Revisiting Matrix Multiplication

6.506 Algorithm Engineering
May 11, 2023
Recap: 6.106 lecture 1 matrix-multiplication case study

As in 6.106, we will use $n = 4096$. 

\[
\begin{pmatrix}
  c_{00} & c_{01} & \cdots & c_{0(n-1)} \\
  c_{10} & c_{11} & \cdots & \vdots \\
  \vdots & \vdots & \ddots & \vdots \\
  c_{(n-1)0} & \cdots & c_{(n-1)(n-1)} \\
\end{pmatrix}
= 
\begin{pmatrix}
  a_{00} & a_{01} & \cdots & a_{0(n-1)} \\
  a_{10} & a_{11} & \cdots & \vdots \\
  \vdots & \vdots & \ddots & \vdots \\
  a_{(n-1)0} & \cdots & a_{(n-1)(n-1)} \\
\end{pmatrix}
\times 
\begin{pmatrix}
  b_{00} & b_{01} & \cdots & b_{0(n-1)} \\
  b_{10} & b_{11} & \cdots & \vdots \\
  \vdots & \vdots & \ddots & \vdots \\
  b_{(n-1)0} & \cdots & b_{(n-1)(n-1)} \\
\end{pmatrix}
\]

\[
c_{ij} = \sum_{k=0}^{n-1} a_{ik} b_{kj}
\]
Final verdict from 6.106 lecture 1

<table>
<thead>
<tr>
<th>Version</th>
<th>Implementation</th>
<th>Running time (s)</th>
<th>Relative speedup</th>
<th>Absolute speedup</th>
<th>GFLOPS</th>
<th>Fraction of peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Python</td>
<td>21,041.67</td>
<td>1</td>
<td>1</td>
<td>0.006</td>
<td>0%</td>
</tr>
<tr>
<td>2</td>
<td>Java</td>
<td>2,387.32</td>
<td>8.8</td>
<td>9</td>
<td>0.058</td>
<td>0.007%</td>
</tr>
<tr>
<td>3</td>
<td>C</td>
<td>1,155.77</td>
<td>2.1</td>
<td>18</td>
<td>0.118</td>
<td>0.014%</td>
</tr>
<tr>
<td>4</td>
<td>+ interchange loops</td>
<td>177.68</td>
<td>6.5</td>
<td>118</td>
<td>0.774</td>
<td>0.093%</td>
</tr>
<tr>
<td>5</td>
<td>+ optimization flags</td>
<td>54.63</td>
<td>3.3</td>
<td>385</td>
<td>2.516</td>
<td>0.301%</td>
</tr>
<tr>
<td>6</td>
<td>Parallel loops</td>
<td>3.04</td>
<td>18</td>
<td>6,921</td>
<td>45.211</td>
<td>5.408%</td>
</tr>
<tr>
<td>7</td>
<td>Parallel divide-and-conquer</td>
<td>1.30</td>
<td>1.4</td>
<td>16,197</td>
<td>105.722</td>
<td>12.646%</td>
</tr>
<tr>
<td>8</td>
<td>+ compiler vectorization</td>
<td>0.70</td>
<td>1.8</td>
<td>30,272</td>
<td>196.341</td>
<td>23.486%</td>
</tr>
<tr>
<td>9</td>
<td>+ AVX intrinsics</td>
<td>0.39</td>
<td></td>
<td>53,292</td>
<td>352.408</td>
<td>41.677%</td>
</tr>
<tr>
<td>10</td>
<td>Intel MKL</td>
<td>0.41</td>
<td></td>
<td>51,497</td>
<td>335.217</td>
<td>40.098%</td>
</tr>
</tbody>
</table>
## Problem: Performance-measurement methodology

