



A “Hands-on” Introduction to OpenMP*

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Preliminaries: Part 1

- Disclosures
 - The views expressed in this tutorial are those of the people delivering the tutorial.
 - We are not 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 .. 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.

Our OpenMP progression

Topic	Exercise	concepts
I. OMP introduction	Install sw, hello_world	Parallel regions
II. Creating threads	Pi_spmd_simple	Parallel, default data environment, runtime library calls
III. Synchronization	Pi_spmd_final	False sharing, critical, atomic
IV. Parallel loops	Pi_loop	For, schedule, reduction,
V. Odds and ends	No Exercise	Single, sections, master, runtime libraries, environment variables, synchronization, etc.
VI. Data environment	Mandelbrot set area	Data environment details, software optimization
VII. OpenMP tasks	Simple tasks, Pi_recur	Explicit tasks in OpenMP
VIII. Wrap-up	Challenge problems	Putting full range of concepts together with more complex problems

Outline

- ➔ • Introduction to OpenMP
 - Creating Threads
 - A brief theoretical interlude: Speedup and Amdahl's law
 - Synchronization
 - Parallel Loops
 - Loop schedules and vectorization
 - Synchronize single masters and stuff
 - Data environment
 - Tasks
 - Challenge Problems

OpenMP* overview:

```
C$OMP FLUSH
```

```
#pragma omp critical
```

```
C$OMP THREADPRIVATE (/ABC/)
```

```
CALL OMP_SET_NUM_THREADS(10)
```

OpenMP: An API for Writing Multithreaded Applications

- A set of compiler directives and library routines for parallel application programmers
- Greatly simplifies writing multi-threaded (MT) programs in Fortran, C and C++
- Standardizes established SMP practice + vectorization and heterogeneous device programming

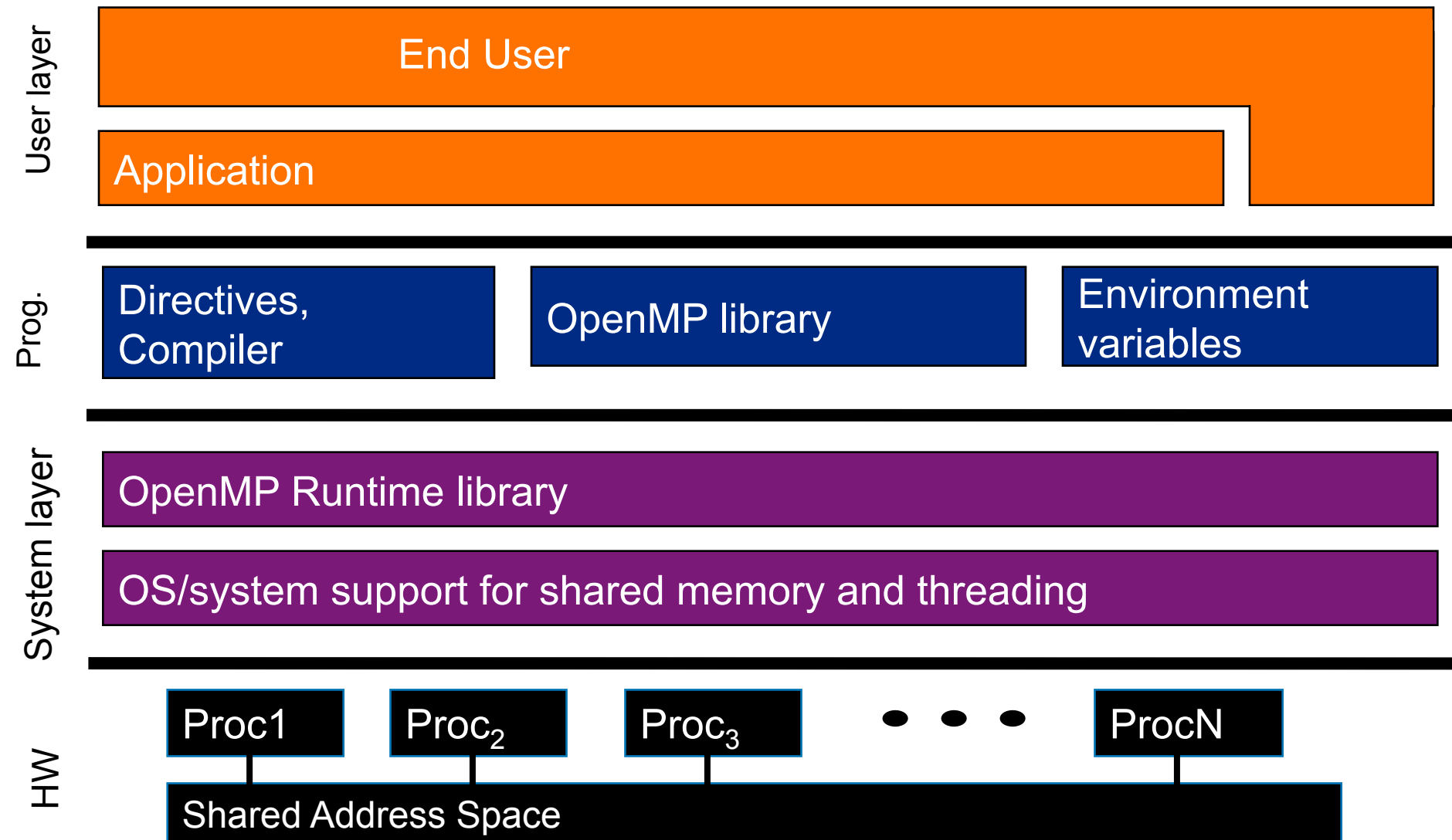
```
C$OMP PARALLEL COPYIN (/blk/)
```

```
C$OMP DO lastprivate (XX)
```

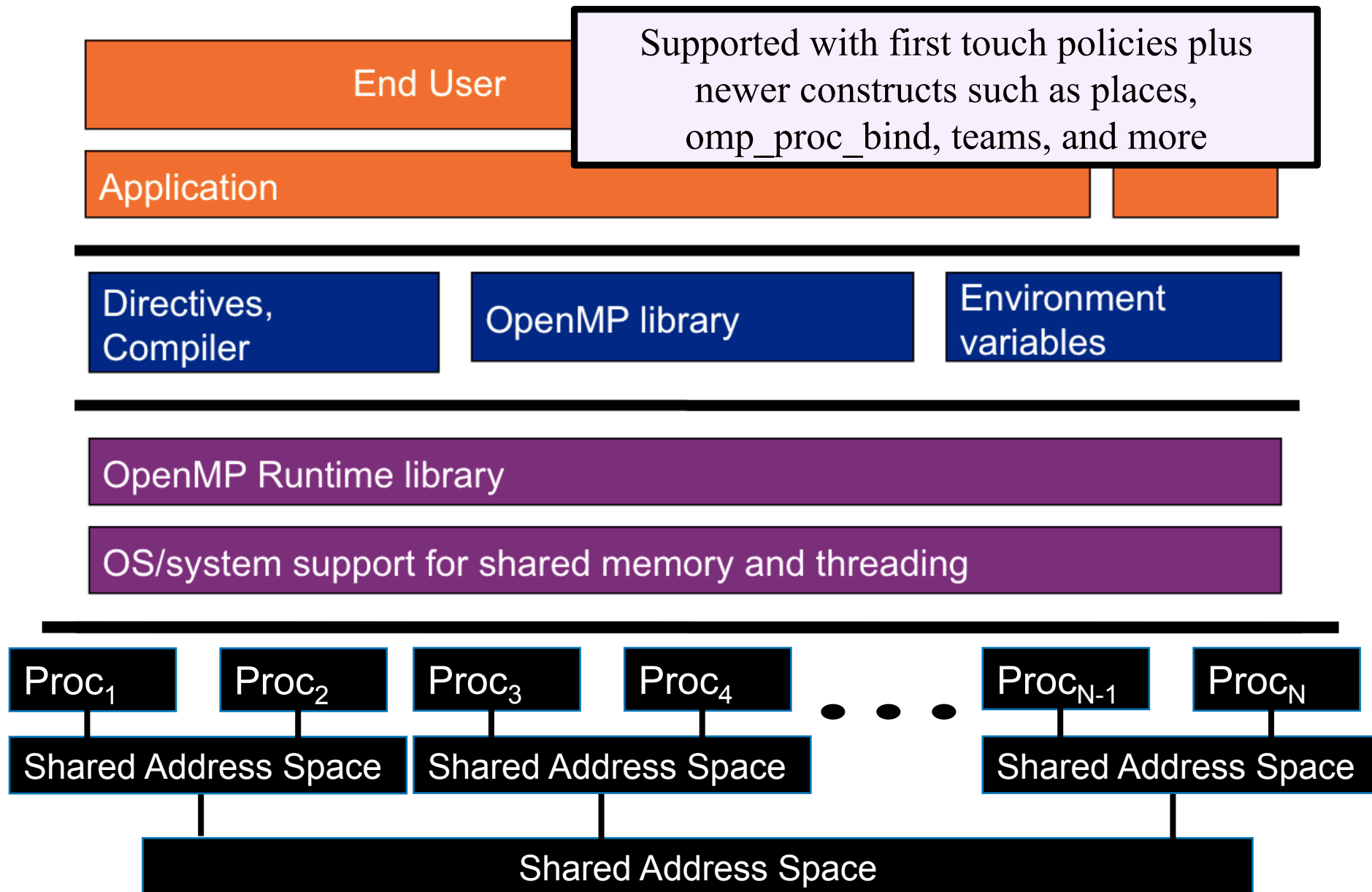
```
Nthrds = OMP_GET_NUM_PROCS()
```

```
omp_set_lock(lck)
```

OpenMP basic definitions: Basic Solution stack

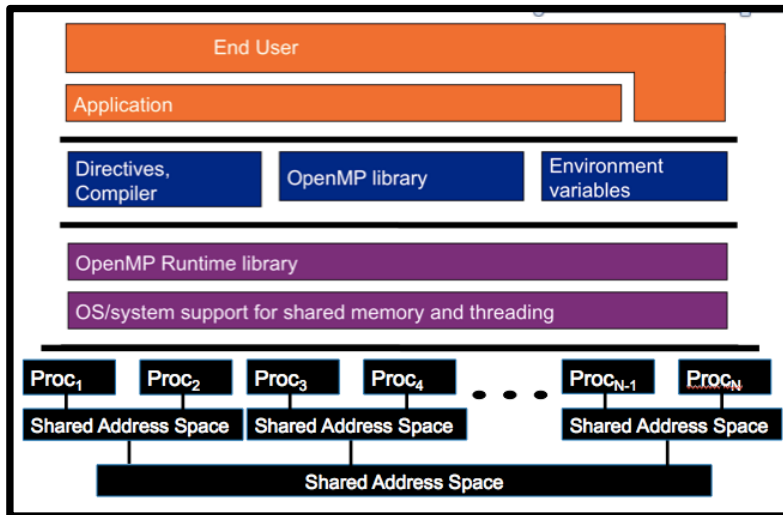


OpenMP basic definitions: NUMA Solution stack

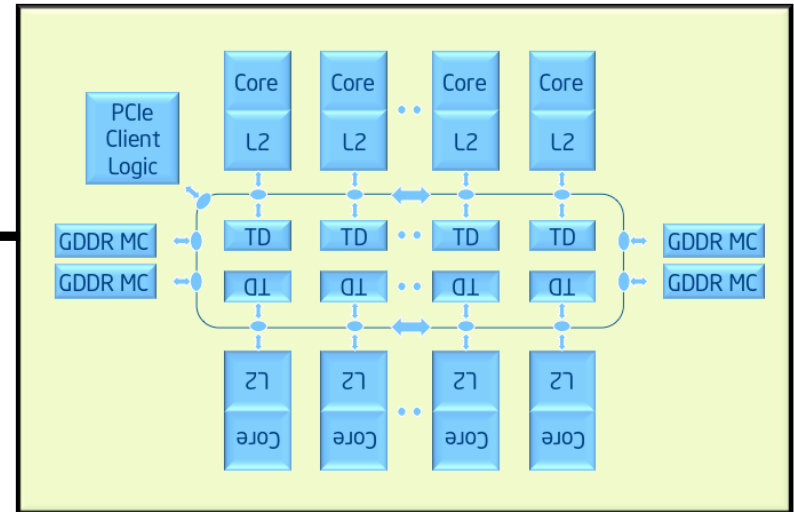


OpenMP basic definitions: Target solution stack

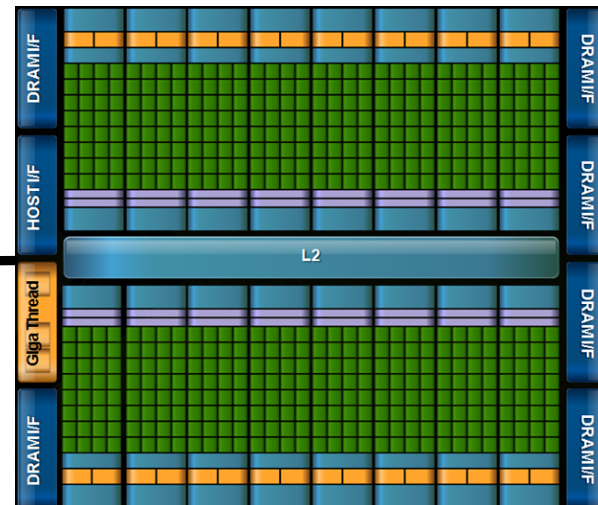
Supported (since OpenMP 4.0)
with target, teams, distribute,
and other constructs



Host



Target Device: Intel® Xeon Phi™ coprocessor



Target Device: GPU

OpenMP core syntax

- Most of the constructs in OpenMP are compiler directives.

#pragma omp construct [clause [clause]...]

- Example

#pragma omp parallel num_threads(4)

- Function prototypes and types in the file:

#include <omp.h>

use omp_lib

- 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 1, Part A: Hello world

Verify that your environment works

- Write a program that prints “hello world”.

```
#include<stdio.h>
int main()
{

    int ID = 0;

    printf(" hello(%d) ", ID);
    printf(" world(%d) \n", ID);

}
```

Exercise 1, Part B: Hello world

Verify that your OpenMP environment works

- Write a multithreaded program that prints “hello world”.

```
#include <omp.h>
#include <stdio.h>
int main()
{
    #pragma omp parallel
    {
        int ID = 0;

        printf(" hello(%d) ", ID);
        printf(" world(%d) \n", ID);
    }
}
```

Switches for compiling and linking

gcc -fopenmp **Linux, OSX**

pgcc -mp **pgi**

icl /Qopenmp **intel (windows)**

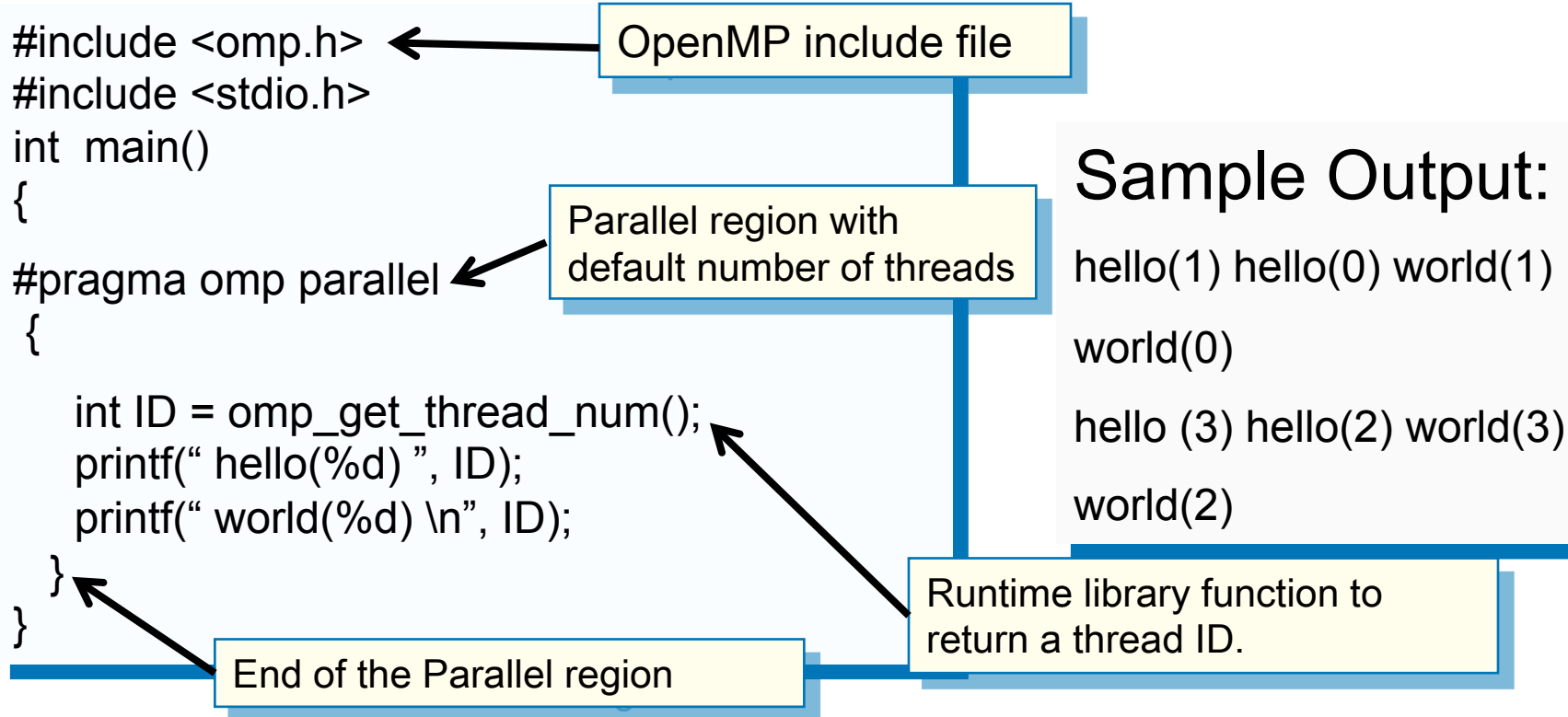
icc -fopenmp **intel (linux)**

lcc -qopenmp **intel ver 16 and beyond**

Exercise 1: Solution

A multi-threaded “Hello world” program

- Write a multithreaded program where each thread prints “hello world”.



OpenMP overview:

How do threads interact?

