Programming and Optimization for Intel® Architecture

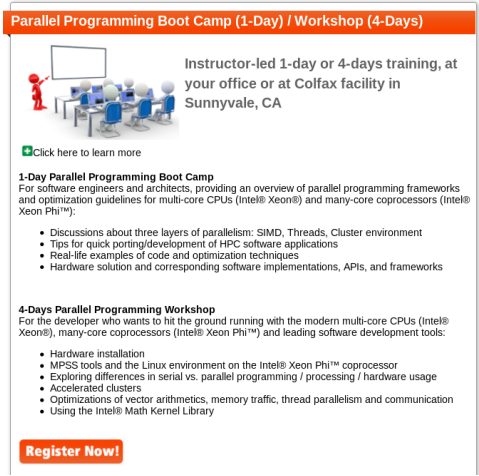
The Hands-On Workshop (HOW) Series

Colfax International — @colfaxintl

July 2016 , Rev. 03a

About This Document

This document represents the materials of a Web-based training “Programming and Optimization with Intel Architecture“ developed and run by Colfax International.



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Course Roadmap

- HOW to Program Intel Architecture
  - 01. Parallelism, specialization, guided tour – July 25
  - 02. Programming Intel Xeon Phi (KNC, KNL) – July 26
- HOW to Express Parallelism
  - 03. Automatic vectorization – July 27
  - 04. Multi-threading with OpenMP – July 28
- HOW to Get Performance
  - 05. Comprehensive demo – July 29
  - 06. Scalar & vectorization tuning – August 1
  - 07. Multi-threading I – August 2
  - 08. Multi-threading II – August 3
  - 09. Memory traffic – August 4
- HOW to Scale
  - 10. Distributed Computing: MPI – August 5

July 2016

S	M	T	W	H	F	S
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17	18	19	20	21	22	23
24	25	26	27	28	29	30
31						

August 2016

S	M	T	W	H	F	S
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28	29	30	31			

— 8:00am UTC Lecture+remote access

HOW Online

Course page: colfaxresearch.com/how-16-07

- 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

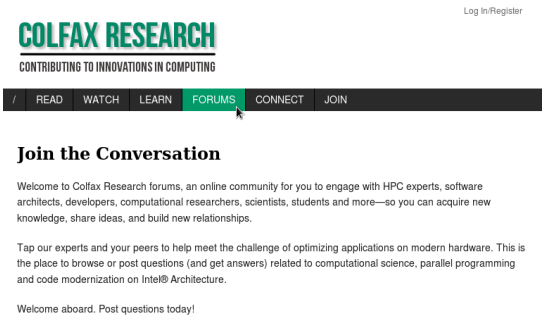
Get Your Questions Answered

Chat (current):

colfaxresearch.com/how-16-07

Forums (technical):

colfaxresearch.com/discussion

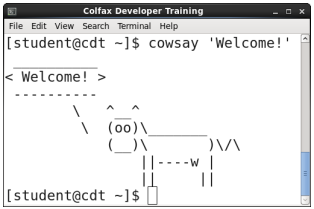


Email (organizational):

`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. Refresh

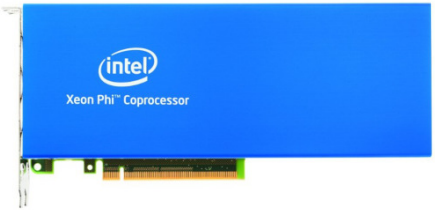
Performance Optimization

Computing Platforms

Intel Xeon Processor

Current: Broadwell
Upcoming: Skylake

Intel Xeon Phi Coprocessor, 1st generation



Knights Corner (KNC)

