# Hardware-aware Performance Engineering

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fall 2019



### Focus of the Lecture

We will learn how to optimize C/C++ code to get more performance from contemporary processors

- maximizing benefit from cache architecture
- writing code taking advantage of compiler auto-vectorization
- using multiple cores efficiently

We will not cover all interesting topics...

- only basic optimizations from each category
- no language-specific optimizations (inlining, proper usage of virtual functions etc.)
- no hardcore, assembly-level optimizations



### Focus of the Lecture

All optimization techniques will be demonstrated on two examples

 so we will see how to change simple code in multiple steps, getting more and more speedup

Timing presented in this lecture will be obtained by using Intel C++

- it has more advanced loop optimization (mainly autovectorization) comparing to competitors
- described optimization methods are of course usable also with different compilers, but it may need some compiler tweaking or writing more complex code
- students can get free license from Intel, anybody from academia can access license via METACentrum



### Motivation

Optimizations will target HW properties, which may change. However, in world of x86 processors:

- caches appear in 80486 (1989), even 80386 had optional off-chip cache
- vector instructions appear in Pentium MMX (1996)
- multiple cores appear in Pentium D (2005), multi-socket configurations much earlier

So, knowledge gathered from this lecture should has sufficiently long lifetime :-).

### Motivation

What if we ignore HW properties and just write good algorithms?

- suppose we have Core i7-5960X processor: 8 cores, Skylake architecture (AVX2 + FMA3 instructions)
- L1 cache latency: 4 cycles, L2: 12 cycles, L3: 42 cycles, RAM about 200 cycles
- vectorized code finishes up to 32 single-precision operations per cycle
- parallelized code take advantage of 8 (or 16 virtual) cores

You can get a lot of speedup by hardware-aware programming.

# Demonstration Examples

We will demonstrate optimization methods using two examples

 I have tried to find as simple as possible computational problems, which still expose a lot of opportunity for various optimization techniques

The code is not very abstract or generic

- in productivity-optimized programming, we want to hide how are algorithms performed, how are data stored etc.
- however, when optimizing code, we have to focus on implementation details, thus, code looks more "old school"
- in practice, usually very small fraction of source code is performance-critical, so different programming style for optimized code is not a problem



Important problem from computational chemistry

- we have a molecule defined by position and charges of its atoms
- the goal is to compute charges at a 3D spatial grid around the molecule

In a given point of the grid, we have

$$V_i = \sum_j \frac{w_j}{4\pi\epsilon_0 r_{ij}}$$

Where  $w_j$  is charge of the j-th atom,  $r_{ij}$  is Euclidean distance between atom j and the grid point i and  $\epsilon_0$  is vacuum permittivity.



#### Initial implementation

- suppose we know nothing about HW, just know C++
- algorithm needs to process 3D grid such that it sums potential of all atoms for each grid point
- we will iterate over atoms in outer loop, as it allows to precompute positions of grid points and minimizes number of accesses into input/output array

```
void coulomb (const sAtom* atoms, const int nAtoms,
    const float gs, const int gSize, float *grid) {
 for (int a = 0; a < nAtoms; a++) {
    sAtom myAtom = atoms[a];
    for (int x = 0; x < gSize; x++) {
      float dx2 = powf((float)x * gs - myAtom.x, 2.0f);
      for (int v = 0; v < gSize; v++) {
        float dy2 = powf((float)y * gs - myAtom.y);
        for (int z = 0; z < gSize; z++) {
          float dz = (float)z * gs - myAtom.z;
          float e = myAtom.w / sqrtf(dx2 + dy2 + dz*dz);
          grid[z*gSize*gSize + y*gSize + x] += e;
```

# Histogram

#### Used in many scientific applications

- computes a frequency of input values occurrence in defined intervals
- in our example, we will compute histogram of population age in uniformly-sized intervals
- input is vector of ages (floating point) and interval size, output is histogram

# Histogram

```
void hist(const float* age, int* const hist, const int n,
    const float group_width, const int m) {
  for (int i = 0; i < n; i++) {
    const int j = (int) ( age[i] / group_width );
    hist[j]++;
  }
}</pre>
```

# Benchmarking

We will benchmark codes on pretty average desktop system

- 4 cores
- AVX2 (256-bit vectors), no FMA

Guess speedup of original codes :-).

