Some elements on
Vectorization

SCIENTIFIC &
DATA-INTENSIVE COMPUTING

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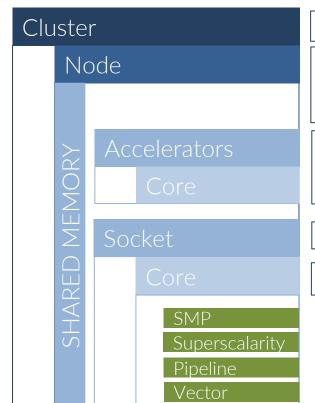I.N.A.F.

Outline

- Introduction

- Understanding the CPU's capability

- Vectorization by compiler's wow effect

- Vectorization by vector types

- Vectorization by OpenMP SIMD

[0]

Introduction

- Recap: the levels of parallelism
- What are vector registers and vector ops
- Why vectorization ?
- Evolution of vector sizes and instructions
- High-level and Low-level approaches for vectorization

Recap: the levels of parallelism

Cluster	Group of nodes connected via a fast network

Node	Set of CPUs and Accelerators connected via fast lanes
	Memory is shared among CPUs; may be shared also with accelerators on new emerging architectures

Accelerators	Special devices specialized for high throughput
Core	massive parallelism of many simple cores

Socket	Set of cores that share levels of cache memory
Core	Group of funtional units that communicate / operate via registers and L1 cache

SHARED MEMORY

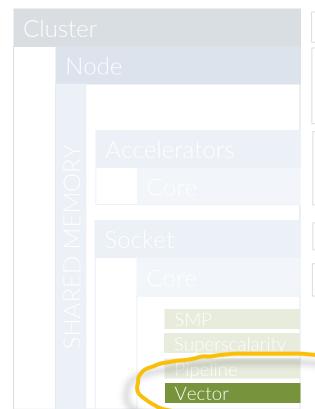| SMP	Group of thread contexts that share functional units
Superscalarity	Group of instructions sharing functional units thanks to out-of-order capability
Pipeline	Multiple instructions sharing functional units
Vector	Single instructions on Multiple Data

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Recap: the levels of parallelism

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Accelerators / Core	Special devices specialized for high throughput — massive parallelism of many simple cores
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SHARED MEMORY

Introduction

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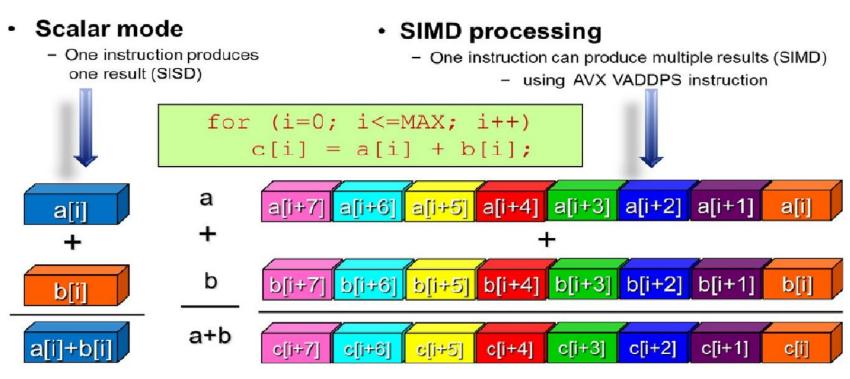
Vector instructions

What is the nature of vector operations ?

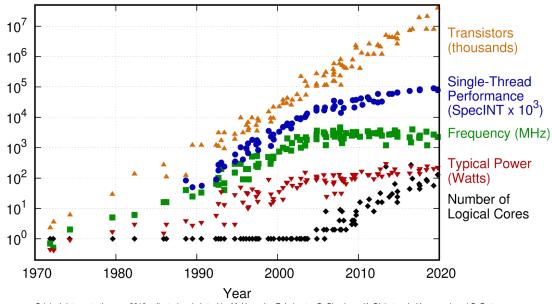taken from "High Performance Parallelism Pearls, vol 2" , ch. 22

Recap: why vectorization ?

Dennard et al. (1974) showed that if MOSFET transistors in a semiconductor device shrink by a factor k in each dimension, then the voltage V and current I required by each circuit element can also be made to decrease by k.
This reduces each element's power consumption (VI) by k^2. But the number of these elements per unit area increases by k^2, so the power dissipated per unit area stays the same.
This means the power and cooling constraints of the overall device remain unaltered. Yet these scaled-down elements can operate at higher frequency, because the delay time TRC per circuit element is reduced by k. (Basic physics: per element, the resistance R=V/I is unchanged, while the capacitance C depends on area/distance and shrinks by k.) Unfortunately, starting around 2005, this favorable Dennard scaling began to run into trouble due to leakage currents that develop at super-small dimensions. As a result, even though transistors are still shrinking in size, the frequency cannot be made to go higher.

Transistors (thousands)

Single-Thread Performance (SpecINT x 10^3)

Frequency (MHz)

Typical Power (Watts)

Number of Logical Cores

1970   1980   1990   2000   2010   2020

Year

Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2019 by K. Rupp

Picture and text quoted from the Cornell Virtual Workshop
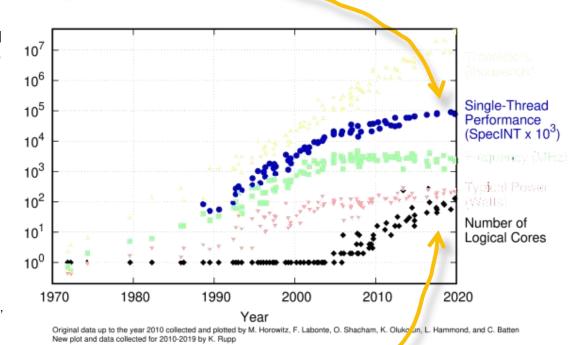
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Recap: why vectorization ?

Dennard et al. (1974) showed that if MOSFET transistors in a semiconductor device shrink by a factor k in each dimension, then the voltage V and current I required by each circuit element can also be made to decrease by k.
This reduces each element's power consumption (VI) by k^2. But the number of these elements per unit area increases by k^2, so the power dissipated per unit area stays the same.
This means the power and cooling constraints of the overall device remain unaltered. Yet these scaled-down elements can operate at higher frequency, because the delay time TRC per circuit element is reduced by k. (Basic physics: per element, the resistance R=V/I is unchanged, while the capacitance C depends on area/distance and shrinks by k.) Unfortunately, starting around 2005, this favorable Dennard scaling began to run into trouble due to leakage currents that develop at super-small dimensions. As a result, even though transistors are still shrinking in size, the frequency cannot be made to go higher.

performance increase partially due to vectorization

Single-Thread Performance (SpecINT x 10^3)

Number of Logical Cores

Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2019 by K. Rupp

More cores to increase parallelism since the frequency has hit the power wall

Vector instructions, evolution
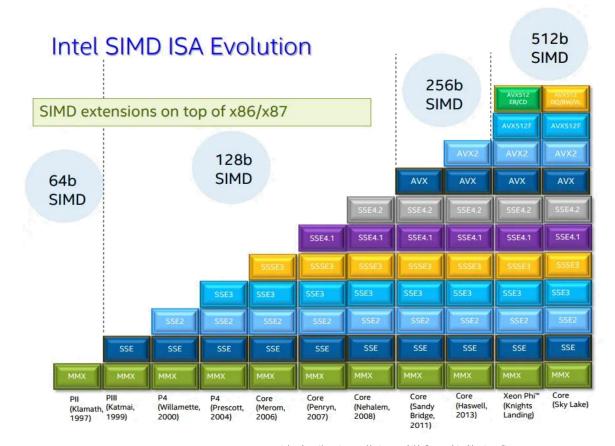
Example for Intel® ISA.
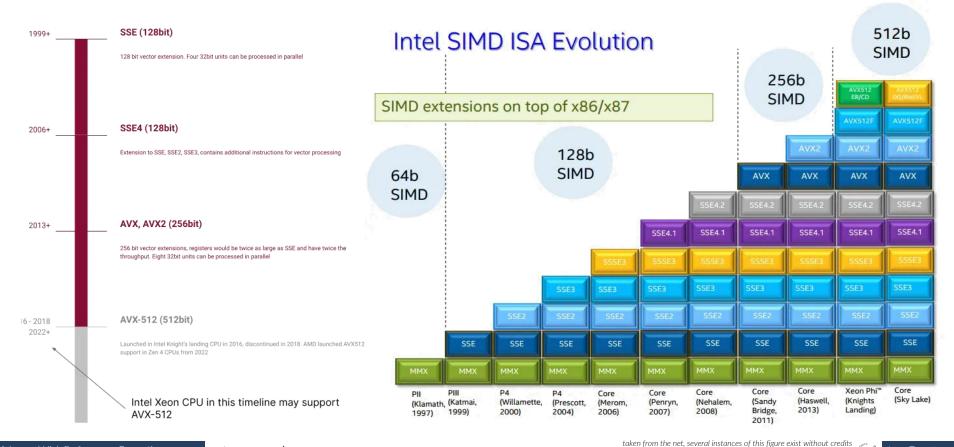AMD® (3dNow®),
ARM® (SVE®, Neon®),
IBM® (AltiVec®),
RISC-V (V), etc,
have their own.