<table>
<thead>
<tr>
<th>Version</th>
<th>Implementation</th>
<th>Running time (s)</th>
<th>Relative speedup</th>
<th>Absolute speedup</th>
<th>GFLOPS</th>
<th>Fraction of peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Python</td>
<td>21,041.67</td>
<td>1</td>
<td>1</td>
<td>0.006</td>
<td>0%</td>
</tr>
<tr>
<td>2</td>
<td>Java</td>
<td>2,387.32</td>
<td>8.8</td>
<td>9</td>
<td>0.058</td>
<td>0.007%</td>
</tr>
<tr>
<td>3</td>
<td>C</td>
<td>1,155.77</td>
<td>2.1</td>
<td>18</td>
<td>0.118</td>
<td>0.014%</td>
</tr>
<tr>
<td>4</td>
<td>+ interchange loops</td>
<td>177.68</td>
<td>6.5</td>
<td>118</td>
<td>0.774</td>
<td>0.093%</td>
</tr>
<tr>
<td>5</td>
<td>+ optimization flags</td>
<td>54.63</td>
<td>3.3</td>
<td>385</td>
<td>2.516</td>
<td>0.301%</td>
</tr>
<tr>
<td>6</td>
<td>Parallel loops</td>
<td>3.04</td>
<td>18</td>
<td>6,921</td>
<td>45.211</td>
<td>5.408%</td>
</tr>
<tr>
<td>7</td>
<td>Parallel divide-and-conquer</td>
<td>1.30</td>
<td>1.4</td>
<td>16,197</td>
<td>105.722</td>
<td>12.646%</td>
</tr>
<tr>
<td>8</td>
<td>+ compiler vectorization</td>
<td>0.70</td>
<td>1.9</td>
<td>30,272</td>
<td>196.341</td>
<td>23.486%</td>
</tr>
<tr>
<td>9</td>
<td>+ AVX intrinsics</td>
<td>0.39</td>
<td>1.8</td>
<td>53,292</td>
<td>352.408</td>
<td>41.677%</td>
</tr>
<tr>
<td>10</td>
<td>Intel MKL</td>
<td>0.41</td>
<td>1</td>
<td>51,497</td>
<td>335.217</td>
<td>40.098%</td>
</tr>
</tbody>
</table>

Each running time is the minimum of 5 runs of a binary.

Each binary runs matrix-multiplication once.
An overlooked performance gap

What happens if the binary runs matrix-multiplication many times?

The first matrix-multiply call is \textbf{slower} than subsequent calls.

Version 9 (AVX intrinsics) takes \(\sim0.39\) seconds.

Intel MKL takes \(\sim0.30\) seconds!

The case study’s conclusions are fine, but MKL is faster than we thought!
## New hardware: AWS c5.metal machine specs

<table>
<thead>
<tr>
<th>Feature</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Microarchitecture</td>
<td>Cascade Lake (Intel Xeon Platinum 8275CL)</td>
</tr>
<tr>
<td>Clock frequency</td>
<td>3.0 GHz</td>
</tr>
<tr>
<td>Processor chips</td>
<td>2</td>
</tr>
<tr>
<td>Processor cores</td>
<td>24 per processor chip</td>
</tr>
<tr>
<td>Floating-point unit</td>
<td>32 double-precision operations, including fused-multiply-add, per core per cycle</td>
</tr>
<tr>
<td>Cache-line size</td>
<td>64 B</td>
</tr>
<tr>
<td>L1 data cache</td>
<td>32 KB private, 8-way set associative</td>
</tr>
<tr>
<td>L2 cache</td>
<td>1 MB private, 16-way set associative</td>
</tr>
<tr>
<td>L3 cache</td>
<td>35.75 MB shared, 11-way set associative</td>
</tr>
<tr>
<td>DRAM</td>
<td>189 GB</td>
</tr>
</tbody>
</table>

**Theoretical peak performance:**

\[
3.0 \text{ GHz} \times 2 \times 24 \times 32 = 4608 \text{ GFLOPS}
\]
Intel oneMKL offers different threading options that give different performance on new hardware.

