# Vectorization 

Aaron Birkland<br>Consultant<br>Cornell CAC

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## What is Vectorization?

- Hardware Perspective: Specialized instructions, registers, or functional units to allow in-core parallelism for operations on arrays (vectors) of data.
- Compiler Perspective: Determine how and when it is possible to express computations in terms of vector instructions
- User Perspective: Determine how to write code in a manner that allows the compiler to deduce that vectorization is possible.


## Vectorization: Hardware

- Goal: parallelize computations over vector arrays
- SIMD: Single Instruction Multiple Data
- Many instances of a single operation executing simultaneously
- Late ‘90s - present, commodity CPUs (x86, x64, PowerPC, etc)
- Small vectors, few cycles per instruction
- Newer CPUs (post Sandy Bridge) can pipeline some SIMD instructions as well - best of both worlds.

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## Vectorization via SIMD: Motivation

- CPU speeds reach a plateau
- Power limitations!
- Many "slow" transistors more efficient than fewer "fast" transistors
- Process improvements make physical space cheap
- Moore's law, $2 x$ every 18-24 months
- Easy to add more "stuff"
- One solution: More cores
- First dual core Intel CPUs appear in 2005
- Increasing in number rapidly (e.g. 8 in Stampede, 61 on MIC)
- Another Solution: More FPU units per core - vector operations
- First appeared on a Pentium with MMX in 1996
- Increasing in vector width rapidly (e.g. 512-bit [8 doubles]) on MIC


## Vectorization via SIMD: History

| Year | Registers | Instruction Set |  |
| :--- | :--- | :--- | :--- |
| ~1997 | 80-bit | MMX | Integer SIMD (in x87 registers) |
| $\sim$ | 1999 | 128-bit | SSE1 | SP FP SIMD (xMM0-8)

## Vector Registers

Floating Point (FP)

## SSE/AVX 128

64-bit
32-bit
AVX-256


MIC-512


4/8

zmm
ymm
xmm

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## Speed

- True SIMD parallelism - Can take 1 cycle per floating point computation on all values in a vector register.
- Exception: Slow operations like division, square roots
- Speedup (compared to no vector) proportional to vector width
- 128-bit SSE $-2 x$ double, $4 x$ single
- 256-bit AVX - $4 x$ double, $8 x$ single
- 512-bit MIC - 8x double, 16x single
- Hypothetical AVX example: 8 cores/CPU * 4 doubles/vector * 2.0 $\mathrm{GHz}=64$ Gflops/CPU DP
- Gets even better with FMA (fused multiply add), $a=a+\left(b^{*} c\right)$. Multiply and add in the same clock cycle (Haswell+).


## Speed

- Clearly memory bandwidth is potential issue, we'll explore this later
- Poor cache utilization, alignment, memory latency all detract from ideal
- SIMD is parallel, so Amdahl's law is in effect!
- Serial/scalar portions of code or CPU are limiting factors
- Theoretical speedup is only a ceiling



## User Perspective

Let's take a step back - how can we leverage this power

- Program in assembly
- Ultimate performance potential, but only for the brave
- Program in intrinsics
- Step up from assembly, useful but risky
- Let the compiler figure it out
- Relatively "easy" for user, "challenging" for compiler
- Less expressive languages like C make compiler's job more difficult
- Compiler may need some hand holding.
- Link to an optimized library that does the actual work
- e.g. Intel MKL, written by people who know all the tricks.
- Get benefits "for free" when running on supported platform


## Vector-aware coding

- Know what makes vectorizable at all
- "for" loops (in C) or "do" loops (in fortran) that meet certain constraints
- Know where vectorization will help
- Evaluate compiler output
- Is it really vectorizing where you think it should?
- Evaluate execution performance
- Compare to theoretical speedup
- Know data access patterns to maximize efficiency
- Implement fixes: directives, compilation flags, and code changes
- Remove constructs that make vectorization impossible/impractical
- Encourage/force vectorization when compiler doesn't, but should
- Better memory access patterns


## Writing Vector Loops

- Basic requirements of vectorizable loops:
- Countable at runtime
- Number of loop iterations is known before loop executes
- No conditional termination (break statements)
- Have single control flow
- No Switch statements
- 'if' statements are allowable when they can be implemented as masked assignments
- Must be the innermost loop if nested
- Compiler may reverse loop order as an optimization!
- No function calls
- Basic math is allowed: pow(), sqrt(), sin(), etc
- Some Inline functions allowed