Different ISA share
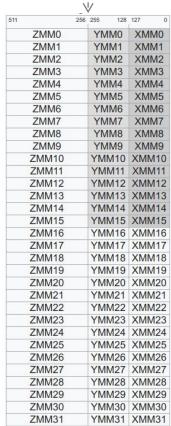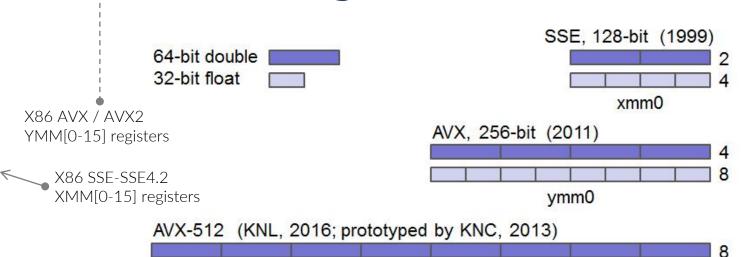several similar features
while having some
peculiar ones.

taken from the net, several instances of this figure exist without credits

Vector instructions, evolution

1999+ — **SSE (128bit)**

128 bit vector extension. Four 32bit units can be processed in parallel

2006+ — **SSE4 (128bit)**

Extension to SSE, SSE2, SSE3, contains additional instructions for vector processing

2013+ — **AVX, AVX2 (256bit)**

256 bit vector extensions, registers would be twice as large as SSE and have twice the throughput. Eight 32bit units can be processed in parallel

|6 - 2018
2022+ — **AVX-512 (512bit)**

Launched in Intel Knight's landing CPU in 2016, discontinued in 2018. AMD launched AVX512 support in Zen 4 CPUs from 2022

Intel Xeon CPU in this timeline may support AVX-512

Intel SIMD ISA Evolution

512b SIMD

256b SIMD

SIMD extensions on top of x86/x87

128b SIMD

64b SIMD

	PII (Klamath, 1997)	PIII (Katmai, 1999)	P4 (Willamette, 2000)	P4 (Prescott, 2004)	Core (Merom, 2006)	Core (Penryn, 2007)	Core (Nehalem, 2008)	Core (Sandy Bridge, 2011)	Core (Haswell, 2013)	Xeon Phi™ (Knights Landing)	Core (Sky Lake)
AVX512 ER/CD / AVX512 DQ/BW/VL										✓	✓
AVX512F										✓	✓
AVX2									✓	✓	✓
AVX								✓	✓	✓	✓
SSE4.2							✓	✓	✓	✓	✓
SSE4.1						✓	✓	✓	✓	✓	✓
SSSE3					✓	✓	✓	✓	✓	✓	✓
SSE3			✓	✓	✓	✓	✓	✓	✓	✓	✓
SSE2		✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
SSE	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
MMX	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

taken from the net, several instances of this figure exist without credits

Vector instructions, registers size

511	256	255	128	127	0
ZMM0		YMM0		XMM0	
ZMM1		YMM1		XMM1	
ZMM2		YMM2		XMM2	
ZMM3		YMM3		XMM3	
ZMM4		YMM4		XMM4	
ZMM5		YMM5		XMM5	
ZMM6		YMM6		XMM6	
ZMM7		YMM7		XMM7	
ZMM8		YMM8		XMM8	
ZMM9		YMM9		XMM9	
ZMM10		YMM10		XMM10	
ZMM11		YMM11		XMM11	
ZMM12		YMM12		XMM12	
ZMM13		YMM13		XMM13	
ZMM14		YMM14		XMM14	
ZMM15		YMM15		XMM15	
ZMM16		YMM16		XMM16	
ZMM17		YMM17		XMM17	
ZMM18		YMM18		XMM18	
ZMM19		YMM19		XMM19	
ZMM20		YMM20		XMM20	
ZMM21		YMM21		XMM21	
ZMM22		YMM22		XMM22	
ZMM23		YMM23		XMM23	
ZMM24		YMM24		XMM24	
ZMM25		YMM25		XMM25	
ZMM26		YMM26		XMM26	
ZMM27		YMM27		XMM27	
ZMM28		YMM28		XMM28	
ZMM29		YMM29		XMM29	
ZMM30		YMM30		XMM30	
ZMM31		YMM31		XMM31	

X86 AVX / AVX2
YMM[0-15] registers

X86 SSE-SSE4.2
XMM[0-15] registers

From the Wikipedia page on AVX-512

64-bit double
32-bit float

SSE, 128-bit (1999)
2
4
xmm0

AVX, 256-bit (2011)
4
8
ymm0

AVX-512 (KNL, 2016; prototyped by KNC, 2013)
8
16
zmm0

From the Cornell Virtual Workshop on Vectorization https://cvw.cac.cornell.edu/vector

A speedup as large as the size of the registers (4x, 8x) may be possible in scientific codes.
However, that result is rarely achieved for a number of reasons that we'll discuss in the next slides.
Also, due to power consumption, normally the CPU frequency is throtthled down when intensive vector operations are running

Strategies for vectorization

How is it possible to achieve the vectorization ?

More Convenience
- *Higher Level*
- *More abstraction*
- *No HW dependence*

- *Less abstraction*
- *HW specific*
- *Lower level*

More Control

OpenMP Vectorization
Compiler Auto-Vectorization

C++ classes

Compiler-dependent vector types

Intrinsics

Assembler

Strategies for vectorization

What we'll see

More Convenience
- *Higher Level*
- *More abstraction*
- *No HW dependence*

✓ **OpenMP Vectorization**
✓ **Compiler Auto-Vectorization**

C++ classes

✓ **Compiler-dependent vector types**

- *Less abstraction*
- *HW specific*
- *Lower level*

More Control

Intrinsics

Assembler

[1]
How to check for SIMD capablities

- Checking the CPU flags from command line
- Checking the CPU capabilities via builtin functions
- Compile code dependent on the capabilities of the target machine

Checking for the right flags

1) statically get the value for your cpu, for instance by
   grep the output of either **lscpu** or **/proc/cpuinfo**

```
Flags:      fpu vme de pse tsc msr pae mce cx8 apic sep mtrr pge mca cmov pat pse36 clflush dts acpi mmx fxsr sse sse2 ss ht
            tm pbe syscall nx pdpe1gb rdtscp lm constant_tsc art arch_perfmon pebs bts rep_good nopl xtopology nonstop_tsc
            cpuid aperfmperf tsc_known_freq pni pclmulqdq dtes64 monitor ds_cpl vmx smx est tm2 ssse3 sdbg fma cx16 xtpr
            pdcm pcid sse4_1 sse4_2 x2apic movbe popcnt tsc_deadline_timer aes xsave avx f16c rdrand lahf_lm abm
            3dnowprefetch cpuid_fault epb ssbd ibrs ibpb stibp ibrs_enhanced tpr_shadow flexpriority ept vpid ept_ad
            fsgsbase tsc_adjust bmi1 avx2 smep bmi2 erms invpcid rdseed adx smap clflushopt clwb intel_pt sha_ni xsaveopt
            xsavec xgetbv1 xsaves split_lock_detect user_shstk avx_vnni dtherm ida arat pln pts hwp hwp_not ify
            hwp_act_window hwp_epp hwp_pkg_req hfi vnmi umip pku ospke waitpkg gfni vaes vpclmulqdq rdpid movdiri movdir64b
            fsrm md_clear serialize arch_lbr ibt flush_l1d arch_capabilities
```

2) discover from the source code at both compile-time and run-time

[1] Check capabilities

Checking for the right flags

How can we check what capabilities has the cpu on which the code runs?

include the relevant header that defines low-level routines

get the cpu data via the cpuid instruction

parse the cpu's flags looking for precise tags

```c
#include <cpuid.h>

int main ( void )
{
  ...
  __builtin_cpu_init();

  if ( __builtin_cpu_supports("avx512f") )
    printf("CPU supports AVX512f\n");
  if ( __builtin_cpu_supports("avx2") )
    printf("CPU supports AVX2\n");
  if ( __builtin_cpu_supports("avx") )
    printf("CPU supports AVX\n");
  if ( __builtin_cpu_supports("sse4.2") )
    printf("CPU supports SSE4.2\n");
  if ( __builtin_cpu_supports("sse4.1") )
    printf("CPU supports SSE4.1\n");
  if ( __builtin_cpu_supports("sse3") )
    printf("CPU supports SSE3\n");
```

[1] Check capabilities

Checking for the right flags

How can we check what capabilities has the cpu on which the code runs?

It is possible to parse the compile-time macros defined by the compiler to check what flags are active on the current cpu.

... however, let's try to run the code `support.c`

to understand that the compiler needs some directives too.

```c
#include <immintrin.h>

#ifdef __AVX512__

#define VD_SIZE ( sizeof( __m512d ) / sizeof(double) )

#elif defined ( __AVX__ ) || defined ( __AVX2__ )

#define VD_SIZE ( sizeof( __m256d ) / sizeof(double) )

#elif defined ( __SSE4__ ) || defined ( __SSE3__ )

#define VD_SIZE ( sizeof( __m128d ) / sizeof(double) )

#else

#define VD_SIZE 1

#endif
```

[1] Check capabilities

Checking for the right flags

How can we check what capabilities has the cpu on which the code runs?

It is possible to parse the compile-time macros defined by the compiler to check what flags are active on the current cpu.

... however, let's try to run the code

→
Vectoriztion/0 .../discover_vector_support.c

to understand that the compiler needs some directives too.

note: including **immintrin.h** is needed to have all the basic intrinsics (for instance, the types __mm512d, __mm256d, ..)

```c
#include <immintrin.h>

#ifdef __AVX512__

#define VD_SIZE ( sizeof( __m512d ) / sizeof(double) )

#elif defined ( __AVX__ ) || defined ( __AVX2__ )

#define VD_SIZE ( sizeof( __m256d ) / sizeof(double) )

#elif defined ( __SSE4__ ) || defined ( __SSE3__ )

#define VD_SIZE ( sizeof( __m128d ) / sizeof(double) )

#else

#define VD_SIZE 1

#endif
```

[1] Check capabilities

Checking for the right flags

How can we check what capabilities has the cpu on which the code runs?

```
:> $ gcc -o discover_vector_support
discover_vector_support.c
:> $ ./discover_vector_support

CPU supports AVX / AVX2
CPU supports SSE4.2
CPU supports SSE4.1
CPU supports SSE3

The double vector size is : 1
```

Why the compiler is able to correctly recognize the CPU's capabilities but actually gets a wrong vector size ?

Also compiling with **-O3** does not make it to behave appropriately

Exercise: compile & run support.c

[1] Check capabilities

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Checking for the right flags

How can we check what capabilities has the cpu on which the code runs?

```
:> $ gcc -march=native -o discover_vector_support discover_vector_support.c
:> $ ./discover_vector_support


CPU supports AVX / AVX2
CPU supports SSE4.2
CPU supports SSE4.1
CPU supports SSE3

The double vector size is : 4
```

We need to instruct the compiler to set the current architecture as a target, instead of a generic **x86_64**

Checking for the right flags

How can we check what capabilities has the cpu on which the code runs?

```
:> $ gcc -msse4.2 -o ...
:> $ ./discover_vector_support

CPU supports AVX / AVX2
CPU supports SSE4.2
CPU supports SSE4.1
CPU supports SSE3

The double vector size is : 2
```

We may ask to support a specific SIMD extension (Intel's and AMD's)
```
-msse
-msse2
...
-msse4.2
-mavx
-mavx2
-mavx512f
```

ARM, POWER, and others have their own specific targets

Exercise: compile with icx and clang

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Checking for the right flags

How can we check what capabilities has the cpu on which the code runs?

