PROGRAMMING AND OPTIMIZATION FOR INTEL® ARCHITECTURE

Hands-On Workshop (HOW) Series "Deep Dive"

Session 7

Colfax International — *colfaxresearch.com*

May 2017

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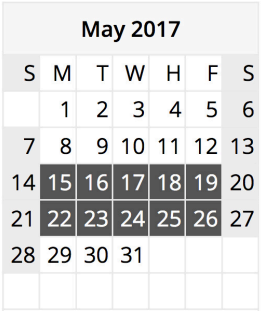
COURSE ROADMAP

- Module I. Programming
  - 01. Intel Architecture and Modern Code – May 15
  - 02. Xeon Phi, Coprocessors, Omni-Path – May 16
- Module II. Expressing Parallelism
  - 03. Automatic vectorization – May 17
  - 04. Multi-threading with OpenMP – May 18
  - 05. Distributed Computing, MPI – May 19
- Module III. Optimization
  - 06. Optimization Overview: N-body – May 22
  - 07. Scalar tuning, Vectorization – May 23
  - 08. Common Multi-threading Problems – May 24
  - 09. Multi-threading, Memory Aspect – May 25
  - 10. Access to Caches and Memory – May 26



HOW SERIES ONLINE

Course page:
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- Code
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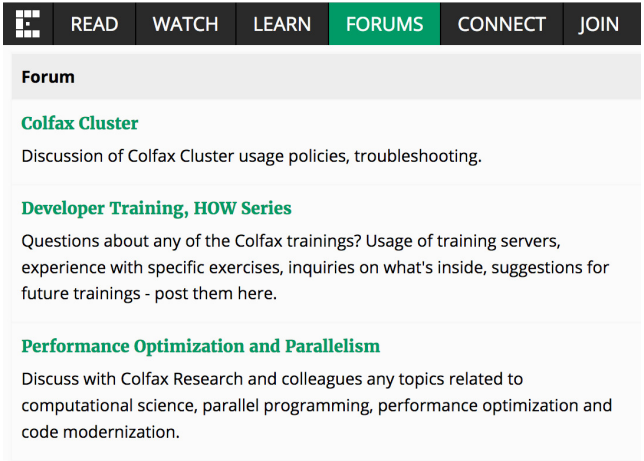


colfaxresearch.com/discussion

HANDS-ON EXERCISES AND REMOTE ACCESS

- All registrants receive an invitation from cluster@colfaxresearch.com
- Queue-based access to Intel Xeon E5, Intel Xeon Phi (KNC and KNL)
- Can access the cluster the entire 2 weeks of the workshop

§2. PERFORMANCE OPTIMIZATION

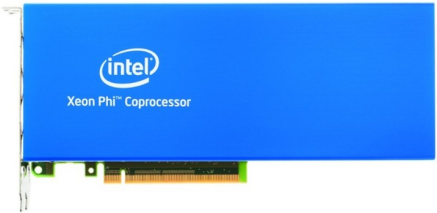
COMPUTING PLATFORMS

Intel Xeon Processor

Current: Broadwell
Upcoming: Skylake

Multi-Core Architecture

Intel Xeon Phi Coprocessor, 1st generation



Knights Corner (KNC)