## Conceptualizing Compiler Vectorization

- Think of vectorization in terms of loop unrolling
- Unroll N interactions of loop, where N elements of data array fit into vector register

$$
\text { for } \begin{aligned}
&(i=0 ; i<N ; i++) \\
& a[i]=b[i]+c[i] ;
\end{aligned}
$$

$$
\}
$$



$$
\text { for } \begin{aligned}
(i= & 0 ; i<N ; i+=4) \quad\{ \\
& a[i+0]=b[i+0]+c[i+0] ; \\
& a[i+1]=b[i+1]+c[i+1] ; \\
& a[i+2]=b[i+2]+c[i+2] ; \\
& a[i+3]=b[i+3]+c[i+3] ;
\end{aligned}
$$

## Compiling Vector loops

- Intel Compiler:
- Vectorization starts at optimization level -02
- Will default to SSE instructions and 128-bit vector width
- use -xAVX to use AVX and 256-bit vector width. Only runs on newer CPUs
- Can embed SSE and AVX instructions in the same binary with -axAVX
- Will run AVX on CPUs with AVX support, SSE otherwise
- -vec-report=<n> for a vectorization report
- GCC
- Vectorization is disabled by default, regardless of optimization level
- Need-ftree-vectorize flag, combined with optimization >-02
- SSE by default, -mavx -march=corei7-avx for AVX
- -ftree-vectorizer-verbose for a vectorization report


## Lab: Simple Vectorization

In this lab you will

- Use the Intel compiler to create vectorized with non-vectorized code
- Compare the performance of vectorized vs non-vectorized code
- Compare performance with different vector widths.
- Take an initial look at compiler vectorization reports
- Bonus: What is the vector efficiency (\% vector instructions) of the test code? Using Amdal's law $\mathrm{P}=\frac{\left(\frac{1}{S}-1\right)}{\left(\frac{1}{n}-1\right)}$ where P is \% parallel (e.g. \% vectorized), S is speedup, n is vector length in number of floats/doubles


## Lab: Simple Vectorization

Host
CPU

| Compile Options | Time | Speedup |
| :--- | :--- | :--- |
| -no-vec -O3 | .67 s | 1 x |
| -O3 | .37 s | 1.8 x |
| -O3-xAVX (or -xhost) | .25 s | 2.7 x |


| MIC | -no-vec -mmic -O3 | 13.22 s | 1 x |
| :--- | :--- | :--- | :--- |
|  | -mmic -O3 | 2.78 s | 4.8 x |

Notes:

- One MIC thread can only use $50 \%$ of a core
- Amdahl's law for $90 \%$ vectorized predicts ( $1 \mathrm{x}, 1.8 \mathrm{x}, 3 \mathrm{x}, 4.7 \mathrm{x}$ )

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## Challenge: Loop Dependencies

- Vectorization changes the order of computation compared to sequential case
- Compiler must be able to prove that vectorization will produce correct result.
- Need to consider independence of unrolled loop operations depends on vector width
- Compiler performs dependency analysis

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## Loop Dependencies: Read After Write

Consider the loop:
$a=\{0,1,2,3,4\}$
b $=\{5,6,7,8,9\}$

$$
\begin{aligned}
& \text { for }(i=1 ; i<N ; i++) \\
& \quad a[i]=a[i-1]+b[i] ;
\end{aligned}
$$

Applying each operation sequentially:

$$
\begin{aligned}
& a[1]=a[0]+b[1] \rightarrow a[1]=0+6 \rightarrow a[1]=6 \\
& a[2]=a[1]+b[2] \rightarrow a[2]=6+7 \rightarrow a[2]=13 \\
& a[3]=a[2]+b[3] \rightarrow a[3]=13+8 \rightarrow a[3]=21 \\
& a[4]=a[3]+b[4] \rightarrow a[4]=21+9 \rightarrow a[4]=30
\end{aligned}
$$

$$
a=\{0,6,13,21,30\}
$$

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## Loop Dependencies: Read After Write

Consider the loop:
$a=\{0,1,2,3,4\}$
$b=\{5,6,7,8,9\}$

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Applying each operation sequentially:
$a[1]=a[0]+b[1] \rightarrow a[1]=0+6 \rightarrow a[1]=6$
$a[2]=a[1]+b[2] \rightarrow a[2]=6+7 \rightarrow a[2]=13$
$a[3]=a[2]+b[3] \rightarrow a[3]=13+8 \rightarrow a[3]=21$
$a[4]=a[3]+b[4] \rightarrow a[4]=21+9 \rightarrow a[4]=30$
$a=\{0,6,13,21,30\}$