Add the directive

`#pragma GCC target("avx2")`

→ Vectoriztion/0 .../declare target.c
at the top of the code
However this goes in the direction of being strongly compiler-dependent, which is not advisable

```
#pragma GCC target("avx2")

#include <immintrin.h>
#include <cpuid.h>

#ifdef __AVX512__

#define VD_SIZE ( sizeof( __m512d ) / sizeof(double) )

#elif defined ( __AVX__ ) || defined ( __AVX2__ )

#define VD_SIZE ( sizeof( __m256d ) / sizeof(double) )

...
```

Exercise: compile with and run with gcc

[1] Check capabilities

[2]

Vector types (via intrinsics)

- Recap of vector types & sizes
- How you can define your own "adaptive" vector types

The vector intrinsics types

Once we include the <immintrin.h> header, we get access to the intrinsincs routines and types

INTEGER types

	types name	int 8bits	int 16bits	int 32bits	int 64bits
64bits	__m64	8x	4x	2x	1x
128bits	__m128i	16x	8x	4x	2x
256bits	__m256i	32x	16x	8x	4x
512bits	__m512i	64x	32x	16x	8x

FLOATING-POINT types

	types name	single precision	double precision
128bits	__m128	4x	-
	__m128d	-	2x
256bits	__m256	8x	-
	__m256d	-	4x
512bits	__m512	16x	-
	__m512d	-	8x

[2] Vector types

Defining vector types via intrinsics

If we want to make explicit use of vector types, and to write a code that adapts to the machine it compiles on, we need to define our own types:

the types
   dvector_t
   fvector_t
   ivector_t

will exist in our code with the correct sizes. As well, we may define our own wrappers for intrinsics operations

see
`Vectorization/0_explore_first_steps/declare_vector_types.c`

```c
// .............................................
#ifdef __AVX512__
typedef __m512d dvector_t;
typedef __m512  fvector_t;
typedef __m512i ivector_t;
// .............................................
#elif defined ( __AVX__ ) || defined ( __AVX2__ )
typedef __m256d dvector_t;
typedef __m256  fvector_t;
typedef __m256i ivector_t;
// .............................................
#elif defined ( __SSE4__ ) || defined ( __SSE3__ )
typedef __m128d dvector_t;
typedef __m128  fvector_t;
typedef __m128i ivector_t;
// .............................................
#else
typedef double dvector_t;
typedef double fvector_t;
typedef double ivector_t;
#endif
// .............................................

#define DV_ELEMENT_SIZE (sizeof( dvector_t ) / sizeof(double) )
#define DV_BIT_SIZE (sizeof( dvector_t ) * 8 )

#define FV_ELEMENT_SIZE (sizeof( fvector_t ) / sizeof(float) )
#define FV_BIT_SIZE (sizeof( fvector_t ) * 8 )

#define IV_ELEMENT_SIZE (sizeof( ivector_t ) / sizeof(int) )
#define IV_BIT_SIZE (sizeof( ivector_t ) * 8 )
```

Defining vector types via intrinsics

What you do in real codes is to have large `#idef` regions in which you define the macros for the precise operations that you need.
This requires to call the `AVX512, AVX, SSEx`, intrinsics that refer to that operations with the suited types.

For instance a "vector summation" for int, double and single precision FP

```
VDSUM (v1, v2, result)
VFSUM (v1, v2, result)
VISUM (v1, v2, result)
```

with a standard call throughout your code

We'll see more details when discussing the usage of intrinsics

```c
// ..............................................
#ifdef __AVX512__
typedef __m512d dvector_t;
typedef __m512  fvector_t;
typedef __m512i ivector_t;
// ..............................................
#elif defined ( __AVX__ ) || defined ( __AVX2__ )
typedef __m256d dvector_t;
typedef __m256  fvector_t;
typedef __m256i ivector_t;
// ..............................................
#elif defined ( __SSE4__ ) || defined ( __SSE3__ )
typedef __m128d dvector_t;
typedef __m128  fvector_t;
typedef __m128i ivector_t;
// ..............................................
#else
typedef double dvector_t;
typedef double fvector_t;
typedef double ivector_t;
#endif
// ..............................................

#define DV_ELEMENT_SIZE (sizeof( dvector_t ) / sizeof(double) )
#define DV_BIT_SIZE (sizeof( dvector_t ) * 8 )

#define FV_ELEMENT_SIZE (sizeof( fvector_t ) / sizeof(float) )
#define FV_BIT_SIZE (sizeof( fvector_t ) * 8 )

#define IV_ELEMENT_SIZE (sizeof( ivector_t ) / sizeof(int) )
#define IV_BIT_SIZE (sizeof( ivector_t ) * 8 )
```

[3]

Auto-vectorization

- Getting insights from a simple example
- Recap on critical path and loop unrolling
- Associative math
- How to use the compiler and Basic requirements for loop vectorization
- What could go wrong ?
  - non-contiguous mem access
  - data dependencies
  - memory ambiguity
- Inefficiencies:
  - unaligned memory
  - SoA vs AoS vs SoAoS

Auto vectorizing a simple loop

Auto-vectorization capabilities of the compilers is a very valuable tools.
However, some general concepts must be understood and analysed because
several factors may hinder the vectoriation

- loop-carried data depencies
- control dependencies and branches
- unaligned memory
- not suited loop structure
- strided memory access
- function calls
- non-vectorizable math functions
- not supported data types
- ...

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Auto vectorizing a simple loop

Let's start with a very simple loop.

Here we perform a simple reduction of an array, with datatype **dtype** that is determined at compile time (either **int** or **float**).

Let's compile the code
`Vectorization/1_simple_loop/sum_loop.c`
for both integer and float data, asking for the vectorization report and generating the assembler:

```
dtype sum_loop ( dtype *array, uint N )
{
  dtype sum = 0;
  for ( uint32_t i = 0; i < N; i++ )
     sum += array[i];
  return sum;
}
```

● options to get the generated assembler in intel syntax

● options for optimization and vectorization

options to get a report on vectorization ●

```
gcc –S –fverbose-asm –masm=intel
–O3 –march=native –mtune=native –ftree-vectorize –funroll_loops
–fopt-info-vec-optimized –fopt-info-vec-missed –fopt-info-loop –fopt-info-loop-missed
–DDTYPE=[INTEGER|FPSP] –o sum_loop.[int|float].s sum_loop.c
```

Auto vectorizing a simple loop

Let's inspect what assembler the compiler issues for `int` type

```
.L4:
# sum_loop_c:51:        sum += array[i];
        vpaddd    ymm0, ymm0, YMMWORD PTR [rax]    # vect_sum_11.16, vect_sum_11.16, MEM <vector(8) unsigned int> [(uint32_t *)_69]
        add       rax, 32                          # ivtmp.22,
        cmp       rdx, rax                         # _53, ivtmp.22
        jne       .L4     #,                                                                    ◄------------------  the actual loop
        vmovdqa   xmm1, xmm0                       # tmp142, vect_sum_11.16
        vextracti128      xmm0, ymm0, 0x1          # tmp143, vect_sum_11.16
        mov       edx, ecx                         # niters_vector_mult_vf.10, N
        vpaddd    xmm0, xmm1, xmm0                 # _41, tmp142, tmp143
        and       edx, -8                          # niters_vector_mult_vf.10,
        test      cl, 7                            # N,
        vpsrldq   xmm1, xmm0, 8                    # tmp145, _41,
        vpaddd    xmm0, xmm0, xmm1                 # _43, _41, tmp145
        vpsrldq   xmm1, xmm0, 4                    # tmp147, _43,
        vpaddd    xmm0, xmm0, xmm1                 # tmp148, _43, tmp147
        vmovd     eax, xmm0                        # <retval>, tmp148
        je        .L15                             #,
        vzeroupper
```

```
vpaddd    ymm0, ymm0, YMMWORD PTR [rax]
add       rax, 32
cmp       rdx, rax
jne       .L4
```

Auto vectorizing a simple loop

Let's inspect what the compiler issues for **int** type

`vpadd target, opA, opB` → `target = opA+opB`
where
- `target`, `opA` and `opB` are `YMMWORD`, i.e. 512bits-wide
- are considered as vectors of `32bits integers`

```
vpaddd    ymm0, ymm0, YMMWORD PTR [rax]
add       rax, 32
cmp       rdx, rax
jne       .L4
```

Addressing mode:
" take 512bits from the address held in `reg rax` "
i.e. the sq brackets [ ] mean "consider what is inside as an address, i.e. a pointer

`rax` works also as a loop counter; compare if it is equal to the final address `rdx`; if not, jump to the begin of the loop body

increment `rax` by `32`, i.e. the address it points to by 32bytes (=256bits)

Auto vectorizing a simple loop

Let's inspect what the compiler issues for `int` type

```
.L4:
# sum_loop.c:51:        sum += array[i];
        vpaddd   ymm0, ymm0, YMMWORD PTR [rax]    # vect_sum_11.16, vect_sum_11.16, ME
        add      rax, 32                          # ivtmp.22,
        cmp      rdx, rax                         # _53, ivtmp.22
        jne      .L4       #,
        vmovdqa  xmm1, xmm0                       # tmp142, vect_sum_11.16
        vextracti128     xmm0, ymm0, 0x1          # tmp143, vect_sum_11.16
        mov      edx, ecx                         # niters_vector_mult_vf.10, N
        vpaddd   xmm0, xmm1, xmm0                 # _41, tmp142, tmp143
        and      edx, -8                          # niters_vector_mult_vf.10,
        test     cl, 7                            # N,
        vpsrldq  xmm1, xmm0, 8                    # tmp145, _41,
        vpaddd   xmm0, xmm0, xmm1                 # _43, _41, tmp145
        vpsrldq  xmm1, xmm0, 4                    # tmp147, _43,
        vpaddd   xmm0, xmm0, xmm1                 # tmp148, _43, tmp147
        vmovd    eax, xmm0                        # <retval>, tmp148
        je       .L15                             #,
        vzeroupper
```

This section get the final single value into `eax`.
In fact, at the end of the loop `ymm0` contains 8 partial results.
The 7 summations are done via 3 `vpaddd` on reshuffled registers

if the iteration space was not exactly divisible by 8, we need to account for the remainder iterations;
otherwise, we jump to a subsequent label

dig more

More details on how to read this assembly in the slides at the end

HINT: a nice repository to explore assembler instructions is
`https://www.felixcloutier.com/x86/`

[3] Auto vectorization

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Auto vectorizing a simple loop