- OpenMP is a multi-threading, shared address model
 - Threads communicate by sharing variables.
- Unintended sharing of data causes race conditions:
 - Race condition: when the program's outcome changes as the threads are scheduled differently.
- To control race conditions:
 - Use synchronization to protect data conflicts.
- Synchronization is expensive so:
 - Change how data is accessed to minimize the need for synchronization.

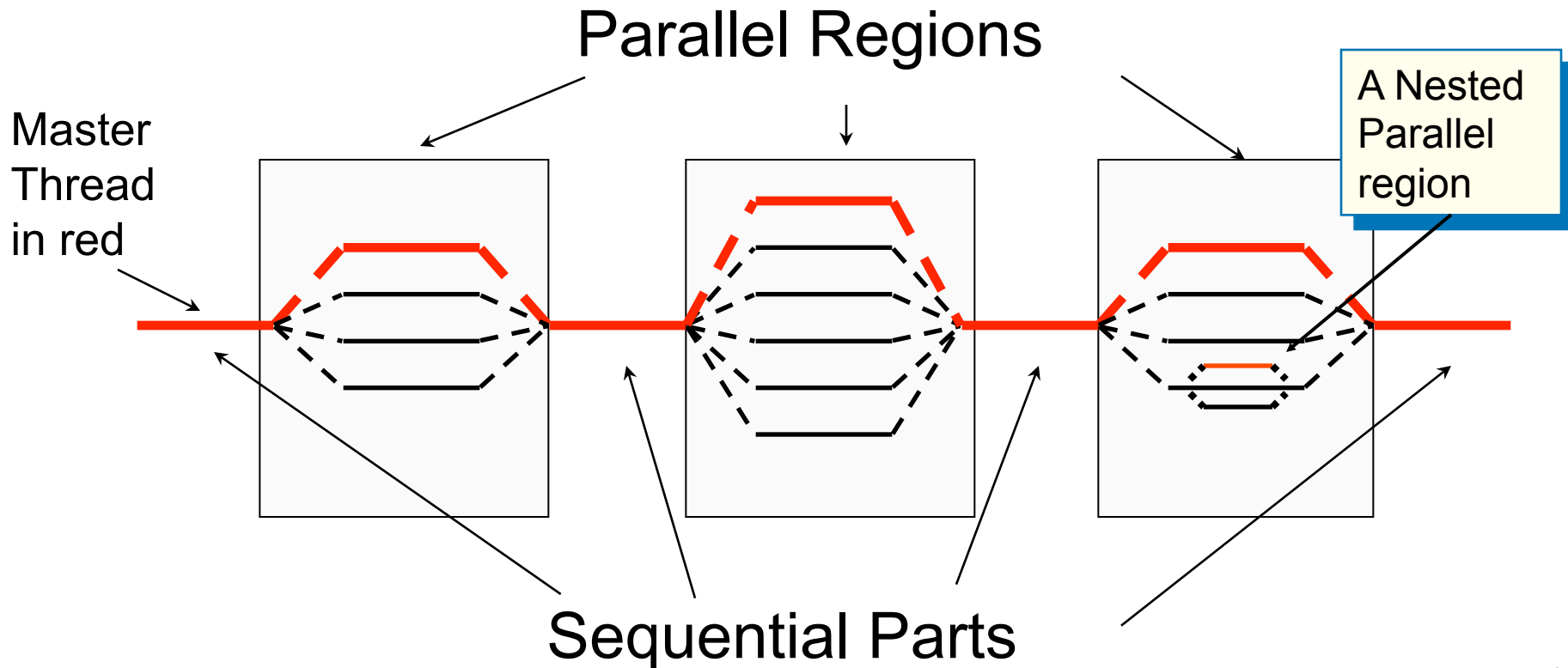
Outline

- Introduction to OpenMP
-  • Creating Threads
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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 returning a thread ID

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

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];
```

```
#pragma omp parallel num_threads(4)
{
    int ID = omp_get_thread_num();
    pooh(ID,A);
}
```

clause to request a certain number of threads

Runtime function returning a thread ID

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

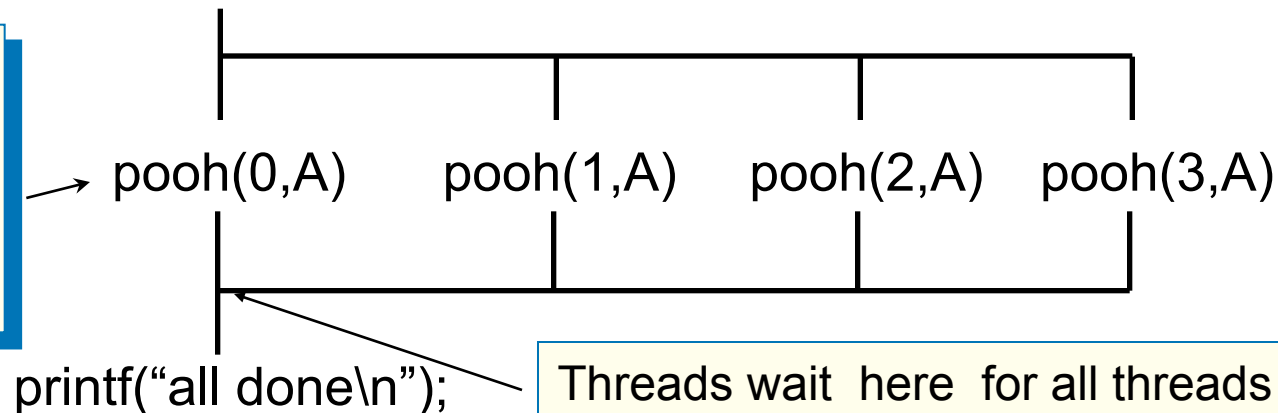
Thread creation: Parallel regions example

- 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");
```

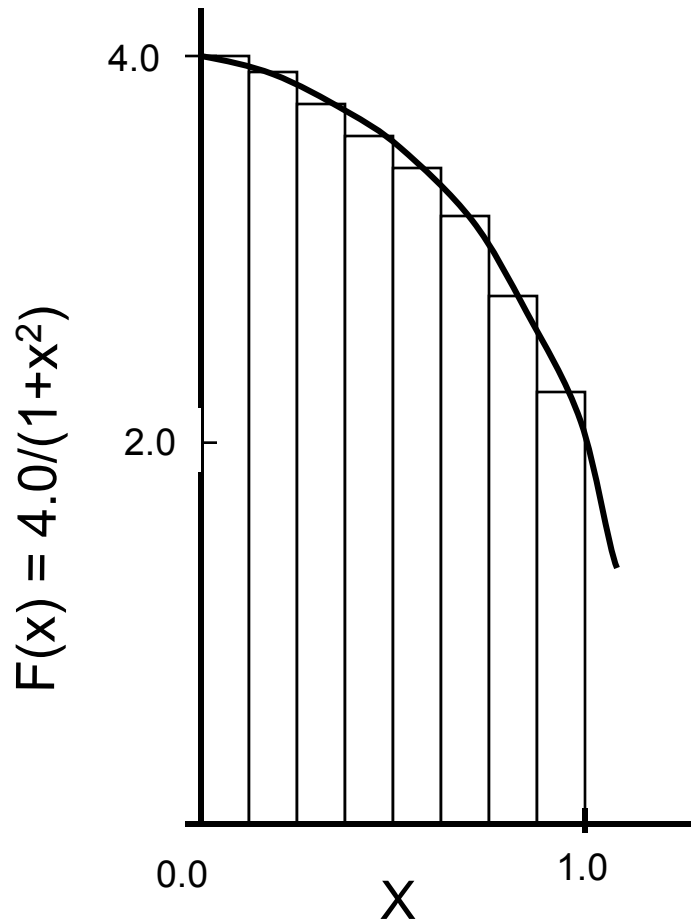
A single copy of A is shared between all threads.



Threads wait here for all threads to finish before proceeding (i.e., a *barrier*)

Exercises 2 to 4:

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 Δx and height $F(x_i)$ at the middle of interval i .

Exercises 2 to 4: 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;
}
```

- #pragma omp parallel.
 - int omp_get_num_threads();
 - int omp_get_thread_num();
 - double omp_get_wtime();
 - omp_set_num_threads();

Exercise 2

- 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();`

Number of threads in the team

– `int omp_get_thread_num();`

Thread ID or rank

– `double omp_get_wtime();`

Time in Seconds since a fixed point in the past

– `omp_set_num_threads();`

Request a number of threads in the team

Exercise 2 (hints)

- 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();`

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 ()
{
    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) nthrds = 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;
    }
}
```

threads	1 st SPMD
1	1.86
2	1.03
3	1.08
4	0.97

*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.

An Example of Parallel Computing

Compute N independent tasks on one processor

Load Data

Compute T_1

...

Compute T_N

Consume Results

$$\text{Time}_{\text{seq}}(1) = T_{\text{load}} + N * T_{\text{task}} + T_{\text{consume}}$$

Compute N independent tasks with P processors

Load Data

Compute T_1

...

Compute T_N

Consume Results

$$\text{Time}_{\text{par}}(P) = T_{\text{load}} + (N/P) * T_{\text{task}} + T_{\text{consume}}$$

Ideally Cut
runtime by $\sim 1/P$
(Note: Parallelism
only speeds-up the
concurrent part)

Talking about performance

- Speedup: the increased performance from running on P processors.
- Perfect Linear Speedup: happens when no parallel overhead and algorithm is 100% parallel.
- Super-linear Speedup: typically due to cache effects ... i.e. as P grows, aggregate cache size grows so more of the problem fits in cache

$$S(P) = \frac{Time_{seq}(1)}{Time_{par}(P)}$$

$$S(P) = P$$

$$S(P) > P$$

Amdahl's Law

- What is the maximum speedup you can expect from a parallel program?
- Approximate the runtime as a part that can be sped up with additional processors and a part that is fundamentally serial.

$$Time_{par}(P) = (serial_fraction + \frac{parallel_fraction}{P}) * Time_{seq}$$

- If serial_fraction is α and parallel_fraction is $(1 - \alpha)$ then the speedup is:

$$S(P) = \frac{Time_{seq}}{Time_{par}(P)} = \frac{Time_{seq}}{(\alpha + \frac{1 - \alpha}{P}) * Time_{seq}} = \frac{1}{\alpha + \frac{1 - \alpha}{P}}$$

- If you had an unlimited number of processors: $P \rightarrow \infty$

- The maximum possible speedup is: $S = \frac{1}{\alpha}$ ←

Amdahl's Law

So now you should understand my silly introduction slide.

Introduction

I'm just a simple kayak instructor

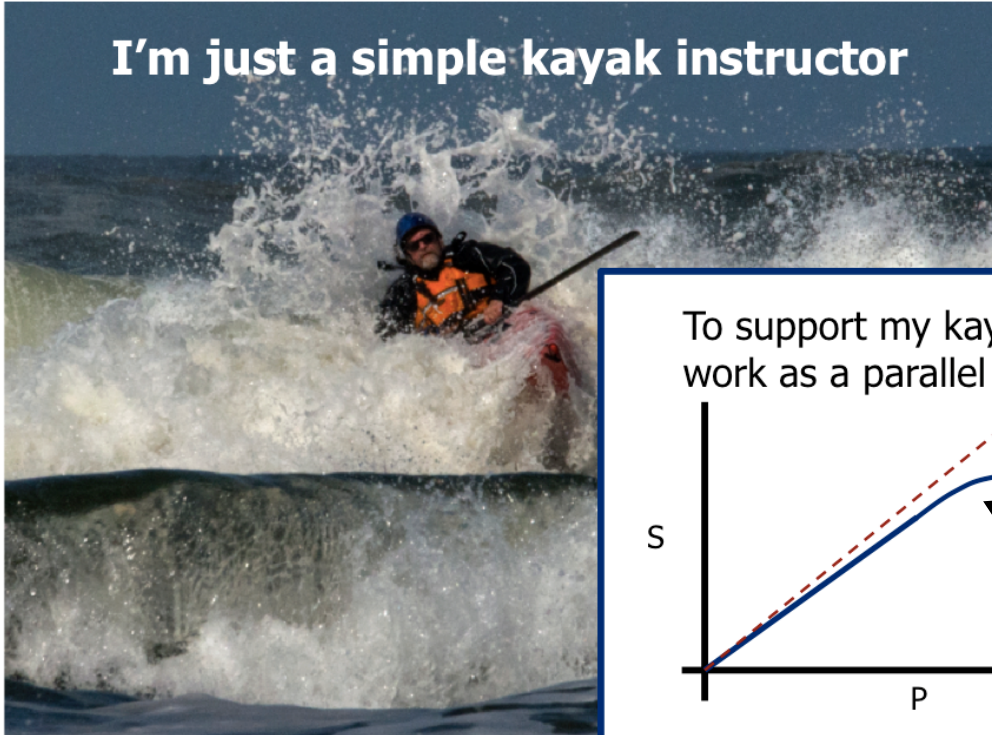
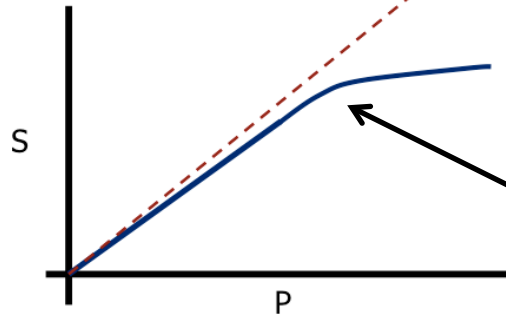


Photo © by Greg Clopton, 2014

We measure our success as parallel programmers by how close we come to ideal linear speedup.

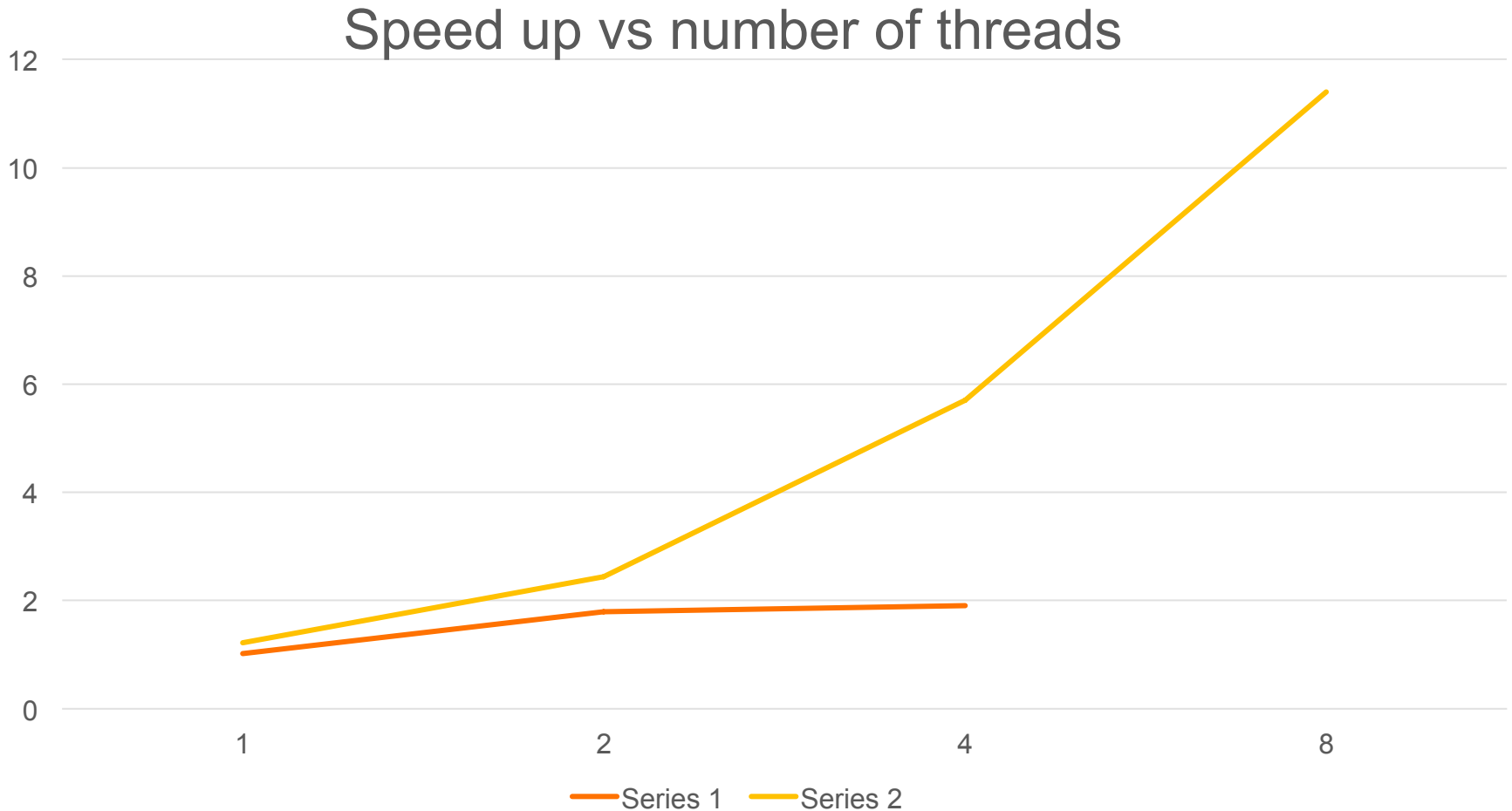
To support my kayaking habit I work as a parallel programmer



Which means I know how to turn math into lines on a speedup plot

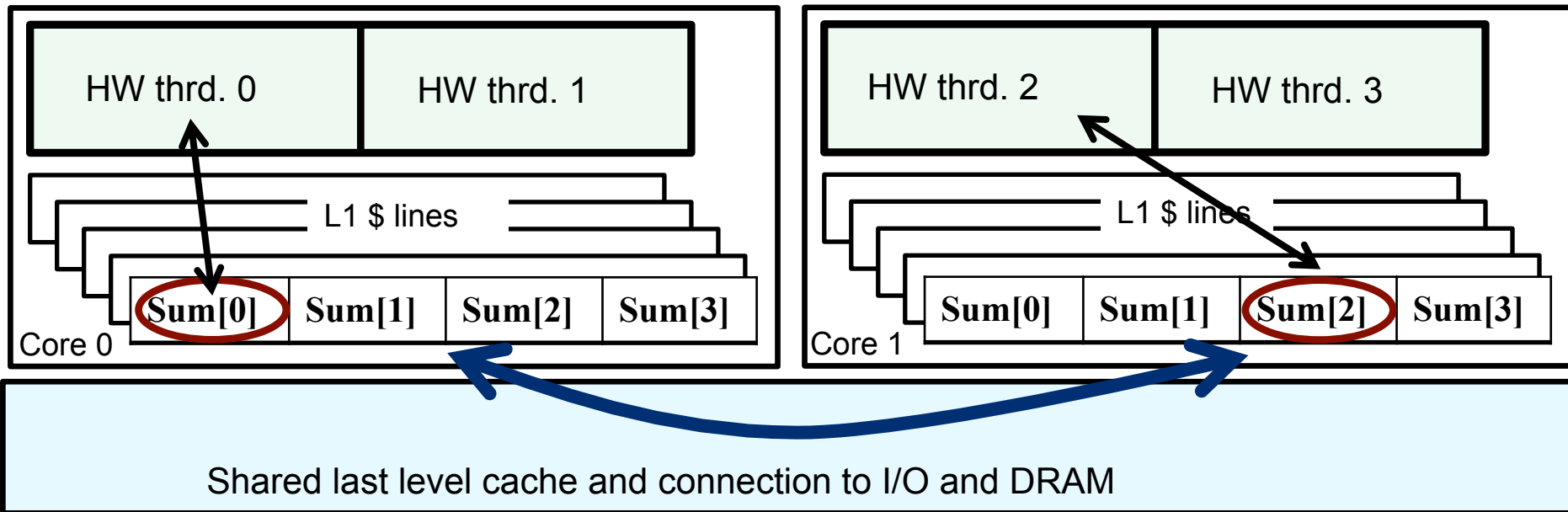
A good parallel programmer always figures out when you fall off the linear speedup curve and why that has occurred.