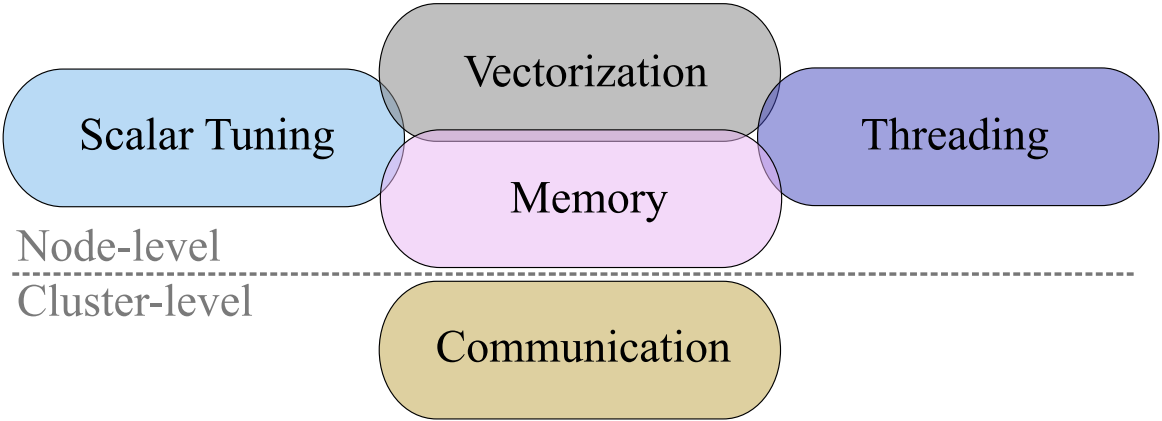
Intel Many Integrated Core (MIC) Architecture

Intel Xeon Phi Processor, 2nd generation*

* socket and coprocessor versions

Knights Landing (KNL)

OPTIMIZATION AREAS



§3. SCALAR TUNING

COMPILER ARGUMENTS

PERFORMANCE-RELATED ARGUMENTS FOR INTEL COMPILERS

`-O<n>` – optimization level (`n`=0, 1, 2, 3 or s)

`-g` – debugging symbols (resets optimization to `-O0`)

`-fp-model <model>` – floating-point semantics (`model=strict`, `precise`, `fast=1` or `fast=2`)

`-fimf-precision=<value>` – transcendental function precision (`value=high`, `medium` or `low`)

`-x<code>` – target arch. (`code=MIC-AVX512`, `CORE-AVX2`, etc., or `host`)

`-ax<code>` – dispatch for multiple target architectures

`-ipo` – inter-procedural optimization

Click above for links in the Intel C++ Compiler User and Reference Guide

Optimization level

Default optimization level `-O2`

- optimization for speed
- automatic vectorization
- inlining
- constant propagation
- dead-code elimination
- loop unrolling

Optimization level `-O3`

- aggressive optimization
- loop fusion
- block-unroll-and-jam
- `if`-statement collapse
- *may or may not be better than* `-O2`

SETTING OPTIMIZATION LEVEL

For the entire file:

```
vega@lyra% icpc -o mycode -O3 source.cc
```

For a specific function:

```
#pragma intel optimization_level 3
void my_function() {
  //...
}
```

PROGRAMMING PRACTICES

STRENGTH REDUCTION

Common Subexpression Elimination.

```
for (int i = 0; i < n; i++)  {
  A[i] /= B;
}
```

```
const float Br = 1.0f/B;
for (int i = 0; i < n; i++)
  A[i] *= Br;
```

Replace division with multiplication.

```
for (int i = 0; i < n; i++)  {
  P[i] = (Q[i]/R[i])/S[i];
}
```

```
for (int i = 0; i < n; i++) {
  P[i] = Q[i]/(R[i]*S[i]);
}
```

Use functions with Hardware support.

```
double r = pow(r2, -0.5);
double v = exp(x);
double y = y0*exp(log(x/x0)*
           log(y1/y0)/log(x1/x0));
```

```
double r = 1.0/sqrt(r2);
double v = exp2(x*1.44269504089);
double y = y0*exp2(log2(x/x0)*
           log2(y1/y0)/log2(x1/x0));
```

PERFORMANCE OF VECTOR INSTRUCTIONS IN KNL

All values in cycles. Lower is better.

