flag variable
  - Reader spins waiting for the new flag value
  - Use flushes to force updates to and from memory

### **Exercise: Producer/consumer**

```
int main()
  double *A, sum, runtime; int numthreads, flag = 0;
  A = (double *)malloc(N*sizeof(double));
  #pragma omp parallel sections
    #pragma omp section
      fill rand(N, A);
      flag = 1;
    #pragma omp section
      while (flag == 0){
      sum = Sum array(N, A);
```

Put the flushes in the right places to make this program race-free.

Do you need any other synchronization constructs to make this work?

# Solution (try 1): Producer/consumer

```
int main()
  double *A, sum, runtime; int numthreads, flag = 0;
  A = (double *)malloc(N*sizeof(double));
  #pragma omp parallel sections
    #pragma omp section
      fill rand(N, A);
      #pragma omp flush
      flag = 1;
      #pragma omp flush (flag)
    #pragma omp section
      #pragma omp flush (flag)
      while (flag == 0){
         #pragma omp flush (flag)
      #pragma omp flush
      sum = Sum array(N, A);
```

Use flag to Signal when the "produced" value is ready

Flush forces refresh to memory; guarantees that the other thread sees the new value of A

Flush needed on both "reader" and "writer" sides of the communication

Notice you must put the flush inside the while loop to make sure the updated flag variable is seen

This program works with the x86 memory model (loads and stores use relaxed atomics), but it technically has a race ... on the store and later load of flag

### The OpenMP 3.1 atomics (1 of 2)

- Atomic was expanded to cover the full range of common scenarios where you need to protect a memory operation so it occurs atomically:
  - # pragma omp atomic [read | write | update | capture]
- Atomic can protect loads
   # pragma omp atomic read
   v = x;
- Atomic can protect stores
   # pragma omp atomic write
   x = expr;
- Atomic can protect updates to a storage location (this is the default behavior ... i.e. when you don't provide a clause)

```
# pragma omp atomic update
    x++; or ++x; or x--; or -x; or
    x binop= expr; or x = x binop expr;
```

This is the original OpenMP atomic

## The OpenMP 3.1 atomics (2 of 2)

 Atomic can protect the assignment of a value (its capture) AND an associated update operation:

# pragma omp atomic capture
statement or structured block

Where the statement is one of the following forms:

$$v = x++;$$
  $v = ++x;$   $v = x--;$   $v = -x;$   $v = x binop expr;$ 

Where the structured block is one of the following forms:

```
{v = x; x binop = expr;} {x binop = expr; v = x;}

{v = x; x = x binop expr;} {X = x binop expr; v = x;}

{v = x; x++;} {v=x; ++x:}

{++x; v=x:} {x++; v = x;}

{v = x; x--;} {v = x;}

{--x; v = x;}
```

The capture semantics in atomic were added to map onto common hardware supported atomic operations and to support modern lock free algorithms

## **Atomics and synchronization flags**

```
int main()
  double *A, sum, runtime;
  int numthreads, flag = 0, flg_tmp;
  A = (double *)malloc(N*sizeof(double));
  #pragma omp parallel sections
    #pragma omp section
    { fill_rand(N, A);
      #pragma omp flush 🛌
      #pragma omp atomic write
           flag = 1;
      #pragma omp flush (flag)
    #pragma omp section
    { while (1){
        #pragma omp flush(flag),
        #pragma omp atomic read
            flg tmp= flag;
         if (flg tmp==1) break;
      #pragma omp flush<
       sum = Sum array(N, A);
```

This program is truly race free ... the reads and writes of flag are protected so the two threads cannot conflict

Still painful and error prone due to all of the flushes that are required

## **OpenMP 4.0 Atomic:** Sequential consistency

- Sequential consistency:
  - The order of loads and stores in a race-free program appear in some interleaved order and all threads in the team see this same order.
- OpenMP 4.0 added an optional clause to atomics
  - #pragma omp atomic [read | write | update | capture] [seq\_cst]
- In more pragmatic terms:
  - If the seq\_cst clause is included, OpenMP adds a flush without an argument list to the atomic operation so you don't need to.
- In terms of the C++'11 memory model:
  - Use of the seq\_cst clause makes atomics follow the sequentially consistent memory order.
  - Leaving off the seq\_cst clause makes the atomics relaxed.

Advice to programmers: save yourself a world of hurt ... let OpenMP take care of your flushes for you whenever possible ... use seq\_cst

## **Atomics and synchronization flags (4.0)**

```
int main()
  double *A, sum, runtime;
  int numthreads, flag = 0, flg_tmp;
  A = (double *)malloc(N*sizeof(double));
  #pragma omp parallel sections
    #pragma omp section
    { fill_rand(N, A);
      #pragma omp atomic write seq_cst
           flag = 1;
    #pragma omp section
    { while (1){
        #pragma omp atomic read seq_cst
             flg tmp= flag;
         if (flg tmp==1) break;
       sum = Sum_array(N, A);
```

This program is truly race free ... the reads and writes of flag are protected so the two threads cannot conflict – and you do not use any explicit flush constructs (OpenMP does them for you)

## **Synchronization: Lock routines**

- Simple Lock routines:
  - A simple lock is available if it is unset.
    - omp\_init\_lock(), omp\_set\_lock(),
       omp\_unset\_lock(), omp\_test\_lock(), omp\_destroy\_lock()
- Nested Locks
  - A nested lock is available if it is unset or if it is set but owned by the thread executing the nested lock function
    - omp\_init\_nest\_lock(), omp\_set\_nest\_lock(),
       omp\_unset\_nest\_lock(), omp\_test\_nest\_lock(),
       omp\_destroy\_nest\_lock()

Note: a thread always accesses the most recent copy of the lock, so you don't need to use a flush on the lock variable.

