Vectorization

November 30, 2022

Principle

Vectorization consists in

- Reformulate algorithms
- So that they operate on vectors
 - ▶ Use only level-1 BLAS...

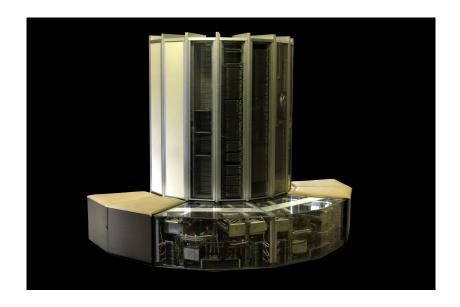
$$\begin{array}{lll} A \leftarrow \lambda B + \mu C & A[i] \leftarrow \lambda B[i] + \mu C[i] \\ A \leftarrow B + C \times D & A[i] \leftarrow B[i] + C[i] \times D[i] & (\textit{Fused Multiply-Add}) \\ A \leftarrow |B| & A[i] \leftarrow |B[i]| \\ A \leftarrow \max(B,C) & A[i] \leftarrow \max(B[i],C[i]) \\ A[B] \leftarrow C & A[B[i]] \leftarrow C[i] & (\textit{scatter}) \\ A \leftarrow C[B] & A[i] \leftarrow C[B[i]] & (\textit{gather}) \\ A \leftarrow B \leq C & A[i] \leftarrow B[i] \leq C[i] \end{array}$$

Why?

Operations on vectors are intrinsically parallel

- Easy way to express parallelism
 - Fortran (≥ 90), numpy natively handle vectors
 - ▶ But not C...
- Vector processors used to rule the HPC world
 - Cray 1 (1975)
 - Cray X-MP (1982)
 - Cray 2 (1985)
 - ► IBM 3090 (1985)
 - Fujitsu VP2000 (1988)
 - ► NEC SX (1992)
 - **...**

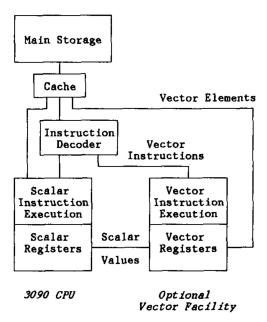
Vector Processors — Before



Vector Processors — Now



IBM 3090 CPU



6

Interest of Vector Instructions

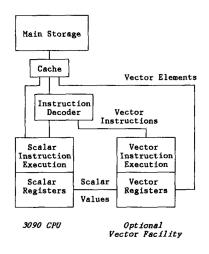
- Possibility of parallel processing
 - Low end = a little
 - ► High-end = a lot
- ► A single instruction gives a lot of work
 - Save on instruction decoding
- ▶ Chained operations → pipelining
 - Power efficiency

Why did it disappear?

- Needs fast memory to transfer the vectors
- Scatter/gather very hard on memory subsystem
- ⇒ (expensive) processors/machines dedicated to HPC
- But trend towards commodity components (ASCI red)

1985 IBM 3090, vector registers of 32Z bits

- Z unspecified, implementation-dependent
- ► Concretely, $Z = 128 \rightsquigarrow 4096$ -bit vectors



