PROGRAMMING AND OPTIMIZATION FOR INTEL® ARCHITECTURE

The Hands-On Workshop (HOW) Series

Session 4

Colfax International — *colfaxresearch.com*

September 2016

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COURSE ROADMAP

- HOW to Program Intel Architecture
  - 01. Parallelism, specialization, guided tour – Sep 26
  - 02. Programming Intel Xeon Phi (KNC, KNL) – Sep 27
- HOW to Express Parallelism
  - 03. Automatic vectorization – Sep 28
  - 04. Multi-threading with OpenMP – Sep 29
- HOW to Get Performance
  - 05. Comprehensive demo – Sep 30
  - 06. Scalar & vectorization tuning – Oct 3
  - 07. Multi-threading: common issues – Oct 4
  - 08. Multi-threading: memory aspect – Oct 5
  - 09. Memory traffic – Oct 6
- HOW to Scale
  - 10. Distributed Computing: MPI – Oct 7

September 2016

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October 2016

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— Webinar+remote access

HOW ONLINE

Course page: colfaxresearch.com/how-16-09

- Slides (including this one), code downloads
- Video of recorded sessions
- Chat (during webinars or offline)

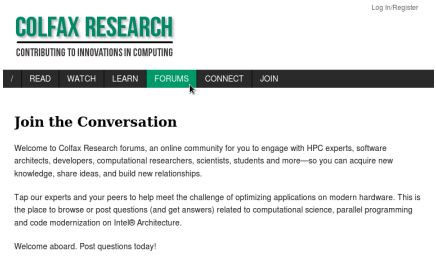
Additional resources:

- More workshops like this one: colfaxresearch.com/training
- Video courses: colfaxresearch.com/video-courses

GET YOUR QUESTIONS ANSWERED

Chat (current):
colfaxresearch.com/how-16-09

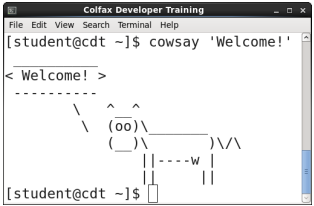
Forums (technical):
colfaxresearch.com/discussion



Email (organizational):
`training@colfax-intl.com`

HANDS-ON EXERCISES AND REMOTE ACCESS

- 96 people receive a remote access token
- Virtualized Intel Xeon CPU, real Intel Xeon Phi coprocessor (1st gen, KNC), SW tools
- Can access the system the entire 2 weeks of the workshop

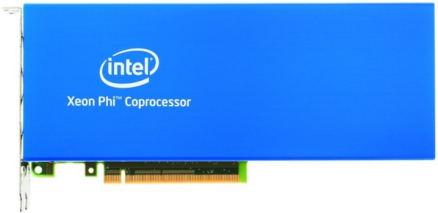


- Not among the 96? Stay tuned: follow along with instructor, use own system, or wait for a seat
- Use it or lose it: if you do not log in for a while, remote access token goes to next student on the list