Locks with hints were added in OpenMP 4.5 to suggest a lock strategy based on intended use (e.g. contended, unconteded, speculative,, unspeculative)

A lock implies a

memory fence (a

visible variables

"flush") of all thread

## Lock Example from Gafort (SpecOMP'2001)

- Genetic algorithm in Fortran
- Most "interesting" loop: shuffle the population.
  - Original loop is not parallel; performs pair-wise swap of an array element with another, randomly selected element. There are 40,000 elements.
  - Parallelization idea:
    - Perform the swaps in parallel
    - Need to prevent simultaneous access to same array element: use one lock per array element → 40,000 locks.

### Parallel loop In shuffle.f of Gafort

Exclusive access to array elements.
Ordered locking prevents deadlock.

```
!$OMP PARALLEL PRIVATE(rand, iother, itemp, temp, my cpu id)
   my cpu id = 1
!$ my cpu id = omp get thread num() + 1
!$OMP DO
   DO j=1,npopsiz-1
    CALL ran3(1,rand,my cpu id,0)
    iother=j+1+DINT(DBLE(npopsiz-j)*rand)
    IF (j < iother) THEN
!$
!$
      CALL omp set lock(lck(j))
      CALL omp set lock(lck(iother))
!$
!$
    ELSE
!$
      CALL omp set lock(lck(iother))
!$
      CALL omp set lock(lck(j))
!$
    END IF
    itemp(1:nchrome)=iparent(1:nchrome,iother)
    iparent(1:nchrome,iother)=iparent(1:nchrome,j)
    iparent(1:nchrome,j)=itemp(1:nchrome)
    temp=fitness(iother)
    fitness(iother)=fitness(j)
    fitness(j)=temp
    IF (j < iother) THEN
!$
      CALL omp unset lock(lck(iother))
!$
      CALL omp unset lock(lck(j))
!$
    ELSE
!$
      CALL omp unset lock(lck(j))
!$
      CALL omp unset lock(lck(iother))
    END IF
  END DO
!$OMP END DO
                                        132
!$OMP END PARALLEL
```

#### **Exercise**

- We provide a program in the file hist.c
- This program tests our random number generator by calling it many times and producing a histogram of the results.
- Parallelize this program.

```
omp_lock_t lck;
omp_init_lock(&lck);
omp_set_lock(&lck);
omp_unset_lock(&lck);
omp_destroy_lock(&lck);
```

### Synchronization: Simple locks

 Example: conflicts are rare, but to play it safe, we must assure mutual exclusion for updates to histogram elements.

```
#pragma omp parallel for
                                            One lock per element of hist
for(i=0;i<NBUCKETS; i++){</pre>
    omp init lock(&hist locks[i]); hist[i] = 0;
#pragma omp parallel for
for(i=0;i<NVALS;i++){</pre>
   ival = (int) sample(arr[i]);
   omp_set_lock(&hist_locks[ival]); 
                                             Enforce mutual
      hist[ival]++;
                                             exclusion on update
   omp_unset_lock(&hist locks[ival]);
                                             to hist array
for(i=0;i<NBUCKETS; i++)
 omp_destroy_lock(&hist_locks[i]);
                                           Free-up storage when done.
```

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## Data sharing: Threadprivate

- Makes global data private to a thread
  - Fortran: COMMON blocks
  - C: File scope and static variables, static class members
- Different from making them PRIVATE
  - with PRIVATE global variables are masked.
  - THREADPRIVATE preserves global scope within each thread
- Threadprivate variables can be initialized using COPYIN or at time of definition (using language-defined initialization capabilities)

## A threadprivate example (C)

Use threadprivate to create a counter for each thread.

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

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

## **Data copying: Copyin**

You initialize threadprivate data using a copyin clause.

```
parameter (N=1000)
   common/buf/A(N)
!$OMP THREADPRIVATE(/buf/)
!$ Initialize the A array
   call init_data(N,A)
!$OMP PARALLEL COPYIN(A)
... Now each thread sees threadprivate array A initialized
... to the global value set in the subroutine init data()
!$OMP END PARALLEL
end
```

## **Data copying: Copyprivate**

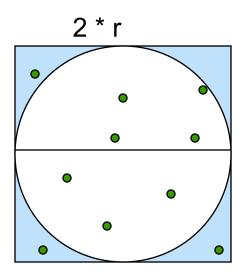
Used with a single region to broadcast values of privates from one member of a team to the rest of the team

```
#include <omp.h>
void input_parameters (int, int); // fetch values of input parameters
void do work(int, int);
void main()
 int Nsize, choice;
 #pragma omp parallel private (Nsize, choice)
    #pragma omp single copyprivate (Nsize, choice)
         input_parameters (*Nsize, *choice);
    do work(Nsize, choice);
```

#### **Exercise: Monte Carlo calculations**

#### Using random numbers to solve tough problems

- Sample a problem domain to estimate areas, compute probabilities, find optimal values, etc.
- Example: Computing π with a digital dart board:



N= 10 
$$\pi$$
 = 2.8  
N=100  $\pi$  = 3.16  
N= 1000  $\pi$  = 3.148

- Throw darts at the circle/square.
- Chance of falling in circle is proportional to ratio of areas:

$$A_c = r^2 * \pi$$
 $A_s = (2*r) * (2*r) = 4 * r^2$ 
 $P = A_c/A_s = \pi/4$ 

 Compute π by randomly choosing points; π is four times the fraction that falls in the circle

## **Exercise: Monte Carlo pi (cont)**

- We provide three files for this exercise
  - pi\_mc.c: the Monte Carlo method pi program
  - random.c: a simple random number generator
  - random.h: include file for random number generator
- Create a parallel version of this program without changing the interfaces to functions in random.c
  - This is an exercise in modular software ... why should a user of your parallel random number generator have to know any details of the generator or make any changes to how the generator is called?
  - The random number generator must be thread-safe.
- Extra Credit:
  - Make your random number generator numerically correct (nonoverlapping sequences of pseudo-random numbers).