### Cache Memories

Why we have cache memories in modern processors?

- main memory is too slow (both latency and bandwidth) comparing to compute cores
- we can build much faster, but also more expensive memory
- cache is fast memory, which temporary keeps parts of larger and slower memories

### Cache Implementation

#### How it is working?

- multiple levels (usually L1 and L2 private for core, L3 shared)
- accessed by cache lines (64 bytes on Intel architectures)
- when data are accessed, they are stored in cache and kept until cache line is needed for another data
- limited associativity (each cache line may cache only defined parts of main memory)
- parallel access into memory cache lines must be somehow synchronized (broadcast, invalidation)

# Optimization for Cache

### Optimization for spatial locality

- access consequent elements
- align data to a multiple of cache line size
- otherwise only part of transfered data is used

#### Optimization for temporal locality

- when data element needs to be accessed multiple times, perform accesses in a short time
- otherwise it may be removed from cache due to its limited capacity or associativity

#### Omit inefficient usage

- conflict misses
- false sharing



```
void coulomb (const sAtom* atoms, const int nAtoms,
    const float gs, const int gSize, float *grid) {
 for (int a = 0; a < nAtoms; a++) {
    sAtom myAtom = atoms[a];
    for (int x = 0; x < gSize; x++) {
      float dx2 = powf((float)x * gs - myAtom.x, 2.0f);
      for (int v = 0; v < gSize; v++) {
        float dy2 = powf((float)y * gs - myAtom.y, 2.0f);
        for (int z = 0; z < gSize; z++) {
          float dz = (float)z * gs - myAtom.z;
          float e = myAtom.w / sqrtf(dx2 + dy2 + dz*dz);
          grid[z*gSize*gSize + y*gSize + x] += e;
```

#### **Evaluation**

We have compiled the code above with vectorization switched off (as we are interested in effects of memory access only)

- 31.6 millions of atoms evaluated per second (MEvals/s) using  $256 \times 256 \times 256$  grid and 4096 atoms
- by changing grid size to  $257 \times 257 \times 257$ , performance changes to 164.7 Mevals/s

#### Interpretation

- strong dependence on input size indicates problems with cache associativity
- even 164.7 Mevals/s is not very good result, considering 8 floating point operations are performed in innermost loop



# Spatial Locality

#### We are interested in the innermost loop

- it defines memory access pattern (i.e. which elements are accessed consequently)
- the innermost loop runs over z, which creates large memory strides in accessing grid
- when grid size is power of two, columns hits the same associativity region

#### Optimization

 $\bullet$  we need to rearrange loops: the innermost loop should iterate through x

# Spatial Locality

```
void coulomb (const sAtom* atoms, const int nAtoms,
    const float gs, const int gSize, float *grid) {
 for (int a = 0; a < nAtoms; a++) {
    sAtom myAtom = atoms[a];
    for (int z = 0; z < gSize; z++) {
      float dz^2 = powf((float)z * gs - myAtom.z, 2.0f);
      for (int v = 0; v < gSize; v++) {
        float dy2 = powf((float)y * gs - myAtom.y, 2.0f);
        for (int x = 0; x < gSize; x++) {
          float dx = (float)x * gs - myAtom.x;
          float e = myAtom.w / sqrtf(dx*dx + dy2 + dz2);
          grid[z*gSize*gSize + y*gSize + x] += e;
```

### **Evaluation**

#### Performance measurement

- 371.8 Mevals/s using  $256 \times 256 \times 256$  grid and 4096 atoms
- no sensitivity to changing grid size (no cache associativity problem)
- much better spatial locality

#### Analysis of cache pattern

- each atom is applied to the whole grid
- poor temporal locality (grid is too large structure)

# Temporal Locality

### Atoms array is much smaller than grid

- we can rearrange loops to iterate over atoms in the innermost loop: z-y-x-a
- alternatively, we may apply atom forces per rows of a grid, creating iteration order z-y-a-x
- or tiling may be used

#### Memory tiling

- we break some loop into nested loops, such that outer loop iterates with step s>1 and those steps are performed in some inner loop
- multiple loops may be tiled
- in our example, we will tile loop running over atoms