Instruction	Latency	1/Throughput
Most vector math and FMA	6	0.5
64-bit exp2a23, rcp28 and rsqrt28	7	2
32-bit exp2a23, rcp28 and rsqrt28	8	3
Floating-point division and sqrt	38	10
Simple integer math	2	2
32-bit scalar division	25	20
64-bit scalar division	40	30
Type conversion (same width)	2	1
Type conversion (different widths)	6	5

CONSISTENCY OF PRECISION: CONSTANTS

```
// Bad: 2 is "int"
long b=a*2;

// Bad: overflow
long n=100000*100000;

// Bad: excessive
float p=6.283185307179586;

// Bad: 2 is "int"
float q=2*p;

// Bad: 1e9 is "double"
float r=1e9*p;

// Bad: 1 is "int"
double t=s+1;
```

```
// Good: 2L is "long"
long b=a*2L;

// Good: correct
long n=100000L*100000L;

// Good: accurate
float p=6.283185f;

// Good: 2.0f is "float"
float q=2.0f*p;

// Good: 1e9f is "float"
float r=1e9f*p;

// Good: 1.0 is "double"
double t=s+1.0;
```

CONSISTENCY OF PRECISION: FUNCTIONS

```
1  // Bad: 3.14 is a double
2  float x = 3.14;
3
4  // Bad: sin() is a
5  // double precision function
6  float s = sin(x);
7
8  // Bad: round() takes double
9  // and returns double
10 long v = round(x);
11
12 // Bad: abs() is not from IML
13 // it takes int and returns int
14 int v = abs(x);
```

```
1  // Good: 3.14f is a float
2  float x = 3.14f;
3
4  // Good: sin() is a
5  // single precision function
6  float s = sinf(x);
7
8  // Good: lroundf() takes float
9  // and returns long
10 long v = lroundf(x);
11
12 // Good: fabsf() is from IML
13 // It takes and returns a float
14 float v = fabsf(x);
```

CONSISTENCY OF PRECISION: FUNCTIONS

Transcendental functions are *not* overloaded (unless in namespace `std` in C++).

```
vega@lyra% ./Scalar-TestFOverload
Proof that exp() is not overloaded:
exp (1.0f)=2.7182818284590451
exp (1.0 )=2.7182818284590451
Exact:   e=2.71828182845904523536...

Proof that expf() gives lower precision:
expf(1.0f)=2.7182817459106445
expf(1.0 )=2.7182817459106445
Exact:   e=2.71828182845904523536...

Overloading in namespace std:
std::exp(1.0f)=2.7182817459106445
std::exp(1.0 )=2.7182818284590451
Exact:       e=2.71828182845904523536...
```

MOVE BRANCHES OUTSIDE OF LOOPS

```
// Elegant, but bad for performance
for (i = 0; i < n; i++) {
  if (i == 0) {
    // Absorbing boundary
    B[i] = 0.0;
  } else if (i == n - 1) {
    // Injection at boundary
    B[i] = A[i] + 1.0;
  } else {
    // Diffusion between boundaries
    B[i] = 0.25*(A[i-1] +
                 2.0*A[i] + A[i+1]);
  }
}
```

```
// Moving branches out of loops


// Absorbing boundary
B[i] = 0.0;

for (i = 1; i < n - 1; i++) {
  // Diffusion between boundaries
  B[i] = 0.25*(A[i-1] + 2.0*A[i] +
                              A[i+1]);
}

// Injection at boundary
B[n-1] = A[n-1] + 1.0;
```

REDUNDANT CODE IS OK

```
1 // Elegant, but bad for performance
2 for (ii = 0; ii < n; ii+=16) {
3   for (i = ii; i < ii+16; i++)
4     // Branch causes unnecessary
5     // masking of vector iterations
6     if (i < n) {
7       A[k*n + i] = ...
8     }
9 }
```

```
1 // Redundant code, but faster
2 const int nTrunc = n - n%16;
3 for (ii = 0; ii < nTrunc; ii+=16) {
4   for (i = ii; i < ii+16; i++)
5       A[k*n + i] = ...
6
7 for (i = nTrunc; i < n; i++)
8   A[k*n + i] = ...
9 }
```

§4. VECTORIZATION

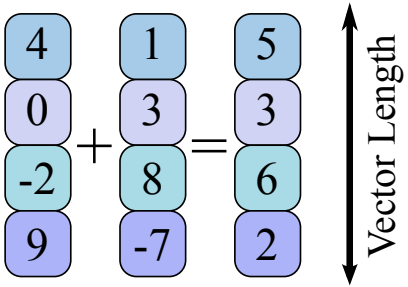
SHORT VECTOR SUPPORT

Vector instructions – one of the implementations of SIMD (Single Instruction Multiple Data) parallelism.