Collect results and plot speedup vs number of threads



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”**.

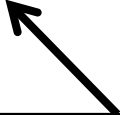


- If you promote scalars to an array to support creation of an SPMD program, the array elements are contiguous in memory and hence share cache lines ... Results in poor scalability.
- Solution: Pad arrays so elements you use are on distinct cache lines.

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
    {
        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][0] += 4.0/(1.0+x*x);
        }
    }

    for(i=0, pi=0.0; i<nthreads; i++) pi += sum[i][0] * step;
}
```



Pad the array so
each sum value is
in a different
cache line

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 ()
{
    int i, nthrds; double pi, sum[NUM_THREADS][PAD];
    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) nthrds = 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<nthrds; i++) pi += sum[i][0] * step;
}
```

threads	1 st SPMD	1 st SPMD padded
1	1.86	1.86
2	1.03	1.01
3	1.08	0.69
4	0.97	0.53

*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.

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Synchronization

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

- High level synchronization:

- critical
- atomic

- barrier
- ordered

- Low level synchronization

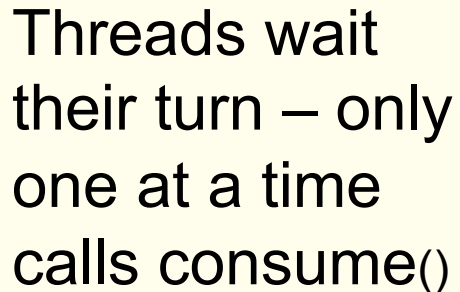
- flush
- locks (both simple and nested)

Discussed later

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){  
        B = big_job(i);  
  
        #pragma omp critical  
        res += consume (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 tmp, B;
    B = DOIT();
    tmp = big_ugly(B);
    #pragma omp atomic
        X += tmp;
}
```

Atomic only protects the read/update of X

Exercise 3

- In exercise 2, 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” from exercise 2 to avoid false sharing due to the sum array.
 - `#pragma omp parallel`
 - `#pragma omp critical`
 - `#pragma omp atomic`
 - `void omp_set_num_threads(int);`
 - `int omp_get_num_threads();`
 - `int omp_get_thread_num();`
 - `double omp_get_wtime();`

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	1 st SPMD
1	1.86
2	1.03
3	1.08
4	0.97

*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
{
    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;
}
}
```

Create a scalar local to each thread to accumulate partial sums.

No array, so no false sharing.

Sum goes “out of scope” beyond the parallel 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>
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
    {
        int i, id, nthrds;  double x, sum;
        id = omp_get_thread_num();
        nthrds = omp_get_num_threads();
        if (id == 0) nthrds = 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 st SPMD	1 st SPMD padded	SPMD critical
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

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    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=0.0; i< num_steps; i=i+nthreads){
        x = (i+0.5)*step;
        #pragma omp critical
        pi += 4.0/(1.0+x*x);
    }
}
pi *= step;
}
```

Be careful where you
put a critical section

What would happen if
you put the critical
section inside the
loop?

Example: Using an atomic 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
```

```
{  
    int i, id, nthrds;  double x, sum;
```

Create a scalar local to each thread to accumulate partial sums.

```
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);
```

No array, so no false sharing.

```
}
```

```
sum = sum*step;
```

```
#pragma omp atomic
```

```
pi += sum ;
```

Sum goes “out of scope” beyond the parallel region ... so you must sum it in here. Must protect summation into pi so updates don't conflict

```
}  
}
```

Outline

- Introduction to OpenMP
- Creating Threads
 - A brief theoretical interlude: Speedup and Amdahl's law
- Synchronization
-  • Parallel Loops
 - Loop schedules and vectorization
- Synchronize single masters and stuff
- Data environment
- Tasks
- Challenge Problems

SPMD vs. worksharing

- A parallel construct by itself creates an SPMD or “Single Program Multiple Data” program ... i.e., each thread redundantly executes the same code.
- How do you split up pathways through the code between threads within a team?
 - Worksharing constructs
 - Loop construct
 - Sections/section constructs
 - Single construct
 - Task constructs

Discussed later

The loop worksharing constructs

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

```
#pragma omp parallel
```

```
{  
#pragma omp for  
    for (l=0;l<N;l++){  
        NEAT_STUFF(l);  
    }  
}
```



Loop construct name:

- C/C++: for
- Fortran: do

The variable `l` is made “private” to each thread by default. You could do this explicitly with a “`private(l)`” clause

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];}
}
```

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];}
```

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

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();  
    }  
}
```

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



These are equivalent

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

```
int i, j, A[MAX];  
j = 5;  
for (i=0; i< MAX; i++) {  
    j += 2;  
    A[i] = big(j);  
}
```

Note: loop index
“i” is private by
default

Remove loop
carried
dependence

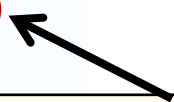
```
int i, A[MAX];  
#pragma omp parallel for  
for (i=0; i< MAX; i++) {  
    int j = 5 + 2*(i+1);  
    A[i] = big(j);  
}
```

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++) {  
        . . . . .  
    }  
}
```



Number of loops
to be
parallelized,
counting from
the outside

- Will form a single loop of length $N \times M$ and then parallelize that.
- Useful if N is $O(\text{no. of threads})$ so parallelizing the outer loop makes balancing the load difficult.

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;
```

- 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;
```

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
^	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 4: 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 parallel for`
 - `#pragma omp for reduction(op:list)`
 - `#pragma omp atomic`
 - `void omp_set_num_threads(int);`
 - `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;
```

```
    step = 1.0/(double) num_steps;
```

```
    #pragma omp parallel
```

```
    {
```

```
        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;
```

```
}
```

Create a team of threads ...
without a parallel construct, you'll
never have more than one thread

Create a scalar local to each thread to hold
value of x at the center of each interval

Break up loop iterations
and assign them to
threads ... setting up a
reduction into sum. Note
... the loop index is local to
a thread by default.

Results*: pi with a loop and a reduction

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

Example: Pi with a

```
#include <omp.h>
static long num_steps = 100000000;
void main ()
{ int i; double x, pi, sum;
  step = 1.0/(double) num_steps;
  #pragma omp parallel
  {
    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;
}
```

threads	1 st SPMD	1 st SPMD padded	SPMD critical	PI Loop
1	1.86	1.86	1.87	1.91
2	1.03	1.01	1.00	1.02
3	1.08	0.69	0.68	0.80
4	0.97	0.53	0.53	0.68

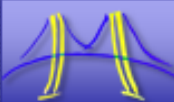
I turned off all optimization to collect these numbers.
Hence, the vector units on the CPU were not utilized.

*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.

MPI Pi program performance

For these numbers, I used `-O3` and hence enabled autovectorization from the compiler

Serial time = 0.43



Pi program in MPI

```
#include <mpi.h>
void main (int argc, char *argv[])
{
    int i, my_id, numprocs; double x, pi, step, sum;
    step = 1.0/(double) num_steps ;
    MPI_Init(&argc, &argv) ;
    MPI_Comm_Rank(MPI_COMM_WORLD,
    MPI_Comm_Size(MPI_COMM_WORLD, &

    for (i=my_id; i<num_steps; ; i=i+numprocs)
    {
        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) ;
}
```

Thread or procs	OpenMP SPMD critical	OpenMP PI Loop	MPI
1	0.85	0.43	0.84
2	0.48	0.23	0.48
3	0.47	0.23	0.46
4	0.46	0.23	0.46

Can you explain the odd performance behavior between these different cases?

*Intel compiler (icpc) with `-O3` 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.

Vectorization before OpenMP 4.0

- Programmers had to rely on automatic-compiler-vectorization...
- ... or to use vendor-specific extensions
 - Programming models (e.g., Intel® Cilk™ Plus)
 - Compiler pragmas (e.g., `#pragma vector`)
 - Low-level constructs (e.g., `_mm_add_pd()`)

#pragma omp parallel for
#pragma vector always
#pragma ivdep

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



You had to trust
the compiler to
do the “right”
thing.

OpenMP SIMD Loop Construct

- Vectorize a loop nest
 - Cut loop into chunks that fit a SIMD vector register

```
#pragma omp simd [clause[,] clause],...  
for-loops
```

```
void sprod(float *a, float *b, int n) {  
    float sum = 0.0f;
```

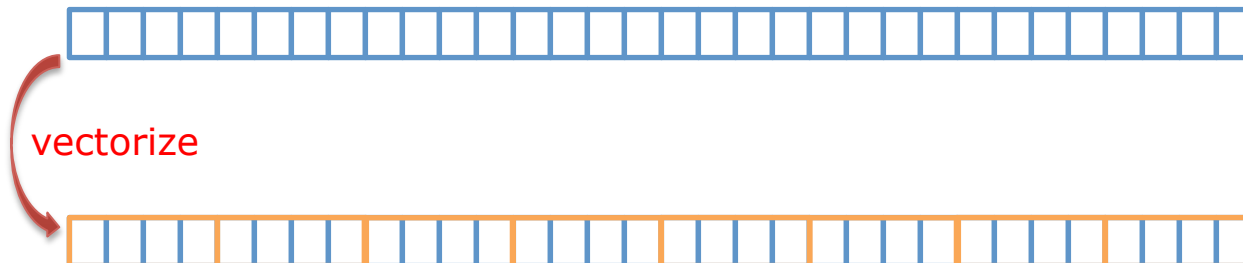
```
    #pragma omp simd reduction(+:sum)
```

```
    for (int k=0; k<n; k++)
```

```
        sum += a[k] * b[k];
```

```
    return sum;
```

```
}
```



Data Sharing Clauses

- **private(*var-list*) :**
Uninitialized vectors for variables in *var-list*



- **firstprivate(*var-list*) :**
Initialized vectors for variables in *var-list*



- **reduction(*op*: *var-list*) :**
Create private variables for *var-list* and apply reduction operator *op* at the end of the construct



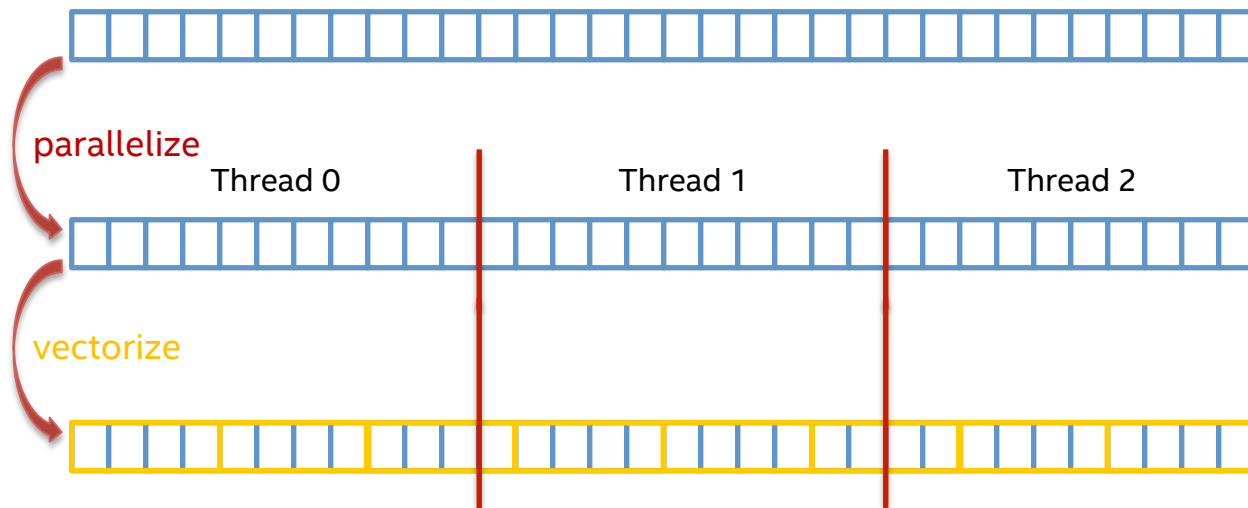
SIMD Loop Clauses

- **safelen** (*length*)
 - Maximum number of iterations that can run concurrently without breaking a dependence
 - in practice, maximum vector length
- **linear** (*list[:linear-step]*)
 - The variable's value is in relationship with the iteration number
$$x_i = x_{\text{orig}} + i * \text{linear-step}$$
- **aligned** (*list[:alignment]*)
 - Specifies that the list items have a given alignment
 - Default is alignment for the architecture
- **collapse** (*n*)

SIMD Worksharing Construct

- Parallelize and vectorize a loop nest
 - Distribute a loop's iteration space across a thread team
 - Subdivide loop chunks to fit a SIMD vector register
- `#pragma omp for simd [clause[,] clause],...`
for-loops

```
void sprod(float *a, float *b, int n) {  
    float sum = 0.0f;  
    #pragma omp parallel for simd reduction(+:sum)  
    for (int k=0; k<n; k++)  
        sum += a[k] * b[k];  
    return sum;  
}
```



SIMD Function Vectorization

- Declare functions to be compiled for calls from a SIMD-parallel loop

```
#pragma omp declare simd [clause[,] clause],...  
function-definition-or-declaration
```

#pragma omp declare simd

```
float min(float a, float b) {  
    return a < b ? a : b;  
}
```



```
vec8 min_v(vec8 a, vec8 b) {  
    return a < b ? a : b;  
}
```

#pragma omp declare simd

```
float distsq(float x, float y) {  
    return (x - y) * (x - y);  
}
```



```
vec8 distsq_v(vec8 x, vec8 y) {  
    return (x - y) * (x - y);  
}
```

```
void example() {
```

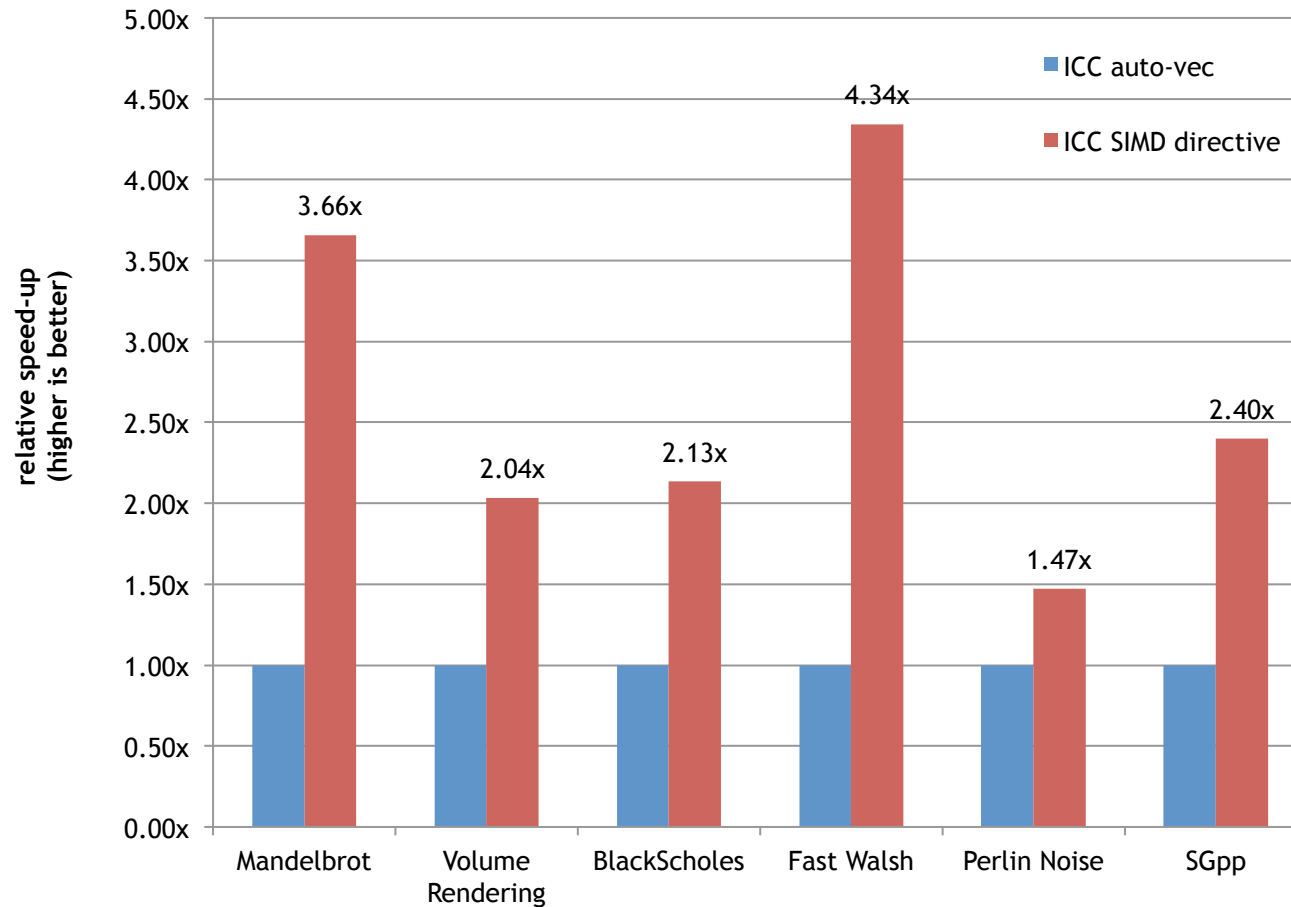
#pragma omp parallel for simd

```
    for (i=0; i<N; i++) {  
        d[i] = min(distsq(a[i], b[i]), c[i]);  
    }  
}
```



```
vd = min_v(distsq_v(va, vb, vc))
```

Performance of the SIMD Constructs



- M. Klemm, A. Duran, X. Tian, H. Saito, D. Caballero, and X. Martorell. Extending OpenMP with Vector Constructs for Modern Multicore SIMD Architectures. In Proc. of the Intl. Workshop on OpenMP, pages 59-72, Rome, Italy, June 2012. LNCS 7312.

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Synchronization: Barrier

- Barrier: Each thread waits until all threads arrive.