Let's inspect what the compiler issues for `float` type

```
.L4:
        vaddss    xmm0, xmm0, DWORD PTR [rax]
        add       rax, 32
        vaddss    xmm0, xmm0, DWORD PTR -28[rax]
        vaddss    xmm0, xmm0, DWORD PTR -24[rax]
        vaddss    xmm0, xmm0, DWORD PTR -20[rax]
        vaddss    xmm0, xmm0, DWORD PTR -16[rax]
        vaddss    xmm0, xmm0, DWORD PTR -12[rax]

        vaddss    xmm0, xmm0, DWORD PTR -8[rax]
        vaddss    xmm0, xmm0, DWORD PTR -4[rax]
        cmp       rax, rcx
        jne       .L4
```

8 `vaddss` calls on xmm0 to itself after having loaded subsequent memory addresses

The loop is then not truly vectorized !

```
vaddss target, opA, opB
```

add the low SP FP from **opB** to **opA** and stores the result in low SP FP of **target**

Auto vectorizing a simple loop

To further test the result of the compilation, let's profile the codes using `perf`
find the details in `Vectorization/1_simple_loop/compile_sum_loop`

For both int and float versions we'll check the events

`cycles:u , instructions:u`

Whereas we'll check che specific events

`int_vec_retired.add_256`

and

`fp_arith_inst_retired.256b_packed_single:u`
`fp_arith_inst_retired.scalar_single:u`

for the int and float version respectively

dig
more

For a recap on Performance
Monitoring Units (PMUs), perf and
the perf profiling, have a look at the
pdf
Materials/profiling_with_perf.pdf
which is the same that you have
seen in the HPC basic course

If you work on a big.LITTLE system,
you may encounter problems in
getting the PMUs working properly.
You need to export a precise
LIBPFM_FORCE_PMU

Auto vectorizing a simple loop

To further test the result of the compilation, let's profile the codes using `perf`

```
Performance counter stats for 'CPU(s) 1':

        11,132,913      cpu_core/cpu-cycles/
        10,143,073      cpu_core/instructions/
           250,000      cpu_core/int_vec_retired.add_256/

    0.000935968 seconds time elapsed
```

```
Performance counter stats for 'CPU(s) 1':

        10,939,564      cpu_core/cpu-cycles/
        10,360,258      cpu_core/instructions/
           250,000      cpu_core/fp_arith_inst_retired.256b_packed_single/
         1,000,000      cpu_core/fp_arith_inst_retired.scalar_single/

    0.005113507 seconds time elapsed
```

Auto vectorizing a simple loop

To further test the result of the compilation, let's profile the codes using `perf`

	integer	float
not vectorized	`0        int_vec.add_256`	`0         vector` `1,000,000 scalar`
vectorized	`250,000 int_vec.add_256`	`250,000    vector` `1,000,000 scalar`

Auto vectorizing a simple loop

...result of the compilation, let's profile the codes using `perf`

	integer	float
not vectorized	0 int_vec.add_256	0 vector 1,000,000 scalar
vectorized	250,000 int_vec.add_256	250,000 vector 1,000,000 scalar

125k are vector ops to initialize the loop.

125k are vec addition in the summation loop

these are the vector ops to initialize the loop.
125k to convert vectors of int into floats, 125k to mov regs in memory

these are the scalar in the summation loop, that are not vectorized at all

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Auto vectorizing a simple loop

Hence, autovectorization works nicely for the integers but not at all for the floats.

Of course that descends from the compiler *not* being entitled to reshuffle operations in the summation loop.

For as we have written it

      `s += a`$_i$

there is a clear critical path on `s`, that must be respected by the compiler.

Let's try by explicitly relaxing the safe math assumption[*] by `-fassociative-math`.

metrics	vectorized	vectorized unsafe-math
	250,000 vector 1,000,000 scalar	375,000 vector 0 scalar

[*] *Note: Intel's compiler by default assumes the relaxed IEEE math*

Critical path

Just a recap about the issue brought in the optimization of loops by the non-commutativity of floating-point airthmetics.
Please get back to the lectures on loop- and pipeline- optimizations given in the basic HPC course for a more comprehensive treatment.

If we excute the loop
```
for ( int i = 0; i < N; i++ )
    S += a[i];
```

we immediately appreciate that it encodes a precise, although obvious, order of operations:

```
i        S                          :
0        a[0]
1        a[0] + a[1]
2        a[0] + a[1] + a[2]
3        a[0] + a[1] + a[2] + a[3]
...      ...
```

Critical path

That pattern is clearly different than that encoded by different loop forms

```
for ( int i = 0; i < N; i+=2 )
    S += (a[i] + a[i+1]);
```

i	S	:
0	a[0] + a[1]	
1	(a[0] + a[1]) + (a[2] + a[3])	

more instruction parallelism is exposed here: `a[2]+a[3]` could be "in flight" at the moment in which `a[0]+a[1]` is being added to S

```
for ( int i = 0; i < N; i+=4 )
    S += (a[i] + a[i+1]) + (a[i+2] + a[i+3]);
```

i	S	:
0	(a[0] + a[1]) + (a[2] + a[3])	
1	(a[4] + a[5]) + (a[6] + a[7])	

and even more instruction parallelism is exposed here: four elements and three adds of the next iteration can be "in flight" while the current iteration is being processed

Critical path

That pattern is clearly different than that encoded by different loop reshapes

```
for ( int i = 0; i < N; i+=2 )
    S += (a[i] + a[i+1]);
```

i	S	:
0	a[0] + a[1]	
1	(a[0] + a[1]) + (a[2] + a[3])	

```
for ( int i = 0; i < N; i+=4 )
    S += (a[i] + a[i+1]) + (a[i+2] + a[i+3]);
```

i	S	:
0	(a[0] + a[1]) + (a[2] + a[3])	
1	(a[4] + a[5]) + (a[6] + a[7])	

However, although much more parallelism has been exposed in these two re-shapings of the loop [NOTE THAT the compiler CAN NOT perform them if not explicitly authorized] there is still a fundamental one.

All the partial summation are added up, in a precise order, to the same variable, the unique accumulator S.

This will lead to the execution of a lot of bit reshuffling and scalar add, in place of clean vector operations

There is an obvious fix for that.

Critical path

That pattern is clearly different than that encoded by different loop reshapes

```
for ( int i = 0; i < N; i+=4 ) {
        S0 += a[i];
        S1 += a[i+2];
        S2 += a[i+2];
        S3 += a[i+3];  }
```

Using more partial accumulators, of course

i	S0	S1	S2	S3	:
0	a[0]	a[1]	a[2]	a[3]	
1	a[0]+a[4]	a[1]+a[5]	a[2]+a[6]	a[3]+a[7]	

...

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Critical path

That pattern is clearly different than that encoded by different loop reshapes

```
for ( int i = 0; i < N; i+=4 ) {
        S0 += a[i];
        S1 += a[i+2];
        S2 += a[i+2];
        S3 += a[i+3];  }
```

Using more partial accumulators, of course

That exposes a natural vector pattern
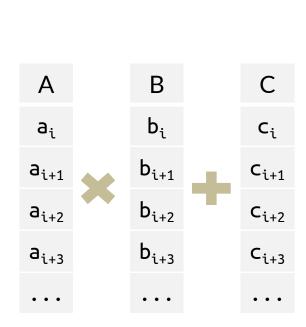
array a

S0-S3
iter 0

iter 1

iter 2

iter 3

Auto vectorizing, 2ⁿᵈ example

```
double kernel ( double *A, double *B, double *C, int N )
{
  double sum = 0;
  for ( int i = 0; i < N; i++ )
     sum += A[i]*B[i] + C[i];
  return sum;
}
```

This case has an higher possible parallelism since the **+**reduction comes after the multiply-and-add vector operation.
It means that a vector of partial results
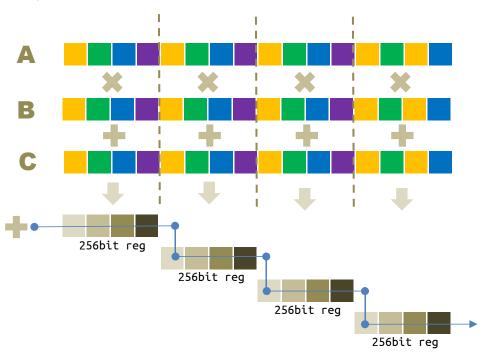
$$D[i:i+n] = A[i:i+n]xB[i:i+n]+C[i:i:n]$$

can be preemptively prepared, waiting for the `D[ ]` entries to be summed up serially

A	B	C
a_i	b_i	c_i
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}
...	...	...

Auto vectorizing, 2ⁿᵈ example

In fact, the compiler opts for this implementation:
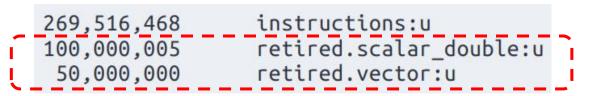
```
double kernel ( double *A, double *B, double *C, int N )
{
  double sum = 0;
  for ( int i = 0; i < N; i++ )
    sum += A[i]*B[i] + C[i];
  return sum;
}
```


A

B

C

256bit reg

256bit reg

256bit reg

256bit reg

64bit scalar register
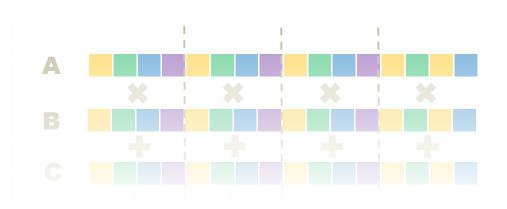
Lots of computation are performed via FMA on vector registers, 256b or 512b depending on what is available on the cpu.

However, lots of reshuffling is needed and all the reduction summations are serial

Auto vectorizing, 2ⁿᵈ example

```
269,516,468      instructions:u
100,000,005      retired.scalar_double:u
 50,000,000      retired.vector:u
```
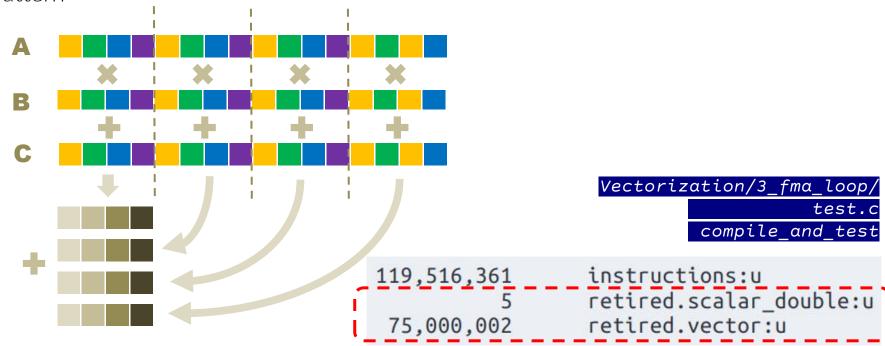
example run with AVX/AVX2
and size 100M elements:
25M + 25M FMA vector ops
                 (delivered in 1ins)
100M summations

[3] Auto vectorization

Auto vectorizing, 2ⁿᵈ example

Opting for either the usage of the "associative math" flags or explicit loop unrolling **(with separated accumulators)** results in a different, fully vectorizable pattern

`Vectorization/3_fma_loop/test.c`

`compile_and_test`

```
119,516,361          instructions:u
          5          retired.scalar_double:u
 75,000,002          retired.vector:u
```

Associative math

Every compiler allows the users to relax the rules for IEEE FP arithmetics.
Many of these rules ensure the correct treatment of under-normal numbers, 0^+ and 0^-, `Inf` and `NaN`. As such, relaxing the checks and the branches that deal with those cases, may incur in some un-correct result.