### **Appendices**

- → Challenge Problems
  - Challenge Problems: solutions
    - Monte Carlo PI and random number generators
    - Molecular dynamics
    - Matrix multiplication
    - Recursive matrix multiplication
  - Mixing OpenMP and MPI
  - Fortran and OpenMP

## Challenge problems

- Long term retention of acquired skills is best supported by "random practice".
  - i.e., a set of exercises where you must draw on multiple facets of the skills you are learning.
- To support "Random Practice" we have assembled a set of "challenge problems"
  - 1. Parallel random number generators
  - 2. Parallel molecular dynamics
  - 3. Optimizing matrix multiplication
  - 4. Recursive matrix multiplication algorithms

### Challenge 1: Parallel Random number generators

- Go back to the monte Carlo pi program we discussed earlier when we covered threadprivate data.
- Make the parallel random number generators correct when used in parallel

## Challenge 2: Molecular dynamics

- The code supplied is a simple molecular dynamics simulation of the melting of solid argon
- Computation is dominated by the calculation of force pairs in subroutine forces (in forces.c)
- Parallelise this routine using a parallel for construct and atomics; think carefully about which variables should be SHARED, PRIVATE or REDUCTION variables
- Experiment with different schedule kinds

## Challenge 2: MD (cont.)

- Once you have a working version, move the parallel region out to encompass the iteration loop in main.c
  - Code other than the forces loop must be executed by a single thread (or workshared).
  - How does the data sharing change?
- The atomics are a bottleneck on most systems.
  - This can be avoided by introducing a temporary array for the force accumulation, with an extra dimension indexed by thread number
  - Which thread(s) should do the final accumulation into f?

## **Challenge 2 MD: (cont.)**

- Another option is to use locks
  - Declare an array of locks
  - Associate each lock with some subset of the particles
  - Any thread that updates the force on a particle must hold the corresponding lock
  - Try to avoid unnecessary acquires/releases
  - What is the best number of particles per lock?

## **Challenge 3: Matrix multiplication**

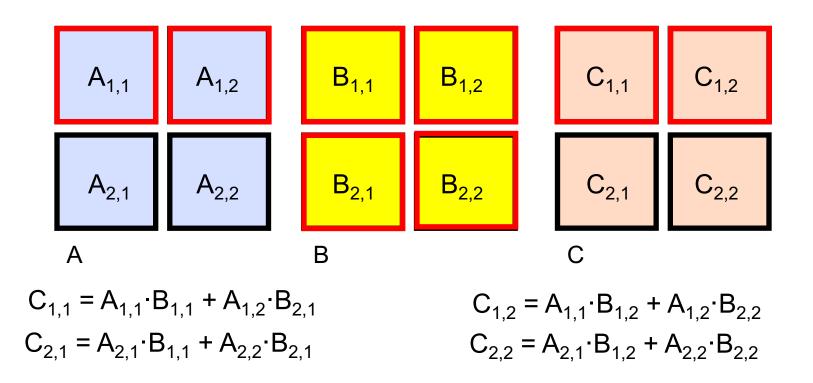
- Parallelize the matrix multiplication program in the file mm\_testbed.c
- Can you optimize the program by playing with how the loops are scheduled?
- Try the following and see how they interact with the constructs in OpenMP
  - Alignment
  - Cache blocking
  - Loop unrolling
  - Vectorization
- Goal: Can you approach the peak performance of the computer?

#### Challenge 4: Recursive matrix multiplication

- The following three slides explain how to use a recursive algorithm to multiply a pair of matrices
- Source code implementing this algorithm is provided in the file matmul\_recur.c
- Parallelize this program using OpenMP tasks

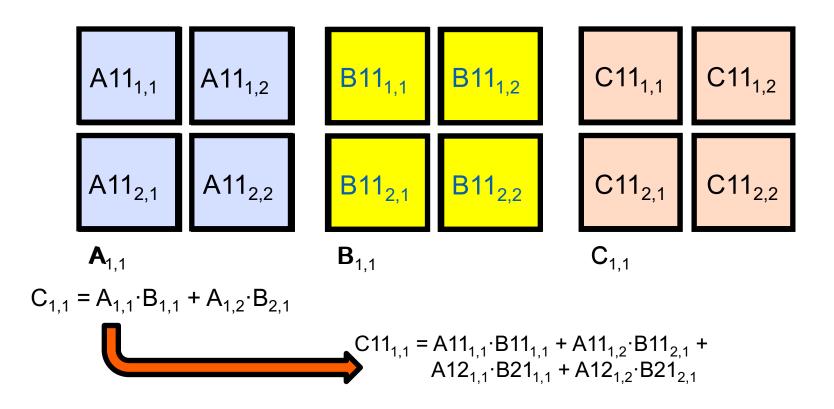
#### Challenge 4: Recursive matrix multiplication

- Quarter each input matrix and output matrix
- Treat each submatrix as a single element and multiply
- 8 submatrix multiplications, 4 additions



## Challenge 4: Recursive matrix multiplication How to multiply submatrices?

- Use the same routine that is computing the full matrix multiplication
  - Quarter each input submatrix and output submatrix
  - Treat each sub-submatrix as a single element and multiply