```
double A[big], B[big], C[big];
```

```
#pragma omp parallel
```

```
{
```

```
    int id=omp_get_thread_num();
```

```
    A[id] = big_calc1(id);
```

```
#pragma omp barrier
```

```
#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); }
```

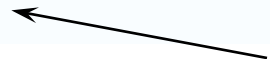
```
    A[id] = big_calc4(id);
```

```
}
```

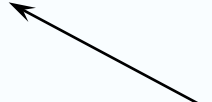
implicit barrier at the end of a for
worksharing construct



implicit barrier at the end
of a parallel region



no implicit barrier
due to nowait



Master construct

- The master construct denotes a structured block that is only executed by the master thread.
- The other threads just skip it (no synchronization is implied).

```
#pragma omp parallel
{
    do_many_things();
    #pragma omp master
        { exchange_boundaries(); }
    #pragma omp barrier
        do_many_other_things();
}
```

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).

```
#pragma omp parallel
{
    do_many_things();
    #pragma omp single
    {   exchange_boundaries();   }
    do_many_other_things();
}
```

Runtime library routines

- Runtime environment routines:
 - Modify/Check the number of threads
 - `omp_set_num_threads()`, `omp_get_num_threads()`,
`omp_get_thread_num()`, `omp_get_max_threads()`
 - Are we in an active parallel region?
 - `omp_in_parallel()`
 - Do you want the system to vary the number of threads dynamically from one parallel construct to another?
 - `omp_set_dynamic()`, `omp_get_dynamic()`;
 - How many processors in the system?
 - `omp_num_procs()`

...plus a few less commonly used routines.

Environment Variables

- Set the default number of threads to use.
 - OMP_NUM_THREADS *int_literal*
- Control how “omp for schedule(RUNTIME)” loop iterations are scheduled.
 - OMP_SCHEDULE “schedule[, chunk_size]”
- Process binding is enabled if this variable is true ... i.e., if true the runtime will not move threads around between processors.
 - OMP_PROC_BIND true | false

... Plus several less commonly used environment variables.

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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**.

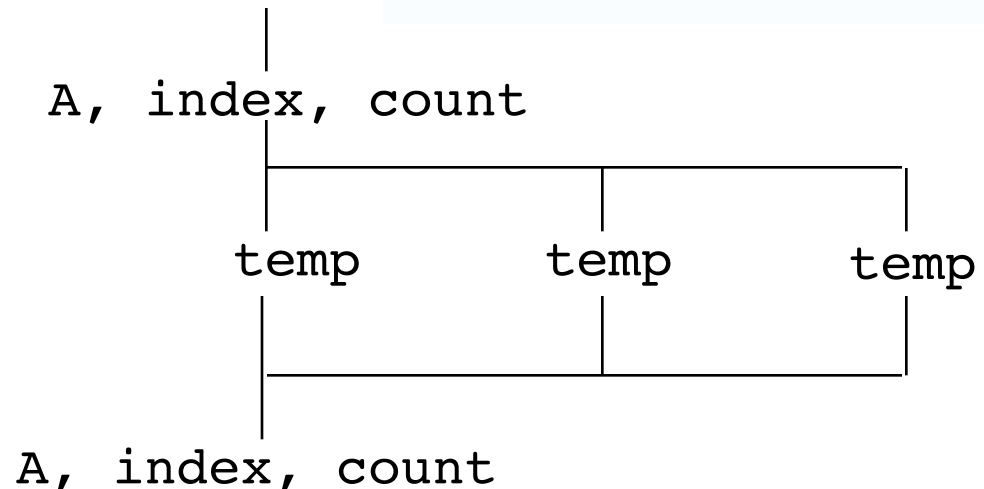
Data sharing: Examples

```
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;
    ...
}
```



Data sharing:

Changing storage attributes

- One can selectively change storage attributes for constructs using the following clauses*
 - SHARED
 - PRIVATE
 - FIRSTPRIVATE
 - The final value of a private variable inside a parallel loop can be transmitted to the shared variable outside the loop with:
 - LASTPRIVATE
 - The default attributes can be overridden with:
 - DEFAULT (PRIVATE | SHARED | NONE)
- DEFAULT(PRIVATE) *is Fortran only*

All the clauses on this page apply to the OpenMP construct NOT to the entire region.

***All data clauses apply to parallel constructs and worksharing constructs except “shared”, which only applies to 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

```
void wrong() {  
    int tmp = 0;  
    #pragma omp parallel for private(tmp)  
    for (int j = 0; j < 1000; ++j)  
        tmp += j;  
    printf("%d\n", tmp);  
}
```

tmp was not
initialized

tmp is 0 here

Data sharing: Private clause

When is the original variable valid?

- 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

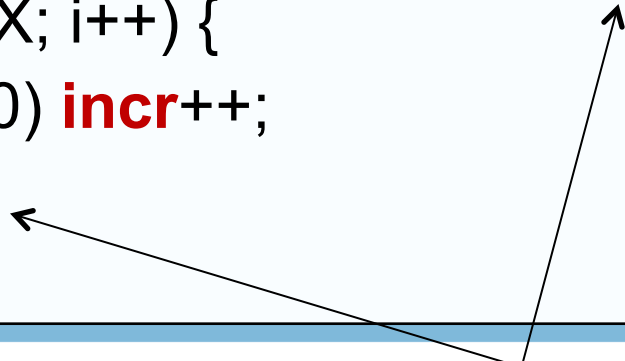
```
extern int tmp;  
void work() {  
    tmp = 5;  
}
```

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;  
}
```



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

Lastprivate clause

- Variables update a shared variable using value from the (logically) last iteration
- C++ objects are updated as if by assignment

```
void sq2(int n, double *lastterm)
{
    double x; int i;
    #pragma omp parallel for lastprivate(x)
    for (i = 0; i < n; i++){
        x = a[i]*a[i] + b[i]*b[i];
        b[i] = sqrt(x);
    }
    *lastterm = x;
}
```

“x” has the value it held for the “last sequential” iteration (i.e., for $i=(n-1)$)

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

- The default storage attribute is `DEFAULT(SHARED)` (so no need to use it)
 - Exception: `#pragma omp task`
- To change default: `DEFAULT(PRIVATE)`
 - *each* variable in the construct is made private as if specified in a private clause
 - mostly saves typing
- `DEFAULT(NONE)`: *no* default for variables in static extent. Must list storage attribute for each variable in static extent. Good programming practice!

Only the Fortran API supports `default(private)`.

C/C++ only has `default(shared)` or `default(none)`.

Data sharing: Default clause example

```
    itotal = 1000
C$OMP PARALLEL PRIVATE(np, each)
    np = omp_get_num_threads()
    each = itotal/np
    .....
C$OMP END PARALLEL
```

These two code
fragments are
equivalent

```
    itotal = 1000
C$OMP PARALLEL DEFAULT(PRIVATE) SHARED(itotal)
    np = omp_get_num_threads()
    each = itotal/np
    .....
C$OMP END PARALLEL
```

Exercise 5: Mandelbrot set area

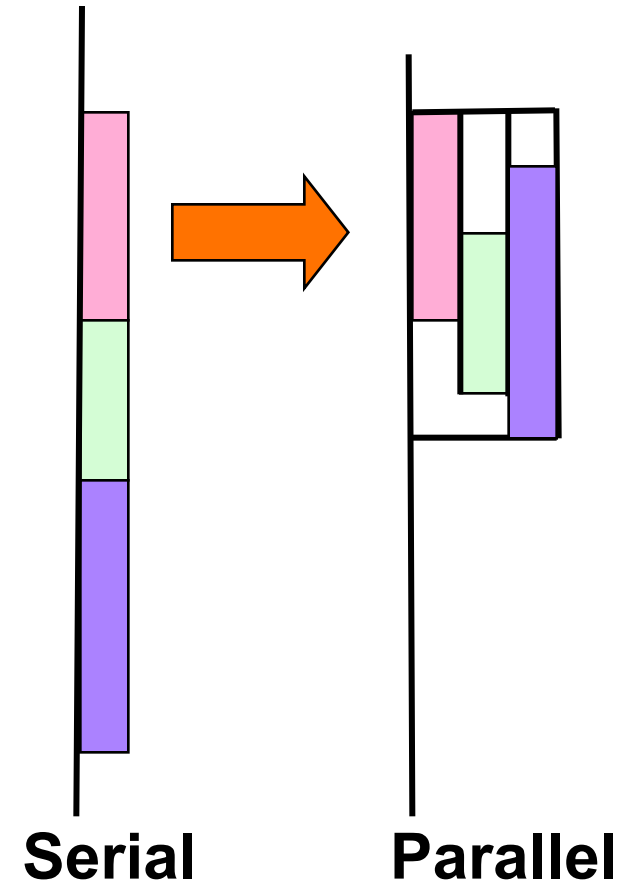
- The supplied program (mandel.c) computes the area of a Mandelbrot set.
- The program has been parallelized with OpenMP, but we were lazy and didn't do it right.
- Find and fix the errors (hint ... the problem is with the data environment).
- Once you have a working version, try to optimize the program.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

Outline

- Introduction to OpenMP
- Creating Threads
 - A brief theoretical interlude: Speedup and Amdahl's law
- Synchronization
- Parallel Loops
 - Loop schedules and vectorization
- Synchronize single masters and stuff
- Data environment
-  • Tasks
- Challenge Problems

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.



OpenMP 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
- Some thread in the parallel region will execute the task at some point in the future
 - note: could be encountering thread, right now
- Tasks can be nested: i.e. a task may itself generate tasks.

task directive

Syntax:

Fortran:

```
! $OMP TASK [clauses]
```

```
    structured block
```

```
! $OMP END TASK
```

C/C++:

```
#pragma omp task [clauses]
```

```
    structured-block
```

Example

```
#pragma omp parallel  
{
```

Create some threads

```
    #pragma omp master  
    {
```

Thread 0 packages tasks

```
        #pragma omp task  
        fred();
```

```
        #pragma omp task  
        daisy();
```

```
        #pragma omp task  
        billy();
```

Tasks executed by
some thread in some
order

```
    }
```

```
}
```

All tasks complete
before this barrier is
released

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.
 - Fortran: **!\$OMP TASKWAIT**
 - C/C++: **#pragma omp taskwait**
 - Note: applies only to tasks generated in the current task, not to “descendants” .
 - The code executed by a thread in a parallel region is considered a task here

When/where are tasks complete?

- At the end of a taskgroup region

- Fortran:

- !\$OMP TASKGROUP

- structured block*

- !\$OMP END TASKGROUP

- C/C++:

- #pragma omp taskgroup

- structured-block*

- wait until all tasks created within the taskgroup have completed
 - applies to all “descendants”

Example

```
#pragma omp parallel
{
    #pragma omp master
    {
        #pragma omp task
        fred();
        #pragma omp task
        daisy();
        #pragma taskwait
        #pragma omp task
        billy();
    }
}
```

fred() and **daisy()**
must complete before
billy() starts



Exercise 6: 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 cars” or “car races” part).
- 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 and programs containing data races are undefined (in OpenMP but also ANSI standards C++’11 and beyond).

`#pragma omp parallel`

`#pragma omp task`

`#pragma omp master`

`#pragma omp single`

Linked list traversal

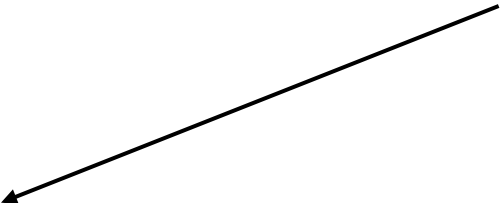
```
p = listhead ;  
while (p) {  
    process(p) ;  
    p=next(p) ;  
}
```

- Classic linked list traversal
- Do some work on each item in the list
- Assume that items can be processed independently
- Cannot use an OpenMP loop directive

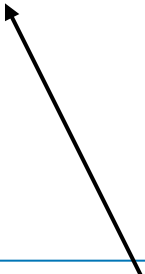
Parallel linked list traversal

```
#pragma omp parallel
{
    #pragma omp master
    {
        p = listhead ;
        while (p) {
            #pragma omp task firstprivate(p)
            {
                process (p) ;
            }
            p=next (p) ;
        }
    }
}
```

Only one thread
packages tasks



makes a copy of **p**
when the task is
packaged



Parallel linked list traversal

Thread 0:

```
p = listhead ;  
while (p) {  
  < package up task >  
  p=next (p) ;  
}  
  
while (tasks_to_do) {  
  < execute task >  
}  
  
< barrier >
```

Other threads:

```
while (tasks_to_do) {  
  < execute task >  
}  
  
< barrier >
```

Parallel pointer chasing on multiple lists

```
#pragma omp parallel
{
    #pragma omp for private(p)
    for ( int i =0; i <numlists; i++) {
        p = listheads[i] ;
        while (p ) {
            #pragma omp task firstprivate(p)
            {
                process(p) ;
            }
            p=next(p) ;
        }
    }
}
```

All threads package
tasks



Data scoping with tasks

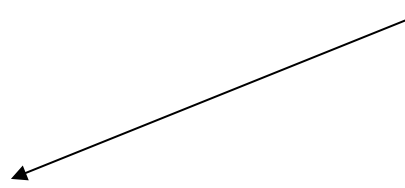
- Variables can be shared, private or firstprivate with respect to task
- These concepts are a little bit different compared with threads:
 - If a variable is **shared** on a task construct, the references to it inside the construct are to the storage with that name at the point where the task was encountered
 - 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
{
    int C;
    compute(A, B, C);
}
}
```

A is shared
B is firstprivate
C is private



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 $O(n^2)$ 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 master
            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!

Using tasks

- Getting the data attribute scoping right can be quite tricky
 - default scoping rules different from other constructs
 - as ever, using `default(none)` is a good idea
- 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

Exercise 6: Pi with tasks

- Consider the program Pi_recur.c. This program implements a recursive algorithm version of the program for computing pi
 - Parallelize this program using OpenMP tasks

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

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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 molecular dynamics
 2. Monte Carlo “pi” program and parallel random number generators
 3. Optimizing matrix multiplication
 4. Traversing linked lists in different ways
 5. Recursive matrix multiplication algorithms

Challenge 1: 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 1: 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?

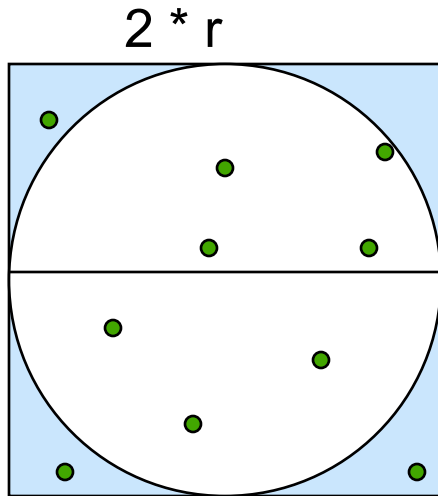
Challenge 1 MD: (cont.)

- 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 2: 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

Challenge 2: 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 (non-overlapping sequences of pseudo-random numbers).

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
 - Cache blocking
 - Loop unrolling
 - Vectorization
- Goal: Can you approach the peak performance of the computer?

Challenge 4: Traversing linked lists

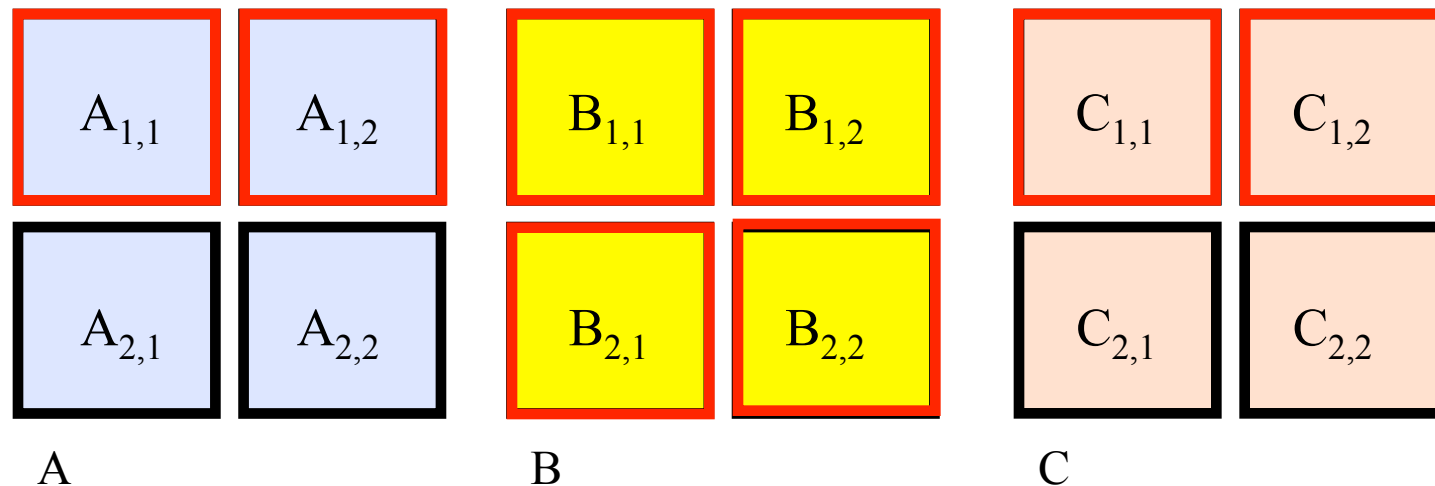
- Consider the program `linked.c`
 - Traverses a linked list, computing a sequence of Fibonacci numbers at each node
- Parallelize this program two different ways
 1. Use OpenMP tasks
 2. Use anything you choose in OpenMP *other than* tasks.
- The second approach (no tasks) can be difficult and may take considerable creativity in how you approach the problem (why its such a pedagogically valuable problem)

Challenge 5: 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 5: Recursive matrix multiplication

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



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

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

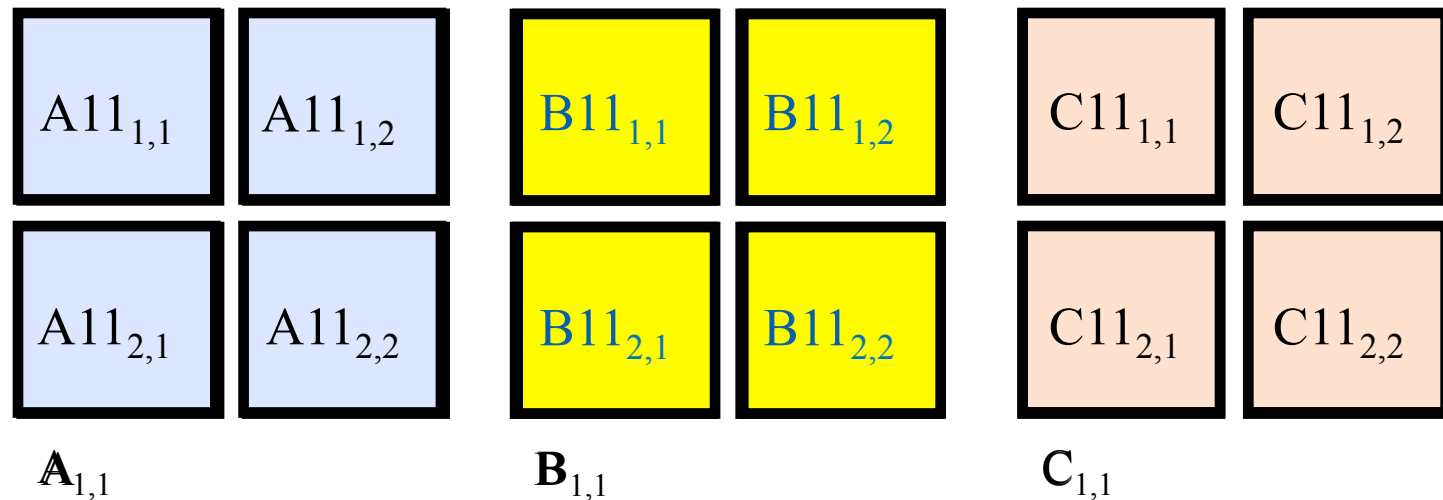
$$C_{1,2} = A_{1,1} \cdot B_{1,2} + A_{1,2} \cdot B_{2,2}$$

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

Challenge 5: 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



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



$$C11_{1,1} = A11_{1,1} \cdot B11_{1,1} + A11_{1,2} \cdot B11_{2,1} + A12_{1,1} \cdot B21_{1,1} + A12_{1,2} \cdot B21_{2,1}$$

Challenge 5: 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