Scalar Instructions

$$4 + 1 = 5$$
$$0 + 3 = 3$$
$$-2 + 8 = 6$$
$$9 + -7 = 2$$

Vector Instructions



DATA STRUCTURES AND MEMORY ACCESS

UNIT-STRIDE ACCESS

Unit-stride access is optimal:

```
1 for (int i = 0; i < n; i++)
2   A[i] += B[i];
```

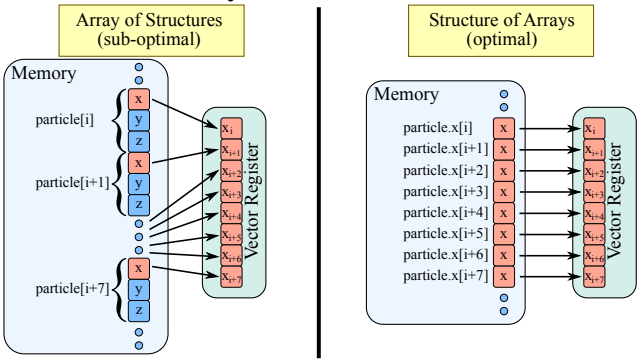
Non-unit stride is slower:

```
1 for (int i = 0; i < n; i++)
2   A[i*stride] += B[i];
```

Stochastic access may be vectorized (but not efficient):

```
1 for (int i = 0; i < n; i++)
2   A[offset[i]] += B[i];
```

It may be a question of changing the order of loop nesting, but sometimes you need to modify data structures:



SUGGESTED EXERCISE

Review lab 4.01 (N-body simulation) or perform lab 4.02 (Coulomb's law calculation) to re-visit the AoS to SoA conversion.

ALIGNMENT AND PADDING

DATA ALIGNMENT REQUIREMENTS

Array `char* p` is `n`-byte aligned if `((size_t)p%n==0)`.

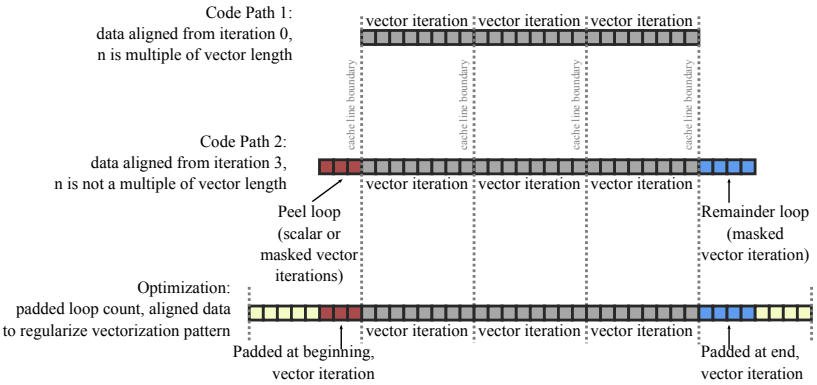
Processor	Operation	Alignment
Xeon (Westmere and earlier)	SSE load, store	16-byte
Xeon (Sandy Bridge and later)	AVX load, store	32-byte (relaxed)
Xeon Phi (1st gen)	IMCI load, store	64-byte (strict)
Xeon Phi (1st gen)	DMA transfer in offload	4096-byte (preferred)
Xeon Phi (2nd gen)	AVX-512 load, store	64-byte (relaxed)

Why align: speed up vector load/stores, avoid false sharing, accelerate RDMA.