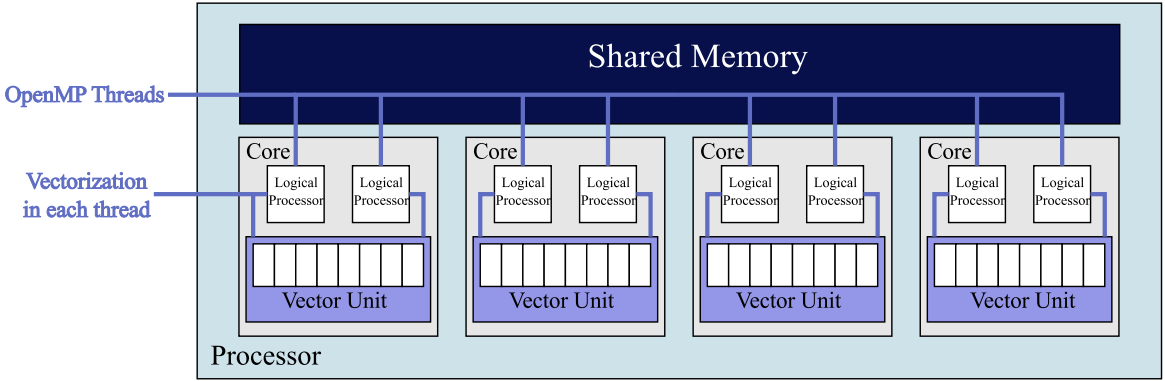
§2. EXPRESSING TASK PARALLELISM

HANDLING MULTIPLE CORES

COMPUTING PLATFORMS

Intel Xeon Processor	Intel Xeon Phi Coprocessor, 1st generation	Intel Xeon Phi Processor, 2nd generation*
		
Current: Broadwell Upcoming: Skylake	Knights Corner (KNC)	* socket and coprocessor versions Knights Landing (KNL)
Multi-Core Architecture	Intel Many Integrated Core (MIC) Architecture	

CO-EXISTENCE WITH VECTORS



Utilize cores: run multiple threads/processes (MIMD)

Utilize vectors: each thread (process) issues vector instructions (SIMD)

SIMULTANEOUS THREADING AND VECTORIZATION

This approach often works:

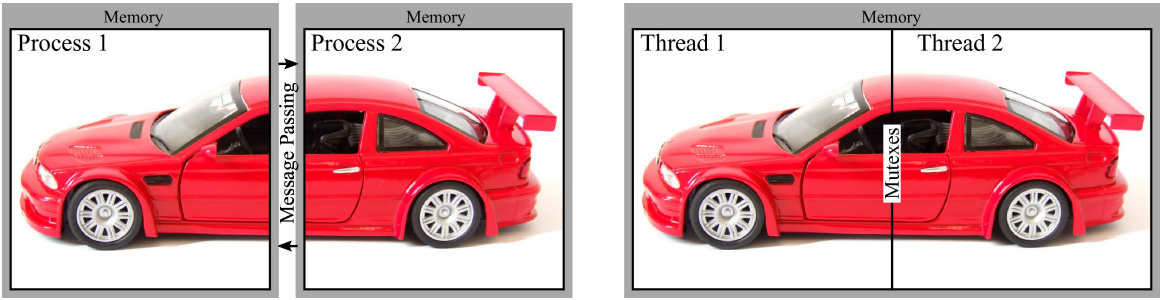
```
#pragma omp parallel for
for (int i = 0; i < n; i++) // Thread parallelism in outer loop
#pragma simd
  for (int j = 0; j < m; j++) // Vectorization in inner loop
    DoSomeWork(A[i][j]);
```

That works as well:

```
#pragma omp parallel for simd
for (int i = 0; i < n; i++) // If the problem is all data-parallel
    DoSomeWork(A[i]);
```

THREADS VERSUS PROCESSES

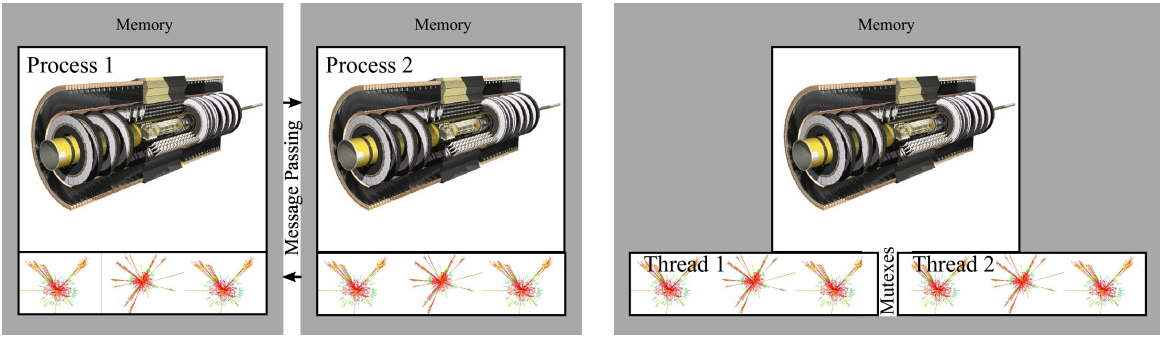
Option 1: Partitioning data set between threads/processes



Examples: computational fluid dynamics (CFD), image processing.