```
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]

  // C11 += A11*B11
  matmultrec(mf, mf+(ml-mf)/2, nf, nf+(nl-nf)/2, pf, pf+(pl-pf)/2, A,B,C);
  // C11 += A12*B21
  matmultrec(mf, mf+(ml-mf)/2, nf, nf+(nl-nf)/2, pf+(pl-pf)/2, pl, A,B,C);
  . . .
}
```

- Also need stopping criteria for recursion

Conclusion

- We have now covered the full sweep of the OpenMP specification
 - We've left off some minor details, but we've covered all major topics ... remaining content you can pick up on your own
- Download the spec to learn more ... the spec is filled with examples to support your continuing education
 - www.openmp.org
- Get involved:
 - Get your organization to join the OpenMP ARB
 - Work with us through cOMPunity

Appendices



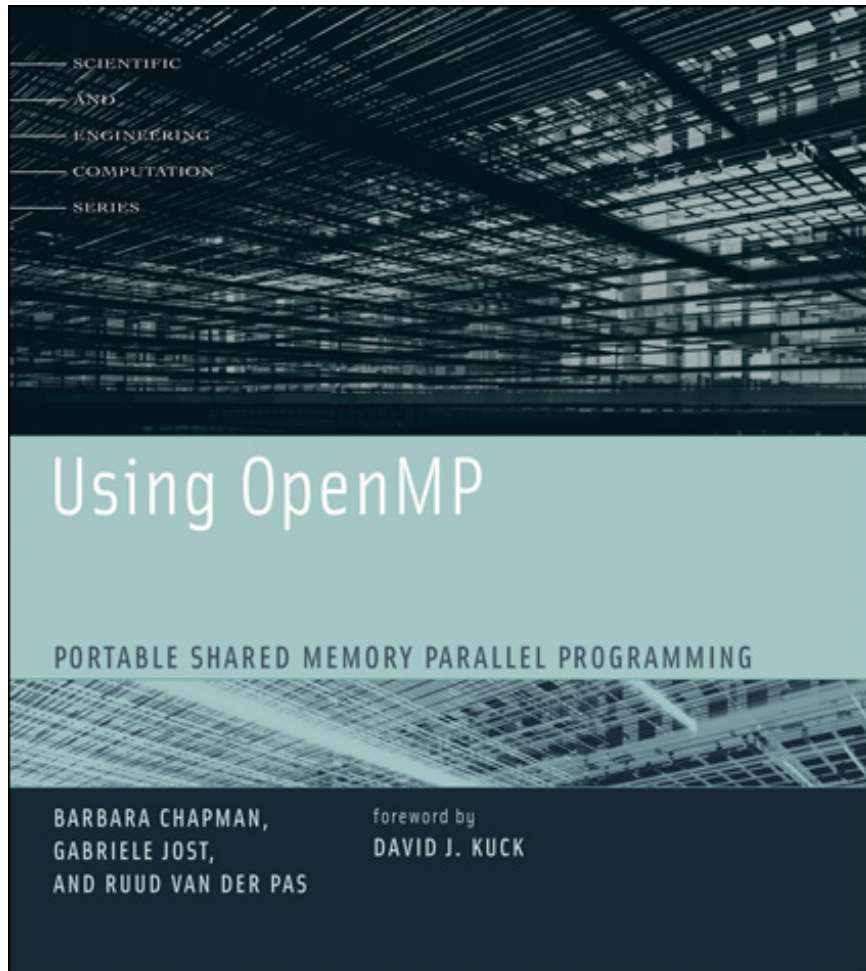
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OpenMP organizations

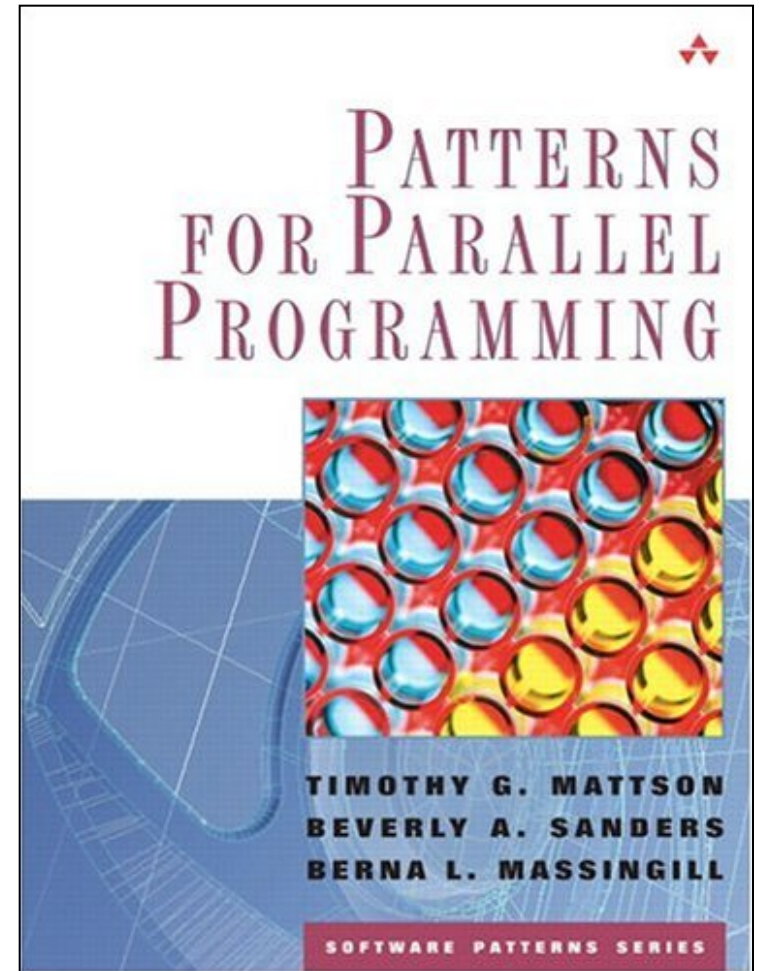
- OpenMP architecture review board URL, the “owner” of the OpenMP specification:
www.openmp.org
- OpenMP User’s Group (cOMPunity) URL:
www.compunity.org

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

Books about OpenMP

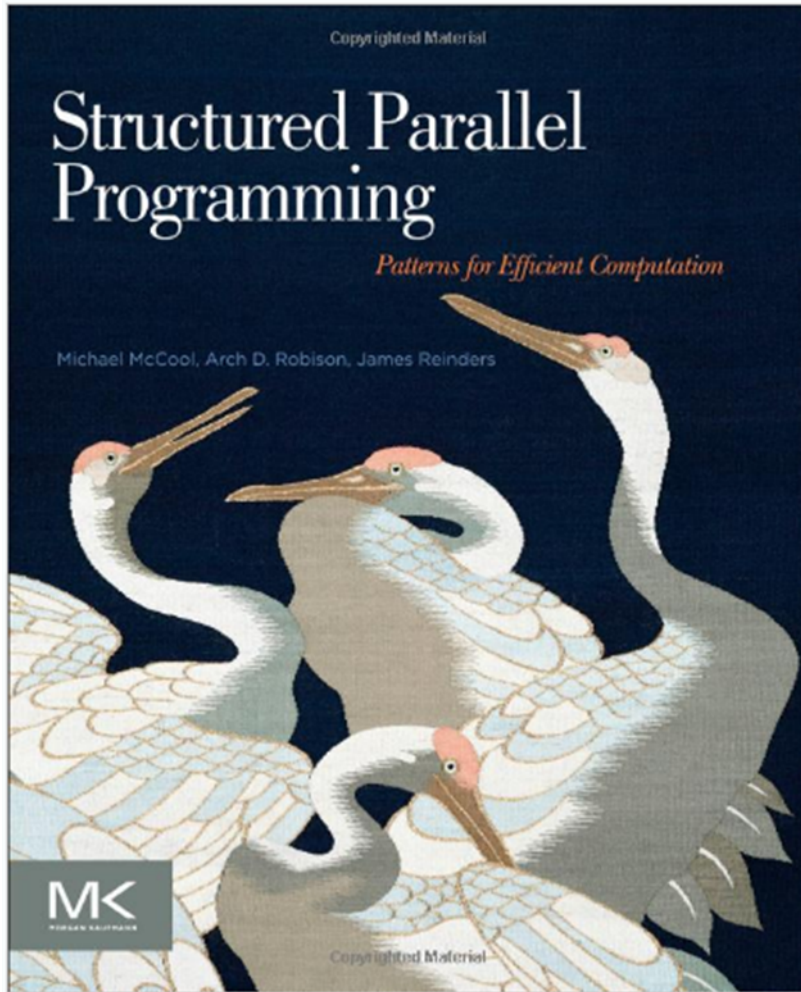


- A book about OpenMP by a team of authors at the forefront of OpenMP's evolution.

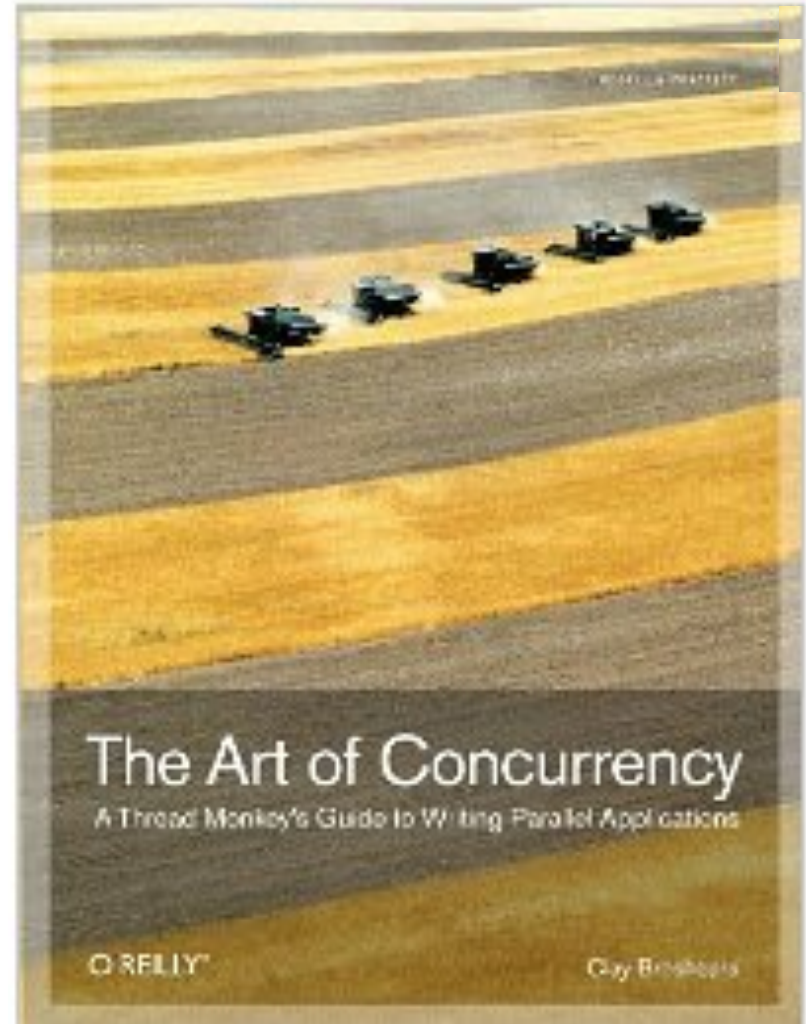


- A book about how to “think parallel” with examples in OpenMP, MPI and java

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)

OpenMP Papers

- Sosa CP, Scalmani C, Gomperts R, Frisch MJ. Ab initio quantum chemistry on a ccNUMA architecture using OpenMP. III. Parallel Computing, vol.26, no.7-8, July 2000, pp.843-56. Publisher: Elsevier, Netherlands.
- Couturier R, Chipot C. Parallel molecular dynamics using OPENMP on a shared memory machine. Computer Physics Communications, vol.124, no.1, Jan. 2000, pp.49-59. Publisher: Elsevier, Netherlands.
- Bentz J., Kendall R., “Parallelization of General Matrix Multiply Routines Using OpenMP”, Shared Memory Parallel Programming with OpenMP, Lecture notes in Computer Science, Vol. 3349, P. 1, 2005
- Bova SW, Breshearsz CP, Cuicchi CE, Demirbilek Z, Gabb HA. Dual-level parallel analysis of harbor wave response using MPI and OpenMP. International Journal of High Performance Computing Applications, vol.14, no.1, Spring 2000, pp.49-64. Publisher: Sage Science Press, USA.
- Ayguade E, Martorell X, Labarta J, Gonzalez M, Navarro N. Exploiting multiple levels of parallelism in OpenMP: a case study. Proceedings of the 1999 International Conference on Parallel Processing. IEEE Comput. Soc. 1999, pp. 172-80. Los Alamitos, CA, USA.
- Bova SW, Breshears CP, Cuicchi C, Demirbilek Z, Gabb H. Nesting OpenMP in an MPI application. Proceedings of the ISCA 12th International Conference. Parallel and Distributed Systems. ISCA. 1999, pp.566-71. Cary, NC, USA.

OpenMP Papers (continued)

- Jost G., Labarta J., Gimenez J., What Multilevel Parallel Programs do when you are not watching: a Performance analysis case study comparing MPI/OpenMP, MLP, and Nested OpenMP, Shared Memory Parallel Programming with OpenMP, Lecture notes in Computer Science, Vol. 3349, P. 29, 2005
- Gonzalez M, Serra A, Martorell X, Oliver J, Ayguade E, Labarta J, Navarro N. Applying interposition techniques for performance analysis of OPENMP parallel applications. Proceedings 14th International Parallel and Distributed Processing Symposium. IPDPS 2000. IEEE Comput. Soc. 2000, pp.235-40.
- Chapman B, Mehrotra P, Zima H. Enhancing OpenMP with features for locality control. Proceedings of Eighth ECMWF Workshop on the Use of Parallel Processors in Meteorology. Towards Teracomputing. World Scientific Publishing. 1999, pp. 301-13. Singapore.
- Steve W. Bova, Clay P. Breshears, Henry Gabb, Rudolf Eigenmann, Greg Gaertner, Bob Kuhn, Bill Magro, Stefano Salvini. Parallel Programming with Message Passing and Directives; SIAM News, Volume 32, No 9, Nov. 1999.
- Cappello F, Richard O, Etiemble D. Performance of the NAS benchmarks on a cluster of SMP PCs using a parallelization of the MPI programs with OpenMP. Lecture Notes in Computer Science Vol.1662. Springer-Verlag. 1999, pp.339-50.
- Liu Z., Huang L., Chapman B., Weng T., Efficient Implementation of OpenMP for Clusters with Implicit Data Distribution, Shared Memory Parallel Programming with OpenMP, Lecture notes in Computer Science, Vol. 3349, P. 121, 2005

OpenMP Papers (continued)

- B. Chapman, F. Bregier, A. Patil, A. Prabhakar, “Achieving performance under OpenMP on ccNUMA and software distributed shared memory systems,” *Concurrency and Computation: Practice and Experience*. 14(8-9): 713-739, 2002.
- J. M. Bull and M. E. Kambites. JOMP: an OpenMP-like interface for Java. Proceedings of the ACM 2000 conference on Java Grande, 2000, Pages 44 - 53.
- L. Adhianto and B. Chapman, “Performance modeling of communication and computation in hybrid MPI and OpenMP applications, *Simulation Modeling Practice and Theory*, vol 15, p. 481-491, 2007.
- Shah S, Haab G, Petersen P, Throop J. Flexible control structures for parallelism in OpenMP; *Concurrency: Practice and Experience*, 2000; 12:1219-1239. Publisher John Wiley & Sons, Ltd.
- Mattson, T.G., How Good is OpenMP? *Scientific Programming*, Vol. 11, Number 2, p.81-93, 2003.
- Duran A., Silvera R., Corbalan J., Labarta J., “Runtime Adjustment of Parallel Nested Loops”, *Shared Memory Parallel Programming with OpenMP*, Lecture notes in Computer Science, Vol. 3349, P. 137, 2005

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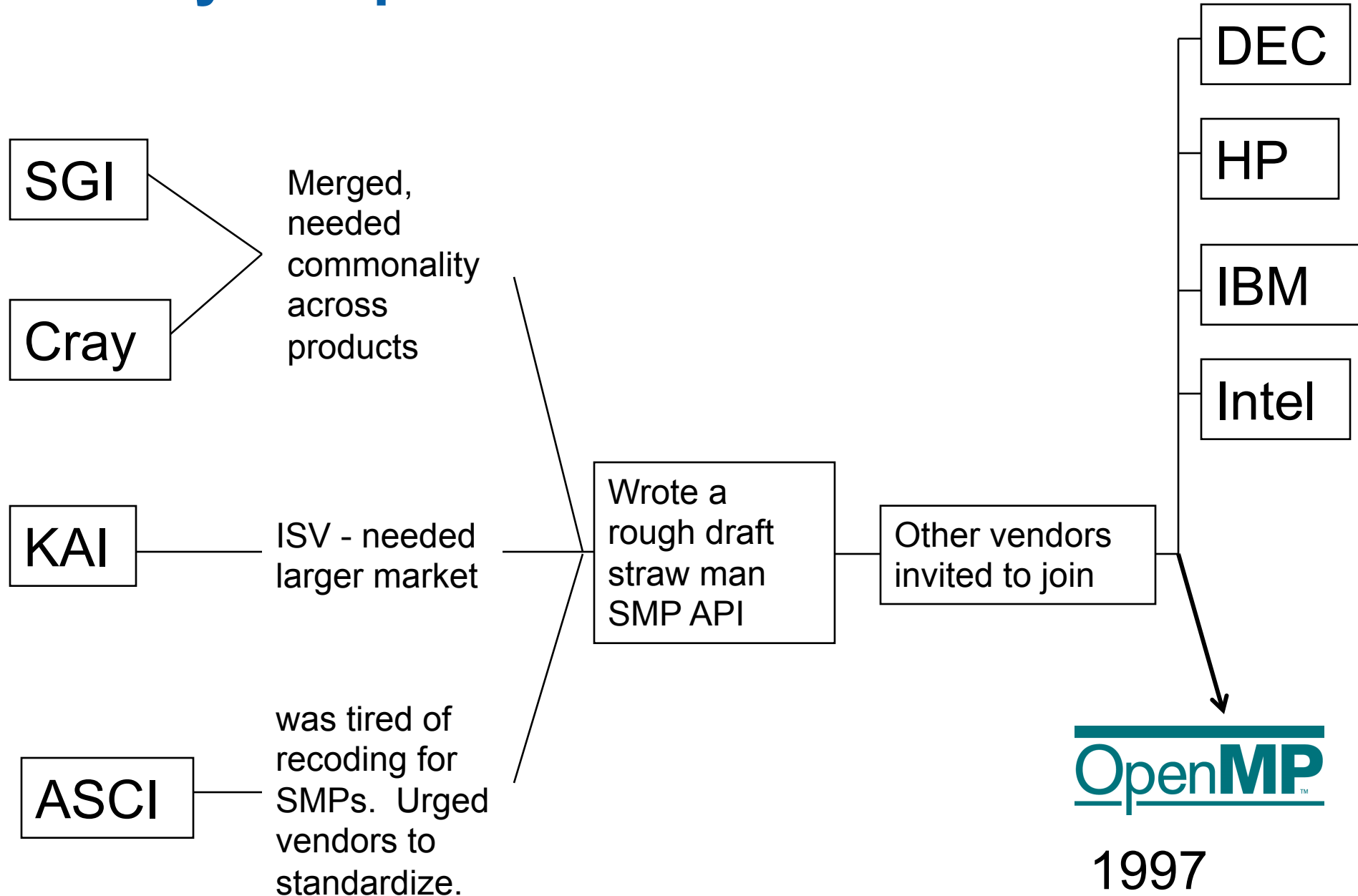
OpenMP pre-history

- OpenMP based upon SMP directive standardization efforts PCF and aborted ANSI X3H5 – late 80's
 - Nobody fully implemented either standard
 - Only a couple of partial implementations
- Vendors considered proprietary API's to be a competitive feature:
 - Every vendor had proprietary directives sets
 - Even KAP, a “portable” multi-platform parallelization tool used different directives on each platform

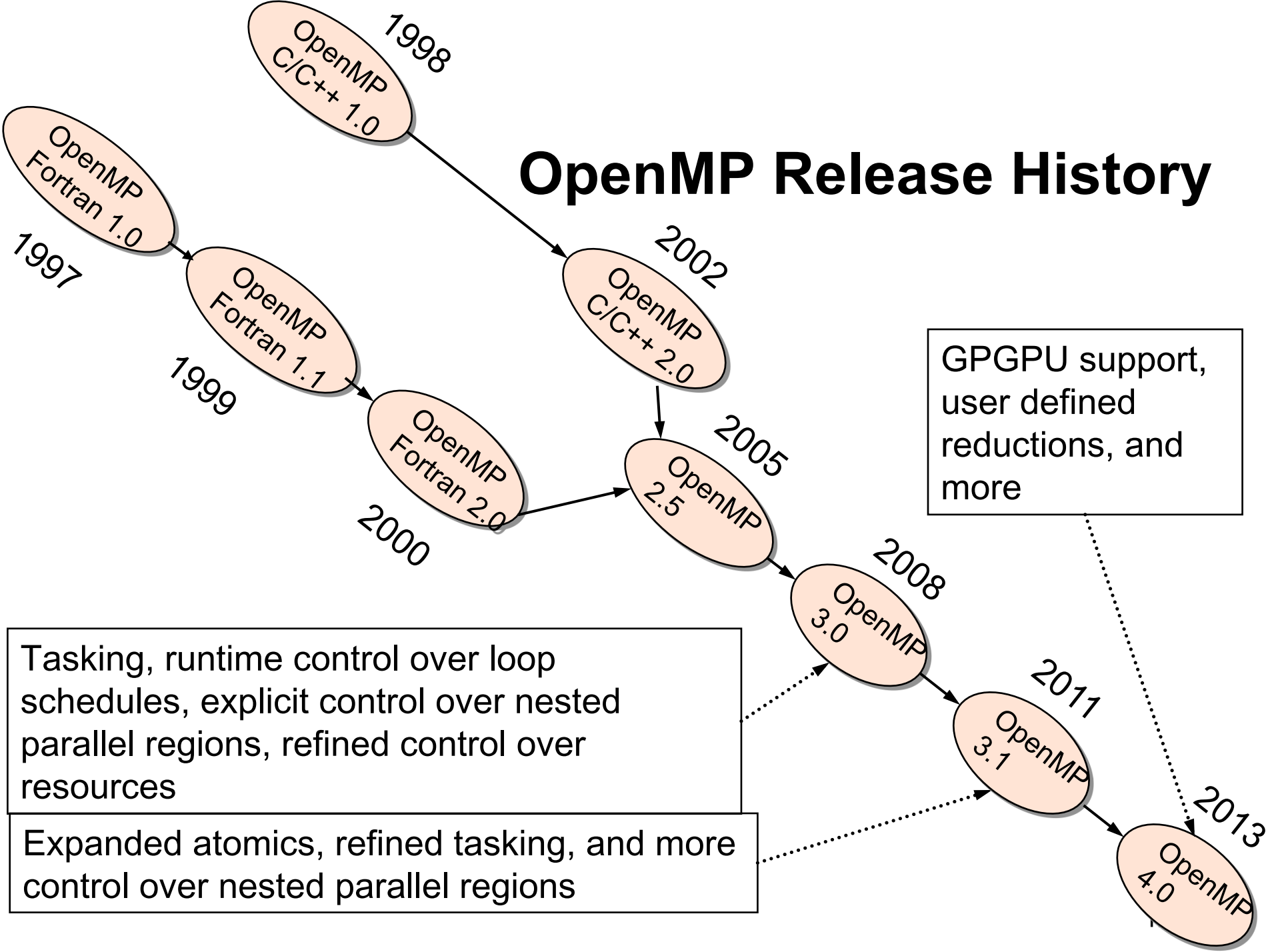
PCF – Parallel computing forum

KAP – parallelization tool from KAI.

History of OpenMP



OpenMP Release History



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Exercise 1: Solution

A multi-threaded “Hello world” program

- Write a multithreaded program where each thread prints “hello world”.