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## Loop Dependencies: Read After Write

Now let's try vector operations:
$a=\{0,1,2,3,4\}$
$b=\{5,6,7,8,9\}$

$$
\begin{aligned}
& \text { for }(i=1 ; i<N ; i++) \\
& \quad a[i]=a[i-1]+b[i] ;
\end{aligned}
$$

Applying vector operations, $\mathrm{i}=\{1,2,3,4\}$ :
$a[i-1]=\{0,1,2,3\} \quad$ (load)
$b[i]=\{6,7,8,9\} \quad$ (load)
$\{0,1,2,3\}+\{6,7,8,9\}=\{6,8,10,12\}$ (operate)
$a[i]=\{6,8,10,12\} \quad$ (store)
$a=\{0,6,8,10,12\} \neq\{0,6,13,21,30\}$ NOT VECTORIZABLE

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## Loop Dependencies: Write after Read

Consider the loop:
$a=\{0,1,2,3,4\}$
$b=\{5,6,7,8,9\}$

$$
\begin{aligned}
& \text { for }(i=0 ; i<N ; i++) \\
& \quad a[i]=a[i+1]+b[i] ;
\end{aligned}
$$

Applying each operation sequentially:
$\mathrm{a}[0]=\mathrm{a}[1]+\mathrm{b}[0] \rightarrow \mathrm{a}[0]=1+5 \rightarrow \mathrm{a}[0]=6$
$a[1]=a[2]+b[1] \rightarrow a[1]=2+6 \rightarrow a[1]=8$
$a[2]=a[3]+b[2] \rightarrow a[2]=3+7 \rightarrow a[2]=10$
$a[3]=a[4]+b[3] \rightarrow a[3]=4+8 \rightarrow a[3]=12$
$a=\{6,8,10,12,4\}$

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## Loop Dependencies: Write after Read

Now let's try vector operations:
$a=\{0,1,2,3,4\}$
$b=\{5,6,7,8,9\}$

$$
\begin{aligned}
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& \quad a[i]=a[i+1]+b[i] ;
\end{aligned}
$$

Applying vector operations, $\mathrm{i}=\{1,2,3,4\}$ :

$$
\begin{aligned}
& \mathrm{a}[\mathrm{i}+1]=\{1,2,3,4\} \quad \text { (load) } \\
& \mathrm{b}[\mathrm{i}]=\{5,6,7,8\} \quad \text { (load) } \\
& \{1,2,3,4\}+\{5,6,7,8\}=\{6,8,10,12\} \quad \text { (operate) } \\
& \mathrm{a}[\mathrm{i}]=\{6,8,10,12\} \quad \text { (store) }
\end{aligned}
$$

$a=\{0,6,8,10,12\}=\{0,6,8,10,12\} \quad$ VECTORIZABLE

## Loop Dependencies

- Read After Write
- Also called "flow" dependency
- Variable written first, then read
- Not vectorizable
- Write after Read
- Also called "anti" dependency
- Variable read first, then written
- vectorizable

$$
\begin{aligned}
& \text { for }(i=1 ; i<N ; i++) \\
& \quad a[i]=a[i-1]+b[i] ;
\end{aligned}
$$

## Loop Dependencies

- Read after Read
- Not really a dependency
- Vectorizable

$$
\begin{aligned}
& \text { for }(i=0 ; i<N ; i++) \\
& \quad a[i]=b[i \circ 2]+c[i] ;
\end{aligned}
$$

- Write after Write
- a.k.a "output" dependency
- Variable written, then re-written
- Not vectorizable

$$
\begin{aligned}
& \text { for }(i=0 ; i<N ; i++) \\
& \quad a[i \circ 2]=b[i]+c[i] ;
\end{aligned}
$$

## Loop Dependencies: Aliasing

- In C, pointers can hide data dependencies!
- Memory regions they point to may overlap
- Is this safe?:

```
void compute(double *a,
    double *b, double *c) {
    for (i=1; i<N; i++) {
    a[i]=b[i]+c[i];
    }
```

- .. Not if we give it the arguments compute (a, $a+1, c)$;
- Effectively, $b$ is really $a[i-1] \rightarrow$ Read after Write dependency
- Compilers can usually cope, add bounds checking tests (overhead)

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## Vectorization Reports

- Shows which loops are or are not vectorized, and why
- Intel: -vec-report=<n>
- 0: None
- 1: Lists vectorized loops
- 2: Lists loops not vectorized, with explanation
- 3: Outputs additional dependency information
- 4: Lists loops not vectorized, without explanation
- 5: Lists loops not vectorized, with dependency information
- Reports are essential for determining where the compiler finds a dependency
- Compiler is conservative, you need to go back and verify that there really is a dependency.