# Tiled Algorithm

```
const int TILE = 16:
sAtom myAtom[TILE]; float dy2[TILE], dz2[TILE];
for (int a = 0; a < nAtoms; a+=TILE) {
 myAtom[0:TILE] = atoms[a:a+TILE];
 for (int z = 0; z < gSize; z++) {
   for (int aa = 0; aa < TILE; aa++)
      dz2[aa] = powf((float)z * gs - myAtom[aa].z, 2.0f);
    for (int y = 0; y < gSize; y++) {
      for (int aa = 0; aa < TILE; aa++)
        dy2[aa] = powf((float)y * gs - myAtom[aa].y, 2.0f);
      for (int x = 0; x < gSize; x++) {
        float e = 0.0f;
        for (int aa = 0; aa < TILE; aa++) {
          float dx = (float)x * gs - myAtom[aa].x;
         e += myAtom[aa].w / sqrtf(dx*dx + dy2[aa] + dz2[aa]);
        grid[z*gSize*gSize + y*gSize + x] += e;
```

### **Evaluation**

Note that autovectorization is switched off for all implementations.

Implementation	Performance	speedup
Naive (grid 257)	164.7	n/a
Spatial loc.	371.8	2.26×
ZYXA	359.7	2.18×
ZYAX	382.2	2.32×
Tiled	476.9	2.9×

Temporal locality brings only minor improvement, but it may change when instructions are optimized/code is parallelized.

### Histogram

```
void hist(const float* age, int* const hist, const int n,
    const float group_width, const int m) {
  for (int i = 0; i < n; i++) {
    const int j = (int) ( age[i] / group_width );
    hist[j]++;
  }
}</pre>
```

Memory access is already consequent in age. The random access into hist cannot be omitted. So, nothing to optimize so far...

### **Vector Instructions**

Modern processors have complex logic preparing instructions

- arithmetical units are relatively cheep
- when instruction is to be executed, it may process multiple data elements in parallel

#### Data-parallel programming

- the same instruction is applied onto multiple data (SIMD model)
- explicit usage: we need to generate vector instructions



### **Vector Instructions**

#### Vector instructions

- the same operation is applied to a short vector
- mainly arithmetic operations, may be masked, may contain support for reduction, binning etc.
- vector length depends on data type and instruction set, e.g. AVX2 works with vector of size 256 bytes, so 8 32-bit numbers or 4 64-bit numbers are processed in parallel

#### Vectorization in C/C++

- explicit: inline assembly or intrinsics
- implicit: compiler generates vector instructions automatically

#### Automatic Vectorization

#### Better portability

- the code can be compiled for any vector instruction set
- Supported in modern compilers
  - however, it is difficult task, so allowing compiler to vectorize code needs programmer assist

#### Automatic Vectorization

#### Current limitations

- only innermost for loops are vectorized
- number of iterations must be known when loop is entered, or (preferably) at compilation time
- memory access must be regular, ideally with unit stride (i.e. consequent elements are accessed in vector instructions)
- vector dependence usually disallows vectorization

### Vector Dependence

#### Vector dependence

- the for loop cannot be vectorized, if there is flow dependence between iterations
- however, compiler may wrongly assume vector dependence (it must by conservative to generate correct code)
- #pragma ivdep (Intel) or #pragma GCC ivdep (gcc) instruct compiler to ignore assumed vector dependences (true dependence still disallows vectorization)

# Vector Dependence

```
float a[n], b[n];
for (int i = 0; i < n; i++)
a[i] = b[i]*2.0f;</pre>
```

No vector dependence, the code is vectorized.

```
void foo(float* a, const float* b, int n) {
  for (int i = 0; i < n; i++)
    a[i] = b[i]*2.0f;
}</pre>
```

The compiler must generate correct code also for pointer aliasing (i.e. when a and b overlaps): it generates vectorized and non-vectorized code with runtime check, or not vectorize at all. We may help the compiler using restrict quantifier with a and b, or use ivdep pragma.