THREADS VERSUS PROCESSES

Option 2: Sharing data set between threads/processes



Examples: particle transport simulation, machine learning (inference).

SCALABILITY EXPECTATIONS (CPU)

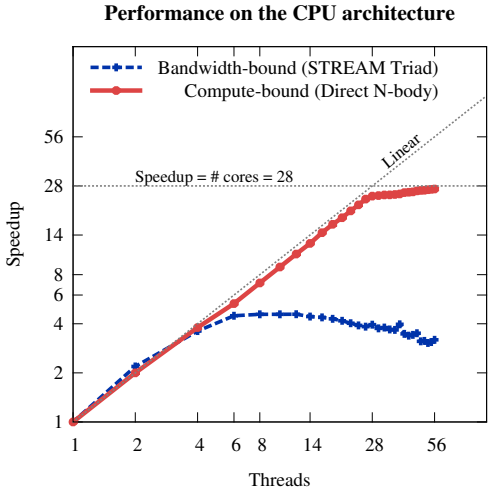
T = number of threads

$$\text{Speedup}(T) = \frac{\text{Performance}(T)}{\text{Performance}(1)}$$

$$\text{Efficiency}(T) = \frac{\text{Speedup}(T)}{T}$$

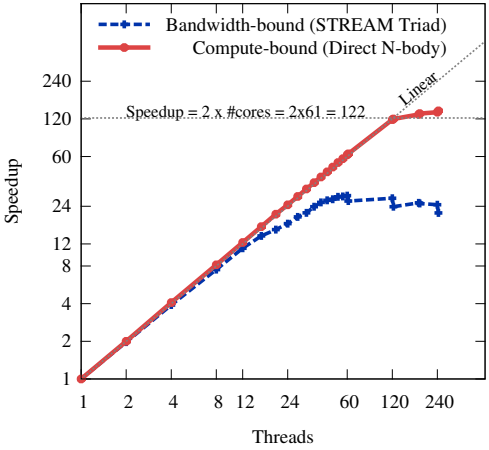
Linear scaling (ideal case, 100% parallel efficiency):

$$\text{Speedup}(T) = T$$

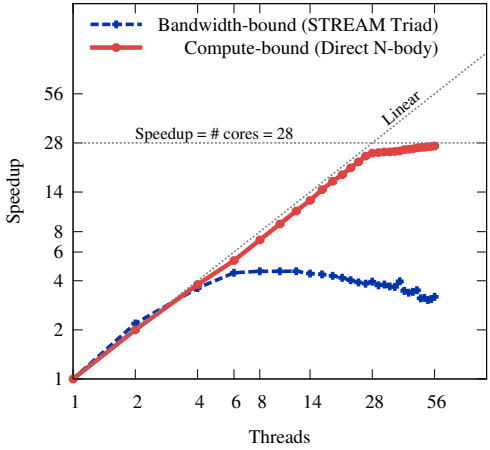


SCALABILITY EXPECTATIONS: MIC VERSUS CPU

Performance on the MIC architecture



Performance on the CPU architecture



THREADING FRAMEWORKS

Framework	Implementation	Complexity	Functionality
POSIX Threads	Various	Simple	Manually control everything
Cilk Plus	Intel, Public	Very simple	Automatic loops and tasks, no user control
TBB	Intel, Public	Complex	Automatic trees of tasks, automatic scheduler
OpenMP	Various	Simple to Complex	HPC-specific functionality, automatic and manual control possible

OPENMP BASICS

"HELLO WORLD" OPENMP PROGRAM

```
1  #include <omp.h>
2  #include <cstdio>
3
4  int main(){
5    // This code is executed by only 1 thread
6    const int nt=omp_get_max_threads();
7    printf("OpenMP with %d threads\n", nt);
8
9  #pragma omp parallel
10   {
11     // This code is executed in parallel
12     // by multiple threads
13     printf("Hello World from thread %d\n",
14                          omp_get_thread_num());
15   }
16 }
```