Version 9 (AVX intrinsics) takes \(~0.12\) seconds.

oneMKL with TBB takes \(~0.11\) seconds.

oneMKL with OpenMP takes \(~0.06\) seconds!
New performance results on a c5.metal instance

<table>
<thead>
<tr>
<th>Implementation</th>
<th>Running time (s)</th>
<th>Relative speedup</th>
<th>Absolute speedup</th>
<th>GFLOPS</th>
<th>Fraction of peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parallel divide-and-conquer</td>
<td>1.091</td>
<td>1</td>
<td>1</td>
<td>125.998</td>
<td>2.734%</td>
</tr>
<tr>
<td>+ AVX2 compiler vectorization</td>
<td>0.878</td>
<td>1.2</td>
<td>1.242</td>
<td>156.511</td>
<td>3.397%</td>
</tr>
<tr>
<td>+ AVX512 compiler vectorization</td>
<td>0.824</td>
<td>1.1</td>
<td>1.324</td>
<td>166.817</td>
<td>3.620%</td>
</tr>
<tr>
<td>+ hand vectorization</td>
<td>0.052</td>
<td>15.9</td>
<td>21.087</td>
<td>2656.893</td>
<td>57.658%</td>
</tr>
<tr>
<td>oneMKL with OpenMP</td>
<td>0.061</td>
<td>0.9</td>
<td>18.002</td>
<td>2268.232</td>
<td>49.224%</td>
</tr>
</tbody>
</table>

Today, we will look at the algorithms and engineering behind these vectorized matrix-multiplication codes.
Outline

• Compiler vectorization
• Vectorization by hand
• Vectorization by hand, another approach
• Performance-engineering the hand-vectorized version
• Intel oneMKL
Outline

- Compiler vectorization
- Vectorization by hand
- Vectorization by hand, another approach
- Performance-engineering the hand-vectorized version
- Intel oneMKL
Recap: Parallel divide-and-conquer matrix multiplication (Version 7)

Matrix-multiply routine

```c
void mmdac(double *restrict C, double *restrict A,
            double *restrict B, size_t size) {
    if (size == S) {
        mmbase(C, A, B);
    } else {
        size_t s00 = 0;
        size_t s01 = size/2;
        size_t s10 = (size/2)*n;
        size_t s11 = (size/2)*(n+1);
        cilk_scope {
            cilk_spawn mmdac(C+s00, A+s00, B+s00, size/2);
            cilk_spawn mmdac(C+s01, A+s00, B+s01, size/2);
            cilk_spawn mmdac(C+s10, A+s10, B+s00, size/2);
                mmdac(C+s11, A+s10, B+s01, size/2);
        }
        cilk_scope {
            cilk_spawn mmdac(C+s00, A+s01, B+s10, size/2);
            cilk_spawn mmdac(C+s01, A+s01, B+s11, size/2);
            cilk_spawn mmdac(C+s10, A+s11, B+s10, size/2);
                mmdac(C+s11, A+s11, B+s11, size/2);
        }
    }
}
```

mmbase() snippet

```c
for (size_t i = 0; i < S; ++i)
    for (size_t k = 0; k < S; ++k)
        for (size_t j = 0; j < S; ++j)
```

For an \(S \times S\) submatrix of \(C\), the base case repeatedly multiplies a row of \(B\) by a value in \(A\) and adds the result to a row of \(C\).
AVX2 and AVX512 vectors

We will use AVX2 and AVX512 vector instructions to speed up this code.

- AVX2 supports 256-bit ymm vector registers (4 doubles).
- AVX512 supports 512-bit zmm vector registers (8 doubles).
- The machine supports 32 ymm and zmm registers.
- All ymm and zmm registers are aliased.
AVX2 and AVX512 vector instructions

Today, we can focus on just a subset of the available vector instructions.

- Vector load and store (aligned and unaligned).
- Element-wise arithmetic, including fused-multiply-add (FMA).
- **Broadcast**: Fill all entries in a vector register with the same value.
- **Shuffle**: Permute the entries in a vector register. (More on this operation later.)

