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 $\mathrm{n}=4096$.

## Final verdict from 6.106 lecture 1

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

## Problem: Performance-measurement methodology

| Version | Implementation | Running time (s) | Relative speedup | Absolute speedup | GFLOPS | Fraction of peak |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | Python | 21,041.67 | 1 |  | 0.006 | 0\% |
| 2 | Java | 2,387.32 | 8.8 | Each running time is the minimum of 5 runs of a binary. |  |  |
| 3 | C | 1,155.77 | 2.1 |  |  |  |
| 4 | + interchange loops | 177.68 | 6.5 |  |  |  |
| 5 | + optimization flags | 54.63 | 3.3 |  |  | T\% |
| 6 | Parallel loops | 3.04 | 18 | Each binary runs matrixmultiplication once. |  |  |
| 7 | Parallel divide-and-conquer | 1.30 | 1.4 |  |  |  |
| 8 | + compiler vectorization | 0.70 | 1.9 | 30,272 | 196.341 | 23.486\% |
| 9 | + AVX intrinsics | 0.39 | 1.8 | 53,292 | 352.408 | 41.677\% |
| 10 | Intel MKL | 0.41 | 1 | 51,497 | 335.217 | 40.098\% |

## An overlooked performance gap

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

The first matrix-multiply call is slower than subsequent calls.

Version 9 (AVX intrinsics) takes $\sim 0.39$ seconds.

Intel MKL takes
$\sim 0.30$ seconds!

| Running time per trial, c4.8xlarge, 48 cores <br> - Version 9 (AVX intrinsics) ■ MKL |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 0.45 |  |  |  |  |  |
|  |  |  |  |  |  |
| $\begin{aligned} & 50.25 \\ & 000 \end{aligned}$ |  |  |  |  |  |
| $0.15$ |  |  |  |  |  |
| 50.1 |  |  |  |  |  |
| 0.05 |  |  |  |  |  |
|  |  |  |  |  |  |
| 0 | 10 | 20 | 30 | 40 | 50 |
| Trial |  |  |  |  |  |

The case study's conclusions are fine, but MKL is faster than we thought!

New hardware: AWS c5.metal machine specs

| Feature | Specification |
| :---: | :---: |
| Microarchitecture | Cascade Lake (Intel Xeon Platinum 8275CL) |
| Clock frequency | 3.0 GHz |
| Processor chips | 2 |
| Processor cores | 24 per processor chip |
| Floating-point unit | 32 double-precision operations, including fused-multiply-add, per core per cycle |
| Cache-line size | 64 B Theor |
| L1 data cache | 32 KB private, 8-way set associa pe |
| L2 cache | 1 MB private, 16-way set associa 3.0 GH |
| L3 cache | 35.75 MB shared, 11-way set asso $=4608$ |
| DRAM | 189 GB |

## Alternative oneMKL threading options

Intel oneMKL offers different threading options that give different performance on new hardware.

Version 9 (AVX intrinsics)
takes $\sim 0.12$ seconds.
oneMKL with TBB takes $\sim 0.11$ seconds.

oneMKL with OpenMP takes $\sim 0.06$ seconds!

New performance results on a c5.metal instance

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

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


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## Recap: Parallel divide-and-conquer matrix multiplication (Version 7)



## AVX2 and AVX512 vectors

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


ZMM

## YMM

- 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 $A V X 512$ 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

- Broadcast: Fill all entries in a vector register with the same value.

- Shuffle: Permute the entries in a

```
c0 c1 c2 c3
c1 c3 c2 c0
``` vector register. (More on this operation later.)

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

\section*{Compiler vectorization}

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)

```


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

\section*{Compiler vectorization}
\$ clang -o mm mm.c -fopencilk -O3 -march=native

Snippet of compiler-vectorized base case


Vector-store into C

\section*{Compiler vectorization}
\$ clang -o mm mm.c -fopencilk -O3 -march=native

Snippet of compiler-vectorized base case
```