WHAT HAPPENS WITHOUT ALIGNMENT

Compiler may implement peel and remainder loops:

```
for (i = 0; i < n; i++)  A[i] = ...
```



CREATING ALIGNED DATA CONTAINERS

- Data alignment on the stack

```
1 float A[n] __attribute__((aligned(64))); // 64-byte alignment applied
```

- Data alignment on the heap

```
1 float *A = (float*) _mm_malloc(sizeof(float)*n, 64);
```

- `A[0]` is aligned on a 64-byte boundary.
- Very high alignment value may lead to wasted virtual memory.
- Fortran: directive or compiler argument `-align array64byte`

PADDING MULTI-DIMENSIONAL CONTAINERS FOR ALIGNMENT

To use aligned instructions, you may need to pad inner dimension of multi-dimensional arrays to a multiple of 16 (in SP) or 8 (DP) elements.

Incorrect:

```
1 // A - matrix of size (n x n)
2 // n is not a multiple of 16
3 float* A =
4  _mm_malloc(sizeof(float)*n*n, 64);
5
6 for (int i = 0; i < n; i++)
7   // A[i*n + 0] may be unaligned
8   for (int j = 0; j < n; j++)
9     A[i*n + j] = ...
```

Correct:

```
1 // ... Padding inner dimension
2 int lda=n + (16-n%16); // lda%16==0
3 float* A =
4  _mm_malloc(sizeof(float)*n*lda, 64);
5
6 for (int i = 0; i < n; i++)
7   // A[i*lda + 0] aligned for any i
8   for (int j = 0; j < n; j++)
9     A[i*lda + j] = ...
```

DATA ALIGNMENT HINTS

Programmer may promise to the compiler (under penalty of segmentation fault) that alignment has been taken care of:

```
1 // Promising that A[i*lda + 0] is aligned for every i
2 // and the same for every other array in this loop
3 #pragma vector aligned
4     for (int j = 0; j < n; j++)
5       A[i*lda + j] -= ...
```

This can lead to significant speedups, because compiler will not implement runtime checks for alignment situation and *peel loops*.

EXAMPLE: LU DECOMPOSITION

EXAMPLE: LU DECOMPOSITION

```
1  void LU_decomp(const int n, float* const A) {
2    // LU decomposition (Doolittle algorithm)
3    // In-place decomposition of form A=LU
4    // L is returned below main diagonal of A
5    // U is returned at and above main diagonal
6    for (int b = 0; b < n; b++) {
7      // Strength reduction:
8      const float recAbb = 1.0f/A[b*n + b];
9      for (int i = b+1; i < n; i++) {
10       A[i*n + b] = A[i*n + b]*recAbb;
11 #pragma simd
12       for (int j = b+1; j < n; j++)
13         A[i*n + j] -= A[i*n + b]*A[b*n + j];
14     }
15   }
16 }
```

LU decomposition for small matrices. ($n \approx 128$)

Based on publication: http://xeonphi.com/papers/

Non-optimal Vectorization Pattern.

- Unaligned
- Irregular loop count

LU DECOMPOSITION: REGULARIZING VECTORIZATION

Before:

```
1  for (int b = 0; b < n; b++) {
2    // ...
3    // ...
4    for (int i = b+1; i < n; i++) {
5      // ...
6      for (int j = b+1; j < n; j++)
7        A[i*n+j] -= A[i*n+b]*A[b*n+j];
8    }
9  }
```

After:

```
1  for (int b = 0; b < n; b++) {
2    // ...
3    const int jMin = (b+1) - (b+1)%16;
4    for (int i = b+1; i < n; i++) {
5      // ...
6      for (int j = jMin; j < n; j++)
7        A[i*n+j] -= L[i*n+b]*A[b*n+j];
8    }
9  }
```