Disclaimer: I will typically illustrate operations using 4-element vectors, but 8-element vectors are used in practice.
Compiler vectorization

Matrix-multiply base case

For each k:
1. \( av = \text{Broadcast}(A[i,k]) \)
2. For \( j \in [0, S) \) by vector width:
   a. \( bv = \text{Vector-load}(B[k,j]) \)
   b. \( cv = \text{Vector-load}(C[i,j]) \)
   c. \( cv += av \times bv \)
   d. \( \text{Vector-store}(cv, C[i,j]) \)
Compiler vectorization

Snippet of compiler-vectorized base case

```llvm
%78 = load double, ptr %59, align 8
%79 = insertelement <4 x double> poison, double %78, i64 0
%80 = shufflevector <4 x double> %79,
    <4 x double> poison, <4 x i32> zeroinitializer
%88 = getelementptr inbounds double, ptr %2, i64 %60
%89 = load <4 x double>, ptr %88, align 8
%96 = load <4 x double>, ptr %16, align 8
%100 = tail call <4 x double> @llvm.fmuladd.v4f64(<4 x double> %80,
...)
```

$ clang -o mm mm.c -fopencilk -O3 -march=native

Load and broadcast a value from A
Vector-load from B
Vector-load from C
FMA
Vector-store into C
Compiler vectorization

$ clang -o mm mm.c -fopencilk -O3 -march=native

Snippet of compiler-vectorized base case

```llvm
%78 = load double, ptr %59, align 8
%79 = insertelement <4 x double> poison, double %78, i64 0
%80 = shufflevector <4 x double> %79,
    <4 x double> poison, <4 x i32> zeroinitializer
%88 = getelementptr inbounds double, ptr %2, i64 %60
%89 = load <4 x double>, ptr %88, align 8
%96 = load <4 x double>, ptr %16, align 8
%100 = tail call <4 x double> @llvm.fmuladd.v4f64(<4 x double> %80,
```

The compiler is using **32-bit** vector registers, but AVX512 offers **64-bit** vector registers!

Why isn’t the compiler using AVX512?
CPU frequency scaling with AVX instructions

It is often hard to get performance out of AVX512 instructions, due to **downclocking**.

- Modern Intel CPUs reduce their clock frequency when they execute AVX512 instructions.
- This downclocking slows down non-AVX instructions running on the core as well.
- Modern compilers are reluctant to use AVX512, because it’s often not worth it.
- This issue has improved on newer CPUs.

https://en.wikichip.org/wiki/intel/frequency_behavior
Compiler vectorization with AVX512

We can make the compiler to use AVX512 with different compiler flags. How much performance do we get?

<table>
<thead>
<tr>
<th>Implementation</th>
<th>Running time (s)</th>
<th>Relative speedup</th>
<th>Absolute speedup</th>
<th>GFLOPS</th>
<th>Fraction of peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parallel divide-and-conquer</td>
<td>1.091</td>
<td>1</td>
<td>1</td>
<td>125.998</td>
<td>2.734%</td>
</tr>
<tr>
<td>+ AVX2 compiler vectorization</td>
<td>0.878</td>
<td>1.2</td>
<td>1.242</td>
<td>156.511</td>
<td>3.397%</td>
</tr>
<tr>
<td>+ AVX512 compiler vectorization</td>
<td>0.824</td>
<td>1.1</td>
<td>1.324</td>
<td>166.817</td>
<td>3.620%</td>
</tr>
</tbody>
</table>

We get a small boost from AVX512, but there’s a still a lot of performance available.
Outline

• Compiler vectorization
• Vectorization by hand
• Vectorization by hand, another approach
• Performance-engineering the hand-vectorized version
• Intel oneMKL
How many loads and stores?

Suppose the base-case size $S$ is 16 and uses 4-element vectors.

The inner loop performs 4 loads from C, 4 loads from B, and 4 stores into C.

Matrix-multiply base case

```
for (size_t i = 0; i < S; ++i)
    for (size_t k = 0; k < S; ++k)
        for (size_t j = 0; j < S; ++j)
```

Computing a row of 16 elements in C requires:

\[ 16 \times (1 + 4 + 4 + 4) = 208 \] loads and stores.
Alternative: Compute outer products

Alternatively, the base case can compute an outer product between a subcolumn of $A$ and a subrow of $B$ to update a submatrix in $C$. 
Vectorizing outer products

For each $k$:
1. $b_v = \text{Vector-load}(B[k,j])$
2. For $x$ in #C-vectors:
   a. $a_v = \text{Broadcast}(A[i+x,k])$
   b. $c_v[x] += a_v * b_v$
Analysis of outer-product base case

Suppose instead that the base case computes 16 elements in a 4×4 block in C using 4-element vectors.