# Contiguous Memory Access

```
struct vec{
   float x,y;
};
vec v[n];
for (int i = 0; i < n; i++)
   v[i].x *= 2.0f;</pre>
```

The loop is vectorized, however, access into v is strided. Typical optimization is transferring array of structures (AoS) to structure of arrays (SoA).

```
struct vec{
   float *x;
   float *y;
};
vec v;
// allocation ...
for (int i = 0; i < n; i++)
   v.x[i] *= 2.0f;</pre>
```

# Loop Strip-mining

If part of the code within a loop cannot be vectorized

- we split loop into two nested loops (similarly to tiling)
- we divide the inner loop according to vectorization possibility into vectorizable loop(s) and non-vectorizable loop(s)

Naive implementation has assumed dependence, which needs to be manually fixed.

```
for (int a = 0; a < nAtoms; a++) {
  sAtom myAtom = atoms[a];
 for (int x = 0; x < gSize; x++) {
    float dx2 = powf((float)x * gs - myAtom.x, 2.0f);
    for (int y = 0; y < gSize; y++) {
      float dy2 = powf((float)y * gs - myAtom.y);
      for (int z = 0; z < gSize; z++) {
        float dz = (float)z * gs - myAtom.z;
        float e = myAtom.w / sqrtf(dx2 + dy2 + dz*dz);
       #pragma ivdep
        grid[z*gSize*gSize + y*gSize + x] += e;
```

#### AZYX and ZYAX Innermost Loop

```
for (int x = 0; x < gSize; x++) {
  float dx = (float)x * gs - myAtom.x;
  float e = myAtom.w / sqrtf(dx*dx + dy2 + dz2);
  grid[z*gSize*gSize + y*gSize + x] += e;
}</pre>
```

The loop is automatically vectorized without problems.

#### ZYXA implementation

```
for (int z = 0; z < gSize; z++) {
 for (int y = 0; y < gSize; y++) {
    for (int x = 0; x < gSize; x++) {
      float e = 0.0f:
      for (int a = 0; a < nAtoms; a++) {
        sAtom myAtom = atoms[a];
        float dx = (float)x * gs - myAtom.x;
        float dy = (float)y * gs - myAtom.y;
        float dz = (float)z * gs - myAtom.z;
        e += myAtom.w / sqrtf(dx*dx + dy*dy + dz*dz);
      grid[z*gSize*gSize + y*gSize + x] += e;
```

### **ZYXA** and Tiled

The innermost loop is difficult to vectorize

- strided memory access into atoms elements
- reduction

Two possible solutions

- AoS to SoA optimization
- vectorization of outer loop running over x

```
for (int z = 0; z < gSize; z++) {
  for (int y = 0; y < gSize; y++) {
    for (int x = 0; x < gSize; x++) {
      float e = 0.0f;
      for (int a = 0; a < nAtoms; a++) {
         float dx = (float)x * gs - atoms.x[a];
         float dy = (float)y * gs - atoms.y[a];
         float dz = (float)z * gs - atoms.z[a];
         e += atoms.w[a] / sqrtf(dx*dx + dy*dy + dz*dz);
      }
    grid[z*gSize*gSize + y*gSize + x] += e;
    }
}</pre>
```

# Outer-loop Vectorization

```
for (int z = 0; z < gSize; z++) {
 for (int y = 0; y < gSize; y++) {
   #pragma simd
   for (int x = 0; x < gSize; x++) {
      float e = 0.0f:
      for (int a = 0; a < nAtoms; a++) {
        sAtom myAtom = atoms[a];
        float dx = (float)x * gs - myAtom.x;
        float dy = (float)y * gs - myAtom.y;
        float dz = (float)z * gs - myAtom.z;
        e += myAtom.w / sqrtf(dx*dx + dy*dy + dz*dz);
      grid[z*gSize*gSize + y*gSize + x] += e;
```

### All implementations

We will use restrict quantifier

 otherwise, compiler may expect aliasing even between atoms and grid and give up vectorization

Implementation	Performance	speedup	(vect. speedup)
Naive (grid 257)	164.7	n/a	n/a
Naive vec. (grid 257)	330.6	2.01×	2.01×
Spatial loc.	1838	11.2×	4.94×
ZYXA outer	2189	13.3×	6.09×
ZYXA SoA	2203	13.4×	6.12×
ZYAX	2197	13.3×	5.75×
Tiled outer	2577	15.6×	5.4×
Tiled SoA	2547	15.5×	5.34×



```
void hist(const float* age, int* const hist, const int n,
    const float group_width, const int m) {
  for (int i = 0; i < n; i++) {
    const int j = (int) ( age[i] / group_width );
    hist[j]++;
  }
}</pre>
```