# Challenge 4: Recursive matrix multiplication Recursively multiply submatrices

$$C_{1,1} = A_{1,1} \cdot B_{1,1} + A_{1,2} \cdot B_{2,1}$$

$$C_{1,2} = A_{1,1} \cdot B_{1,2} + A_{1,2} \cdot B_{2,2}$$

$$C_{2,1} = A_{2,1} \cdot B_{1,1} + A_{2,2} \cdot B_{2,1}$$

$$C_{2,2} = A_{2,1} \cdot B_{1,2} + A_{2,2} \cdot B_{2,2}$$

Need range of indices to define each submatrix to be used

Also need stopping criteria for recursion

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  - Fortran and OpenMP

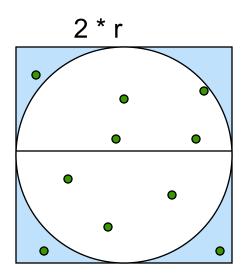
#### **Computers and random numbers**

- We use "dice" to make random numbers:
  - Given previous values, you cannot predict the next value.
  - There are no patterns in the series ... and it goes on forever.
- Computers are deterministic machines ... set an initial state, run a sequence of predefined instructions, and you get a deterministic answer
  - By design, computers are not random and cannot produce random numbers.
- However, with some very clever programming, we can make "pseudo random" numbers that are as random as you need them to be ... but only if you are very careful.
- Why do I care? Random numbers drive statistical methods used in countless applications:
  - Sample a large space of alternatives to find statistically good answers (Monte Carlo methods).

#### **Monte Carlo Calculations**

#### Using Random numbers to solve tough problems

- Sample a problem domain to estimate areas, compute probabilities, find optimal values, etc.
- Example: Computing π with a digital dart board:



$$N=10$$
  $\pi=2.8$   $N=100$   $\pi=3.16$   $N=1000$   $\pi=3.148$ 

- Throw darts at the circle/square.
- Chance of falling in circle is proportional to ratio of areas:

$$A_c = r^2 * \pi$$
 $A_s = (2*r) * (2*r) = 4 * r^2$ 
 $P = A_c/A_s = \pi/4$ 

 Compute π by randomly choosing points, count the fraction that falls in the circle, compute pi.

#### Parallel Programmers love Monte Carlo Embarrassingly parallel: the

parallelism is so easy its

algorithms

```
#include "omp.h"
                                                    embarrassing.
static long num trials = 10000;
                                                 Add two lines and you have a
int main ()
                                                    parallel program.
  long i; long Ncirc = 0; double pi, x, y; double pi, x, y;
  double r = 1.0; // radius of circle. Side of squrare is 2*r
  seed(0,-r, r); // The circle and square are centered at the origin
  #pragma omp parallel for private (x, y) reduction (+:Ncirc)
  for(i=0;i<num trials; i++)</pre>
    x = random(); y = random();
    if (x^*x + y^*y) \le r^*r Ncirc++;
  pi = 4.0 * ((double)Ncirc/(double)num_trials);
  printf("\n %d trials, pi is %f \n",num_trials, pi);
```

## **Linear Congruential Generator (LCG)**

LCG: Easy to write, cheap to compute, portable, OK quality

```
random_next = (MULTIPLIER * random_last + ADDEND)% PMOD;
random_last = random_next;
```

- If you pick the multiplier and addend correctly, LCG has a period of PMOD.
- Picking good LCG parameters is complicated, so look it up (Numerical Recipes is a good source). I used the following:
  - ◆ MULTIPLIER = 1366
  - ◆ ADDEND = 150889
  - ◆ PMOD = 714025

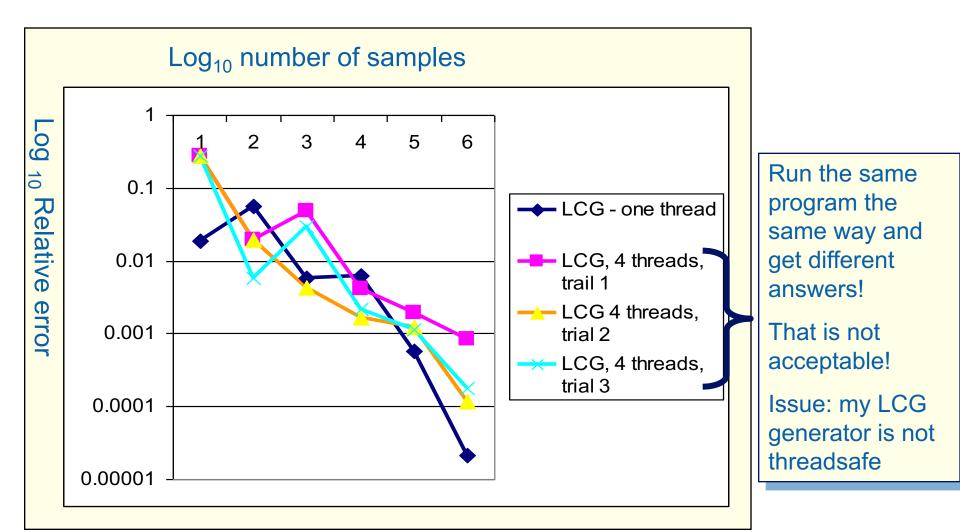
#### LCG code

```
static long MULTIPLIER = 1366;
static long ADDEND = 150889;
static long PMOD = 714025;
long random_last = 0;
double random ()
{
    long random_next;

    random_next = (MULTIPLIER * random_last + ADDEND)% PMOD;
    random_last = random_next;

    return ((double)random_next/(double)PMOD);
}
```