If \( S = 16 \), then computing a 4×4 block of elements requires:
\[
4 + 4 + 16 \times (1 + 4)
= 88 \text{ loads and stores.}
\]

Computing a 4×4 block requires 4 loads from C, 4 stores into C, and, for each \( k \), 4 loads from A and 1 load from B.

Less than half the loads and stores!
Advantages over compiler vectorization

This base case performs **fewer loads and stores** than the compiler-vectorized base case.

- Vector registers storing the C submatrix act like an **additional, faster cache**.
- Processing a C submatrix results in **better data locality**.

This base case performs fewer loads and stores than the compiler-vectorized base case.
Implementation using the GCC vector extension

// Vector type
typedef double vdouble __attribute__((vector_size(sizeof(double) * 8)));

// Zero-initialize the C-submatrix vectors.
vdouble cv[8];
for (int ivec = 0; ivec < 8; ++ivec)
    cv[ivec] = (vdouble){0.0};

// Loop over k.
for (int k = 0; k < BC; ++k) {
    // Load a vector from B.
    vdouble bv = *(const vdouble *)(&B[B_index(k, j, BC)]);
    for (int ivec = 0; ivec < 8; ++ivec)
        // Load a value from A, broadcast that value, and perform FMA.
        cv[ivec] += bv * A[A_index(i + ivec, k, BC)];
}

// Add the C-submatrix vectors to the C.
Budgeting the AVX512 vector registers

Each \texttt{zmm} register stores 8 doubles.

To compute an $8 \times 8$ C submatrix requires 10 registers:

- 8 registers to store the C submatrix;
- 1 register for a value from A; and
- 1 register for a vector from B.

There are 32 registers available, so compute a larger C submatrix!

- An $8 \times 24$ C submatrix requires 24 registers for C, 3 registers for B, and 1 register for A.
Instruction comparison in practice

We can use **performance counters** on the machine to compare the operations of these different implementations in practice.

<table>
<thead>
<tr>
<th>Implementation</th>
<th>Instructions</th>
<th>L1 loads</th>
</tr>
</thead>
<tbody>
<tr>
<td>AVX512 compiler vectorization</td>
<td>1.40E+10</td>
<td>1.00E+10</td>
</tr>
<tr>
<td>Broadcast outer product</td>
<td>1.68E+10</td>
<td>5.3E+09</td>
</tr>
</tbody>
</table>

Broadcast outer-product base case performs approximately half the L1 loads in practice!
Outline

- Compiler vectorization
- Vectorization by hand
- Vectorization by hand, another approach
- Performance-engineering the hand-vectorized version
- Intel oneMKL
Can we do even better?

Currently, the code performs many scalar loads from A for each vector-load from B.

Scalar and vector loads have the same cost, but vector loads handle more data.

Can we vectorize the loads from A?
Using a vector from A

Supposing we can efficiently vector-load a subcolumn of A, there are other concerns.

How do we get the other values in the C submatrix?

**Answer:** Vector shuffle instructions

The element-wise vector product produces a **diagonal** of the C submatrix!
Vector shuffle instructions

AVX2 and AVX512 offer **vector-shuffle** instructions for shuffling elements in arbitrary ways.

- Some shuffles operate on 1 vector register, while others operate on 2.
- Some shuffles have specialized instructions, while others use a register to describe the shuffle.
- Some shuffles are more expensive than others.
What shuffles do we need?