Intel Xeon Phi Processor, 2nd generation*

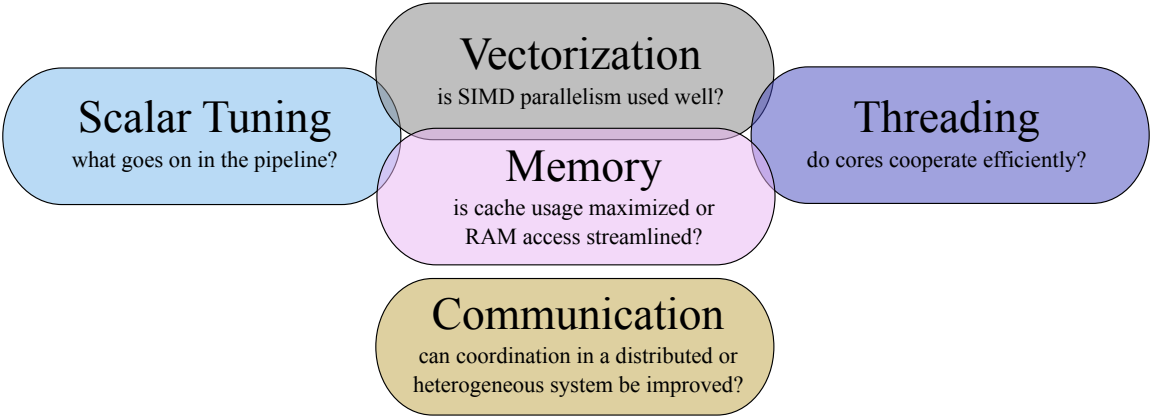
* socket and coprocessor versions

Knights Landing (KNL)