#### Running the PI\_MC program with LCG generator



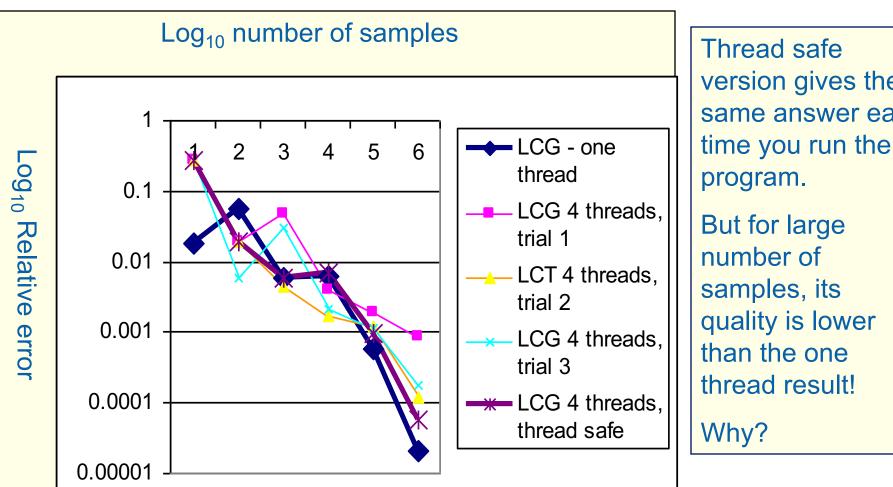
Program written using the Intel C/C++ compiler (10.0.659.2005) in Microsoft Visual studio 2005 (8.0.50727.42) and running on a dual-core laptop (Intel T2400 @ 1.83 Ghz with 2 GB RAM) running Microsoft Windows XP.

#### LCG code: threadsafe version

```
between random number
static long MULTIPLIER = 1366;
static long ADDEND = 150889;
                                                computations,
static long PMOD = 714025;
                                                To make the generator
long random last = 0;
#pragma omp threadprivate(random_last)
                                                threadsafe, make
double random ()
                                                random_last threadprivate
                                                so each thread has its
  long random next;
                                                own copy.
  random_next = (MULTIPLIER * random_last + ADDEND)% PMOD;
  random last = random next;
 return ((double)random next/(double)PMOD);
```

random\_last carries state

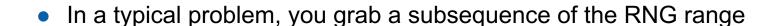
### Thread safe random number generators



version gives the same answer each time you run the

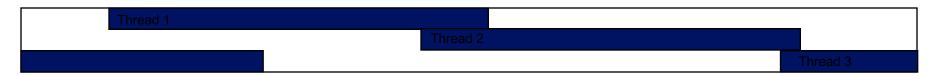
## Pseudo Random Sequences

 Random number Generators (RNGs) define a sequence of pseudo-random numbers of length equal to the period of the RNG



Seed determines starting point

- Grab arbitrary seeds and you may generate overlapping sequences
  - ◆ E.g. three sequences ... last one wraps at the end of the RNG period.



 Overlapping sequences = over-sampling and bad statistics ... lower quality or even wrong answers!

### Parallel random number generators

- Multiple threads cooperate to generate and use random numbers.
- Solutions:
  - Replicate and Pray
  - Give each thread a separate, independent generator
  - Have one thread generate all the numbers.
  - Leapfrog ... deal out sequence values "round robin" as if dealing a deck of cards.
  - Block method ... pick your seed so each threads gets a distinct contiguous block.
- Other than "replicate and pray", these are difficult to implement. Be smart ... get a math library that does it right.

Intel's Math kernel Library supports a wide range of parallel random number generators.

If done right, can generate the same sequence regardless of the number of threads ...

Nice for debugging, but not really needed scientifically.

For an open alternative, the state of the art is the Scalable Parallel Random Number Generators Library (SPRNG): <a href="http://www.sprng.org/">http://www.sprng.org/</a> from Michael Mascagni's group at Florida State University.

## MKL Random number generators (RNG)

- MKL includes several families of RNGs in its vector statistics library.
- Specialized to efficiently generate vectors of random numbers

#define BLOCK 100
double buff[BLOCK];

VSLStreamStatePtr stream;

vslNewStream(&ran\_stream, VSL\_BRNG\_WH, (int)seed\_val);

vdRngUniform (VSL\_METHOD\_DUNIFORM\_STD, stream,
BLOCK, buff, low, hi)

Fill buff with BLOCK pseudo rand.

Delete the stream when you are done

vslDeleteStream( &stream );

nums, uniformly distributed with values

between lo and hi.

## Wichmann-Hill generators (WH)

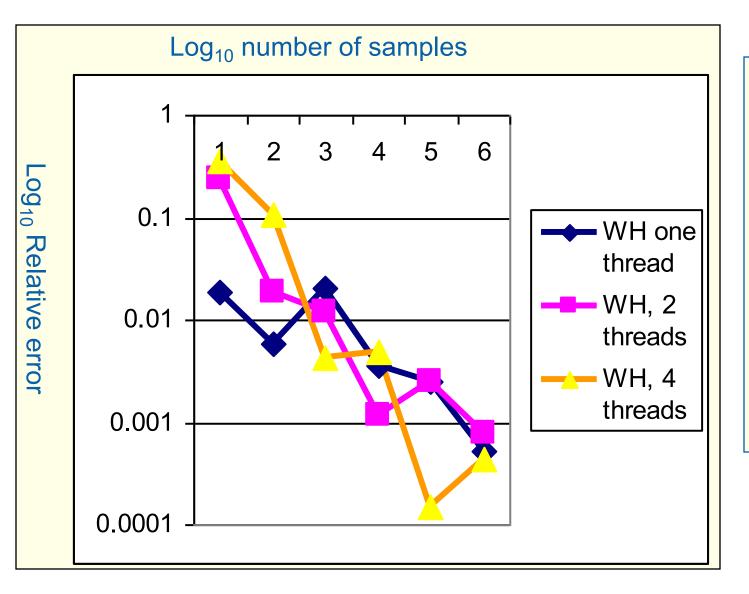
- WH is a family of 273 parameter sets each defining a nonoverlapping and independent RNG.
- Easy to use, just make each stream threadprivate and initiate RNG stream so each thread gets a unique WG RNG.

```
VSLStreamStatePtr stream;

#pragma omp threadprivate(stream)
...

vslNewStream(&ran_stream, VSL_BRNG_WH+Thrd_ID, (int)seed);
```

## Independent Generator for each thread



Notice that once you get beyond the high error, small sample count range, adding threads doesn't decrease quality of random sampling.