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```
1996 Intel Pentium MMX: 64 bit-vectors (8*int8/4*int16)
```

- 1999 Intel SSE: 128-bit vectors, 4*float only
- 2001 Intel SSE2: more types, int and double
- 2004 Intel SSE3: more operations
- 2007 Intel SSE4: more operations
- 2010 Intel AVX: 256-bit vectors, 8*float only
- 2010 Intel AVX2: more types, int and double + gather
- 2017 Intel AVX512: 512-bit, all types + scatter/gather/mask

ISA	Accronym	Name	Year	# regs	regs
IBM 3090		Vector Facility	1985	16	variable
x86-64	MMX	Multi Media eXtensions	1996	8	64
	3DNow!		1998	8	64
	SSE	Streaming SIMD Extensions	1999	16	128
	SSE2		2001		
	SSE3		2004		
	SSSE3		2004		
	SSE4		2007		
	AVX	Advanced Vector eXtensions	2010	16	256
	AVX2		2013		
	AVX512		2017	32	512
PowerPC	Altivec		1999	32	128
ARM v7	NEON Advanced SIMD extension	Advanced SIMD extension	2005	16	128
ARM v8		2011	32	120	
	SVE	Scalable Vector Extensions	2020	32	variable

- ARMv8 SVE : registers of (128Z)-bit ($1 \le Z \le 16$)
 - fugaku has SVE with 512-bit registers
 - ► AWS graviton has SVE with 256-bit registers
- ▶ RISC-V has an "old school" vector extension (IBM 3090-like)

Two Styles

"Real" (old-school) vector architectures

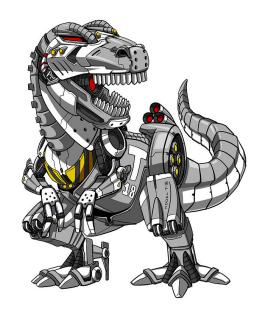
- Unknown register size, or no registers at all
- Functionality: Scatter + Gather + masks
- ► Revival: ARMv8 SVE, RISC-V, AVX-512, ...

SIMD Instructions available in consumer CPUs

- Fixed register size
- Stacking of successive generations
- Constrained memory access

In between / besides: GPUs

Vector Processors — Revival?



- ARM Neon is there in all smartphones
 - And recent Apple macbooks
- Nearly all x86 CPUs presently have AVX2
- AVX512 is not for everybody
 - ► Intel Xeon bronze/silver/gold (since 2017)
 - Intel Some core i7/i9 ("X" or "extreme")
 - AMD EPYC "Zen 4"
- ► AVX512 @ g5k:
 - dahu (Grenoble)
 - gros (Nancy)

chbouillaguet@gros-70:~\$ cat /proc/cpuinfo

model name : Intel(R) Xeon(R) Gold 5220 CPU @ 2.20GHz

. . .

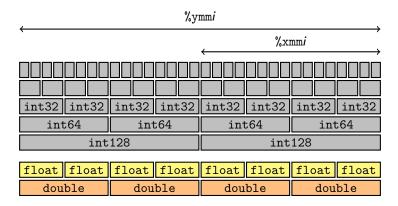
: fpu vme de pse tsc msr pae mce cx8 apic sep mtrr pge flags mca cmov pat pse36 clflush dts acpi mmx fxsr sse sse2 ss ht tm pbe syscall nx pdpe1gb rdtscp lm constant_tsc art arch_perfmon pebs bts rep_good nopl xtopology nonstop_tsc cpuid aperfmperf pni pclmulqdq dtes64 monitor ds_cpl vmx smx est tm2 ssse3 sdbg fma cx16 xtpr pdcm pcid dca sse4_1 sse4_2 x2apic movbe popcnt tsc_deadline_timer aes xsave avx f16c rdrand lahf_lm abm 3dnowprefetch cpuid_fault epb cat_13 cdp_13 invpcid single pti intel ppin ssbd mba ibrs ibpb stibp tpr shadow vnmi flexpriority ept vpid ept ad fsgsbase tsc adjust bmi1 hle avx2 smep bmi2 erms invpcid rtm cgm mpx rdt a avx512f avx512dg rdseed adx smap clflushopt clwb intel pt avx512cd avx512bw avx512vl xsaveopt xsavec xgetbv1 xsaves cqm llc cqm occup llc cqm mbm total cqm mbm local dtherm ida arat pln pts pku ospke flush 11d

Problems with SIMD Instruction Sets

Their multiplicity makes them hard to use

- Needs recompilation at each new iteration
 - Even rewrite code / change algorithms...
- Makes code non-portable
 - Does the CPU that will run it have AVX-xxx?
 - Query the CPU at runtime...
 - ... and choose appropriate function (sigh)

SSEx + AVX + AVX2



Instructions	registers	size	
SSEx	%xmm0,, %xmm15	128-bit	
AVX + AVX2	%ymm0,, %ymm15	256-bit	
AVX512	%zmm0,, %zmm31	512-bit	
ΑνΑΣΙΖ	%k0,, %k7	64-bit	

SIMD Instructions Nomenclature

Floating-point SIMD instructions have compound names:

```
<prefix><op><simd or not><type>
```

where

E.g. vmaxpd, vmulss, etc.

Practical Vectorization

General Principle

- 1. Load data into vector registers
- 2. Use vector instructions
- 3. Write result back to memory

(minimise these transfers is an important goal)

Use cases

- Happens inside a single thread
 - Parallelization = distribute over several cores
 - Vectorization = use SIMD instructions inside ONE core
- Only small code chunks can (usually) be vectorized
 - ► Tight **loops** (limits of the instruction set)
 - ⇒ Target the innermost loops

Obstacles

Data dependencies (dependent iterations)

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

- No possible parallel processing
- → Must change the algorithm
- Conditional instructions (if)

```
for (int i = 1; i < n; i++)
  if (a[i] != 0)
     a[i] = 1 / a[i];</pre>
```

- Potentially manageable (overhead to avoid if possible)
- Complex memory access pattern and/or alignment problems
 - Loading contiguous array slices only
- Complex operations (sin, cos, log, exp, my_function, ...)

Data Alignment

Rule of thumb

xxx-bytes vector must be located at an address multiple of xxx

Solutions

- double A[n] __attribute__ ((aligned(32)));
 - This is valid C code
- int posix_memalign(void **ptr, size_t align, size_t size);
- void *aligned_alloc(size_t alignment, size_t size);
 - Included in C11

Complex memory access pattern

Array of struct

```
struct point {
     double x, y, z;
};
struct point *A;
xyzxyzxyzxyzxyzxyz....
```

Struct of Array

Vectorizing Simple Loops: strip-mining

Original code

```
for (int i = 0; i < n; i++)
    u[i] = u[i] + alpha * v[i];</pre>
```

Transformed code

```
int m = n - (n % 4);
/* Processing in batches of 4 with SIMD instructions */
for (i = 0; i != m; i += 4) {
    u[i + 0] = u[i + 0] + alpha * v[i + 0];
    u[i + 1] = u[i + 1] + alpha * v[i + 1];
    u[i + 2] = u[i + 2] + alpha * v[i + 2];
    u[i + 3] = u[i + 3] + alpha * v[i + 3];
}
/* epilogue when n is not a multiple of 4 */
for (int i = m; i < n; i ++)
    u[i] = u[i] + alpha * v[i];</pre>
```

- Potentially: prologue to ensure alignment
- The epilogue can be avoided with padding

strip-mining?



Algorithmic Modifications

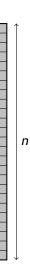
Starting Point

Transformed code

- ► Loop is now vectorizable
- ► Small overhead in epilogue

Sequential Algorithm ${\cal A}$

- Applies to an array X
- "data-oblivious": sequence id instructions independent of the values



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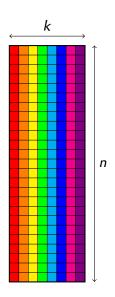


Sequential Algorithm $\mathcal A$

- Applies to an array X
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Apply *k* times the algorithm in parallel

- ightharpoonup scalars ightharpoonup vectors of size k
- ▶ scalar operations → SIMD

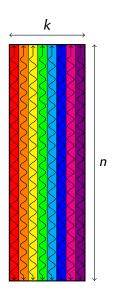


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How to Use SIMD / Vector Instructions?

- 1. Write assembler code directly
- 2. Use "instrinsics" offered by compilers
- 3. Let the compiler do it (automatic vectorization)
- 4. Provide vectorization directives (OpenMP \geq v4.0)
- 5. Use gcc-specific vector extensions

Using the Intrinsics

- Introduced by Intel, later adopted by other compilers
- Pseudo-functions that emit one SIMD instructions
- Need to know the instruction set(s)

Headers

Data Types for the *Intrinsics*

```
Match the hardware "vectors"
    m512 512 bits (16 float)
   m512d 512 bits (8 double)
   m512i 512 bits (ints)
           + __mmask8, __mmask16, __mmask32, __mmask64
    m256 256 bits (8 float)
   m256d 256 bits (4 double)
   m256i 256 bits (ints)
    m128 128 bits (4 float)
   m128d 128 bits (2 double)
   m128i 128 bits (ints)
```

Examples (AVX2)

- _mm256_set1_ps
- _mm256_load_pd
- _mm256_xor_si256
- _mm256_srli_epi32
- mm256_i32gather_mask_pd
- _mm256_cmpeq_epi32
- _mm256_movemask_epi8
- **...**

General Nomenclature