Explore two resources to have a better comprehension of this

https://simonbyrne.github.io/notes/fastmath/
https://kristerw.github.io/2021/10/19/fast-math/

Appreciate that also explicit tests as `isinf(x)` or `isnan(x)` will be disabled. As such, to be confident in activating those switches, you must be sure that your code is not incurring in those cases. However, by definition, the tests performed without those flags are not definitive because once the operations are re-shuffled, which is due exactly to those flags, the results may be different.

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Auto vectorization of loops

As we have just seen, to express the whole inherent loop data- and instruction- parallelism is of primary importance to either

authorizing the compiler to **re-shuffle floating-point** operations

or

unroll the loops to expose more instruction- and data- parallelism

Since the flag "just reorder ops associatively" does not exist, my personal advice is to opt for the manual refactoring of the code.
This way, in fact, you can reliably test for the correctness of the results while achieving the same vectorization.

references:
- *A guide to Vectorization with Intel® C++ compiler*
- *Requirements for vectorizable loops (Intel)*
- *Loop Independence, Compiler Vectorization and Threading of Loops, Intel®*
- *Vectorization with compilers, G. Zitzlsberger @ IT4I*
- *Cornell Virtual Workshop on Vectorization*

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Loops Auto-vectorization

`Vectorization/headers/vector_pragmas.h`

Tipically **-O2** or even **-O3** are required to vectorize for all compilers, in addition to explicit compiler-dependent options (why not to opt for **O3**, anyway?).

GCC

`-ftree-vectorize`	enables loops vectorization
`-funroll-loops`	enables the loop unrolling (may or may not issue faster code)
`-march=native`	specifies the current one as target architecture
`-mtune=native`	ask maximum code tuning for the host architecture

clang

`-mllvm` `-force-vector-width=4`	

Intel

`-xHost`	enables the maximum vectorization available on the target cpu
`-axFLAG1 -axFLAG2 ...`	enables code for multiple targets

Auto vectorization of loops

Ask the compiler to report on optimizations and vectorization

GCC

`-fopt-info-vec-optimized`	reports on the successful vectorizations
`-fopt-info-vec-missed`	reports on the reasons for unsuccessful vectorization

clang

`-Rpass=loop-vectorize`	identifies loops that were successfully vectorized
`-Rpass-missed=loop-vectorize`	identifies loops that were NOT successfully vectorized
`-Rpass-analysis=loop-vectorize`	dentifies the statements that caused vectorization to fail. If in addition -fsave-optimization-record is provided, multiple causes of vectorization failure may be listed

Intel

`-qopt-report=<n>` `-qopt-report-file=`*name*	enables the output of diagnosis n = 1 loops succesfully vectorized n = 2 loops not vectorized, and the reasons for n = 3 dependency informations n = 4 reports vectorization issues only n = 5 reports vect. issues with dependency infos

Auto vectorization of loops

- **`countable loops, with no data-dependent control flow`**
  The iteration space must be known at run-time. The end of the loop can not depend on data (i.e.: loops without break instructions)

  example of non-vectorizable loops
  (from Intel's guide) with data-dependent exit point
  Note that a countable while loop is vectorizable
  as a for loop is

```
int i = 0.;
while (i < 100)
{
    a[i] = b[i] * c[i];
    if (a[i] < 0.0)
        break;
    ++i;
}
```

```
for ( int i = 0; i < size_of_data(); i++ )
{
    ....
}
```

example of non-vectorizable for loop, due to unpredictable iteration space

Auto vectorization of loops

- **`countable loops, with no data-dependent control flow`**
  The iteration space must be known at run-time.

- **`loops without branching`**
  Since the SIMD instructions are meant to perform exactly the same operation on multiple data, different iterations can not have different control flows.
  if statements are admitted if they can result in a mask - like implementation (hile instructions are executed for all the elements, the results are propagated only for those whose mask entry is true)

```
for ( int i = 0; i < N; i++ )
{
    float tmp = a[i]*b[i] - a[i]/b[i];
    if ( tmp > 1 ) {
        c[i] = tmp }
    else { c[i] = sqrt(tmp) - exp(tmp); }
}
```

example of vectorizable loop

Auto vectorization of loops

- **`countable loops, with no data-dependent control flow`**
  The iteration space must be known at run-time.

- **`loops without branching`**
  since the SIMD instructions are meant to perform exactly the same operation on multiple data, different iterations can not have different control flows.
  if statements are admitted if they can result in a mask - like implementation (hile instructions are executed for all the elements, the results are propagated only for those whose mask entry is true)

- **`avoid function calls`**
  Obvious, for the same reason mentioned above.
  Vectorizable functions are an exception.

Auto vectorization of loops

- **`non-contiguous memory access`**
  loops that access data with a non-unit stride, or even worse with an irregular pattern, are rarely vectorized.
  That is because while consecutive data can be loaded in a single cache line, or in a register, with a single memory operation, sparse memory access need separate loads and data gathering; if the compiler estimates that this overhead is larger than the benefits, the loop is not vectorized

  → `Vectorization/2_loop_dependencies/non_contiguous_access.c`

Auto vectorization of loops

What could go wrong ?

- `non-contiguous memory access`

memory segments mapped to cache lines
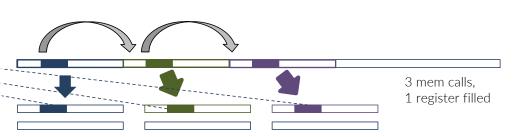
contiguous memory access results in fetching and using of entire lines of cache; the bandwidth utilization is optimal

3 mem calls,
3 cache lines,
3 register filled

registers

strided memory access results in gathering sparse memory location, accessed with separate memory calls, with a lot of overhead in memory calls and in mem moves from/to registers

3 mem calls,
1 register filled

These loops **could** be vectorized but the compiler may evaluate that the cost of the memory overhead exceeds the gain from the vectorization.

[3] Auto vectorization

Auto vectorization of loops

What could go wrong ?

- `non-contiguous memory access`
  loops that access data with a stride, or even worse with an irregular non-contiguous pattern, are rarely vectorized.

- `Data dependencies`
  fundamental fact : a loop is vectorizable if there are no cyclic dependencies chains among different iterations within the vector length.
  For practical purposes, any dependency beyond the vector length does not hinder vectorization.

  note: AVX512-CD implements Conflict-Detection

  1. Read-After-Write
  2. Write-After-Read
  3. Write-After-Write
  4. Memory ambiguity

Auto vectorization of loops

- **Read-After-Write (flow-dependency)**   → `Vectorization/2_loop_dependencies/raw.c`
  A variable is written in an interation and read on a subsequent one

  ```
  for ( int i = 1; i < N; i++ )
     a[i]= a[i-1] + c[i];
  ```

  This loop can NOT be vectorized without leading to wrong results.

  However, let's consider the following 2D case:

  ```
  for ( int i = 1; i < M; i++ ) {
     a[i][0] = c[i][0];
     for ( int j = 1; j < N; j++)
        a[i][j]= a[i][j-1] + c[i][j];
  ```
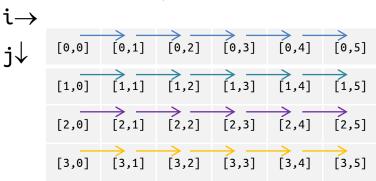
  The dependency is carried in the *inner* loop, while the *outer* loop iterations do not exhibit any dependency and the <u>outer loop vectorization</u> can be performed.

Auto vectorization of loops
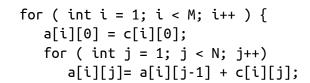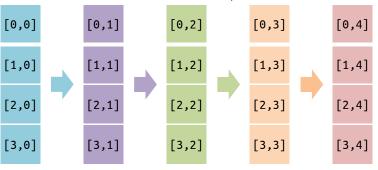
- `Read-After-Write (flow-dependency)`

  Consider the dependency graph of the iteration space. It clearly shows that there are no vertical dependencies (i.e. carried in the outer loop).

```
for ( int i = 1; i < M; i++ ) {
    a[i][0] = c[i][0];
    for ( int j = 1; j < N; j++)
        a[i][j]= a[i][j-1] + c[i][j];
```

4 (or 8) outer iterations can be executed together because there are no vertical dependencies

i→

j↓

However, if the elements are stored in memory in row-major order that require a lot of memory gather and scatter opearations. If not supported in hw, they must be emulated, which is even more expensive.
We may consider to write the data column-major, if possibile (it depends on the context).
The compiler tipically will not be able to perform this optimization.

[3] Auto vectorization

Auto vectorization of loops

- **Read-After-Write (flow-dependency)**   → `Vectorization/2_loop_dependencies/raw.c`
  A variable is written in an interation and read on a subsequent one

- **Write-After-Read (anti-dependency)**   → `Vectorization/2_loop_dependencies/war.c`
  A variable is read in one iteration and written in a subsequent one.
  Unsafe for parallelism (no strict order among iterations assigned to tasks), normally safe
  for vectorization

```
for ( int i = 1; i < N; i++ )
   a[i-1]= a[i] + c[i];
```

This loop can be vectorized

```
for ( int i = 1; i < N; i++ ){
   a[i-1]= a[i] + c[i];
   sum += a[i]; }
```

*This loop can NOT be vectorized because
it's unclear if `a[i]` may be overwritten
before the summation to `sum`*

```
#pragma ivdep
 for ( int i = 1; i < N; i++ ){
   a[i-1]= a[i] + c[i];
   sum += a[i+4]; }
```

This loop can be vectorized

Auto vectorization of loops

- **Read-After-Write (flow-dependency)**
  A variable is written in an interation and read on a subsequent one

- **Write-After-Read (anti-dependency)**
  A variable is read in one iteration and written in a subsequent one.
  Unsafe for parallelism (no strict order among iterations assigned to tasks), normally safe for vectorization

- **Write-After-Write (output dependecy)**
  The same variable is written in more than one iteration.
  Generally unsafe both in parallelization and in vectorization.

```
double sum = 0;
for ( int i = 1; i < N; i++ ) {
    a[i-1] = function1(i);
    a[i]   = function2(i); }
```

[3] Auto vectorization

Auto vectorization of loops

- **Read-After-Write (flow-dependency)**
  A variable is written in an interation and read on a subsequent one

- **Write-After-Read (anti-dependency)**
  A variable is read in one iteration and written in a subsequent one.
  Unsafe for parallelism (no strict order among iterations assigned to tasks), normally safe for vectorization

- **Write-After-Write (output dependecy)**
  The same variable is written in more than one iteration.
  Generally unsafe both in parallelization and in vectorization.