The loop cannot be vectorized due to dependency in hist. We will use strip-mining.

```
void hist(const float* restrict age, int* const restrict hist,
    const int n, const float group_width, const int m) {
    const int vecLen = 16;
    //XXX: this algorithm assumes n%vecLen == 0.
    for (int ii = 0; ii < n; ii += vecLen) {
        int histIdx[vecLen];
        for (int i = ii; i < ii + vecLen; i++)
            histIdx[i-ii] = (int) ( age[i] / group_width );
        for (int c = 0; c < vecLen; c++)
            hist[histIdx[c]]++;
    }
}</pre>
```

Division is heavy-weight operation, we will remove it.

```
void hist(const float* restrict age, int* const restrict hist,
    const int n, const float group_width, const int m) {
    const int vecLen = 16;
    const float invGroupWidth = 1.0f/group_width;
    //XXX: this algorithm assumes n%vecLen == 0.
    for (int ii = 0; ii < n; ii += vecLen) {
        int histIdx[vecLen];
        for (int i = ii; i < ii + vecLen; i++)
            histIdx[i-ii] = (int) ( age[i] * invGroupWidth );
        for (int c = 0; c < vecLen; c++)
            hist[histIdx[c]]++;
    }
}</pre>
```

Implementation	Performance	speedup
Naive	1020 MB/s	n/a
Vectorized	2455 MB/s	2.41×
Removed div.	4524 MB/s	4.44×



#### **Parallelization**

#### Why we have multicore processors?

- processors frequency is no longer substantially improved due to energy requirements
- however, with new manufacturing processes, it is possible to build smaller cores, thus, multiple cores can be integrated into a die

#### Programming multiple cores

- coarse-grained parallelism (compared to vectorization)
- threads are asynchronous by default (MIMD model), synchronization is explicit and relatively expensive



# Parallelization in C/C++

#### Thread-level parallelism in C/C++

- many possible ways to parallelize a code: pthreads, Boost threads, TBB etc.
- we will use OpenMP in our examples, as it broadly-supported standard and it requires only small changes in our code
- however, optimization principles are general and can be used with any parallelization interface

# OpenMP

#### OpenMP standard

- for shared-memory parallelism
- uses pragmas to declare, which parts of the code runs in parallel
- very easy to use, but writing efficient code may be challenging (much like in other interfaces)
- implements fork-join model
- standard, implemented in all major C/C++ compilers

# **OpenMP**

# The parallel region of the code is declared by #pragma omp parallel

```
//serial code
const int n = 100;
#pragma omp parallel
{
    //parallel code
    printf("Hello from thread %d\n", omp_get_thread_num());
    //parallel loop, iterations order is undefined
    #pragma omp for
    for (int i = 0; i < n; i++) {
        //iteration space is distributed across all threads
        printf("%d ", i);
    }
}
//serial code</pre>
```

# **OpenMP**

#### We can define private and shared variables

- #pragma omp parallel for private(a) shared(b)
- variables declared before parallel block are shared by default
- private statement creates private copy for each thread

#### Thread synchronization

- we can define critical section by #pragma omp critical
- or use lightweight atomic operations, which are restricted to simple scalar operations, such as + - \* /

# Electrostatic Potential Map

#### Which loop can be parallelized?

- AZYX: loop running over atoms would need synchronization, so we prefer to parallelize loop running over Z, Y or X
- ZYXA: we can parallelize up to three outermost loops
- ZYAX: we can parallelize up to two outermost loops
- tiled: we can parallelize loop running over Z, Y and X

#### Which loop to parallelize?

- enter and exit of the loop is synchronized
- we want to minimize number of synchronizations, so we will parallelize loops performing more work
- to scale better, we may collapse n perfectly-nested loops using #pragma omp for collapse(n)



# **ZYXA** Example

```
#pragma omp parallel for
for (int z = 0; z < gSize; z++) {
 for (int y = 0; y < gSize; y++) {
   #pragma simd
    for (int x = 0; x < gSize; x++) {
      float e = 0.0f:
      for (int a = 0; a < nAtoms; a++) {
        sAtom myAtom = atoms[a];
        float dx = (float)x * gs - myAtom.x;
        float dy = (float)y * gs - myAtom.y;
        float dz = (float)z * gs - myAtom.z;
        e += myAtom.w / sqrtf(dx*dx + dy*dy + dz*dz);
      grid[z*gSize*gSize + y*gSize + x] += e;
```