#### **Leap Frog method**

- Interleave samples in the sequence of pseudo random numbers:
  - Thread i starts at the i<sup>th</sup> number in the sequence

random\_last = (unsigned long long) pseed[id];

- Stride through sequence, stride length = number of threads.
- Result ... the same sequence of values regardless of the number of threads.

```
#pragma omp single
  nthreads = omp_get_num_threads();
   iseed = PMOD/MULTIPLIER; // just pick a seed
                                                                 One thread
   pseed[0] = iseed;
                                                                 computes offsets
   mult n = MULTIPLIER;
                                                                 and strided
                                                                 multiplier
   for (i = 1; i < nthreads; ++i)
     iseed = (unsigned long long)((MULTIPLIER * iseed) % PMOD);
     pseed[i] = iseed;
                                                           LCG with Addend = 0 just
     mult_n = (mult_n * MULTIPLIER) % PMOD;
                                                           to keep things simple
                                                         Each thread stores offset starting
```

point into its threadprivate "last

random" value

## Same sequence with many threads.

 We can use the leapfrog method to generate the same answer for any number of threads

Steps	One thread	2 threads	4 threads
1000	3.156	3.156	3.156
10000	3.1168	3.1168	3.1168
100000	3.13964	3.13964	3.13964
1000000	3.140348	3.140348	3.140348
10000000	3.141658	3.141658	3.141658

Used the MKL library with two generator streams per computation: one for the x values (WH) and one for the y values (WH+1). Also used the leapfrog method to deal out iterations among threads.



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## Molecular dynamics: Solution

Compiler will warn you if you have missed some variables **#pragma omp parallel for default (none)** shared(x,f,npart,rcoff,side) \ reduction(+:epot,vir) \ schedule (static,32) for (int i=0; i<npart\*3; i+=3) { Loop is not well load balanced: best schedule has to be found by experiment.

### Molecular dynamics : Solution (cont.)

```
#pragma omp atomic
     f[j] -= forcex;
#pragma omp atomic
     f[j+1] = forcey;
#pragma omp atomic
     f[j+2] = forcez;
#pragma omp atomic
   f[i] += fxi;
#pragma omp atomic
   f[i+1] += fyi;
#pragma omp atomic
   f[i+2] += fzi;
```

All updates to f must be atomic

## Molecular dynamics: With orphaning

#### #pragma omp single Implicit barrier needed to avoid race vir = 0.0;condition with update of reduction variables at end of the for construct epot = 0.0; #pragma omp for reduction(+:epot,vir) schedule (static,32) for (int i=0; i< npart\*3; i+=3) { All variables which used to be shared here are now

implicitly determined

## Molecular dynamics: With array reduction

```
ftemp[myid][j] -= forcex;
 ftemp[myid][j+1] = forcey;
 ftemp[myid][j+2] = forcez;
ftemp[myid][i]
             += fxi;
ftemp[myid][i+1] += fyi;
ftemp[myid][i+2] += fzi;
```

Replace atomics with accumulation into array with extra dimension

## Molecular dynamics: With array reduction

```
Reduction can be done
#pragma omp for
                                   in parallel
  for(int i=0;i<(npart*3);i++){
       for(int id=0;id<nthreads;id++){
          f[i] += ftemp[id][i];
         ftemp[id][i] = 0.0;
                                        Zero ftemp for next time
                                        round
```

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## **Challenge: Matrix Multiplication**

- Parallelize the matrix multiplication program in the file matmul.c
- Can you optimize the program by playing with how the loops are scheduled?
- Try the following and see how they interact with the constructs in OpenMP
  - Cache blocking
  - Loop unrolling
  - Vectorization
- Goal: Can you approach the peak performance of the computer?

### **Matrix multiplication**

There is much more that can be done. This is really just the first and most simple step

- On a dual core laptop
  - •13.2 seconds 153 Mflops one thread
  - •7.5 seconds 270 Mflops two threads



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#### Recursive matrix multiplication