- **Unclear dependencies**
  Tipically due to memory aliasing

Auto vectorization of loops

- **Unclear dependencies**
  Tipically due to memory aliasing

  ```
  void function ( int *a, int *b, int *c, int N )
   {
     for ( int i = 0; i < N; i++ )
       c[i]= a[i] + b[i];
   }
  ```

It may be impossible for the compiler to decide whether, for some value of i, $a[i]$, $b[i]$ and $c[i]$ will somehow overlap.

If that is the case, it will not issue a vector code.

*When it is possible, the compiler will issue **more than one** version of the loop **and** a code that performs an overlap test among the pointers.*
Then the execution will be routed to the correct version at run-time

Auto vectorization of loops

- **Unclear dependencies**
  Tipically due to memory aliasing

```
void function ( int *a, int *b, int *c, int N )
 {
   for ( int i = 0; i < N; i++ )
     c[i]= a[i] + b[i];
 }
```

you can easily **disambiguate**:

```
void function ( const int * restrict a, const int * restrict b, int * restrict c, const int N )
 {
   for ( int i = 0; i < N; i++ )
     c[i]= a[i] + b[i];
 }
```

The `restrict` *keyword grants to the compiler that every restrict pointer will never overlap with any other pointer*

The `const` *qualifier adds important hints about what to optimize and how. Also add clarity for the programmers.*

Note: a pointer to constant data is different than a costant pointer to data and than a constant pointer to constant data...

Auto vectorization of loops

A variable is said to be *aligned* in memory when its first byte's address is a multiple of the variable's type size:

`short int`	2 bytes: 0, 2, 4, 6, 8 .. are aligned placements
`int / float`	4 bytes: 0, 4, 8, 12, 16 .. are aligned placements
`long long / double`	8 bytes: 0, 8, 16, 24 .. are aligned placements

Consequently, an aligned variable is also aligned w.r.t the cache line it belongs to: it means that an aligned variable will never cross 2 cache lines.

Auto vectorization of loops

However, let's imagine that you allocate a bunch of memory, and you consider it as an array of elements with byte size s_B. Let's say that
- its starting byte is aligned at a_B bytes (actually, that is usually expressed in bits)
- you access this array by vectors of element-size V_L (meaning that every vecot has V_L elements); hence, you will access $V_L \times s_B$ bits every time.

Then if
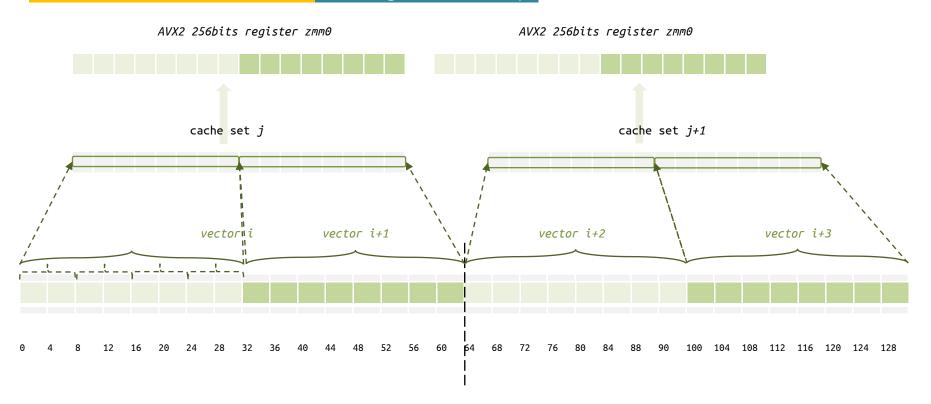
$$(a_B + V_L \times s_B) \, \% \, C_L == 0 \qquad (C_L \text{ being the cache capacity in terms of elements})$$

all the vectors will stay in the same cache line and will require 1 load;
otherwise, a vector will be mapped into two different cache lines and will require 2 loads.

Let's examine two examples in the following slides.

Auto vectorization of loops
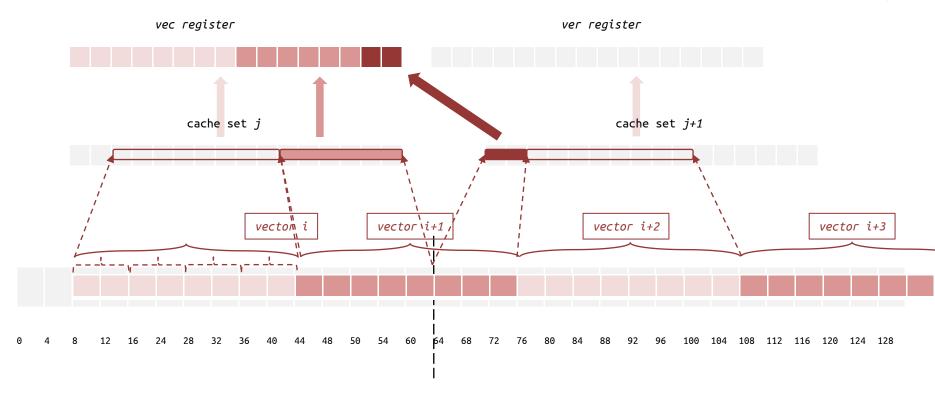
an array of float aligned at **64bits** accessed as vector of size 4
(cache capacity is 16 with a std cache line of 64B)
$a_B = 8B$, $V_L = 4$, $s_B = 4$, $C_L = 16$
every vector will occupy exactly 1 cache line

What could be inefficient?   Unaligned memory

AVX2 256bits register zmm0

AVX2 256bits register zmm0

cache set *j*

cache set *j+1*

vector i   *vector i+1*   *vector i+2*   *vector i+3*

0   4   8   12   16   20   24   28   32   36   40   44   48   52   56   60   64   68   72   76   80   84   88   90   100   104   108   112   116   120   124   128

[3] Auto vectorization

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Auto vectorization of loops

an array of float aligned at **16bits** accessed as vector of size 4
(cache capacity is 16 with a std cache line of 64B)
$a_B = 8B$, $V_L = 4$, $s_B = 4$, $C_L = 16$

What could be inefficient?   Unaligned memory

vec register

ver register

cache set *j*

cache set *j+1*

vector i   vector i+1   vector i+2   vector i+3

0   4   8   12   16   24   28   32   36   40   44   48   50   54   60   64   68   72   76   80   84   88   92   96   100   104   108   112   116   120   124   128

[3] Auto vectorization

Auto vectorization of loops

- Keep together data that are used together in vector operations
  (see slides "SoA vs AoS")

- The smallest the data type you use, the larger the number of data that you
  can fit in cache and in the vector registers

- Do not mix same-type different-size data

  ```
  func ( float *A, float *B, double *C, int N) {
     for ( int i = 0; i < N; i++ )
        A[i] = B[i]*C[i]; }
  ```

  the type conversion renders things less efficient.
  `long double` type is NOT supported on GPUs.

Auto vectorization of loops

Very commonly the data are multi-dimensional and hence the most natural representation is by a structure that encapsulates all the quantities for a single data point.
Every entry of the array that contains all the data points is then a structure:

```
data[i].pos[3], data[i].acceleration[3], data[i].mass, data[i].composition[n_elements], ...
```

That is called an "Array of Structures" (AoS) and is a very convenient representation in many respects. For instance, when you perform a domain decomposition it is very immediate to send and receive data points.

However, when the structures collects many and diverse data, the SoA have several inconvenience too when computational performance is considered.

Auto vectorization of loops

To understand why, consider the example of this structures that occupies 96bytes.

```
struct Particle {
        double pos[3], accel[3], vel[3];
        double mass;
        long long int ID;
        float composition[n_el]; }
```

As a first consideration, even a single particle could not fit in a cache line.
Second, most probably `pos[3]` will be used, likely with mass, to get `accel[3]` and then `vel[3]` will be update.

Auto vectorization of loops

Very likely every of these calculation may have a high degree of vectorization.
However, there is no way in which those quantities can be loaded from memory to
vector register efficiently without lots of overhead, either using gathering
instructions or allocating additional memory and moving there only the variables
used for every calculation.

So, a very first step consist in opting for **S**tructures **o**f **A**rrays **o**f (small)**S**tructures
(**SoAoS**) :

```
struct Ppos        { double pos[3], double mass; };     PPos   *mpositions;
struct Paccel      { double accel[3]; };                Paccel *accelerations;
struct Pvel        { vel[3]; }                          Pvel   *velocities;
struct Pchemistry  { float elements[n_el]; };           Pelems *Pchemistry;
                                                        long long int *PIds;
```

Auto vectorization of loops

```
struct Ppos       { double pos[3], double mass; };
struct Paccel     { double accel[3]; };
struct Pvel       { vel[3]; }
struct Pchemistry { float elements[n_el]; };
```

```
PPos   *mpositions;
Paccel *accelerations;
Pvel   *velocities;
Pelems *Pchemistry;
long long int *PIds;
```

Clearly that alleviates the aforementioned issues but it is still sub-optimal.
For instance, considering a force computation between 2 particles, we would have

Vector reg of size 4 double

| regA: PPos[i] | pos[0] | pos[1] | pos[2] | m |

| regA: PPos[j] | pos[0] | pos[1] | pos[2] | m |

| regC:
PPos[i] - PPos[j] | $x_i - x_j$ | $y_i - y_j$ | $z_i - z_j$ | $m_i - m_j$ |

[3] Auto vectorization

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Auto vectorization of loops

What could be inefficient ?   **SoA over AoS**

A vector subtraction returns in `regC` the 1d distance in every dimension.
However, its fourth entry would contains a to-be-discarded value (the mass difference).