- OpenMP = “Open Multi-Processing” = computing-oriented framework for shared-memory programming
- Threads – streams of instructions that share memory address space
- Distribute threads across CPU cores for parallel speedup

COMPILING THE "HELLO WORLD" OPENMP PROGRAM

```
vega@lyra% icpc -qopenmp hello_omp.cc
vega@lyra% export OMP_NUM_THREADS=5
vega@lyra% ./a.out
OpenMP with 5 threads
Hello World from thread 0
Hello World from thread 3
Hello World from thread 1
Hello World from thread 2
Hello World from thread 4
```

`OMP_NUM_THREADS` controls number of OpenMP threads (default: logical CPU count)

CONTROL OF VARIABLE SHARING

Method 1: using clauses in pragma omp parallel (C, C++, Fortran):

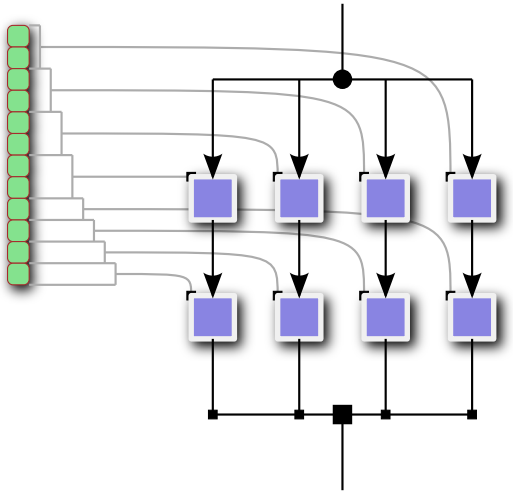
```
1 int A, B; // Variables declared at the beginning of a function
2 #pragma omp parallel private(A) shared(B)
3   {
4     // Each thread has its own copy of A, but B is shared
5   }
```

Method 2: using scoping (only C and C++):

```
1 int B; // Variable declared outside of parallel scope - shared by default
2 #pragma omp parallel
3   {
4     int A; // Variable declared inside the parallel scope - always private
5     // Each thread has its own copy of A, but B is shared
6   }
```

LOOP-CENTRIC PARALLELISM: FOR-LOOPS IN OPENMP

- Simultaneously launch multiple threads
- Scheduler assigns loop iterations to threads
- Each thread processes one iteration at a time



Parallelizing a `for`-loop.

LOOP-CENTRIC PARALLELISM: FOR-LOOPS IN OPENMP

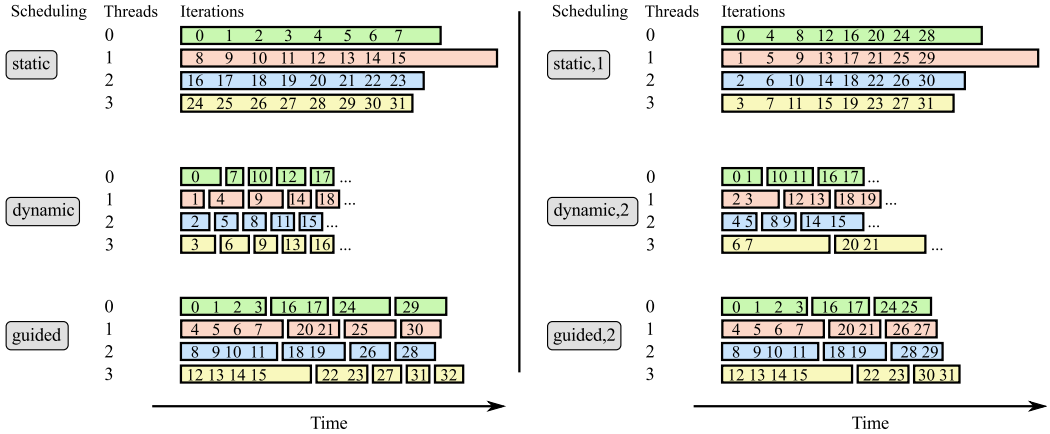
The OpenMP library will distribute the iterations of the loop following the `#pragma omp parallel for` across threads.

```
1 #pragma omp parallel for
2 for (int i = 0; i < n; i++) {
3   printf("Iteration %d is processed by thread %d\n",
4          i, omp_get_thread_num());
5   // ... iterations will be distributed across available threads...
6 }
```