```
#include "omp.h"
void main()
```

```
{
#pragma omp parallel
{
    int ID = omp_get_thread_num();
    printf(" hello(%d) ", ID);
    printf(" world(%d) \n", ID);
}
}
```

OpenMP include file

Parallel region with default number of threads

Sample Output:

```
hello(1) hello(0) world(1)
world(0)
hello (3) hello(2) world(3)
world(2)
```

Runtime library function to return a thread ID.

End of the Parallel region

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The SPMD pattern

- The most common approach for parallel algorithms is the SPMD or Single Program Multiple Data pattern.
- Each thread runs the same program (Single Program), but using the thread ID, they operate on different data (Multiple Data) or take slightly different paths through the code.
- In OpenMP this means:
 - A parallel region “near the top of the code”.
 - Pick up thread ID and num_threads.
 - Use them to split up loops and select different blocks of data to work on.

Exercise 2: A simple SPMD 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;
}
```

Promote scalar to an array dimensioned by number of threads to avoid race condition.



Only one thread should copy the number of threads to the global value to make sure multiple threads writing to the same address don't conflict.



This is a common trick in SPMD programs to create a cyclic distribution of loop iterations



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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.
 - Result ... poor scalability
- Solution:
 - When updates to an item are frequent, work with local copies of data instead of an array indexed by the thread ID.
 - Pad arrays so elements you use are on distinct cache lines.

Exercise 3: SPMD pi without false sharing

```
#include <omp.h>
```

```
static long num_steps = 100000;    double step;
```

```
#define NUM_THREADS 2
```

```
void main ()
```

```
{    double pi;    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)    nthrds = nthrds;  
    id = omp_get_thread_num();  
    nthrds = omp_get_num_threads();
```

```
    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;
```

```
}  
}
```

← Create a scalar local to each thread to accumulate partial sums.

← No array, so no false sharing.

← Sum goes “out of scope” beyond the parallel region ... so you must sum it in here. Must protect summation into pi in a critical region so updates don’t conflict



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Exercise 4: Solution

```
#include <omp.h>
static long num_steps = 100000;      double step;
void main ()
{   int i;   double x, pi, sum = 0.0;
    step = 1.0/(double) num_steps;
#pragma omp parallel
{
    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;
}
```

Exercise 4: Solution

```
#include <omp.h>
```

```
static long num_steps = 100000;    double step;
```

```
void main ()
```

```
{    int i;    double x, pi, sum = 0.0;  
    step = 1.0/(double) num_steps;
```

```
#pragma omp parallel for private(x) reduction(+:sum)
```

```
    for (i=0;i< num_steps; i++){  
        x = (i+0.5)*step;  
        sum = sum + 4.0/(1.0+x*x);
```

i private by
default

```
    }  
    pi = step * sum;
```

```
}
```

For good OpenMP
implementations,
reduction is more
scalable than critical.

Note: we created a parallel
program without changing
any code and by adding 2
simple lines of text!

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Exercise 5: The Mandelbrot area program

```
#include <omp.h>
# define NPOINTS 1000
# define MXITR 1000
void testpoint(void);
struct d_complex{
    double r;    double i;
};
struct d_complex c;
int numoutside = 0;

int main(){
    int i, j;
    double area, error, eps = 1.0e-5;
#pragma omp parallel for default(shared) \
                    private(c,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();
        }
    }
    area=2.0*2.5*1.125*(double)(NPOINTS*NPOINTS-numoutside)/
(double)(NPOINTS*NPOINTS);
    error=area/(double)NPOINTS;
}
```

```
void testpoint(void){
    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) {
            numoutside++;
            break;
        }
    }
}
```

When I run this program, I get a different incorrect answer each time I run it ... there is a race condition!!!!

Exercise 5: Area of a Mandelbrot set

- Solution is in the file `mandel_par.c`
- Errors:
 - `Eps` is private but uninitialized. Two solutions
 - It's read-only so you can make it shared.
 - Make it `firstprivate`
 - The loop index variable `j` is shared by default; make it private
 - The variable `c` has global scope so “testpoint” may pick up the global value rather than the private value in the loop; solution ... pass `c` as an arg to `testpoint`
 - Updates to “numoutside” are a race; protect with an atomic.

Debugging parallel programs

- Find tools that work with your environment and learn to use them; a good parallel debugger can make a huge difference
- But parallel debuggers are not portable and you will assuredly need to debug “by hand” at some point
- There are tricks to help you; the most important is to use the `default(none)` pragma

```
#pragma omp parallel for default(none) private(c, 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();
    }
}
```

Using `default(none)` generates a compiler error that `j` is unspecified.

Exercise 5: 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 default(shared) private(c, j) \
firstprivate(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 atomic
            numoutside++;
            break;
        }
    }
}
```

Other errors found using a debugger or by inspection:

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



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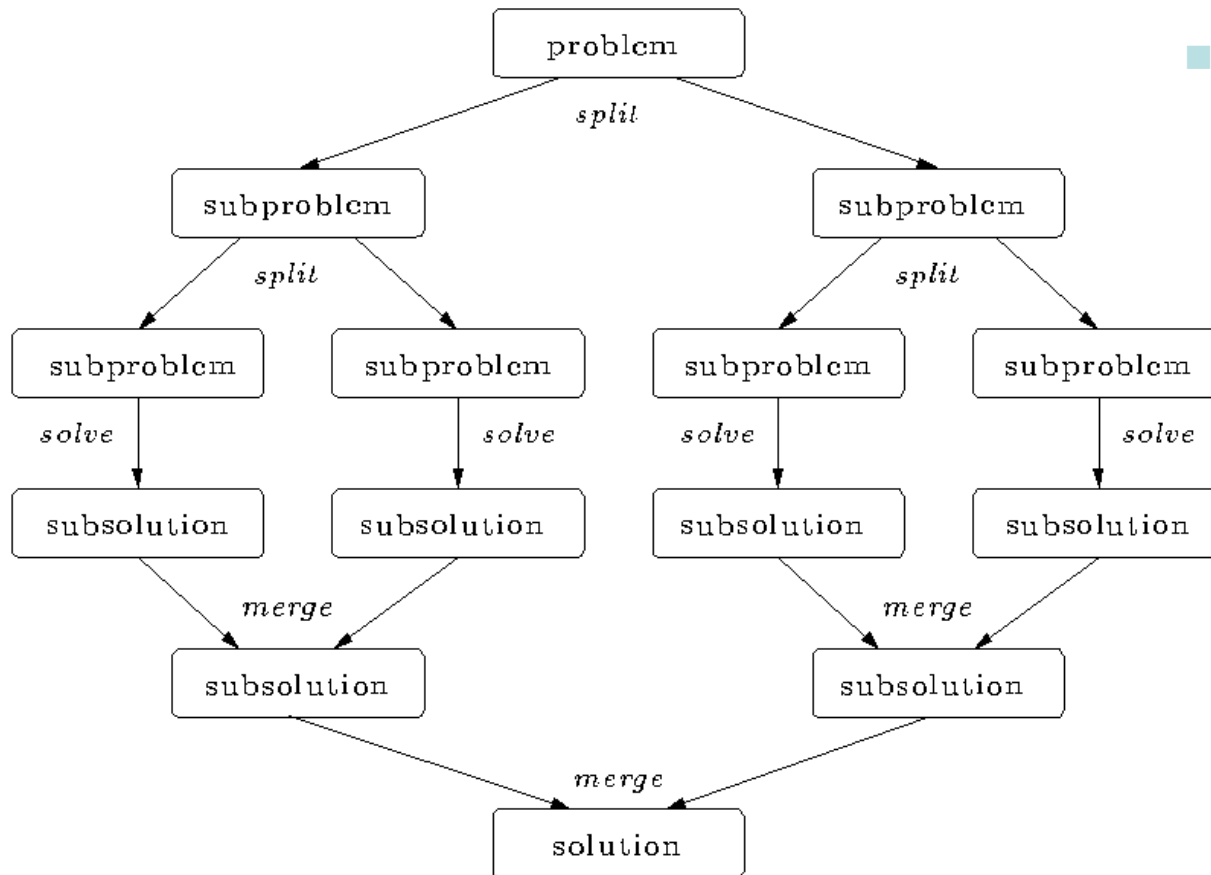
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Divide and conquer pattern

- Use when:
 - A problem includes a method to divide into subproblems and a way to recombine solutions of subproblems into a global solution
- Solution
 - Define a split operation
 - Continue to split the problem until subproblems are small enough to solve directly
 - Recombine solutions to subproblems to solve original global problem
- Note:
 - Computing may occur at each phase (split, leaves, recombine)

Divide and conquer

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



■ 3 Options:

- Do work as you split into sub-problems
- Do work only at the leaves
- Do work as you recombine

Program: OpenMP tasks (divide and conquer pattern)

```
include <omp.h>

static long num_steps = 100000000;
#define MIN_BLK 10000000

double pi_comp(int Nstart,int Nfinish,double step)
{  int i,iblk;
   double x, sum = 0.0,sum1, sum2;
   if (Nfinish-Nstart < MIN_BLK){
       for (i=Nstart;i< Nfinish; i++){
           x = (i+0.5)*step;
           sum = sum + 4.0/(1.0+x*x);
       }
   }
   else{
       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;
}
```

```
int main ()
{
   int i;
   double step, pi, sum;
   step = 1.0/(double) num_steps;
   #pragma omp parallel
   {
       #pragma omp single
       sum =
           pi_comp(0,num_steps,step);
   }
   pi = step * sum;
}
```

Results*: pi with tasks

threads	1 st 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

*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.



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Challenge 1: 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.



Challenge 1: 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;  
}  
}
```

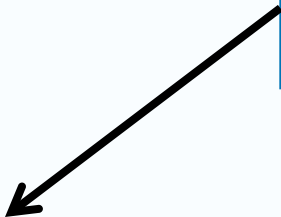
All updates to f must be
atomic

Challenge 1: With orphaning

```
#pragma omp single
```

```
{  
    vir    = 0.0;  
    epot   = 0.0;  
}
```