# **ZYXA** Example

```
#pragma omp parallel for collapse(2)
for (int z = 0; z < gSize; z++) {
 for (int y = 0; y < gSize; y++) {
   #pragma simd
    for (int x = 0; x < gSize; x++) {
      float e = 0.0f:
      for (int a = 0; a < nAtoms; a++) {
        sAtom myAtom = atoms[a];
        float dx = (float)x * gs - myAtom.x;
        float dy = (float)y * gs - myAtom.y;
        float dz = (float)z * gs - myAtom.z;
        e += myAtom.w / sqrtf(dx*dx + dy*dy + dz*dz);
      grid[z*gSize*gSize + y*gSize + x] += e;
```

Implementation	Performance	speedup	(par. speedup)
Naive (grid 257)	164.7	n/a	n/a
Spatial loc.	2272	13.8×	1.24×
ZYXA outer	7984	48.5×	3.62×
ZYAX	8092	49.1×	3.68×
Tiled SoA	9914	60.2×	3.92×



```
void hist(const float* restrict age, int* const restrict hist,
    const int n, const float group_width, const int m) {
    const int vecLen = 16;
    const float invGroupWidth = 1.0 f/group_width;
    for (int ii = 0; ii < n; ii += vecLen) {
        int histIdx[vecLen];
        for (int i = ii; i < ii + vecLen; i++)
            histIdx[i-ii] = (int) ( age[i] * invGroupWidth );
        for (int c = 0; c < vecLen; c++)
            hist[histIdx[c]]++;
    }
}</pre>
```

We can parallelize the outer loop and atomically update hist.

```
void hist(const float* restrict age, int* const restrict hist,
    const int n, const float group_width, const int m) {
    const int vecLen = 16;
    const float invGroupWidth = 1.0f/group_width;
    #pragma omp parallel for
    for (int ii = 0; ii < n; ii += vecLen) {
        int histIdx[vecLen];
        for (int i = ii; i < ii + vecLen; i++)
            histIdx[i-ii] = (int) ( age[i] * invGroupWidth );
        for (int c = 0; c < vecLen; c++)
            #pragma omp atomic
            hist[histIdx[c]]++;
    }
}</pre>
```

Implementation	Performance	speedup
Naive	1020 MB/s	n/a
Vectorized	2455 MB/s	2.41×
Removed div.	4524 MB/s	4.44×
Parallel	290.2 MB/s	0.28×

So, overhead of atomic operations is too high...



```
void hist(const float* restrict age, int* const restrict hist,
    const int n, const float group_width, const int m) {
 const int vecLen = 16:
  const float invGroupWidth = 1.0f/group_width;
 #pragma omp parallel
    int histPriv[m];
   histPriv[:] = 0;
    int histIdx[vecLen];
   #pragma omp for
   for (int ii = 0; ii < n; ii += vecLen) {
      for (int i = ii; i < ii + vecLen; i++)
        histIdx[i-ii] = (int) (age[i] * invGroupWidth);
      for (int c = 0; c < vecLen; c++)
        histPriv[histIdx[c]]++;
    for (int c = 0; c < m; c++)
     #pragma omp atomic
      hist[c] += histPriv[c];
```

Implementation	Performance	speedup
Naive	1020 MB/s	n/a
Vectorized	2455 MB/s	2.41×
Removed div.	4524 MB/s	4.44×
Parallel	290.2 MB/s	0.28×
Parallel opt.	20086 MB/s	19.7×



#### This implementation is OK on our system

- however, combination of small m (wide groups, for which the histogram is computed) and highly-parallel system decreases performance significantly
- false sharing issue!

#### False sharing

- array histPriv is created by all threads
- if the array is small, multiple arrays may share the same cache line
- so write access to the independent array causes frequent synchronization of the cache
- very simple optimization: padding histPriv array



#### Conclusion

We have demonstrated basic hardware-aware optimization methods

- there is still a lot of uncovered topics
- however, knowledge of basic optimization methods can still make a big difference in performance

We have demonstrated optimization on two examples

- electrostatic potential map: up to 60× speedup
- histogram: up to 20× speedup
- this is much more, than people usually expect...

#### More info

- Intel/AMD optimization manuals
- Colfax Research courses