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## Loop Dependencies: Vectorization Hints

- Compiler must prove there is no data dependency that will affect correctness of result
- Sometimes, this is impossible
- e.g. unknown index offset, complicated use of pointers
- Intel compiler solution: IVDEP (Ignore Vector DEPendencies) hint.
- Tells compiler "Assume there are no dependencies"

```
subroutine
vecl(sl,M,N,x)
```

!DEC\$ IVDEP
do $i=1, N$
$x(i)=x(i+M)+s 1$
end do

```
void vecl(double s1,int M,
    int N, double *x) {
```

\#pragma IVDEP
for (i=0; i<N;i++) $x[i]=x[i+M]+s 1$;

## Compiler hints affecting vectorization

- For Intel compiler only
- Affect whether loop is vectorized or not
- \#pragma ivdep
- Assume no dependencies.
- Compiler may vectorize loops that it would otherwise think are not vectorizable
- \#pragma vector always
- Always vectorize if technically possible to do so.
- Overrides compiler's decision to not vectorize based upon cost
- \#pragma novector
- Do not vectorize


## Loop Dependencies: Language Constructs

- C99 introduced 'restrict' keyword to language
- Instructs compiler to assume addresses will not overlap, ever

```
void compute(double * restrict a,
        double * restrict b, double * restrict c) {
    for (i=1; i<N; i++) {
        a[i]=b[i]+c[i];
    }
}
```

- May need compiler flags to use, e.g. -restrict, -std=c99


## Cache and Alignment

$$
\begin{gathered}
{\left[\begin{array}{c}
z_{1} \\
z_{2} \\
z_{3} \\
\vdots \\
z_{n}
\end{array}\right]} \\
\operatorname{ymm} 2
\end{gathered} \underset{a^{*}}{\left[\begin{array}{c}
x_{1} \\
x_{2} \\
x_{3} \\
\vdots \\
x_{n}
\end{array}\right]}+\left[\begin{array}{c}
y_{1} \\
y_{2} \\
y_{3} \\
\vdots \\
y_{n}
\end{array}\right]
$$

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$$
\begin{gathered}
y 1, y 2, y 3, \ldots y n x 1, x 2, x 3, \ldots x n \\
z 1, z 2, z 3, \ldots z n
\end{gathered}
$$

- Optimal vectorization requires concerns beyond SIMD unit!
- Registers: Alignment of data on 128, 256 bit boundaries
- Cache: Cache is fast, memory is slow
- Memory: Sequential access much faster than random/strided


## Strided access

- Fastest usage pattern is "stride 1 ": perfectly sequential
- Best performance when CPU can load L1 cache from memory in bulk, sequential manner
- Stride 1 constructs:
- Iterating Structs of arrays vs arrays of structs
- Multi dimensional array:
- Fortran: stride 1 on "inner" dimension
- C/C++: Stride 1 on "outer" dimension

$$
\begin{aligned}
& \text { do } j=1, n ; \text { do } i=1, n \\
& a(i, j)=b(i, j) * s \\
& \text { enddo; endo }
\end{aligned}
$$

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## Strided access

- Striding through memory reduces effective memory bandwidth!
- For DP, roughly 1-stride/8
- Worse than non-aligned access. Lots of memory

Cost of Memory-Strided Summation
 operations to populate a cache line, vector register

$$
\begin{aligned}
& \text { do } i=1,4000000 * i s t r i d e, ~ i s t r i d e \\
& \text { a(i) }=b(i)+c(i) * \text { sfactor } \\
& \text { enddo }
\end{aligned}
$$

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## Diagnosing Cache and Memory deficiencies

- Obviously bad stride patterns may prevent vectorization at all:
- In vector report: "vectorization possible but seems inefficient"
- Otherwise, may be difficult to detect
- No obvious assembly instructions, other than a proliferation of loads and stores
- Vectorization performance farther away from ideal than expected
- Profiling tools can help
- PerfExpert (available at TACC)
- Visualize CPU cycle waste spent in data access (L1 cache miss, TLB misses, etc)

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## Conclusion

- Vectorization occurs in tight loops "automatically" by the compiler
- Need to know where vectorization should occur, and verify that compiler is doing that.
- Need to know if a compiler's failure to vectorize is legitimate
- Fix code if so, use \#pragma if not
- Need to be aware of caching and data access issues
- Very fast vector units need to be well fed.