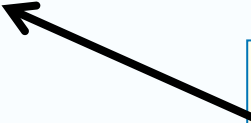
Implicit barrier needed to avoid race condition with update of reduction variables at end of the for construct



```
#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



Challenge 1: 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

Challenge 1: With array reduction

....

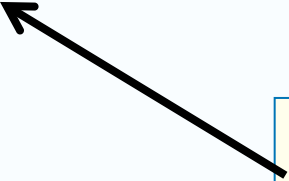
#pragma omp for

```
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;  
    }  
}
```

Reduction can be done in parallel



Zero ftemp for next time round



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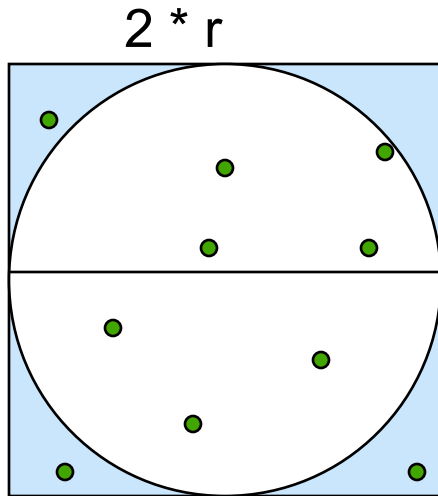
Computers and random numbers

- 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 algorithms

```
#include "omp.h"
```

```
static long num_trials = 10000;
```

```
int main ()
```

```
{  
    long i;    long Ncirc = 0;    double pi, x, y;  
    double r = 1.0; // radius of circle. Side of square 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++)
```

```
{  
    x = random();    y = random();  
    if ( x*x + y*y <= r*r) Ncirc++;  
}
```

```
pi = 4.0 * ((double)Ncirc/((double)num_trials);
```

```
printf("\n %d trials, pi is %f \n",num_trials, pi);
```

```
}
```

Embarrassingly parallel: the parallelism is so easy its embarrassing.

Add two lines and you have a parallel program.

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

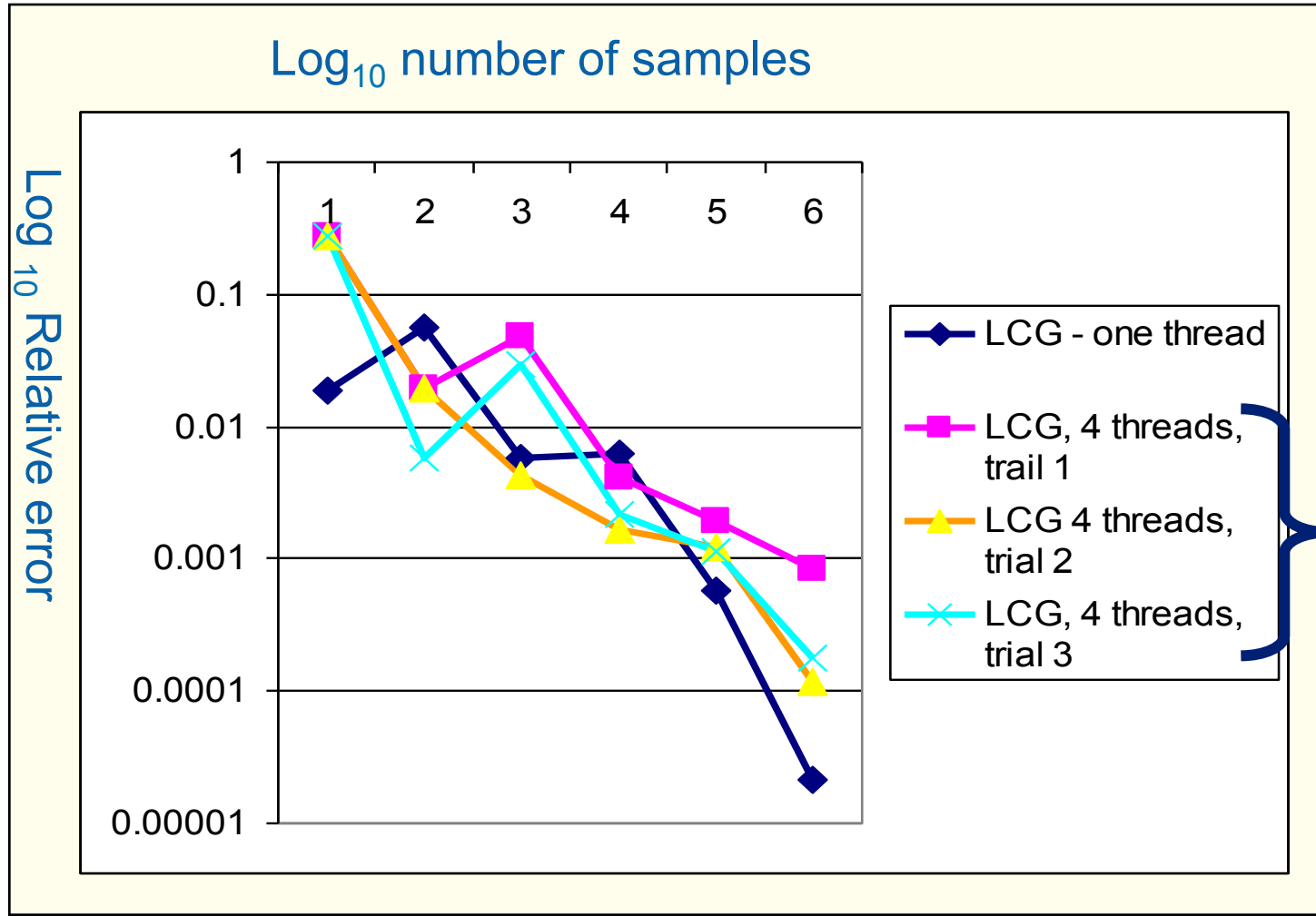
```
static long MULTIPLIER = 1366;
static long ADDEND     = 150889;
static long PMOD       = 714025;
long random_last = 0;
double random ()
{
    long random_next;

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

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

Seed the pseudo random
sequence by setting
random_last

Running the PI_MC program with LCG generator



Run the same program the same way and get different answers!

That is not acceptable!

Issue: my LCG generator is not threadsafe

LCG code: threadsafe version

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

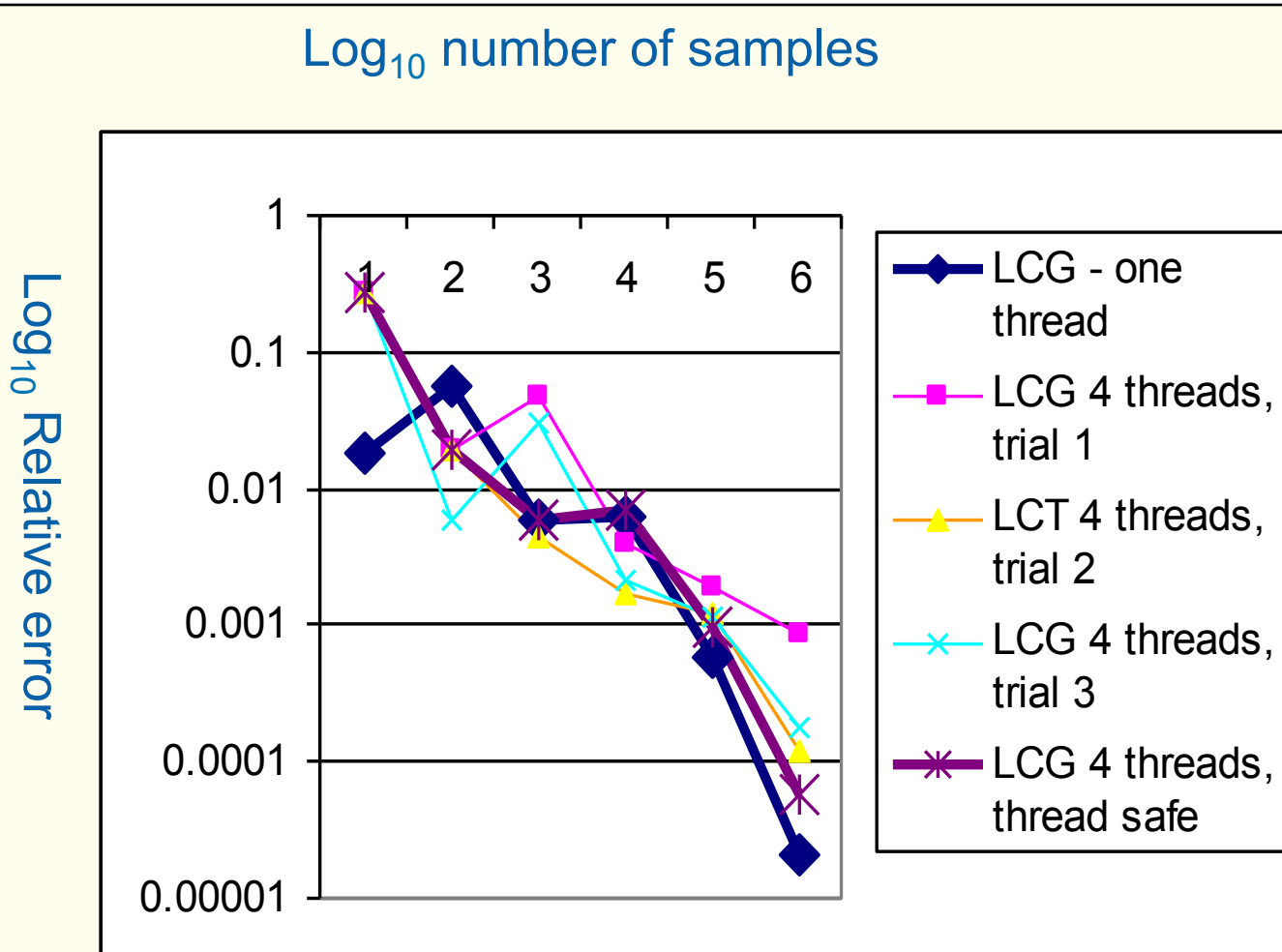
    random_next = (MULTIPLIER * random_last + ADDEND);
    random_last = random_next;

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

random_last carries state between random number computations,

To make the generator threadsafe, make random_last threadprivate so each thread has its own copy.

Thread safe random number generators



Thread safe version gives the same answer each time you run the program.

But for large number of samples, its quality is lower than the one thread result!

Why?

Pseudo Random Sequences

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

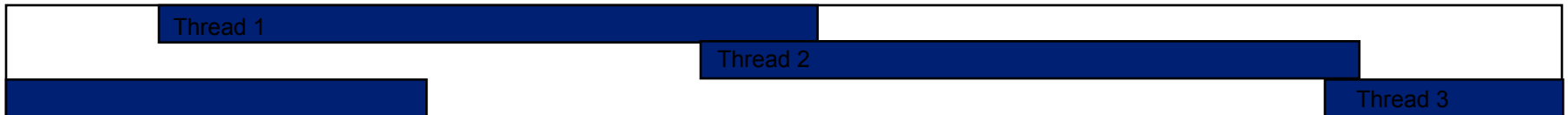


- In a typical problem, you grab a subsequence of the RNG range



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 ... buy a math library that does it right.

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

...

Nice for debugging, but not really needed scientifically.

Intel's Math kernel Library supports all of these methods.

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)
```

```
vslDeleteStream( &stream );
```

Select type of RNG
and set seed

Initialize a
stream or
pseudo
random
numbers

Fill buff with BLOCK pseudo rand.
nums, uniformly distributed with values
between lo and hi.

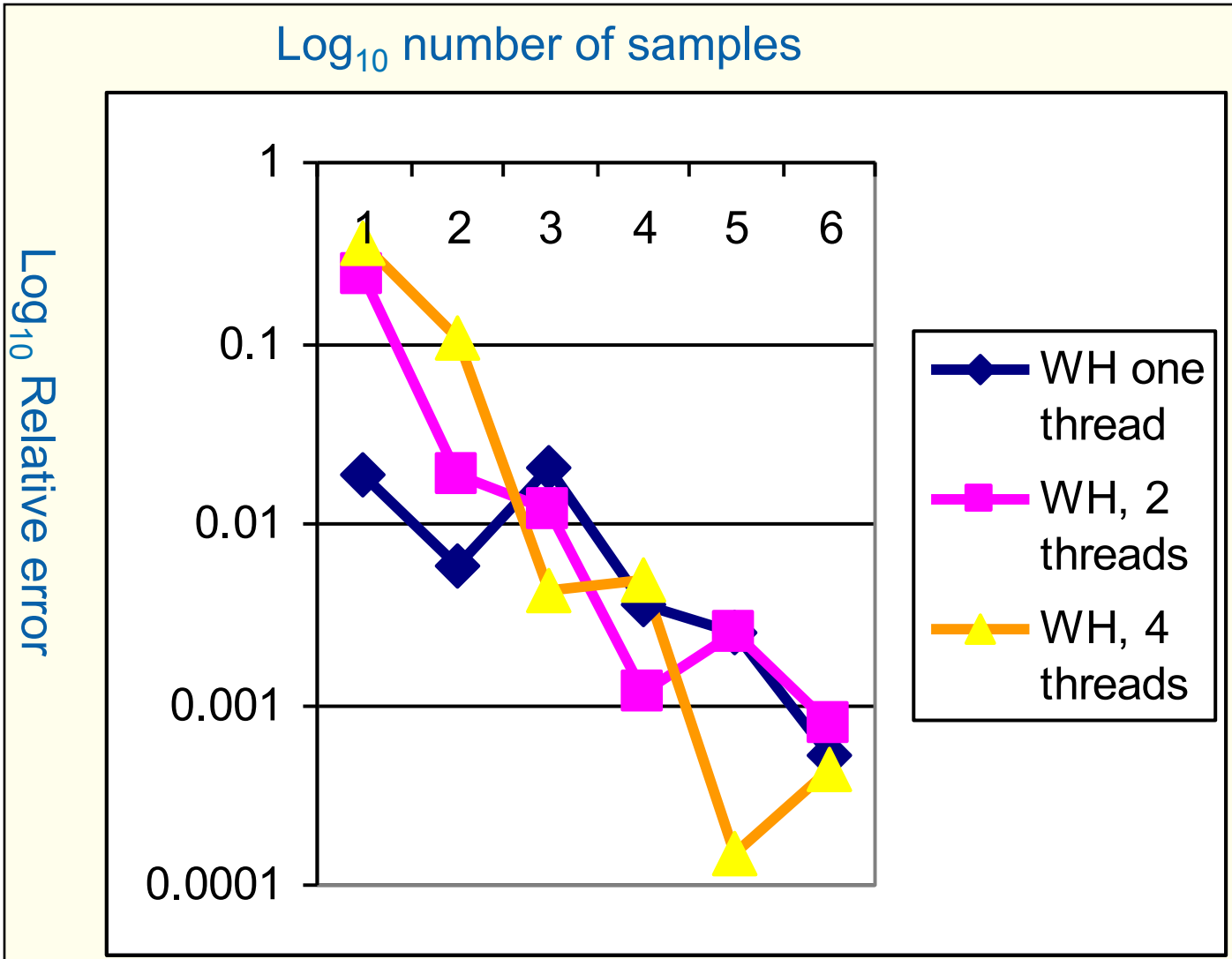
Delete the stream when you are done

Wichmann-Hill generators (WH)

- WH is a family of 273 parameter sets each defining a non-overlapping 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^{th} number in the sequence
 - 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
    pseed[0] = iseed;
    mult_n = MULTIPLIER;
    for (i = 1; i < nthreads; ++i)
    {
        iseed = (unsigned long long)((MULTIPLIER * iseed) % PMOD);
        pseed[i] = iseed;
        mult_n = (mult_n * MULTIPLIER) % PMOD;
    }
}

random_last = (unsigned long long) pseed[id];
```

One thread
computes offsets
and strided
multiplier

LCG with Addend = 0 just
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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Challenge 3: 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

```
#pragma omp parallel for private(tmp, i, j, k)
```

```
for (i=0; i<Ndim; i++){  
    for (j=0; j<Mdim; j++){  
        tmp = 0.0;  
        for(k=0;k<Pdim;k++){  
            /* C(i,j) = sum(over k) A(i,k) * B(k,j) */  
            tmp += *(A+(i*Ndim+k)) * *(B+(k*Pdim+j));  
        }  
        *(C+(i*Ndim+j)) = tmp;  
    }  
}
```

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

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Challenge 4: traversing linked lists

- Consider the program `linked.c`
 - Traverses a linked list computing a sequence of Fibonacci numbers at each node.
- Parallelize this program two different ways
 - ➔ 1. Use OpenMP tasks
 - 2. Use anything you choose in OpenMP *other than* tasks.
- The second approach (no tasks) can be difficult and may take considerable creativity in how you approach the problem (hence why its such a pedagogically valuable problem).

Linked lists with tasks (OpenMP 3)

- See the file Linked_omp3_tasks.c

```
#pragma omp parallel
{
    #pragma omp single
    {
        p=head;
        while (p) {
            #pragma omp task firstprivate(p)
            processwork(p);
            p = p->next;
        }
    }
}
```



Creates a task with its own copy of “p” initialized to the value of “p” when the task is defined

Challenge 4: traversing linked lists

- Consider the program `linked.c`
 - Traverses a linked list computing a sequence of Fibonacci numbers at each node.
- Parallelize this program two different ways
 1. Use OpenMP tasks
 -  2. Use anything you choose in OpenMP *other than* tasks.
- The second approach (no tasks) can be difficult and may take considerable creativity in how you approach the problem (hence why its such a pedagogically valuable problem).