Loop in `j` always starts on a multiple of 64 → aligned access to `A` and `L`

LU DECOMPOSITION: COMPILER HINTS

- Data alignment hint: `#pragma vector aligned`

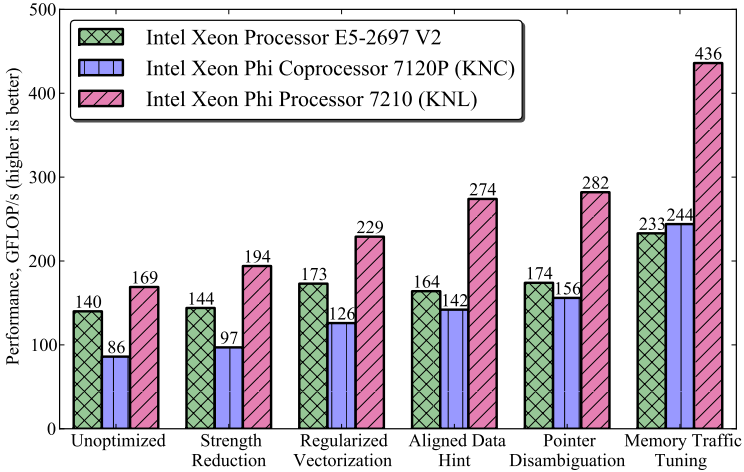
Before:

```
1  for (int b = 0; b < n; b++) {
2    const int jMin = (b+1)-(b+1)%tile;
3    const float recAbb = 1.0f/A[b*n+b];
4    for (int i = b+1; i < n; i++) {
5      L[i*n + b] = A[i*n + b]*recAbb;
6
7
8  #pragma simd
9      for (int j = jMin; j < n; j++)
10       A[i*n+j] -= L[i*n+b]*A[b*n+j];
11   }
12 }
```

After:

```
1  for (int b = 0; b < n; b++) {
2    const int jMin = (b+1)-(b+1)%tile;
3    const float recAbb = 1.0f/A[b*n+b];
4    for (int i = b+1; i < n; i++) {
5      L[i*n + b] = A[i*n + b]*recAbb;
6  #pragma vector aligned
7  #pragma ivdep
8  #pragma simd
9      for (int j = jMin; j < n; j++)
10       A[i*n+j] -= L[i*n+b]*A[b*n+j];
11   }
12 }
```

LU DECOMPOSITION: PERFORMANCE



Paper: http://xeonphi.com/papers/lu

STRIP-MINING FOR VECTORIZATION

STRIP-MINING FOR VECTORIZATION

- Programming technique that turns one loop into two nested loops.
- Used to expose vectorization opportunities.

Original:

```
1 for (int i = 0; i < n; i++) {
2   // ... do work
3 }
```

Strip-mined:

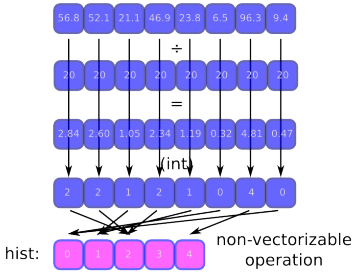
```
1 const int STRIP=1024;
2 const int nPrime = n - n%STRIP;
3 for (int ii=0; ii<nPrime; ii+=STRIP)
4   for (int i=ii; i<ii+STRIP; i++)
5     // ... do work
6
7 for (int i=nPrime; i<n; i++)
8   // ... do work
```

EXAMPLE: BINNING

EXAMPLE: BINNING PROBLEM

```
1  void Histogram(
2    // Ages, values from 0.0f to 100.0f:
3    const float* age,
4    // Size of array age, n=100000000:
5    const int n,
6    // Output: counts in groups:
7    int* const hist,
8    // Size of array hist, m=5:
9    const int m,
10   const float grpWidth) {
11     for (int i = 0; i < n; i++) {
12       const int j = int(age[i]/grpWidth);
13       hist[j]++;
14     }
15 }
```