After that, we need to take the square invert of `regC` and to perform an horizontal addition over it to get $1/r^2$.
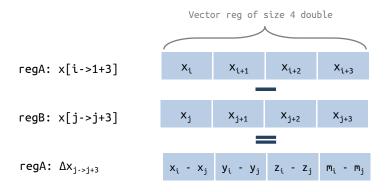
Eventually, we'll need to multiply `regA×regB` to get $m_i \times m_j$ (this time wasting 3 out of 4 entries), and to multiply the result by the scalar value of $1/r^2$ to have the force between two particles.

| regA: PPos[i] | pos[0] | pos[1] | pos[2] | m |

| regA: PPos[j] | pos[0] | pos[1] | pos[2] | m |

| regC: PPos[i] - PPos[j] | $x_i - x_j$ | $y_i - y_j$ | $z_i - z_j$ | $m_i - m_j$ |

Auto vectorization of loops

If, instead, we opt for a **S**tructure **o**f **A**rrays (**SoA**) approach:

```
double    *x, *y, z*, *mass, *xacc, *yacc, *zacc, *xvel, *yvel, *zvel;
long long *ids;
```
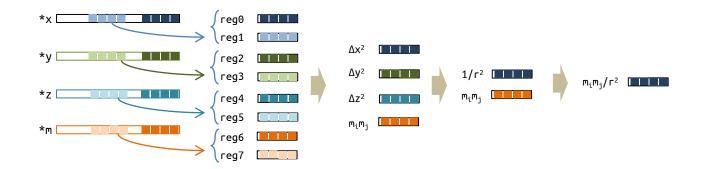
the possible vectorization is definitely higher:

Vector reg of size 4 double

regA: x[i->1+3]

| x_i | x_{i+1} | x_{i+2} | x_{i+3} |

regB: x[j->j+3]

| x_j | x_{j+1} | x_{j+2} | x_{j+3} |

regA: $\Delta x_{j->j+3}$

| $x_i - x_j$ | $y_i - y_j$ | $z_i - z_j$ | $m_i - m_j$ |

With 3 vec `sub` we'll get $\Delta x, \Delta y, \Delta z$ among four particles; four additional vec `mul` would convey $\Delta x^2, \Delta y^2, \Delta z^2$ and [$m_i m_j$, $m_{i+1} m_{j+1}$, ...].

A final vec `mul` will convey the force beween **four particles**.

Auto vectorization of loops

Data rearranged in **SoA** approach definitely would expose more, and more efficient, vectorization opportunities.
That said, however, what is really convenient in every specific case may depend on several additional factors and that, in the context of this lecture, hinders more than just mentioning and explaining the vectorization advantage of SoA.

Auto vectorization of loops

Give hints and directions to the compiler

GCC

`#pragma GCC ivdep`	ignore potential loop-carried dependencies that are not formally proven
`#pragma GCC unroll n`	unroll the subseuquent loop body n times

clang

`#pragma clang ivdep`	ignore potential loop-carried dependencies
`#pragma clang vectorize (<enable|disable>)`	enable the vectorization of the following loop
`#pragma clang vectorize_width ( N )`	specifies the VL
`#pragma clang interleave (<enable|disable>)`	enable the unrolling of the following loop
`#pragma clang interleav_count ( N )`	specifies how many iterations are to be unrolled

check the compiler's manual for comprehensive and updated descriptions

[3] Auto vectorization

Auto vectorization of loops

Give hints and directions to the compiler

Intel

`#pragma ivdep`	`ignore potential loop-carried dependencies`
`#pragma vector always`	`vectorize even if the estimated gain is low or negative`
`#pragma vector aligned`	`assume aligned data`
`#pragma vector unliagned`	`assume unaligned data`

check the compiler's manual for comprehensive and updated descriptions

Auto vectorization of loops

Give hints and directions to the compiler

```
#define STRINGIFY(X) #X
#define _DO_PRAGMA(x) _Pragma (#x)

#if defined(__GNUC__) && !defined(__clang__)
#pragma message "using GCC"
#define IVDEP                _Pragma("GCC ivdep")
#define LOOP_VECTORIZE       _Pragma("GVV ivdep")
#define LOOP_VECTOR_LENGTH(N)
#define LOOP_UNROLL          _Pragma("GCC unroll")
#define LOOP_UNROLL_N(N)     _DO_PRAGMA(GCC unroll N)

#elif defined(__clang__)
#define IVDEP                _Pragma("clang ivdep")
#define LOOP_VECTORIZE       _DO_PRAGMA(clang loop vectorize( enable ))
#define LOOP_VECTOR_LENGTH(N) _DO_PRAGMA(clang vectorize_width( N ))
#define LOOP_UNROLL          _DO_PRAGMA(clang loop interleave( enable ))
#define LOOP_UNROLL_N(N)     _DO_PRAGMA(clang loop interleave_count( N ))

#elif defined(__ICC)
#define IVDEP              _Pragma("ivdep")
#define LOOP_VECTORIZE     _Pragma("ivdep")
#define VECTOR_ALWAYS      _Pragma("vector always")
#define VECTOR_ALIGNED     _Pragma("vector aligned")
#define VECTOR_UNALIGNED   _Pragma("vector unaligned")
```

check the example file
`Vectorization/headers/vector_pragmas.h`
to have an example of how you may define
your own pragmas without bothering about
which compiler you're using

Auto vectorization of loops

[>   Challenges   <]

1. write a code to generate the **Mandelbrot set** for a given region of the complex plane, and compare the naive version with a vectorized one.

2. write a code for a **convolution kernel** (for instance, to blur an image), and compare the naive version and the vectorized one

3. write a very simple **N-body code** that performs the estimate of the $1/r^2$ force among N_p particles, updates their accelerations and their velocity in a timestep **Δ**t.
   As above, try to vectorize the code and compare the relative performance.

[4]

Vectorization by vector types

- How to define a vector type
- Memory alignment
- In practice
- Unrolling by hands
- Conditional evaluations

Vector types in C/C++

De facto standard to declare vector types in C / C++ (*)

```
typedef type name __attribute__ ((vector_size ( bytes ) ));
```

type	the basic type for every element of the vector
name	the name with which you will refer to the type in your code
bytes	the vector width in bytes

vector of 4 double
```
typedef double v4d __attribute__ ((vector_size ( 4*sizeof(double) ) ));
```
vector of 8 double
```
typedef double v8d __attribute__ ((vector_size ( 8*sizeof(double) ) ));
```
vector of 4 integers
```
typedef int v4i __attribute__ ((vector_size ( 4*sizeof(int) ) ));
```

(*) There are third-party libraries that provide interfaces to low-level types and intrinsics, especially for C++. Check
Highway, EVE, xsimd, VCL (Vector Class Library)

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Vector types in C/C++

Let's say that we declare a vector of 4 double

```
typedef double v4d __attribute__ ((vector_size ( 4*sizeof(double) ) ));
```

Is it possible to access singularly each one of the double in the vector?
No, exactly as you can not access the single bytes in a double.
However, there a standard way to do that:

```
typedef union {
  v4d    V;
  double v[VD_SIZE];
}v4d_u;
```

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Vector types in C/C++

Declare a vector of 4 double

```
typedef double v4d __attribute__ ((vector_size ( 4*sizeof(double) ) ));
```

and by using

```
  typedef union {
    v4d     V;
    double v[VD_SIZE];
  }v4d_u;
```

find the order of elements in the vector: is the first double placed at the lowest or at the highest memory address ?

Vector types :: memory alignment

- It is mandatory that memory regions accessed by vector instructions are aligned (see this slide)
  32B for AVX/AVX2 and 64B for AVX512 (on x86_64 architecture)

- Loops are translated by the compiler:
  - ▶ **Peeling** - scalar until aligned addresses are reached
  - ▶ **Main body** - well vectorized from aligned addresses
  - ▶ **Remainder** - scalar ops if the number of elements is not a multiple of the VL

Vector types :: memory alignment

- It is mandatory that memory regions accessed by vector instructions are **aligned**.

- Loops translated by the compiler consist of three sections:
  - ▶ **Peeling loop** - scalar until aligned addresses are reached
    - → avoided by proper alignment
  - ▶ **Main body** - well vectorized from aligned addresses
  - ▶ **Remainder loop** - scalar ops if the number of elements is not a multiple of the VL
    - → (maybe) avoided by hinting the compiler

    e.g. `__attribute((__assume(N%4==0)))`
    or by accounting for the main body and the remainder explicitly

Vector types :: memory alignment

Controlling the alignment

- Allocated memory
    - ▶ C11
      ```
      void * aligned_alloc (size_t alignment, size_t size)
      ```

    - ▶ POSIX
      ```
      int posix_memalign (void **memptr, size_t alignment, size_t size)
      ```

- Static allocation (i.e. variables or automatic arrays)
  ```
  __attribute__ ((aligned(base))) <var>
  ```

- Assuming alignment
  ```
  __assume_aligned(<array>, base)
  ```

Vector types :: in practice

Re-implement the following loop using the vector types and check what changes in the generated assembler code and in the run-time

```
double kernel( double *data, int N )
  {
      double sum = 0;
      for ( int i = 0; i < N; i++ )
        sum += data[i];

      return sum;
  }
```

Unrolling loops by hands

When unrolling a loop by hands, which you tipically do in order to expose more parallelism as we have discussed in the previous slides, you also need to separately handle the main loop and the remind loop.

```
for (int i = 0; i < N; i++ ) ...
```

becomes

```
int N4 = (N/4)*4;   --> integer division ensures that N4 is the largets
                        multiple of 4 that is smaller than N

for ( int i = 0; i < N4; i+=4 ) ...         main body

for ( int i = N4; i < N; i++ ) ...          remaind
```

Unrolling loops by hands

You can give some additional hint to the compiler so that to avoid the issuing of additional codes to check the peeling

The line
```
int N4 = (N/4)*4;
```

→ Vectorization/3_fma_loop/hint_compiler<..>.c

can be rewritten as
```
N4 = N&0xFFFFFFFC;   --> use 0xFFFFFFF8 for 8
                     --> use 0xFFFFFFFFFFFFFFFF<C|8> for 64bits integers
```

this will (may, on some compilers) hint the compiler that N4 is a multiple of 4, without need of issuing additional code.
Alternatively,
```
N4 __attribute((__assume(N4 % 4 == 0)));
```
may also work (on some compilers)

Vector types :: in practice

1) define the appropriate vector variables

```
#define VD_SIZE 4
 typedef double v4df __attribute__ ((vector_size (VD_SIZE*sizeof(double))));
 typedef union
  {
    v4df   V;
    double v[VD_SIZE];
  } v4df_u;


v4df *vA  = (v4df*)A;
v4df *vB  = (v4df*)B;
v4df *vC  = (v4df*)C;
v4df vsum = {0};
```