Multi-Core Architecture

Intel Many Integrated Core (MIC) Architecture

Optimization Areas

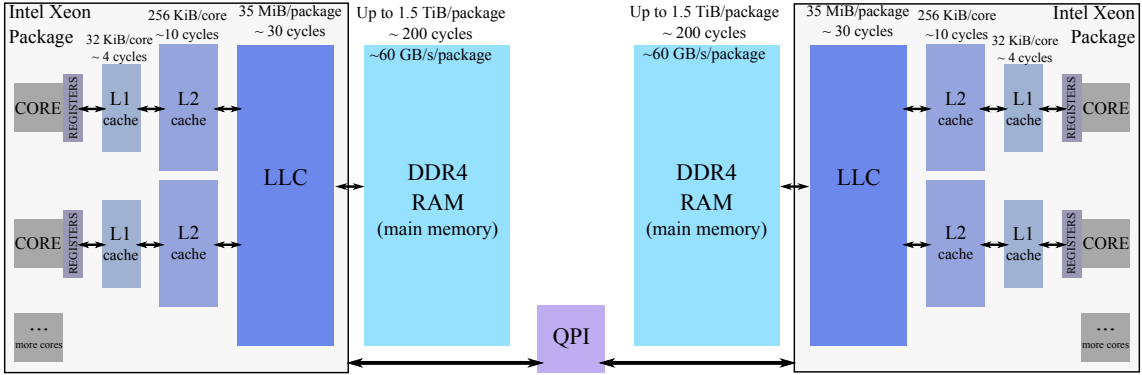


§3. Memory Traffic Tuning

Memory Hierarchy

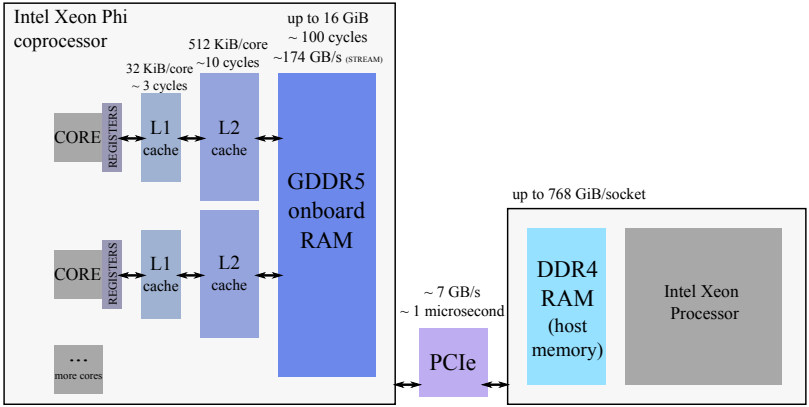
Intel Xeon CPU: Memory Organization

- Hierarchical cache structure
- Two-way processors have NUMA architecture



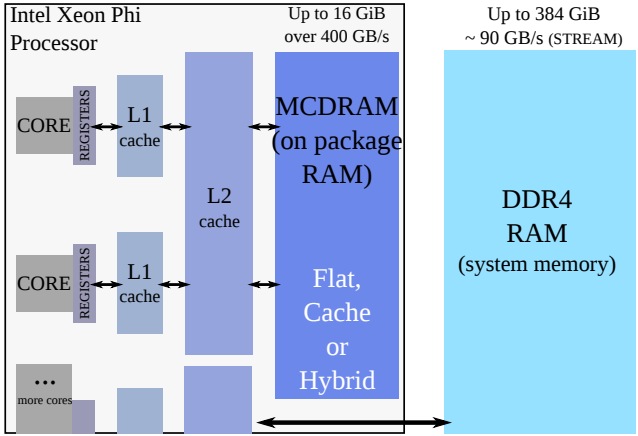
KNC Memory Organization

- Direct access to ≤ 16 GiB of cached GDDR5 memory on board
- No access to system DDR4, connected to host via PCIe



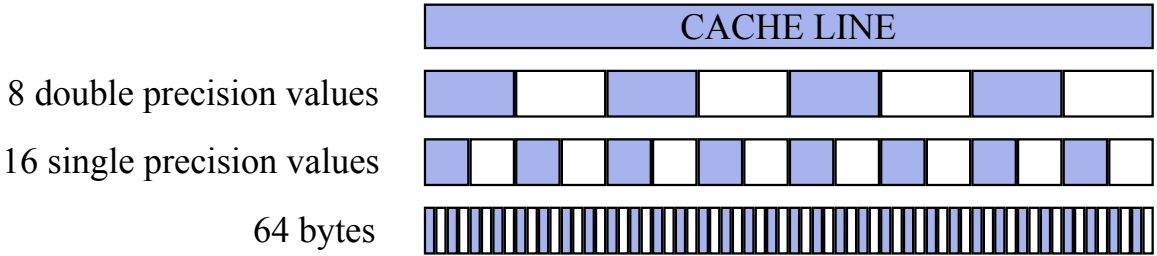
KNL Memory Organization

- Direct access to on-package MCDRAM *and* system DDR4 (socket)
- Use MCDRAM as cache, in flat mode, or as hybrid



Cache Lines

- Minimal block of data transferred between memory and cache
- 64 bytes long in Intel Architecture
- Aligned on 64-byte boundaries in memory



Memory Re-Use and Algorithms

Loop Was Vectorized, Now What?

1. Ensure unit stride access
2. Align data
3. Pad multi-dimensional containers
4. Eliminate peel loops
5. Eliminate multiversioning
6. **Optimize data re-use in caches**

Good to Know

Vector FLOPs are cheap compared to memory access.

If your data is served by RAM and not caches, it does not matter if you have vectorization: you will be bottlenecked by memory access.

How Cheap are FLOPs?

Theoretical estimates, Intel Xeon E5-2697 V3 processor

$$\text{Performance} = 28\,\text{cores} \times 2.7\,\text{GHz} \times (256/64)\,\text{vec.lanes} \times 2\,\text{FMA} \times 2\,\text{FPU} \approx 1.2\,\text{TFLOP/s}$$

$$\text{Required Data Rate} = 1.2\,\text{TFLOP/s} \times 8\,\text{bytes} \approx 10\,\text{TB/s}$$

$$\text{Memory Bandwidth} = \eta \times 2 \times 59.7 \approx 0.1\,\text{TB/s}$$

$$\text{Ratio} = 10/0.1 \approx 100\ \text{(FLOPs)/(Memory Access)}$$

If the Arithmetic Intensity is...

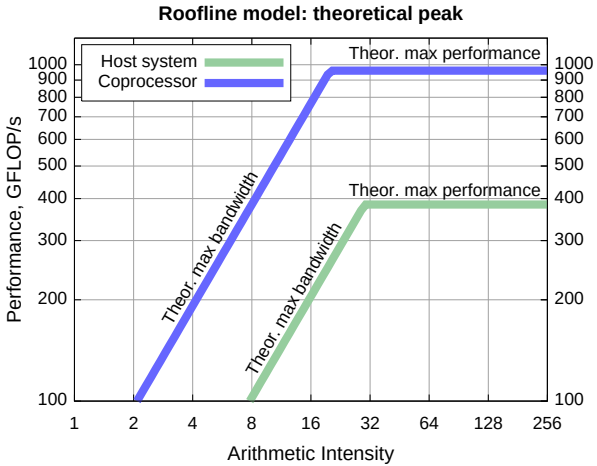
- > 100 (FLOPs)/(Memory Access) — Compute Bound Application
- < 100 (FLOPs)/(Memory Access) — Bandwidth Bound Application