\[
\begin{array}{c|cccc}
\alpha & b_{k0} & b_{k1} & b_{k2} & b_{k3} \\
\hline
a_0 & c_{00} & & & \\
a_1 & & c_{11} & & \\
a_2 & & & c_{22} & \\
a_3 & & & & c_{33}
\end{array}
\]

\[
\begin{array}{c|cccc}
\beta & b_{k0} & b_{k1} & b_{k2} & b_{k3} \\
\hline
a_0 & c_{01} & & & \\
a_1 & & c_{10} & & \\
a_2 & & & c_{23} & \\
a_3 & & & & c_{32}
\end{array}
\]

\[
\begin{array}{c|cccc}
\gamma & b_{k0} & b_{k1} & b_{k2} & b_{k3} \\
\hline
a_0 & & c_{02} & & \\
a_1 & & & c_{13} & \\
a_2 & & c_{20} & & \\
a_3 & & c_{31} & &
\end{array}
\]

\[
\begin{array}{c|cccc}
\delta & b_{k0} & b_{k1} & b_{k2} & b_{k3} \\
\hline
a_0 & & & c_{03} & \\
a_1 & & & & c_{12} \\
a_2 & & & c_{21} & \\
a_3 & & c_{30} & &
\end{array}
\]
For each k:

1. \(bv = \text{Vector-load}(B[k,j])\)
2. \(av = \text{Vector-load}(A[i,k])\)
3. \(cv[0] += av \times bv\)
4. \(av' = \text{Shuffle}(av, 1,0,3,2)\)
5. \(cv[1] += av' \times bv\)
6. \(bv' = \text{Shuffle}(bv, 2,3,0,1)\)
7. \(cv[2] += av \times bv'\)
8. \(cv[3] += av' \times bv'\)
Comparison against broadcast base case

- The shuffle base case performs fewer loads than the broadcast base case.
- Shuffles operate entirely on registers.
- More shuffles are needed to write the results to C, but that happens rarely.
Generalizing to 8-element vectors

We can generalize this idea to use 4 permutations of 8-element vectors to compute an $8 \times 8$ C submatrix, such as by using the following 4 permutations:
Implementing the shuffle base case using the GCC vector extension

```c
// Vector type
typedef double vdouble __attribute__((vector_size(sizeof(double) * 8)));

// Zero-initialize the C-submatrix vectors…

// Loop over k.
for (int k = 0; k < BC; ++k) {
    // Load vectors from A and B.
    vdouble bv = *(const vdouble *)(&B[B_index(k, j, BC)]);
    vdouble av = *(const vdouble *)(&A[A_index(i, k, BC)]);
    // av_p = A1 A0 A3 A2 A5 A4 A7 A6
    vF a_p = __builtin_shufflevector(av, av, 1, 0, 3, 2, 5, 4, 7, 6);
    // bv_p0 = B2 B3 B0 B1 B6 B7 B4 B5
    vF bv_p0 = __builtin_shufflevector(bv, bv, 2, 3, 0, 1, 6, 7, 4, 5);
    cv[0] += av * bv;
    cv[1] += av_p * bv;
    // bv_p1 = B4 B5 B6 B7 B0 B1 B2 B3
    vF bv_p1 = __builtin_shufflevector(bv, bv, 4, 5, 6, 7, 0, 1, 2, 3);
    cv[2] += av * bv_p0;
    cv[3] += av_p * bv_p0;
    // bv_p2 = B6 B7 B4 B5 B2 B3 B0 B1
    vF bv_p2 = __builtin_shufflevector(bv_p0, bv_p0, 4, 5, 6, 7, 0, 1, 2, 3);
    cv[4] += av * bv_p1;
    cv[5] += av_p * bv_p1;
}
```

Type definition for a vector of 8 doubles.

Vector-loads from A and B.

Shuffle A.

Shuffle B.

Shuffle B again.

Shuffle B yet again.
Budgeting the AVX512 vector registers for the shuffle base case

Each of the 32 \texttt{zmm} registers stores 8 doubles.

To compute an 8$\times$8 C submatrix requires 14 registers:
- 8 registers to store the C submatrix;
- 2 registers for A and its permutation; and
- 4 registers for B and its permutations.

Can we compute an 8$\times$24 C submatrix?
- An 8$\times$24 C submatrix seems to require 34 registers: 24 for C, 6 for A and its permutations, and 4 for B and its permutations.
- If we order the operations carefully, we can reuse registers for different permutations and require just 2 registers for B.
Comparison in practice

How do the broadcast and shuffle outer-product base cases compare in practice?