%78 = load double, ptr %59, align 8 LLLVM IR
%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_alin}
%96 = load <4x double>, ptr %16, align 8
%100 = tail call <4 x double> @|vm.fmuladd.v4f64(<4x double> %80,

```

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 17

\section*{Compiler vectorization with AVX512}

We can make the compiler to use AVX512 with different compiler flags. How much performance do we get?
\begin{tabular}{|c|rrrrr|}
\hline Implementation & \begin{tabular}{c} 
Running \\
time (s)
\end{tabular} & \begin{tabular}{c} 
Relative \\
speedup
\end{tabular} & \begin{tabular}{l} 
Absolute \\
speedup
\end{tabular} & GFLOPS & \begin{tabular}{c} 
Fraction of \\
peak
\end{tabular} \\
\hline Parallel divide-and-conquer & 1.091 & 1 & 1 & 125.998 & \(2.734 \%\) \\
\hline + AVX2 compiler vectorization & 0.878 & 1.2 & 1.242 & 156.511 & \(3.397 \%\) \\
\hline + AVX512 compiler vectorization & 0.824 & 1.1 & 1.324 & 166.817 & \(3.620 \%\) \\
\hline
\end{tabular}

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

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- Vectorization by hand, another approach
- Performance-engineering the hand-vectorized version
- Intel oneMKL

\section*{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 * \((1+4+4+4)\)
\(=208\) loads and stores.

\section*{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


\section*{Analysis of outer-product base case}

Suppose instead that the base case computes 16 elements in a \(4 \times 4\) block in C using 4-element vectors.


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

If \(S=16\), then computing a elements \(4 \times 4\) block of elements requires:
\(4+4+16\) * \((1+4)\)
\(=88\) loads and stores.

Less than half the
loads and stores!

\section*{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.

\section*{Implementation using the GCC vector extension}

```

// 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.
Vector-load from B.
Broadcast from A and
perform FMA.
cv[ivec] += bv * A[A_index(i + ivec, k, BC)];
}
Store into C.

## Budgeting the AVX512 vector registers

Each 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 $\mathrm{C}, 3$ 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.

| Implementation | Instructions |
| :---: | ---: |
| L1 loads |  |
| AVX512 compiler vectorization | $1.40 \mathrm{E}+10$ |
| Broadcast outer product | $1.00 \mathrm{E}+10$ |
|  |  |
| Broadcast outer-product base case <br> performs approximately half the L1 <br> loads in practice! |  |

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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?

| $\alpha$ | $b_{k 0}$ | $b_{k 1}$ | $b_{k 2}$ | $b_{k 3}$ |
| :---: | :---: | :---: | :---: | :---: |
| $a_{0 k}$ | $c_{00}$ |  |  |  |
| $a_{1 k}$ |  | $c_{11}$ |  |  |
|  |  |  |  |  |
| $a_{2 k}$ |  |  | $c_{22}$ |  |
|  | $a_{3 k}$ |  |  |  |


| $\beta$ | $\mathrm{b}_{k 0}$ | $\mathrm{~b}_{k 1}$ | $\mathrm{~b}_{k 2}$ | $\mathrm{~b}_{k 3}$ |
| :--- | :--- | :--- | :--- | :--- |
| $\mathrm{a}_{0 k}$ |  | $\mathrm{c}_{01}$ |  |  |
| $\mathrm{a}_{1 k}$ | $\mathrm{c}_{10}$ |  |  |  |
| $\mathrm{a}_{2 k}$ |  |  |  |  |
| $\mathrm{a}_{3 k}$ |  |  | $\mathrm{c}_{23}$ |  |


| $\gamma$ | $b_{k 0}$ | $b_{k 1}$ | $b_{k 2}$ | $b_{k 3}$ |
| :--- | :--- | :--- | :--- | :--- |
| $a_{0 k}$ |  |  | $c_{02}$ |  |
| $a_{1 k}$ |  |  |  | $c_{13}$ |
| $a_{2 k}$ | $c_{20}$ |  |  |  |
| $a_{3 k}$ |  | $C_{31}$ |  |  |


| $\delta$ | $\mathrm{b}_{k 0}$ | $\mathrm{~b}_{k 1}$ | $\mathrm{~b}_{\mathrm{k} 2}$ | $\mathrm{~b}_{k 3}$ |
| :---: | :---: | :---: | :---: | :---: |
| $\mathrm{a}_{0 k}$ |  |  |  | $c_{03}$ |
| $\mathrm{a}_{1 k}$ |  |  | $\mathrm{c}_{12}$ |  |
| $\mathrm{a}_{2 k}$ |  | $\mathrm{c}_{21}$ |  |  |
| $\mathrm{a}_{3 \mathrm{k}}$ | $\mathrm{c}_{30}$ |  |  |  |



Outer products with shuffles


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:


## Implementating the shuffle base case using the GCC vector extension



## Budgeting the AVX512 vector registers for the shuffle base case

Each of the 32 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 $\mathrm{C}, 6$ 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?

| Outer-product base case | Instructions | L1 loads | Running t |
| :--- | :--- | :--- | :--- |
| Broadcast | $1.68 \mathrm{E}+10$ | $5.30 \mathrm{E}+09$ | 0.052 |
| Shuffle | $1.64 \mathrm{E}+10$ | $2.53 \mathrm{E}+09$ | 0.063 |

## 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

Cascade Lake execution engine schematic


On Intel CPUs, different ports support different functional units.