LOOP-CENTRIC PARALLELISM: FOR-LOOPS IN OPENMP

```
1  #pragma omp parallel
2  {
3    // Code placed here will be executed by all threads.
4
5    // Alternative way to specify private variables:
6    // declare them in the scope of pragma omp parallel
7    int private_number=0;
8
9  #pragma omp for
10   for (int i = 0; i < n; i++) {
11     // ... iterations will be distributed across available threads...
12   }
13   // ... code placed here will be executed by all threads
14 }
```

LOOP SCHEDULING MODES IN OPENMP

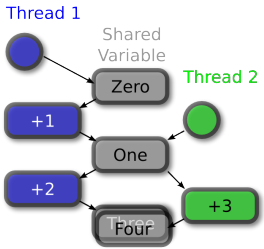


THREAD SYNCHRONIZATION

RACE CONDITIONS AND UNPREDICTABLE PROGRAM BEHAVIOR

```
1  #include <omp.h>
2  #include <cstdio>
3  int main() {
4    const int n = 1000;
5    int total = 0;
6  #pragma omp parallel for
7    for (int i = 0; i < n; i++) {
8      total = total + i; // Race condition
9    }
10   printf("total=%d (must be %d)\n", total,
11                                   ((n-1)*n)/2);
12 }
```

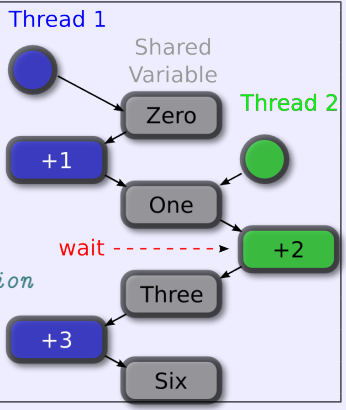
```
vega@lyra% icpc -o app omp-race.cc -qopenmp
vega@lyra% ./app
total=208112 (must be 499500)
```



- Occurs when 2 or more threads access the same memory address, and at least one of these accesses is for writing

PROTECTING RACE CONDITIONS WITH A CRITICAL SECTION

```
1  #include <omp.h>
2  #include <cstdio>
3  int main() {
4    const int n = 1000;
5    int total = 0;
6  #pragma omp parallel for
7    for (int i = 0; i < n; i++) {
8  #pragma omp critical
9      { // Only one thread at a time can execute this section
10       total = total + i;
11     }
12 } }
```




```
vega@lyra% icpc -o omp-critical omp-critical.cc -qopenmp
vega@lyra% ./omp-critical
total=499500 (must be 499500)
```

AVOIDING RACES WITH ATOMIC OPERATIONS

This parallel fragment of code has predictable behavior, because the race condition was eliminated with *an atomic operation*:

```
#pragma omp parallel for
for (int i = 0; i < n; i++)
{ // Lightweight synchronization
#pragma omp atomic
  total += i;
}
```

LIMITATIONS OF ATOMIC OPERATIONS

Read : operations in the form `v = x`

Write : operations in the form `x = v`

Update : operations in the form `x++`, `x--`, `--x`, `++x`, `x` *binop*`=` *expr* and `x = x` *binop expr*

Capture : operations in the form `v = x++`, `v = x-`, `v = -x`, `v = ++x`, `v = x` *binop expr*

- Here `x` and `v` are scalar variables
- *binop* is one of `+`, `*`, `-`, `- /`, `&`, `^` , `|`, `«`, `»`.
- No "trickery" is allowed for atomic operations:
  - no operator overload,
  - no non-scalar types,
  - no complex expressions.