<table>
<thead>
<tr>
<th>Outer-product base case</th>
<th>Instructions</th>
<th>L1 loads</th>
<th>Running time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Broadcast</td>
<td>1.68E+10</td>
<td>5.30E+09</td>
<td>0.052</td>
</tr>
<tr>
<td>Shuffle</td>
<td>1.64E+10</td>
<td>2.53E+09</td>
<td>0.063</td>
</tr>
</tbody>
</table>

The shuffle base case performs fewer instructions and half the L1 loads, but runs slower!
Why wasn’t it faster?

**Problem:** We’re running out of **functional units** on the core to perform arithmetic and shuffles.

**Recall complex pipelining:**
A processor core in a modern multicore chip has **many** functional units on different paths through the execution pipeline.
Not enough ports

On Intel CPUs, different ports support different functional units.

- Ports 0/1 and 5 handle FMA operations.
- Ports 2 and 3 load from memory.
- Port 5 handles all shuffle instructions.

Source: https://en.wikichip.org/wiki/intel/microarchitectures/cascade_lake
Hope remains!

"Note that on 3rd Gen…and 4th Gen Intel Xeon Scalable processors…, port 1 also can execute some shuffle instructions…”

The shuffle outer-product base case might be faster on the next generation of CPU hardware.
Outline

• Compiler vectorization

• Vectorization by hand

• Vectorization by hand, another approach

• Performance-engineering the hand-vectorized version

• Intel oneMKL
Order of memory accesses

For each k, the base case accesses a **subcolumn** of elements of A.

For each k, the base case accesses a **subrow** of elements of B.

Ideally, the base case should access all memory **in order**.
Can we get the ideal data layouts for A and B?
**Local buffers**

Idea: At the start of the base case, move the relevant entries in A and B into small, local buffers.

![Diagram showing the movement of entries into local buffers](image)

- **A**:
  - Local buffer: a0 a0 a0
  - Copy and transpose subcolumns of A.

- **B**:
  - Local buffer: b0 b0 b0 b0
  - Copy subrows of B.

**Notes:**
- The diagram illustrates the process of moving relevant entries from matrices A and B into local buffers to optimize subsequent computations.
Indexing buffers for A and B

To index matrix elements in these local buffers, **interleave the bits** of the matrix index.

Index calculation for A buffer

```c
int64_t A_index(int64_t i, int64_t k, int64_t BC) {
    return ((i / 8) * BC * 8) + (k * 8) + (i % 8);
}
```

The compiler can optimize the divisions by constants in these index calculations.

Index calculation for B buffer

```c
int64_t B_index(int64_t j, int64_t k, int64_t BC) {
    return ((j / 24) * BC * 24) + (k * 24) + (j % 24);
}
```

In the loop over k in the base case, these addresses simply increase.
What do these buffers cost?

How much work does this filling a local buffer add to the base case of size $S$?

- In theory, $\Theta(S^2)$, which the $\Theta(S^3)$ work of the base case dominates.
- In practice, after optimizing the $\Theta(S^3)$ base-case work, this cost is noticeable.
void mmdac(double *restrict C, double *restrict A, double *restrict B, size_t size) {
if (size == S) {
mmbase(C, A, B);
} else {
size_t s00 = 0;
size_t s01 = size / 2;
size_t s10 = (size / 2) * n;
size_t s11 = (size / 2) * (n + 1);
cilk_scope {
  cilk_spawn mmdac(C+s00, A+s00, B+s00, size/2);
  cilk_spawn mmdac(C+s01, A+s00, B+s01, size/2);
  cilk_spawn mmdac(C+s10, A+s10, B+s00, size/2);
  mmdac(C+s11, A+s10, B+s01, size/2);
}
cilk_scope {
  cilk_spawn mmdac(C+s00, A+s01, B+s10, size/2);
  cilk_spawn mmdac(C+s01, A+s01, B+s11, size/2);
}
}

Avoiding unnecessary work

How can we reduce the extra work of filling local buffers?