On Computational Complexity of Algorithms

Type	Properties	Examples
$O(N)$	Each data element is used a fixed number of times. Memory-bound unless the number of times is large.	Array scaling, image brightness adjustment, vector dot-product.
$O(N^\alpha)$	Each element is used $N^{\alpha-1}$ times. A lot of data reuse for $\alpha \gtrsim 2$. Good implementation can be compute-bound, poor one – memory-bound.	Matrix-matrix multiplication: $O\left(N^{3/2}\right)$ (N = amount of data in matrix), direct N-body calculation: $O\left(N^2\right)$
$O(N \log N)$	Each element is used $\log N$ times. For small problems – memory-bound, for very large problems transitions to compute-bound	Fast Fourier transform, merge sort
$O(\log N)$	Always memory-bound.	Binary search

N = data size

Arithmetic Intensity and Roofline Model

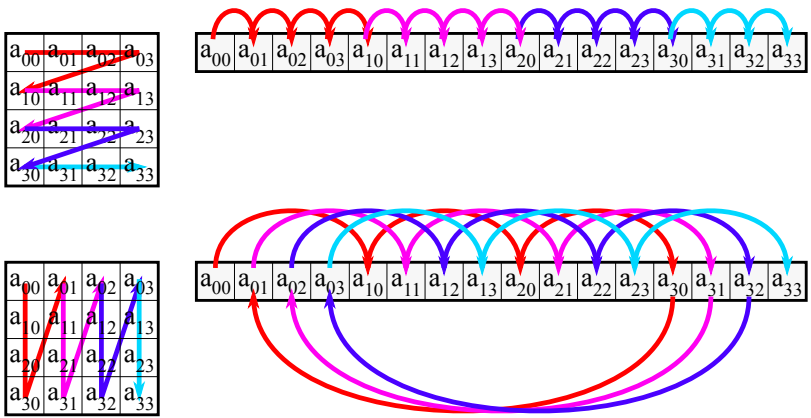


More on roofline model: Williams et al.

Loop Permutation

Principle

Choose loop order to maintain unit-stride memory access



Compiler may or may not be able to automate loop permutation.

Example: Over-simplified Matrix-Matrix Multiplication

$$C = AB \quad \Leftrightarrow \quad C_{ij} = \sum_{k=0}^{n-1} A_{ik} B_{kj}$$

Before:

```
1 #pragma omp parallel for
2 for (int i = 0; i < n; i++)
3   for (int j = 0; j < n; j++)
4 #pragma vector aligned
5     for (int k = 0; k < n; k++)
6       C[i*n+j]+=A[i*n+k]*B[k*n+j];
```

After:

```
1 #pragma omp parallel for
2 for (int i = 0; i < n; i++)
3   for (int k = 0; k < n; k++)
4 #pragma vector aligned
5     for (int j = 0; j < n; j++)
6       C[i*n+j]+=A[i*n+k]*B[k*n+j];
```


Principle

- The order of nested loops must be chosen for best locality of data access
- At `-O2` and above, the compiler automatically interchanges loops in some cases
- In other cases, loop interchange must be investigated manually

Loop Fusion

Loop Fusion Technique

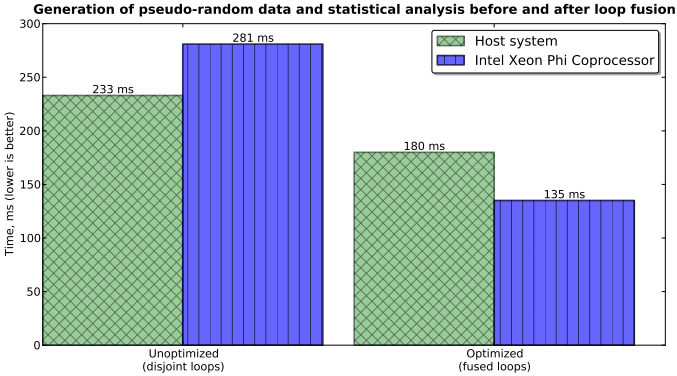
Re-use data in cache by fusing loops in a data processing pipeline

```
1  MyDataType* data = new MyDataType(n);
2
3  for (int i = 0; i < n; i++)
4    Initialize(data[i]);
5
6  for (int i = 0; i < n; i++)
7    Stage1(data[i]);
8
9  for (int i = 0; i < n; i++)
10   Stage2(data[i]);
```

```
1  MyDataType* data = new MyDataType(n);
2
3  for (int i = 0; i < n; i++) {
4
5    Initialize(data[i]);
6
7    Stage1(data[i]);
8
9    Stage2(data[i]);
10 }
```

Potential positive side-effect: less data to carry between stages, reduced memory footprint, improved performance (see, e.g., this paper).