PARALLEL REDUCTION

REDUCTION CLAUSE IN PARALLEL REGION

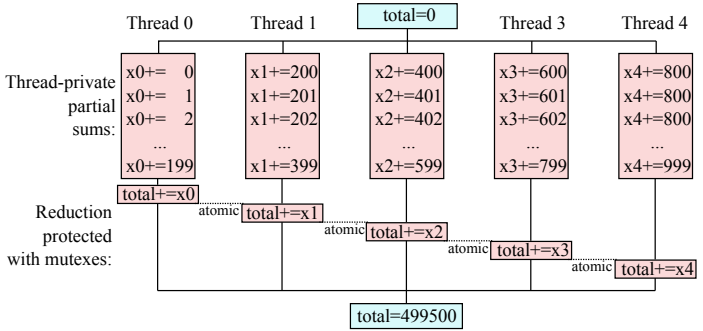
```
1  #include <omp.h>
2  #include <cstdio>
3
4  int main() {
5    const int n = 1000;
6    int total = 0;
7  #pragma omp parallel for reduction(+: total)
8    for (int i = 0; i < n; i++) {
9      total = total + i;
10   }
11   printf("total=%d (must be %d)\n", total, ((n-1)*n)/2);
12 }
```

```
vega@lyra% icpc -o omp-reduction omp-reduction.cc -qopenmp
vega@lyra% ./omp-reduction
total=499500 (must be 499500)
```

AVOIDING RACES WITH THREAD-PRIVATE STORAGE

Correct and efficient code:

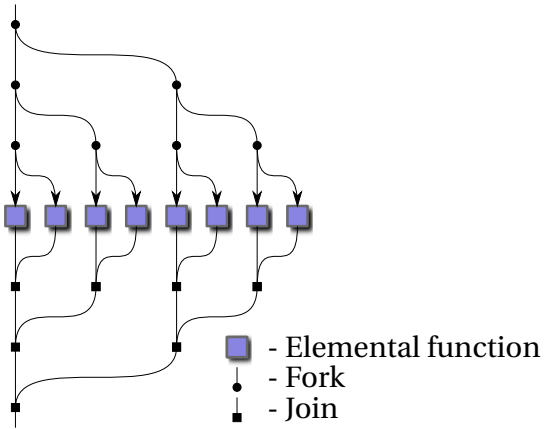
```
1  int total = 0;
2  #pragma omp parallel
3  {
4    int total_thr = 0;
5  #pragma omp for
6    for (int i=0; i<n; i++)
7      total_thr += i;
8
9  #pragma omp atomic
10   total += total_thr;
11
12 }
```



TASKS IN OPENMP

FORK-JOIN MODEL OF PARALLEL EXECUTION

- Each thread can spawn daughter threads
- Available threads pick up queued tasks
- Expresses algorithms that cannot be expressed in the loop model (e.g., parallel recursion)



Fork-join model of parallel execution.

(`#pragma omp task` functionality)

TASKS IN OPENMP: EXAMPLE

```
// Starting the first task:
#pragma omp parallel
{ // Enter a parallel region
#pragma omp single
  { // Start the first task
    // from only one thread
    RecursiveWorkload(args);
  }
}
```

```
// Recursive task spawning:
void RecursiveWorkload(Arg* args) {
  if (args->size > threshold) {
    // Split work
    Arg* args1=args->FirstHalf();
    Arg* args2=args->SecondHalf();

    // Parallel divide-and-conquer
#pragma omp task firstprivate(args1)
    { RecursiveWorkload(args1); }
#pragma omp task firstprivate(args2)
    { RecursiveWorkload(args2);  }
  } else {
    // End of recursion
    args->ProcessSmallestSubTask();
  }
}
```

RECIPES FOR SUCCESS

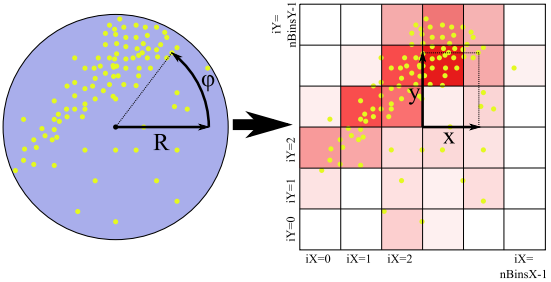
RECIPE FOR SUCCESS: ``TAKE A DEEP BREATH''