- Vector dependence in `hist[j]++`
- Strip-mine or use conflict detection



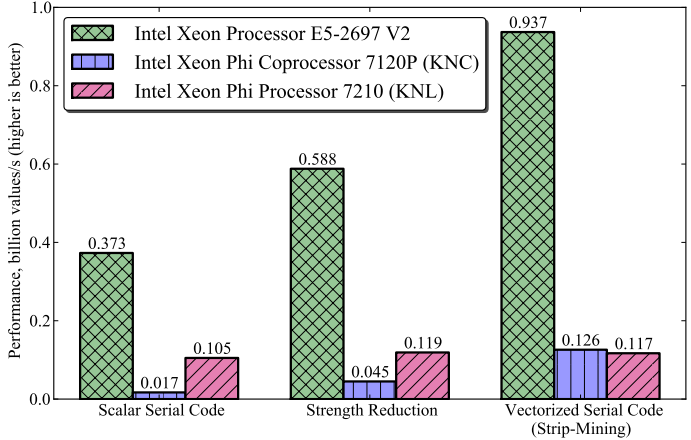
THE SAME CALCULATION, STRIP-MINED, VECTORIZED

```
1  const float recGrpWidth = 1.0f/grpWidth; // precompute the reciprocal
2
3  for (int ii = 0; ii < n; ii += 16) { // strip-mining
4
5    int index[16]; // a block of indices
6    for (int i = ii; i < ii + 16; i++) // vectorizable
7      index[i-ii] = (int) ( age[i] * recGrpWidth ); // unit-stride access
8
9    for (int c = 0; c < 16; c++) // not vectorizable
10     hist[index[c]]++; // indirect access
11 }
```

STRIP-MINING FOR VECTORIZATION

Vectorization improves performance.

More work is needed to take advantage of multiple cores.



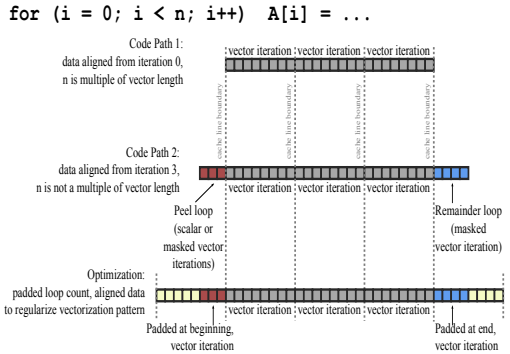
§5. REVIEW AND WHAT'S NEXT

SUMMARY

1. Vector-Friendly Data Structures
   - Use data structures that allow for unit-stride vector load.
2. Regularization of Vectorization Pattern
   - Align data to 64-byte boundaries
   - Pad data containers and loop bounds
3. Remove Run-time Checks
   - Disable run-time checks for alignment and aliasing with compiler hints
4. Strip-Mining for Vectorization
   - Use strip-mining expose vectorization opportunities.

LOOP WAS VECTORIZED, NOW WHAT?

1. Unit-stride access
2. Data alignment
3. Container padding
4. Eliminate peel loops
5. Eliminate multiversioning
6. **Optimize data re-use in caches**



LOOP WAS VECTORIZED, NOW WHAT?

1. Unit-stride access
2. Data alignment
3. Container padding
4. Eliminate peel loops
5. Eliminate multiversioning
6. **Optimize data re-use in caches**

Vector Arithmetics is Cheap, Memory Access is Expensive

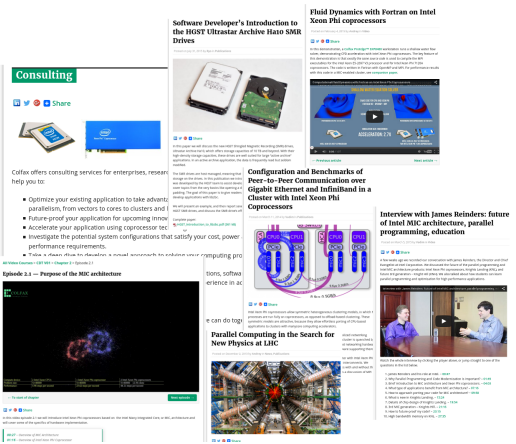
If you don't optimize cache usage, vectorization will not matter.
You will be bottlenecked by memory access.

NEXT SESSION

Next class: optimization of thread parallelism, common issues.

1. Controlling synchronization in parallel reduction
2. Eliminating false sharing
3. Dealing with insufficient parallelism

COLFAX RESEARCH



http://colfaxresearch.com/