Example Application – Performance



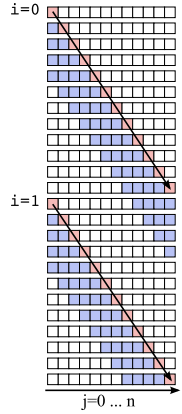
See `labs/4/4.09-memory-loop-fusion-statistics/`

Loop Tiling

Loop Tiling

Original:

```
for (i=0; i<m; i++)
  for (j=0; j<n; j++)
    ...=...*b[j];
```



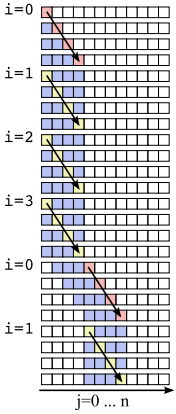
- cached, LRU eviction policy
- cache miss (read from memory, slow)
- cache hit (read from cache, fast)

Cache size: 4
TILE=4
(must be tuned to cache size)

Cache hit rate without tiling: 0%
Cache hit rate with tiling: 75%

Tiled:

```
for (jj=0; jj<n; jj+=TILE)
  for (i=0; i<m; i++)
    for (j=jj; j<jj+TILE; j++)
      ...=...*b[j];
```



Loop Tiling (Cache Blocking) – Procedure

```
for (int i = 0; i < m; i++)  // Original code:
  for (int j = 0; j < n; j++)
    compute(a[i], b[j]); // Memory access is unit-stride in j
```

```
// Step 1: strip-mine inner loop
for (int i = 0; i < m; i++)
  for (int jj = 0; jj < n; jj += TILE)
    for (int j = jj; j < jj + TILE; j++)
      compute(a[i], b[j]); // Same order of operation as original
```

```
// Step 2: permute
for (int jj = 0; jj < n; jj += TILE)
  for (int i = 0; i < m; i++)
    for (int j = jj; j < jj + TILE; j++)
      compute(a[i], b[j]); // Re-use to j=jj sooner
```


Loop Tiling (Unroll-and-Jam/Register Blocking)

```
1   for (int i = 0; i < m; i++)  // Original code:
2     for (int j = 0; j < n; j++)
3       compute(a[i], b[j]); // Memory access is unit-stride in j
```

```
1   // Step 1: strip-mine outer loop
2   for (int ii = 0; ii < m; ii += TILE)
3     for (int i = ii; i < ii + TILE; i++)
4       for (int j = 0; j < n; j++)
5         compute(a[i], b[j]); // Same order of operation as original
```

```
1   // Step 2: permute and vectorize outer loop
2   for (int ii = 0; ii < m; ii += TILE)
3 #pragma simd
4     for (int j = 0; j < n; j++)
5       for (int i = ii; i < ii + TILE; i++)
6         compute(a[i], b[j]); // Use each vector in b[j] a total of TILE times
```


Loop Tiling (Unroll-and-Jam) – Alternative Implementation

```
1  for (int i = 0; i < m; i++)    // Original code:
2    for (int j = 0; j < n; j++)
3      compute(a[i], b[j]); // Memory access is unit-stride in j
```

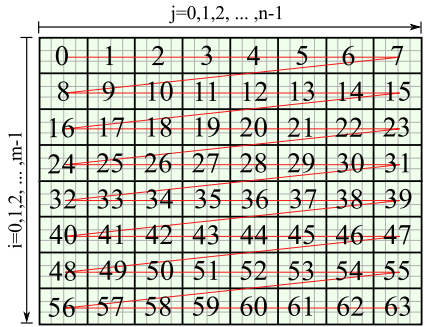
```
1  // Step 1: strip-mine both loops
2  for (int ii = 0; ii < m; ii += TILE)
3    for (int i = ii; i < ii + TILE; i++)
4      for (int jj = 0; jj < n; jj += VECLEN)
5        for (int j = jj; j < jj + VECLEN; j++)
6          compute(a[i], b[j]); // Same order of operation as original
```