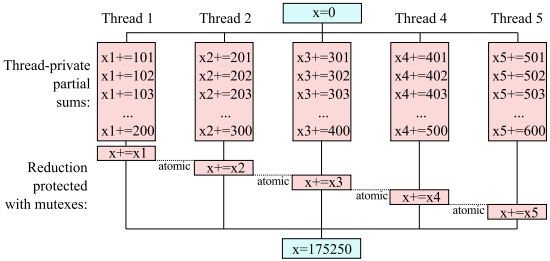
Where is parallelism in your application?

See also full interview with James Reinders at Colfax Research

SUGGESTED ADDITIONAL READING

Colfax Research tutorial on multi-threading in a binning code





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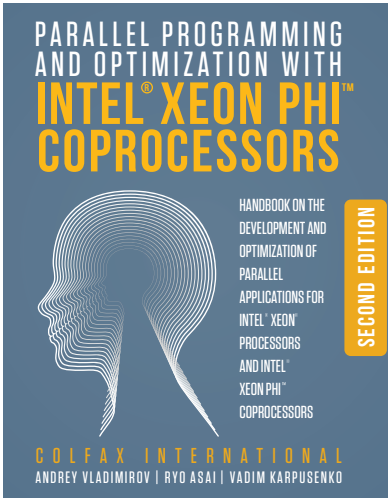
ADDITIONAL MATERIALS ON OPENMP

1. OpenMP Specifications
2. Intel's OpenMP Video Course
3. LLNL tutorial: OpenMP
4. Book: "Parallel Programming and Optimization with Intel Xeon Phi Coprocessors" by Colfax.



SUMMARY

Discussed today:

- Cores can run independent programs
- Use threads to scale across cores
- OpenMP – well-established parallel framework for HPC
- Data races lead to incorrect, unpredictable results
- Mutexes control data races at cost of performance
- Co-exist with have vectorization in each thread

Next session: introduction into optimization for Xeon and Xeon Phi.

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TEXTBOOK

ISBN: 978-0-9885234-0-1 (508 pages, Electronic or Print)

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Handbook on the Development and
Optimization of Parallel Applications
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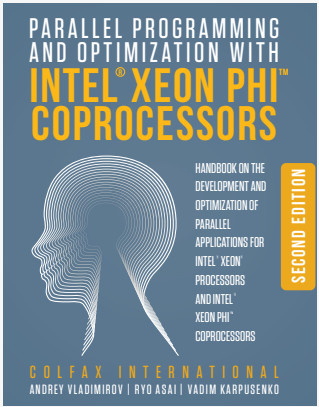
and Intel® Xeon Phi™ Coprocessors



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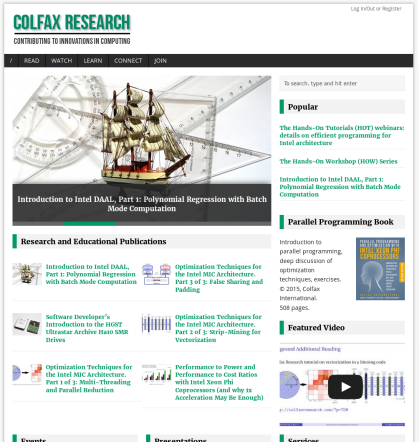

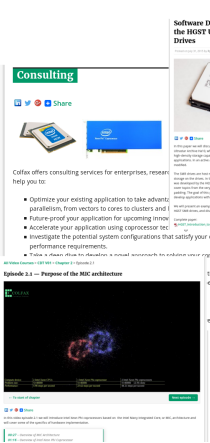

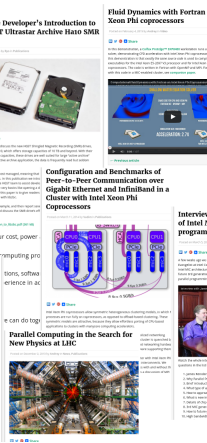

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