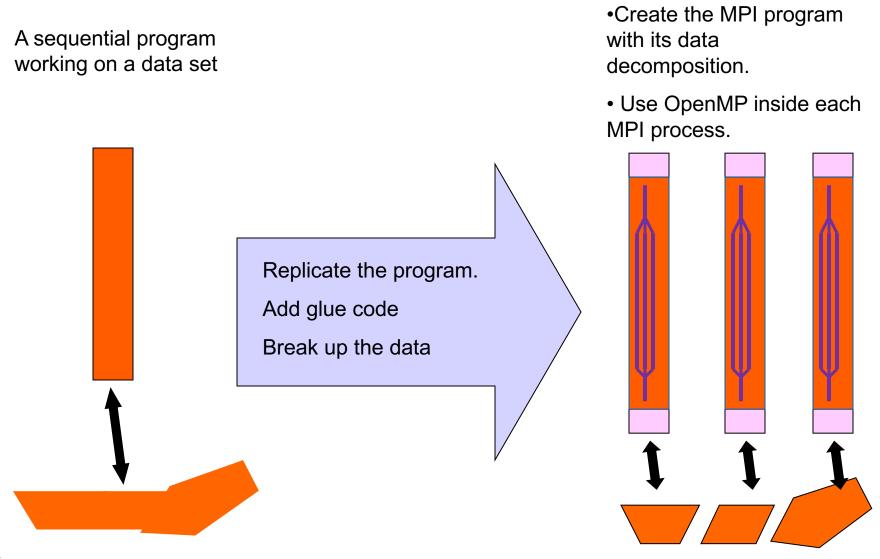
- Could be executed in parallel as 4 tasks
  - Each task executes the two calls for the same output submatrix of C
- However, the same number of multiplication operations needed

```
// product size below which simple matmult code is called
#define THRESHOLD 32768
void matmultrec(int mf, int ml, int nf, int nl, int pf, int pl,
                double **A, double **B, double **C)
// Dimensions: A[mf..ml][pf..pl] B[pf..pl][nf..nl] C[mf..ml][nf..nl]
  if ((ml-mf)*(nl-nf)*(pl-pf) < THRESHOLD)</pre>
     matmult (mf, ml, nf, nl, pf, pl, A, B, C);
   else
#pragma omp task firstprivate(mf,ml,nf,nl,pf,pl)
     matmultrec(mf, mf+(ml-mf)/2, nf, nf+(nl-nf)/2, pf, pf+(pl-pf)/2, A, B, C); // C11 += A11*B11
     matmultrec(mf, mf+(ml-mf)/2, nf, nf+(nl-nf)/2, pf+(pl-pf)/2, pl, A, B, C); // C11 += A12*B21
}
#pragma omp task firstprivate(mf,ml,nf,nl,pf,pl)
     matmultrec(mf, mf+(ml-mf)/2, nf+(nl-nf)/2, nl, pf, pf+(pl-pf)/2, A, B, C); // C12 += A11*B12
     matmultrec(mf, mf+(ml-mf)/2, nf+(nl-nf)/2, nl, pf+(pl-pf)/2, pl, A, B, C); // C12 += A12*B22
#pragma omp task firstprivate(mf,ml,nf,nl,pf,pl)
     matmultrec(mf+(ml-mf)/2, ml, nf, nf+(nl-nf)/2, pf, pf+(pl-pf)/2, A, B, C); // C21 += A21*B11
     matmultrec(mf+(ml-mf)/2, ml, nf, nf+(nl-nf)/2, pf+(pl-pf)/2, pl, A, B, C); // C21 += A22*B21
#pragma omp task firstprivate(mf,ml,nf,nl,pf,pl)
     matmultrec(mf+(ml-mf)/2, ml, nf+(nl-nf)/2, nl, pf, pf+(pl-pf)/2, A, B, C); // C22 += A21*B12
     matmultrec(mf+(ml-mf)/2, ml, nf+(nl-nf)/2, nl, pf+(pl-pf)/2, pl, A, B, C); // C22 += A22*B22
#pragma omp taskwait
```

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## How do people mix MPI and OpenMP?



# Pi program with MPI and OpenMP

Get the MPI part done first, then add OpenMP pragma where it makes sense to do so

```
#include <mpi.h>
#include "omp.h"
void main (int argc, char *argv[])
        int i, my id, numprocs; double x, pi, step, sum = 0.0;
        step = 1.0/(double) num steps;
        MPI Init(&argc, &argv);
        MPI_Comm_Rank(MPI_COMM_WORLD, &my_id);
        MPI_Comm_Size(MPI_COMM_WORLD, &numprocs);
        my_steps = num_steps/numprocs;
#pragma omp parallel for reduction(+:sum) private(x)
        for (i=my id*my steps; i<(m id+1)*my steps; i++)
                 x = (i+0.5)*step;
                 sum += 4.0/(1.0+x*x);
        sum *= step;
        MPI_Reduce(&sum, &pi, 1, MPI_DOUBLE, MPI_SUM, 0,
                MPI_COMM_WORLD);
```

## Key issues when mixing OpenMP and MPI

- 1. Messages are sent to a process not to a particular thread.
  - Not all MPIs are threadsafe. MPI 2.0 defines threading modes:
    - MPI\_Thread\_Single: no support for multiple threads
    - MPI\_Thread\_Funneled: Mult threads, only master calls MPI
    - MPI\_Thread\_Serialized: Mult threads each calling MPI, but they
      do it one at a time.
    - MPI\_Thread\_Multiple: Multiple threads without any restrictions
  - Request and test thread modes with the function:
     MPI\_init\_thread(desired\_mode, delivered\_mode, ierr)
- 2. Environment variables are not propagated by mpirun. You'll need to broadcast OpenMP parameters and set them with the library routines.

## **Dangerous Mixing of MPI and OpenMP**

 The following will work only if MPI Thread Multiple is supported ... a level of support I wouldn't depend on. MPI Comm Rank(MPI COMM WORLD, &mpi id); #pragma omp parallel int tag, swap\_neigh, stat, omp\_id = omp\_thread\_num(); long buffer [BUFF\_SIZE], incoming [BUFF\_SIZE]; big ugly calc1(omp id, mpi id, buffer); // Finds MPI id and tag so neighbor(omp\_id, mpi\_id, &swap\_neigh, &tag); // messages don't conflict MPI\_Send (buffer, BUFF\_SIZE, MPI\_LONG, swap\_neigh, tag, MPI COMM WORLD); MPI\_Recv (incoming, buffer\_count, MPI\_LONG, swap\_neigh, tag, MPI COMM WORLD, &stat); big ugly calc2(omp id, mpi id, incoming, buffer); #pragma critical consume(buffer, omp\_id, mpi\_id);

# Messages and threads

- Keep message passing and threaded sections of your program separate:
  - Setup message passing outside OpenMP parallel regions (MPI\_Thread\_funneled)
  - Surround with appropriate directives (e.g. critical section or master)
     (MPI\_Thread\_Serialized)
  - For certain applications depending on how it is designed it may not matter which thread handles a message. (MPI\_Thread\_Multiple)
    - Beware of race conditions though if two threads are probing on the same message and then racing to receive it.