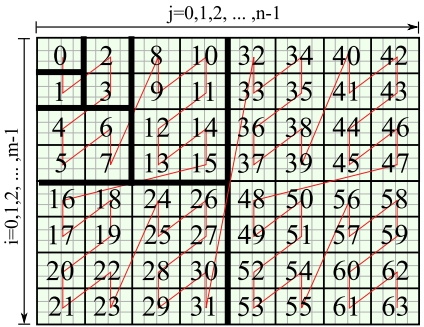
```
1  // Step 2: permute middle two loops
2  for (int ii = 0; ii < m; ii += TILE)
3    for (int jj = 0; jj < n; jj += VECLEN)
4      for (int i = ii; i < ii + TILE; i++)
5        for (int j = jj; j < jj + VECLEN; j++)
6          compute(a[i], b[j]); // Use each vector in b[j] a total of TILE times
```


Cache-Oblivious Recursion

Principle

Matrix A

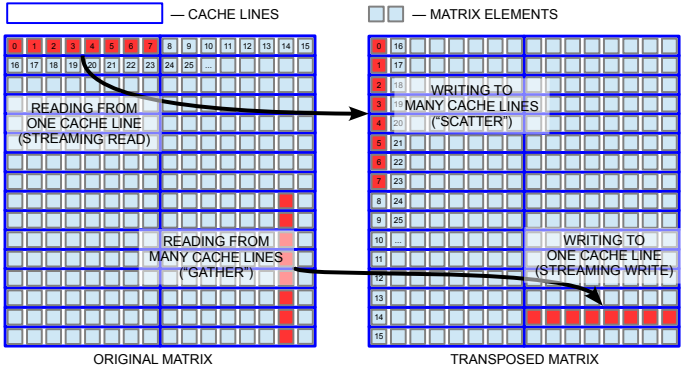




Example 1: Matrix Transposition, Tiling

Example: Matrix Transposition

$$B = A^T \quad \Leftrightarrow \quad B_{ij} = A_{ji}$$



See also this paper.

Matrix Transposition

Before:

```
1 #pragma omp parallel for
2 for (int i = 0; i < n; i++)
3   for (int j = 0; j < n; j++)
4     B[i*n + j] = A[j*n + i];
```

After:

```
1 const int tile = 200;
2 if (n%tile != 0) exit(1);
3
4 #pragma omp parallel for
5 for (int ii=0; ii<n; ii+=tile)
6  for (int jj=0; jj<n; jj+=tile)
7   for (int i=ii; i<ii+tile; i++)
8    for (int j=jj; j<jj+tile; j++)
9     B[i*n + j] = A[j*n + i];
```


Example 2: Matrix-Vector Multiplication, Tiling

Example: Matrix-vector Multiplication

$$c_i = \sum_{j=0}^{n} A_{ij} b_j, \quad i = 0, 1, \ldots, (m-1). \tag{1}$$

```
void Multiply(const double* const A, const double* const b,
              double* const c, const long n, const long m){
  assert(n%64 == 0);
#pragma omp parallel for
  for (long i = 0; i < m; i++)
#pragma vector aligned
    for (long j = 0; j < n; j++) // Each value of A[i*n+j] is used only once
      c[i] += A[i*n+j] * b[j];   // Each value of b[j] is used a total of m times
}
```

Non-optimal performance due to inefficient cache use

Applying Tiling

```
1   const long jTile = 4096L; assert(n%jTile == 0);
2 #pragma omp parallel
3   {
4     double temp_c[m] __attribute__((aligned(64)));
5     temp_c[:] =0;
6 #pragma omp for
7     for (long jj =0; jj < n; jj+=jTile) // Loop Tiling in j
8       for (long i = 0; i < m; i++)
9 #pragma vector aligned
10        for (long j =jj; j < jj+jTile; j++)
11          temp_c[i] += A[i*n+j] * b[j];
12
13    for(long i = 0; i < m; i++) { // Reduction
14 #pragma omp atomic
15      c[i]+= temp_c[i];
16 } } }
```