- Ports $0 / 1$ and 5 handle FMAs.
- Ports 2 and 3 load from memory.
- Port 5 handles all shuffle instructions.
Inte ${ }^{\circledR}$ Advanced Vector Extensions 512 (Inte ${ }^{\circledR}$ AVX-512)- Permuting Data Within and Between AVXRegisters


## intel.

## Hope remains!

| Technology Guide |  |
| :---: | :---: |
| Inte ${ }^{\circledR}$ Advanced Vector Extensions 512 (Intel ${ }^{\circledR}$ AVX-512)-Permuting Data Within and Between AVXRegisters |  |
| Author |  |

"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.

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## 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.

## Ideal data layouts for $A$ and $B$


a0 a1 a2 as a0 a1 a2 as à a0 a1 a2 as
Can we get the ideal data layouts for A and B ?
b0 b0 b0 b0 b1 b1 b1 b1 b2 b2 b2 b2

## Local buffers

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


## 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
int64_t A_index(int64_t i, int64_t k, int64_t BC) \{ return ((i / 8) * BC * 8) + (k * 8) + (i \% 8);

Index calculation for B buffer
int64_t B_index(int64_t j, int64_t k, int64_t BC) \{ return $((j / 24)$ * $B C$ * 24$)+(k$ * 24$)+(j$ \% 24);

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

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, $\Theta\left(S^{2}\right)$, which the $\Theta\left(S^{3}\right)$ work of the base case dominates.
- In practice, after optimizing the $\Theta\left(S^{3}\right)$ base-case work, this cost is noticeable.




## Avoiding unnecessary work

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

| Matrix-multiply routine |
| :--- |
| void mmdac(double *restrict C, double *restrict A, <br> $\quad$ double *restrict B, size_t size) \{ <br> if (size == S) \{ <br> mmbase(C, A, B); <br> \} else \{ <br> size_t s00 = 0; <br> size_t s01 = size/2; <br> size_t s10 = (size/2)*n; <br> size_t s11 = (size/2)*(n+1); <br> cilk_scope \{ <br> cilk_spawn mmdac(C+s00, A+s00, B+s00, size/2); <br> cilk_spawn mmdac(C+s01, A+s00, B+s01, size/2); <br> cilk_spawn mmdac(C+s10, A+s10, B+s00, size/2); <br> mmdac(C+s11, A+s10, B+s01, size/2); <br> \} cilk_scope \{ <br> cilk_spawn mmdac(C+s00, A+s01, B+s10, size/2); <br> cilk_spawn mmdac(C+s01, A+s01, B+s11, size/2); |

A new subdivision strategy

1. Divide the k dimension into large pieces.

2. Divide the i dimension into medium pieces.

| $\substack{i \\ \hline \\ c 00 \\ \hline c 10 \\ \hline c 20 \\ \hline c 30 \\ \hline}$ |
| :---: |


3. Divide the j dimension into small pieces.


## Why does this subdivision strategy work?

1. Divide the k dimension into large pieces.


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

It's cheaper to copy from B than
to copy and transpose from A.
2. Divide the i dimension into medium pieces.

| $\stackrel{j}{\square}$ |
| :---: |
| $C 00$ |
| $C 10$ |
| $C 20$ |
| $C 30$ |



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

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## Performance results versus oneMKL

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

| Implementation | Running <br> time (s) | GFLOPS | Fraction of <br> peak |
| :---: | :---: | :---: | :---: |
| Cilk, hand-vectorization | 0.052 | 2656.893 | $57.658 \%$ |
| oneMKL with OpenMP | 0.061 | 2268.232 | $49.224 \%$ |

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

What's causing this performance difference?

| Implementation | Running <br> time (s) | GFLOPS | Fraction of <br> peak |
| :---: | ---: | :---: | :---: |
| Cilk, hand-vectorization | 0.092 | 1494.807 | $32.439 \%$ |
| oneMKL with OpenMP | 0.082 | 1670.604 | $36.254 \%$ |

## 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


## 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)

```
// 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.
    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 * Ar^ indnv/i , ivmnlvonlr.
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 highperformance 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?