Vector types :: in practice

2) Re-define the iteration space

```
int N4  = N&0xFFFFFFFC;
for ( int i = 0 ; i < N4; i++ )         // main body
   vsum += vA[i] * vB[i] + vC[i];

v4df_u *vsum_u = (v4df_u*)&vsum;        // summation of the 4 entries of vsum
vsum_u->v[0] += vsum_u->v[1] +          // vsum[0] will contain the scalar sum
              (vsum_u->v[2] + vsum_u->v[3]);

for ( int i = N4*4; i < N; i++ )        // remind loop
   sum += A[i]*B[i] + C[i];             // sum up the final elements

sum += vsum_u->v[0];
```
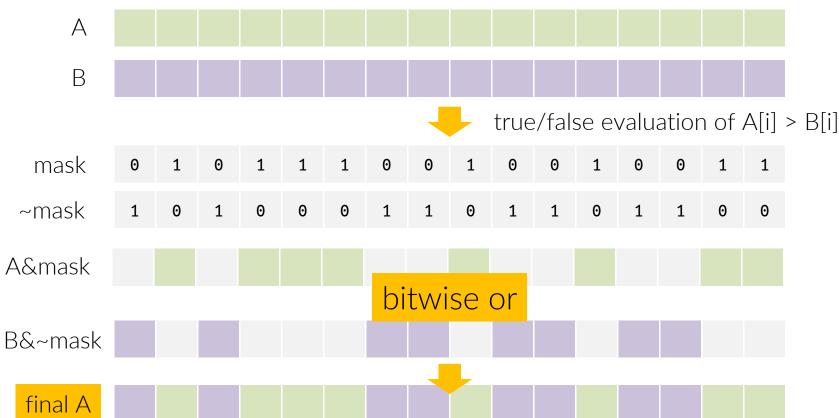
Vector types :: conditional evaluation

Although life is a long sequence of IF-THIS-THEN-THAT and we stated at the begin of these series of lectures that the conditionals hinder the vectorization, or at least render it much more difficult.
The only "easily" vectorizable if-conditions are those solvable as "masquerable" events

```
void kernel( double * restrict A, double * restrict B, const int N )
    // element-wise swap of A and B so that
    //   A[i] > B[i] for every i
    {
        for ( int i = 0; i < N; i++ )
          if ( A[i] < B[i] ) swap(A, B);
        return;
    }
```

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Vector types :: conditional → masking

A

B

true/false evaluation of A[i] > B[i]

| mask | 0 | 1 | 0 | 1 | 1 | 1 | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 1 | 1 |

| ~mask | 1 | 0 | 1 | 0 | 0 | 0 | 1 | 1 | 0 | 1 | 1 | 0 | 1 | 1 | 0 | 0 |

A&mask

bitwise or

B&~mask

final A

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Vector types :: conditional evaluation → masking

The concept of vectorized conditional flow can really be thought as "projecting" through a mask so that the final values that are "impressed" in the memory positions pass through the "transparent" entries and are blocked by "opaque" ones.

Many "projected" values could of course overlap by using multiple masks combines with bit-wise operators.

West rose window, Zodiac, 1220/25 - Cathedral de NôtreDame de Paris

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Vector types :: conditional / 1

Actually this code can be easily fully vectorized by the compiler itself with the appropriate compilation flags.

We use it as a testbed to experiment how the conditionals could be expressed using vector types.

```c
void kernel( double *A, double *B, int N )
   // element-wise swap of A and B so that
   //   A[i] > B[i] for every i
   {
      for ( int i = 0; i < N; i++ ) {
        double min = (A[i]>B[i] ? B[i] : A[i]);
        double max = (A[i]>=B[i] ? A[i] : B[i]);
        A[i] = max;
        B[i] = min;  }
   return;
   }
```

→ Vectorization/3_conditionals/vector_conditionals.a.c

Vector types :: conditional / 1

```
void kernel( double *restrict A, double *restrict B, const int N )
```

```
for ( int i = 0; i < N; i++ )
  {
    double min = (A[i]>B[i] ? B[i] : A[i]);
    double max = (A[i]>=B[i] ? A[i] : B[i]);
    A[i] = max;
    B[i] = min;
  }
```

```
dvector_t *vA = (dvector_t *)__builtin_assume_aligned(A, VALIGN);
dvector_t *vB = (dvector_t *)__builtin_assume_aligned(B, VALIGN);

int VN = (N/DVSIZE)&0xFFFFFFFC;
IVDEP
LOOP_VECTORIZE
LOOP_UNROLL_N(4)
for ( int i = 0; i < VN; i++ )
  {
    dvector_t a    = vA[i];
    dvector_t b    = vB[i];
    llvector_t keep = (vA[i]>=vB[i]);
    vA[i] = (dvector_t)(((llvector_t)a & keep) |
                        ((llvector_t)b & ~keep));
    vB[i] = (dvector_t)(((llvector_t)b & keep) |
                        ((llvector_t)a & ~keep));
  }

int j = VN*DVSIZE;
process ( &A[j], &B[j], N-j+1);
```

plain version

version A

→ /Vector/4_conditional/vector_conditional.a.c::vprocessA

Vector types :: conditional / 1

cast to pointers to vector type
assume memory alignment
(note: the arrays *must* have been allocated aligned)

```
void kernel( double *restrict A, double *restrict B, const int N )

1  dvector_t *vA = (dvector_t *)__builtin_assume_aligned(A, VALIGN);
2  dvector_t *vB = (dvector_t *)__builtin_assume_aligned(B, VALIGN);
3
4  int VN = (N/DVSIZE)&0xFFFFFFFC;
5  IVDEP
6  LOOP_VECTORIZE
7  LOOP_UNROLL_N(4)
8  for ( int i = 0; i < VN; i++ )
9    {
10     dvector_t a     = vA[i];
11     dvector_t b     = vB[i];
12     llvector_t keep = (vA[i]>=vB[i]);
13
14     vA[i] = (dvector_t)(((llvector_t)a & keep) |
15                          ((llvector_t)b & ~keep));
16     vB[i] = (dvector_t)(((llvector_t)b & keep) |
17                          ((llvector_t)a & ~keep));
18    }
19
20  int j = VN*DVSIZE;
21  process ( &A[j], &B[j], N-j+1);
```

version A

remap the iteration space & signal that no peeling is needed

unroll & vectorization hints / requests

build the mask as a vector of integers - the bitfield must have the same than the data you will mask

make it local - i.e. suggest that data should be resident in registers

final masking: (a & keep) will contain a's entries where mask==1 and 0 elsewhere; at the opposite, (b & ~keep) will contain b's entries where the mask==0.
The | is blending the two in one.

```
dvector_t
VALIGN
DVSIZE
IVDEP
LOOP_VECTORIZE
LOOP_UNROLL_N
are defined in /Vector/header/*_pragmas.h
```

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[4] Vector types
→ /Vector/4_conditional/vector_conditional.a.c::vprocessA
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Vector types :: conditional / 1

cast to pointers to vector type

assume memory alignment
(note: the arrays *must* have been allocated aligned)

remap the iteration space & signal that no peeling is needed

unroll & vectorization hints / requests

make it local using union type: we will be able to access individual elements

masking is done individually via the union trick

reassign to array's elements

```
    void kernel( double *restrict A, double *restrict B, const int N )

1   dvector_t *vA = (dvector_t *)__builtin_assume_aligned(A, VALIGN);
2   dvector_t *vB = (dvector_t *)__builtin_assume_aligned(B, VALIGN);
3
4   int VN = (N/DVSIZE)&((-(int)DVSIZE);
5   IVDEP
6   LOOP_VECTORIZE
7   LOOP_UNROLL_N(4)
8   for ( int i = 0; i < VN; i++ )
9     {
10      dvector_u vAu, vBu;
11      vAu.V = vA[i];
12      vBu.V = vB[i];
13      for ( int j = 0; j < DVSIZE; j++ ) {
14        vAu.v[j] = ( vAu.v[j] >= vBu.v[j]? vAu.v[j] : vBu.v[j]);
15        vBu.v[j] = ( vAu.v[j] >= vBu.v[j]? vBu.v[j] : vAu.v[j]); }
16      vA[i] = vAu.V;
17      vB[i] = vBu.V;
18    }
19
20  int j = VN*DVSIZE;
21  process ( &A[j], &B[j], N-j+1);
```

version B

[> Exercise <]
Inspect the assembler code and find that the issued code is basically the same in the three cases

→ /Vector/4_conditional/vector_conditional.a.c::vprocessB

Vector types :: conditional /2

```
void kernel( double *restrict A, double *restrict B, const int N )
```

```
double sum = 0;
for ( int i = 0; i < N; i++ )
  {
    double tmp = A[i]*B[i];
    if ( tmp > 0.5 ) sum += B[i];
  }
return sum;
```

[> Exercise <]

Let's analyze that together

plain version

```
 1  dvector_t *vA = (dvector_t *)__builtin_assume_aligned(A, VALIGN);
    dvector_t *vB = (dvector_t *)__builtin_assume_aligned(B, VALIGN);
 2
 3  int VN = (N/DVSIZE)&0xFFFFFFFC;
 4  IVDEP
 5  LOOP_VECTORIZE
 6  LOOP_UNROLL_N(4)
 7  for ( int i = 0; i < VN; i++ )
 8      {
 9        dvector_t a     = vA[i]*vB[i];
10        dvector_t b     = vB[i];
11        llvector_t keep = (a > 0.5);
12        vsum += (dvector_t)( (llvector_t)b & keep );
13      }
14
15    dvector_u *vsum_u = (dvector_u*)&vsum;
16    vsum_u->v[0] += vsum_u->v[1] + (vsum_u->v[2] + vsum_u->v[3]);
17
18    int j = VN*DVSIZE;
19    double sum = 0;
20
21    sum += process ( &A[j], &B[j], N-j+1);
      sum += vsum_u->v[0];
```

version A

→ /Vector/4_conditional/vector_conditional.b.c::vprocess

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[5]

Vectorization by OpenMP SIMD directive

- How to define a vector type
- Memory alignment
- In practice
- Unrolling by hands
- Conditional evaluations

Addressing modes in x64 assembly

TBD

Main sources

- [Intel®'s Intrinsics Guide](#)

- [Cornell's Virtual Workshop on Vectorization](#) *(cited as VWV)*

- [SIMD at Algorithmica.org](#)

- High Performance Parallelism Pearls, Volume 1 & 2

- Materials and examples uploaded in the git

That`s all folks, have fun