Matrix-multiply routine

If we use the same input submatrix between calls to mmbase(), we don’t need to refill the corresponding buffer.

Reorder the calls to the base case to avoid refilling buffers!
A new subdivision strategy

1. Divide the k dimension into large pieces.

2. Divide the i dimension into medium pieces.

3. Divide the j dimension into small pieces.
Why does this subdivision strategy work?

1. Divide the k dimension into large pieces.

2. Divide the i dimension into medium pieces.

3. Divide the j dimension into small pieces.

It’s cheaper to copy from B than to copy and transpose from A.

Larger k for the base case means fewer loads and stores from C.

Base-cases fill local buffers with 1 copy and transpose from A and many copies from B.

1. Divide the k dimension into large pieces.

2. Divide the i dimension into medium pieces.

3. Divide the j dimension into small pieces.
Outline

• Compiler vectorization

• Vectorization by hand

• Vectorization by hand, another approach

• Performance-engineering the hand-vectorized version

• Intel oneMKL
Performance results versus oneMKL

On 48 cores, this hand-vectorized implementation outperforms the latest version of Intel oneMKL with OpenMP threads.

<table>
<thead>
<tr>
<th>Implementation</th>
<th>Running time (s)</th>
<th>GFLOPS</th>
<th>Fraction of peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cilk, hand-vectorization</td>
<td>0.052</td>
<td>2656.893</td>
<td>57.658%</td>
</tr>
<tr>
<td>oneMKL with OpenMP</td>
<td>0.061</td>
<td>2268.232</td>
<td>49.224%</td>
</tr>
</tbody>
</table>

But on 24 cores on 1 chip, the performance difference is reversed!

<table>
<thead>
<tr>
<th>Implementation</th>
<th>Running time (s)</th>
<th>GFLOPS</th>
<th>Fraction of peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cilk, hand-vectorization</td>
<td>0.092</td>
<td>1494.807</td>
<td>32.439%</td>
</tr>
<tr>
<td>oneMKL with OpenMP</td>
<td>0.082</td>
<td>1670.604</td>
<td>36.254%</td>
</tr>
</tbody>
</table>

What’s causing this performance difference?
Intel oneMKL

Intel oneMKL uses the same broadcast outer-product base case and local buffers, but it subdivides the problem differently.

Intel oneMKL matrix subdivision on 1 thread

Base case for A: 4096x384

Total base-case size: ~12MB

Base case for B: 384x24

In comparison, L2 is 1MB.
Software prefetching

Intel oneMKL’s base case uses **software prefetching** to speed up memory accesses.

- The base case mixes a few software-prefetch operations to load locations in A and B local buffers to be accessed in the future.
- During the last few iterations before storing into C, the base case software-prefetches locations in C.

Snippet of broadcast-based matrix-multiply base case (simplified)

```c
// Loop over k.
for (int k = 0; k < BC; ++k) {
    // Prefetch from A.
    __builtin_prefetch(&A[A_index(i, k + 4, BC)]);
}

// Load a vector from B.
vdoubles bv = *(const vdouble *)(&B[B_index(k, j, BC)]);
for (int ivec = 0; ivec < 8; ++ivec)
    // Load a value from A, broadcast that value, // and perform FMA.
    cv[ivec] += bv * A[A_index(i + ivec, k, BC)];
```

Load a value from A that will be used in a future loop iteration.
My experience with software prefetching

Software prefetch instructions are tricky to use.

- Software prefetches increase instruction counts, memory traffic, and data in residing in cache.
- Software prefetches can only improve performance if their use hides memory latency more effectively than the hardware prefetchers.

Careful uses of software prefetch instructions can improve performance by a few percent, but poor uses can hurt performance.
Takeaways

- One can use OpenCilk to implement parallel programs with state-of-the-art performance that competes with professionally engineered high-performance software.

- Many theoretically good algorithms can have the performance impact that theory predicts, but many systems issues need to be handled first.

- Even when most of a program’s running time is spent in a small amount of the code, the keys to optimizing that hot spot might lie elsewhere in the code.

- Check your performance-testing methodology and your raw performance data!
Questions?