Linked lists without tasks

- See the file `Linked_omp25.c`

```
while (p != NULL) {  
    p = p->next;  
    count++;  
}
```

Count number of items in the linked list

```
p = head;  
for(i=0; i<count; i++) {  
    parr[i] = p;  
    p = p->next;  
}
```

Copy pointer to each node into an array

```
#pragma omp parallel  
{  
    #pragma omp for schedule(static,1)  
    for(i=0; i<count; i++)  
        processwork(parr[i]);  
}
```

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 without tasks: C++ STL

- See the file `Linked_cpp.cpp`

```
std::vector<node *> nodelist;  
for (p = head; p != NULL; p = p->next)  
    nodelist.push_back(p);  
  
int j = (int)nodelist.size();  
#pragma omp parallel for schedule(static,1)  
    for (int i = 0; i < j; ++i)  
        processwork(nodelist[i]);
```

Copy pointer to each node into an array

Count number of items in the linked list

Process nodes in parallel with a for loop

	C++, default sched.	C++, (static,1)	C, (static,1)
One Thread	37 seconds	49 seconds	45 seconds
Two Threads	47 seconds	32 seconds	28 seconds

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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

```
#define THRESHOLD 32768    // product size below which simple matmult code is called

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)
        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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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
```

A structured block

```
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
```

Not A structured block

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 PARREL
 - CRITICAL ... END CRITICAL
 - SECTION ... END SECTION
 - SECTIONS ... END SECTIONS
 - SINGLE ... END SINGLE
 - MASTER ... END MASTER

Runtime library routines

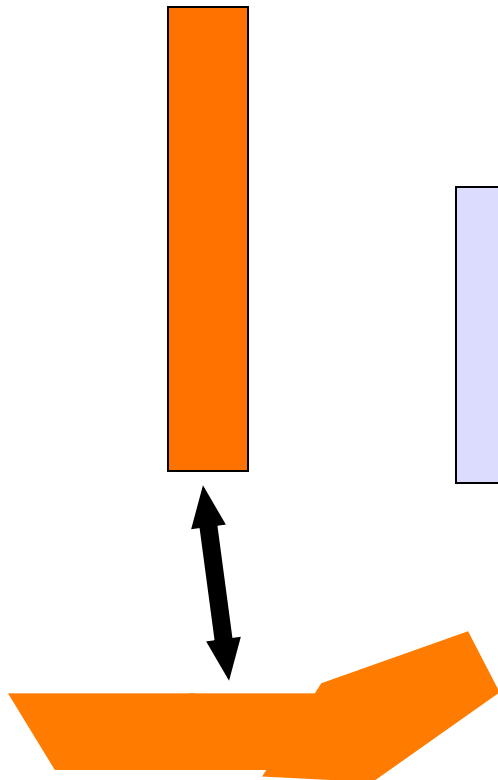
- The include file or module defines parameters
 - Integer parameter `omp_lock_kind`
 - Integer parameter `omp_nest_lock_kind`
 - Integer parameter `omp_sched_kind`
 - Integer parameter `openmp_version`
 - With value that matches C's `_OPENMP` macro
- Fortran interfaces are similar to those used with 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)`

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- Fortran and OpenMP
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- Some Important topics we skipped

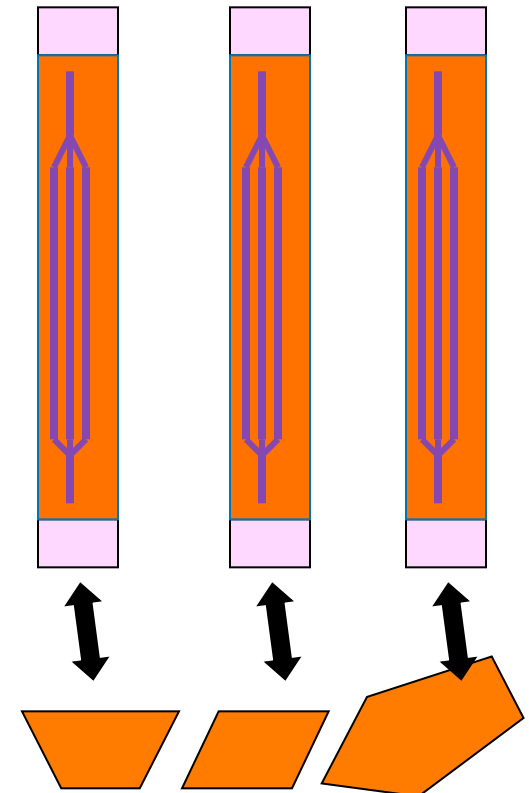
How do people mix MPI and OpenMP?

A sequential program
working on a data set



Replicate the program.
Add glue code
Break up the data

- Create the MPI program with its data decomposition.
- Use OpenMP inside each MPI process.



Pi program with MPI and OpenMP

```
#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<(my_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) ;
}
```

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

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 (l=0;l<N;l++) {  
    U[l] = big_calc(l);  
}
```

```
    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 (l=0;l<N;l++) {  
    U[l] = other_big_calc(l, incoming);  
}
```

```
consume(U, mpi_id);
```

Technically Requires
MPI_Thread_funneled, but I
have never had a problem with
this approach ... even with pre-
MPI-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
```

```
#pragma omp parallel
{
    #pragma omp for
        for (l=0;l<N;l++)    U[l] = big_calc(l);

    #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 (l=0;l<N;l++)    U[l] = other_big_calc(l, incoming);

    #pragma omp master
        consume(U, mpi_id);
}
```

Technically Requires
MPI_Thread_funneled, but I
have never had a problem with
this approach ... even with pre-
MPI-2.0 libraries.

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.

*L. Adhianto and Chapman, 2007

Appendices

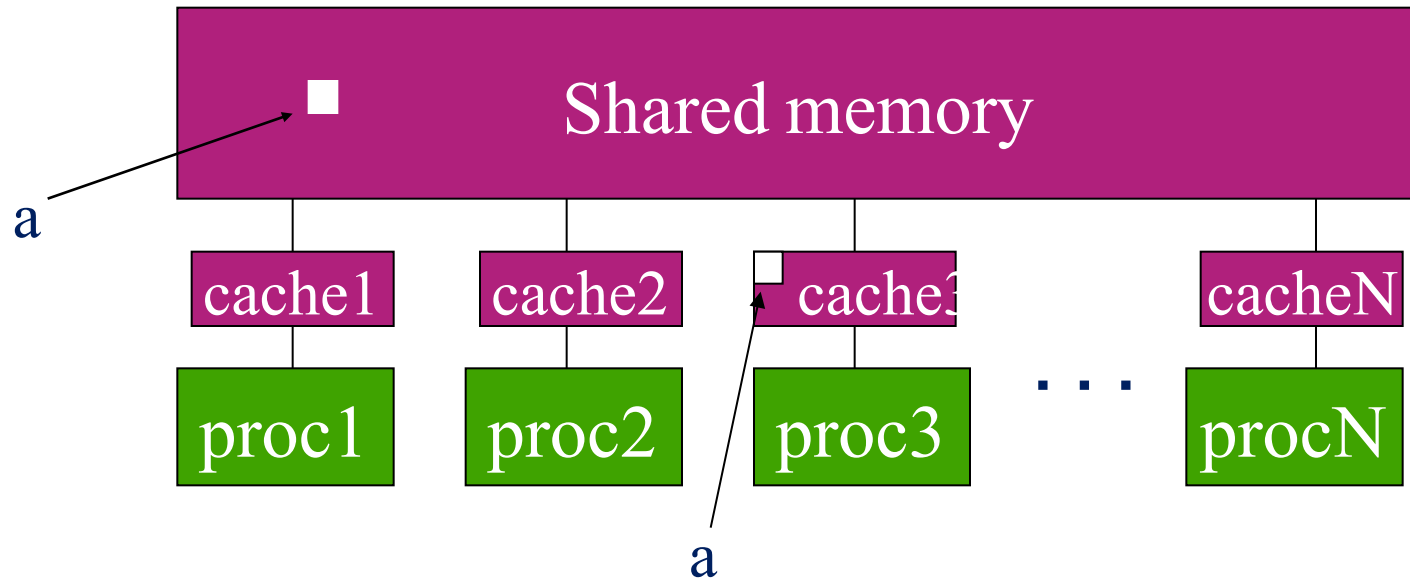
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Some important topics we skipped

- ➔ • Memory model
 - Threadprivate Data
 - Recent additions and future OpenMP directions

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

Synchronization: flush example

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

```
double A;  
  
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)

What is the BIG DEAL with flush?

- Compilers routinely reorder instructions implementing a program
 - Can better exploit the functional units, keep the machine busy, hide memory latencies, etc.
- Compiler generally cannot move instructions:
 - Past a barrier
 - Past a flush on all variables
- But it can move them past a flush with a list of variables so long as those variables are not accessed
- Keeping track of consistency when flushes are used can be confusing ... especially if “flush(list)” is used.

Note: the flush operation does not actually synchronize different threads. It just ensures that a thread's variables are made consistent with main memory

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

Example: 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

The problem is this program 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;}

{--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 flush

Some important topics we skipped

- Memory model
-  • Threadprivate Data
- Recent additions and future OpenMP directions

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/)
```

```
C 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);
    }
}
```

Some important topics we skipped

- Memory model
- Threadprivate Data
-  • Recent additions and future OpenMP directions

OpenMP 4.0 ratified July 2013

- End of a long road? A brief rest stop along the way...
- Addresses several major open issues for OpenMP
- Do not break existing code unnecessarily
- Includes 106 passed tickets
 - Focused on major tickets initially
 - Builds on two comment drafts (“RC1” and “RC2”)
 - Many small tickets after RC2, a few large ones

Overview of major 4.0 additions

- Device constructs
- SIMD constructs
- Cancellation
- Task dependences and task groups
- Thread affinity control
- User-defined reductions
- Initial support for Fortran 2003
- Support for array sections (including in C and C++)
- Sequentially consistent atomics
- Display of initial OpenMP internal control variables

OpenMP 4.0 provides support for a wide range of devices

- Use `target` directive to offload a region

```
#pragma omp target [clause [[,] clause] ...]
```

- Creates new data environment from enclosing device data environment
- Clauses support data movement and conditional offloading
 - `device` supports offload to a device other than default
 - Does not assume copies are made – memory may be shared with host
 - Does not copy if present in enclosing device data environment
 - `if` supports running on host if amount of work is small
- Other constructs support device data environment
 - `target data places map` list items in device data environment
 - `target update` ensures variable is consistent in host and device

Several other device constructs support full-featured code

- Use `target declare` directive to create device versions

```
#pragma omp declare target
```

- Can be applied to functions and global variables
 - Required for UDRs that use functions and execute on device
- `teams` directive creates multiple teams in a `target` region

```
#pragma omp teams [clause [[,] clause] ...]
```

- Work across teams only synchronized at end of `target` region
 - Useful for GPUs (corresponds to thread blocks)
- Use `distribute` directive to run loop across multiple teams

```
#pragma omp distribute [clause [[,] clause] ...]
```

- Several combined/composite constructs simplify device use

Example: OpenMP support for devices

Jacobi iteration

```
#pragma omp target data map(A, Anew)
while (err>tol && iter < iter_max){
    err = 0.0;
#pragma omp target teams distribute parallel for reduction(max:err)
    for(int j=1; j< n-1; j++){
        for(int i=1; i<M-1; i++){
            Anew[j][i] = 0.25* (A[j][i+1] + A[j][i-1]+
                                A[j-1][i] + A[j+1][i]);
            err = max(err,abs(Anew[j][i] - A[j][i]));
        }
    }
#pragma omp target teams distribute parallel for
    for(int j=1; j< n-1; j++){
        for(int i=1; i<M-1; i++){
            A[j][i] = Anew[j][i];
        }
    }
    iter ++;
}
```

← Create a data region on the device. Map A and Anew onto the target device

← Copy A back out to host ... but only once

The "target teams" construct tells the compiler to pick the number of teams ... which translates to thread blocks for CUDA.

OpenMP 4.0 provides portable SIMD constructs

- Use `simd` directive to indicate a loop should be SIMDized

```
#pragma omp simd [clause [[,] clause] ...]
```

- Execute iterations of following loop in SIMD chunks
 - Region binds to the current task, so loop is not divided across threads
 - SIMD chunk is set of iterations executed concurrently by a SIMD lanes
- Creates a new data environment
- Clauses control data environment, how loop is partitioned
 - `safelen(length)` limits the number of iterations in a SIMD chunk
 - `linear` lists variables with a linear relationship to the iteration space
 - `aligned` specifies byte alignments of a list of variables
 - `private`, `lastprivate`, `reduction`, `collapse` – usual meanings

The declare simd construct generates SIMD functions

```
#pragma omp declare simd notinbranch
float min (float a, float b) {
    return a < b ? a : b; }
```

```
#pragma omp declare simd notinbranch
float distsq (float x, float y) {
    return (x - y) * (x - y); }
```

Notinbranch tells the compiler you can assume this function will not be called inside a branch statement .. i.e. all vector lanes will execute this function

- Compile library and use functions in a SIMD loop

```
void minex (float *a, float *b, float *c, float *d) {
    #pragma omp parallel for simd
    for (i = 0; i < N; i++)
        d[i] = min (distsq(a[i], b[i]), c[i]);
}
```

- Creates implicit tasks of `parallel` region
- Divides loop into SIMD chunks
- Schedules SIMD chunks across implicit tasks
- Loop is fully SIMDized by using SIMD versions of functions

A simple UDR example

- Declare the reduction operator

```
#pragma omp declare reduction (merge : std::vector<int> :  
    omp_out.insert(omp_out.end(), omp_in.begin(), omp_in.end()))
```

- Use the reduction operator in a `reduction` clause

```
void schedule (std::vector<int> &v, std::vector<int> &filtered) {  
    #pragma omp parallel for reduction (merge : filtered)  
    for (std::vector<int>::iterator it = v.begin(); it < v.end(); it++)  
        if ( filter(*it) )    filtered.push_back(*it);  
}
```

- Private copies created for a reduction are initialized to the identity that was specified for the operator and type
 - Default identity defined if `identity` clause not present
- Compiler uses `combiner` to combine private copies
 - `omp_out` refers to private copy that holds combined value
 - `omp_in` refers to the other private copy

A simple UDR example

- Declare the reduction operator

```
#pragma omp declare reduction (merge : std::vector<int> :  
    omp_out.insert(omp_out.end(), omp_in.begin(), omp_in.end()))
```

- Use the reduction operator in a `reduction` clause

```
void schedule (std::vector<int> &v, std::vector<int> &filtered) {  
    #pragma omp parallel for reduction (merge : filtered)  
    for (std::vector<int>::iterator it = v.begin(); it < v.end(); it++)  
        if ( filter(*it) )    filtered.push_back(*it);  
}
```

- Private copies created for a reduction are initialized to the identity that was specified for the operator and type
 - Default identity defined if `identity` clause not present
- Compiler uses `combiner` to combine private copies
 - `omp_out` refers to private copy that holds combined value
 - `omp_in` refers to the other private copy

OpenMP 4.0 includes initial support for Fortran 2003

- Added to list of base language versions
- Have a list of unsupported Fortran 2003 features
 - List initially included 24 items (some big, some small)
 - List has been reduced to 14 items
 - List in specification reflects approximate OpenMP Next priority
 - Priorities determined by importance and difficulty
- Plan: Reduce list and ideally provide full support in 5.0
 - Many small changes throughout; Support:
 - Procedure pointers
 - Renaming operators on the `USE` statement
 - `ASSOCIATE` construct
 - `VOLATILE` attribute
 - Structure constructors
 - Will support Fortran 2003 object-oriented features next
 - The biggest issue
 - Considering concurrent reexamination of C++ support

Plan for OpenMP specifications

- OpenMP Tools Interface Technical Report
 - Released in March 2014
 - Working towards adoption in 5.0
- TR3: Initial OpenMP 4.1 Comment Draft
 - Changes adopted in time frame of SC14
 - Provided clear guidance to begin 4.1 implementations
- Final OpenMP 4.1 Comment Draft: Released Late Last Month
- OpenMP 4.1
 - Clarifications, refinements and minor extensions to existing specification
 - Major focus is device construct refinements
 - Do not break existing code
 - Will be released by SC15
- OpenMP 5.0
 - Address several major open issues for OpenMP
 - Expect less significant advance than 4.0 from 3.1/3.0
 - Do not break existing code unnecessarily
 - Targeting release for SC17 (somewhat ambitious)

OpenMP 4.1 will include many refinements to recent additions

- 92 tickets have been passed
 - Many refinements to device support
 - Reflects improved efficiency due to LaTeX conversion
- Many clarifications and minor enhancements
 - Handled several items from Fortran 2003 list
 - SIMD and tasking extensions and refinements
 - Reductions for C/C++ arrays and templates
 - Runtime routines to support cancelation and affinity
- Some new features are being added
 - Support for DOACROSS loops
 - Can divide loop into tasks with `taskloop` construct

TR3 (initial OpenMP 4.1 comment draft) refines device constructs

- Adds flush to several device constructs
- Supports unstructured data movement
- Can now require update/assignment for map (`always`)
- Improves asynchronous execution
 - In 4.0, could have a `task` region with only a `target` region
 - `target` and other device regions are now tasks
 - By default, undeferred
 - Can use `nowait` and `depend` clauses
- Many clarifications and minor corrections

Final OpenMP 4.1 comment draft

further refines device constructs

- `memcpy` API to support manual mapping
- Device pointers (provides interoperability with CUDA and OpenCL libraries)
- Mapping structure elements
- Tweaks to device environment support, including:
 - Default for scalar variables: `firstprivate`
 - `link` clause for `declare target` construct
- New combined constructs
- Other miscellaneous usability features

More significant topics are being considered for OpenMP 5.0

- Updates to support latest C/C++ standards
- More tasking advances (support for event loops)
- General error model
- Continued improvements to device support
- Performance and debugging tools support
- Interoperability and composability
- Locality and affinity
- Transactional memory
- Additional looping constructs and refinements

Preliminaries: Part 0 (use your own laptop)

- You can use your Apple laptops running OS-X
 - Use the gnu compilers
 - Download xcode with command line tools (from Apple) and macports (from macports.org)
 - `sudo port install gcc5`
 - `sudo port select --set gcc mp-gcc5`
 - `gcc -fopenmp <<file names>>`
 - copy exercises from github onto your own laptops
 - `git clone https://github.com/tgmattso/OpenMP_Exercises.git`

OpenMP constructs

- `#pragma omp parallel`
- `#pragma omp for`
- `#pragma omp critical`
- `#pragma omp atomic`
- `#pragma omp barrier`
- Data environment clauses
 - `private (variable_list)`
 - `firstprivate (variable_list)`
 - `lastprivate (variable_list)`
 - `reduction(+:variable_list)`
- Tasks (remember ... private data is made firstprivate by default)
 - `pragma omp task`
 - `pragma omp taskwait`
- `#pragma threadprivate(variable_list)`
- Runtime library routines:
 - `int omp_get_num_threads()`
 - `int omp_get_thread_num()`
 - `double omp_get_wtime()`

Where variable list is a comma separated list of variables

Print the value of the macro

`_OPENMP`

And its value will be

`yyyymm`

For the year and month of the spec the implementation used