Cache Blocking + Strip-Mine and Collapse

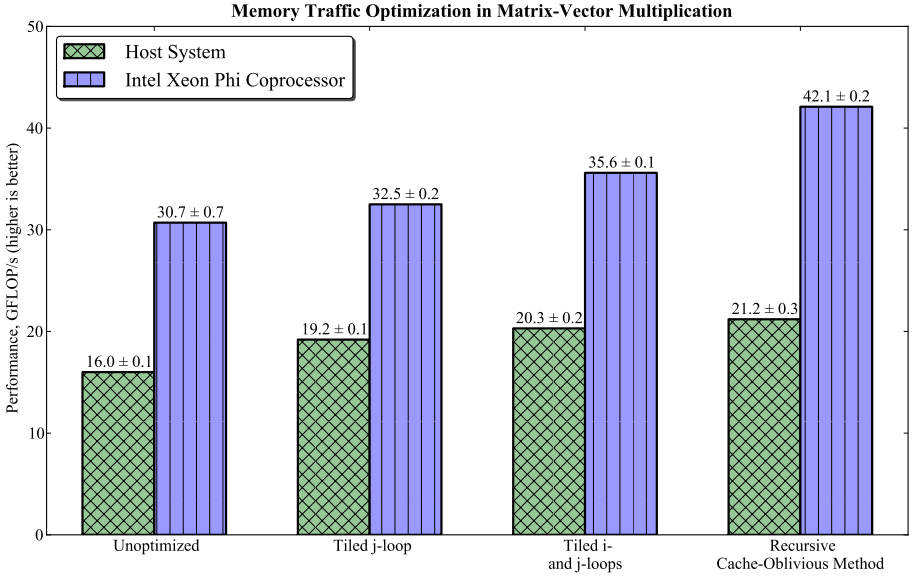
```
1   const long iTile = 64L;   assert(m%iTile == 0);
2   const long jTile = 4096L; assert(n%jTile == 0);
3  #pragma omp parallel
4   {
5     double temp_c[m] __attribute__((aligned(64))); temp_c[:] =0;
6  #pragma omp for collapse(2)
7     for (long ii = 0; ii < m; ii += iTile)
8       for (long jj = 0; jj < n; jj += jTile)
9         for (long i = ii; i < ii+iTile; i++)
10 #pragma vector aligned
11          for (long j =jj; j < jj+jTile; j++)
12            temp_c[i] += A[i*n+j] * b[j];
13
14    for(long i = 0; i < m; i++) {
15 #pragma omp atomic
16      c[i]+= temp_c[i];
17 } } }
```


Example 3: Matrix-Vector Multiplication, Recursion

Example: Matrix-Vector Multiplication

```
1  void RecursMultiply(const double* const A, const double* const b,
2        double* const c, const long n, const long m, const long lda){
3    const long jThreshold = 8192L; assert(n%jThreshold == 0);
4    const long iThreshold = 64L;   assert(m%iThreshold == 0);
5    if ((m<=iThreshold) && (n<=jThreshold)) { // Recursion threshold
6      // .... Base Case: Compute the result inside the tile ... //
7    } else { // Recursive divide-and-conquer
8      if (m*jThreshold > n*iThreshold) { // Split i-wise
9        double c1[m/2] __attribute__((aligned(64)));
10 #pragma omp task
11       { RecursMultiply(&A[0*lda + 0], &b[0], c1, n, m/2, lda); }
12       double c2[m/2] __attribute__((aligned(64)));
13       RecursMultiply(&A[(m/2)*lda + 0], &b[m/2], c2, n, m/2, lda);
14 #pragma omp taskwait
15       c[0:m/2] += c1[0:m/2]; c[m/2:m/2] += c2[0:m/2]; // Reduction
16     } else { // .... Split j-wise .... // }
17 } }
```