## Safe Mixing of MPI and OpenMP

#### **Put MPI in sequential regions**

```
MPI Init(&argc, &argv); MPI Comm Rank(MPI COMM WORLD, &mpi id);
// a whole bunch of initializations
#pragma omp parallel for
for (I=0;I<N;I++) {
   U[I] = big calc(I);
   MPI Send (U, BUFF SIZE, MPI DOUBLE, swap neigh,
           tag, MPI COMM WORLD);
   MPI Recv (incoming, buffer count, MPI DOUBLE, swap neigh,
           tag, MPI COMM WORLD, &stat);
#pragma omp parallel for
for (I=0;I<N;I++) {
   U[I] = other_big_calc(I, incoming);
consume(U, mpi id);
```

Technically Requires
MPI\_Thread\_funneled, but I
have never had a problem with
this approach ... even with preMPI-2.0 libraries.

## Safe Mixing of MPI and OpenMP

#### Protect MPI calls inside a parallel region

```
MPI Init(&argc, &argv); MPI Comm Rank(MPI COMM WORLD, &mpi id);
// a whole bunch of initializations
                                                 Technically Requires
#pragma omp parallel
                                                 MPI_Thread_funneled, but I
#pragma omp for
                                                 have never had a problem with
  for (I=0;I<N;I++) U[I] = big calc(I);
                                                 this approach ... even with pre-
                                                 MPI-2.0 libraries.
#pragma master
  MPI Send (U, BUFF SIZE, MPI DOUBLE, neigh, tag, MPI COMM WORLD);
  MPI Recv (incoming, count, MPI DOUBLE, neigh, tag, MPI COMM WORLD,
                                                                    &stat);
#pragma omp barrier
#pragma omp for
  for (I=0;I<N;I++) U[I] = other big calc(I, incoming);
#pragma omp master
  consume(U, mpi_id);
```

#### Hybrid OpenMP/MPI works, but is it worth it?

- Literature\* is mixed on the hybrid model: sometimes its better, sometimes
   MPI alone is best.
- There is potential for benefit to the hybrid model
  - MPI algorithms often require replicated data making them less memory efficient.
  - Fewer total MPI communicating agents means fewer messages and less overhead from message conflicts.
  - Algorithms with good cache efficiency should benefit from shared caches of multi-threaded programs.
  - The model maps perfectly with clusters of SMP nodes.
- But really, it's a case by case basis and to large extent depends on the particular application.

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# Fortran and OpenMP

- We were careful to design the OpenMP constructs so they cleanly map onto C, C++ and Fortran.
- There are a few syntactic differences that once understood, will allow you to move back and forth between languages.
- In the specification, language specific notes are included when each construct is defined.

# **OpenMP:**

## Some syntax details for Fortran programmers

- Most of the constructs in OpenMP are compiler directives.
  - For Fortran, the directives take one of the forms:

```
C$OMP construct [clause [clause]...]
!$OMP construct [clause [clause]...]
*$OMP construct [clause [clause]...]
```

The OpenMP include file and lib module

```
use omp_lib
Include omp_lib.h
```

# **OpenMP: Structured blocks (Fortran)**

- Most OpenMP constructs apply to structured blocks.
  - Structured block: a block of code with one point of entry at the top and one point of exit at the bottom.
  - The only "branches" allowed are STOP statements in Fortran and exit() in C/C++.

```
C$OMP PARALLEL

10 wrk(id) = garbage(id)

res(id) = wrk(id)**2

if(conv(res(id)) goto 10

C$OMP END PARALLEL

print *,id
```

```
C$OMP PARALLEL

10 wrk(id) = garbage(id)

30 res(id)=wrk(id)**2
    if(conv(res(id))goto 20
    go to 10

C$OMP END PARALLEL
    if(not_DONE) goto 30

20 print *, id
```

# **OpenMP:**

#### **Structured Block Boundaries**

 In Fortran: a block is a single statement or a group of statements between directive/end-directive pairs.

```
C$OMP PARALLEL

10 wrk(id) = garbage(id)

res(id) = wrk(id)**2

if(conv(res(id)) goto 10

C$OMP END PARALLEL
```

```
C$OMP PARALLEL DO

do I=1,N

res(I)=bigComp(I)

end do

C$OMP END PARALLEL DO
```

- The "construct/end construct" pairs is done anywhere a structured block appears in Fortran. Some examples:
  - DO ... END DO
  - PARALLEL ... END PARALLEL
  - CRICITAL ... END CRITICAL
  - SECTION ... END SECTION

- SECTIONS ... END SECTIONS
- SINGLE ... END SINGLE
- MASTER ... END MASTER

# Runtime library routines

- The include file or module defines parameters
  - Integer parameter omp\_lock\_kind
  - Integer parameter omp\_nest\_lock\_kind
  - Integer parameter omp\_sched\_kind
  - Integer parameter openmp\_version
    - With value that matches C's OPEMMP macro
- Fortran interfaces are similar to those used with C
  - Subroutine omp\_set\_num\_threads (num\_threads)
  - Integer function omp get num threads()
  - Integer function omp\_get\_thread\_num()\
  - Subroutine omp\_init\_lock(svar)
    - Integer(kind=omp\_lock\_kind) svar
  - Subroutine omp\_destroy\_lock(svar)
  - Subroutine omp\_set\_lock(svar)
  - Subroutine omp\_unset\_lock(svar)