Performance of Matrix Vector Multiplication

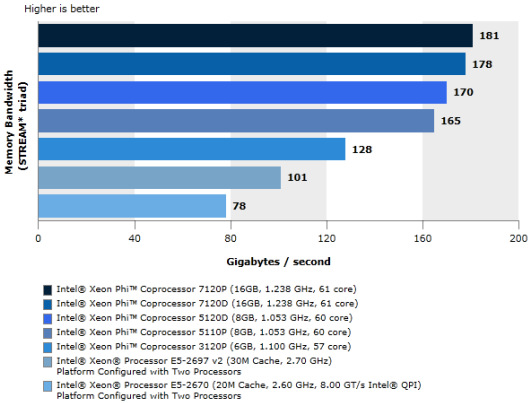


Bandwidth Tuning

STREAM Benchmark

- Industry-standard tool for memory bandwidth measurement
- 4 tests: COPY, ADD, SCALE and TRIAD
- Download from Dr. John McCalpin's site: www.cs.virginia.edu/stream

Expected for KNL: ≈400 GB/s



STREAM Benchmark on Tuning

- Set 1 thread per core on all platforms (-1 for offload)
- Set affinity “scatter”: white paper (Colfax Research)
- Tune prefetching: white paper (Intel)

In addition, secret sauce for your own STREAM-like application:

- Parallel first touch (see NUMA discussion in Session 08)
- Essential element – streaming stores: discussion

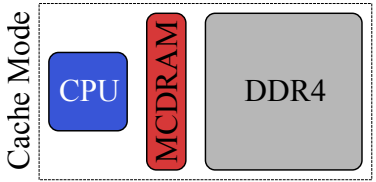
Using High-Bandwidth Memory (MCDRAM) in KNL

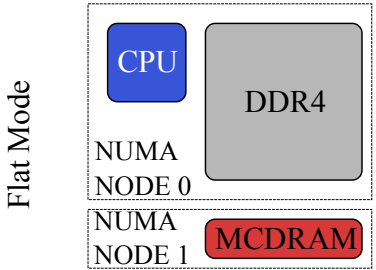
Option 1 : cache/hybrid mode

- Treat it as LLC
- Data locality techniques
- Miss latency 2x the direct DDR4 access

Option 2 : flat mode

- Application fits in 16 GiB? `numactl`
- More than 16 GiB data? Use special allocators (e.g., `memkind`)





Binding to NUMA Nodes with `numactl`

- `numactl` – a Linux tool for controlling NUMA policy for processes

```
vega@lyra% numactl --hardware
available: 2 nodes (0-1)
node 0 cpus: 0 1 2 3 4 5 12 13 14 15 16 17
node 0 size: 65457 MB
node 0 free: 24426 MB
node 1 cpus: 6 7 8 9 10 11 18 19 20 21 22 23
node 1 size: 65536 MB
node 1 free: 53725 MB
node distances:
node   0   1
  0:  10  21
  1:  21  10
vega@lyra% numactl --membind=<nodes> --cpunodebind=<nodes> ./myApplication
```


HBM in Knights Landing

- Finding HBM (MCDRAM) in an Intel Xeon Phi processor x200 (KNL):

```
user@knl% # In Flat mode with All-to-All or Quadrant
user@knl% numactl -H
available: 2 nodes (0-1)
node 0 cpus: 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 ... 249 250 251 252 253 254 255
node 0 size: 98207 MB
node 0 free: 94798 MB
node 1 cpus:
node 1 size: 16384 MB
node 1 free: 15991 MB
```

- Binding the application to HBM (Flat/Hybrid)

```
user@knl% numactl --membind 1 ./runme
// ... Application running in HBM ... //
```


§4. Review and What's Next

Summary

This session:

1. Memory traffic optimization: spatial and temporal data locality
2. Loop tiling: cache blocking and unroll-and-jam
3. Cache-oblivious recursion
4. First-touch allocation in NUMA systems
5. Loop fusion

Next session: distributed computation with MPI, specifics of message passing with coprocessors.

Learn More

HOW Series: Knights Landing

colfaxresearch.com/how-knl/

Textbook

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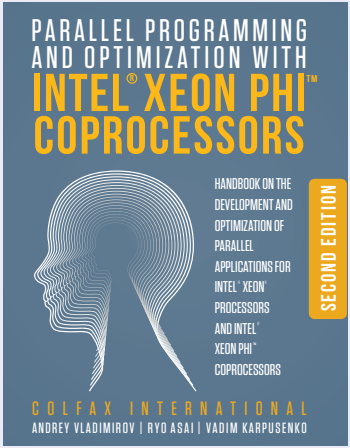
Parallel Programming
and Optimization with
Intel® Xeon Phi™
Coprocessors

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



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