```
_mm_<operation>_<suffix>(param1, param2)
_mm256_<operation>_<suffix>(param1, param2, param3)
_mm512_<operation>_<suffix>(param1, param2, param3)
```

Two-part <suffix>

- 1st part
 - p (packed) and ep (extended packed): SIMD
 - s (scalar): only 1st vector element is active
- 2nd part (type)
 - ▶ [s/d]: single- or double-precision float
 - [i/u]nnn: signed or unsigned nnn-bits integer (nnn is 512, 256, 128, 64, 32, 16, or 8)

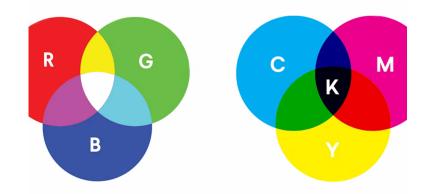
Example

Original Code

```
double alpha;
double u[], v[];
// ...
for (int i = 0; i < n; i++)
    u[i] = u[i] + alpha * v[i];</pre>
```

Vectorized code (AVX2)

Non-Trivial Example: Colorimetric Conversions



Non-Trivial Example: Colorimetric Conversions

R, G, B, C, M, Y, K = floats in [0; 1]

Easy Direction

$$\begin{cases} R = (1 - C) \times (1 - K) \\ G = (1 - M) \times (1 - K) \\ B = (1 - Y) \times (1 - K) \end{cases}$$

Problematic direction

- ► If (R, G, B) = (0, 0, 0) then (C, M, Y, K) = (0, 0, 0, 1)
- Otherwise

$$\begin{cases} K = 1 - \max(R, G, B) \\ C = 1 - R/(1 - K) \\ M = 1 - G/(1 - K) \\ Y = 1 - B/(1 - K) \end{cases}$$

Problems with Conditional Instructions

Example: $RGB \rightarrow CMYK$

```
If K < 1
__m256 vC = _mm256_sub_ps(vone, _mm256_div_ps(vR, vmax));
__m256 vM = _mm256_sub_ps(vone, _mm256_div_ps(vG, vmax));
__m256 vY = _mm256_sub_ps(vone, _mm256_div_ps(vB, vmax));</pre>
```

Problems with Conditional Instructions

Example: $RGB \rightarrow CMYK$

Intructions for shuffling data inside registers:

▶ blend, blendv, broadcast, extract, insert, permute, permutevar, shuffle, unpackhi, unpacklo, ...

Problems with Conditional Instructions

Example: $RGB \rightarrow CMYK$

```
// R. G. B. C. M. Y. K must be aligned
m256 vone, vzero, vmask, vR, vG, vB, vC, vM, vY, vK;
vone = mm256 \text{ set1 ps}(1.0);
                                   // (1, 1, 1, 1, 1, 1, 1, 1)
                                       // (0. 0. 0. 0. 0. 0. 0. 0)
vzero = _mm256_setzero_ps();
for (int i = 0; i < n; i += 8) {
    vR = mm256 load ps(&R[i]);
    vG = _mm256_load_ps(\&G[i]);
    vB = mm256 load ps(\&B[i]);
    vmax = _mm256_max_ps(_mm256_max_ps(vR, vG), vB);
    vK = _mm256_sub_ps(vone, vmax);
    vC = mm256 \text{ sub ps}(vone, mm256 div ps}(vR, vmax));
    vM = _mm256_sub_ps(vone, _mm256_div_ps(vG, vmax));
    vY = _mm256_sub_ps(vone, _mm256_div_ps(vB, vmax));
    vmask = _mm256_cmp_ps(vK, vone, _CMP_EQ_OQ);
    vC = _mm256_blendv_ps(vzero, vC, vmask);
    vM = _mm256_blendv_ps(vzero, vM, vmask);
    vY = _mm256_blendv_ps(vzero, vY, vmask);
    _mm256_store_ps(&C[i], vC);
    mm256 store ps(&M[i], vM);
    _mm256_store_ps(&Y[i], vY);
    _mm256_store_ps(&K[i], vK);
```

OpenMP simd Directive

OpenMP reminder

- requires compiling with -fopenmp
- fopenmp-simd enables SIMD but not threads

```
#pragma omp simd
for (int i = 0; i < n; i++)
...</pre>
```

- Groupe iterations in chunks of size N
 - ▶ Do the computation using *N*-wide SIMD instructions
- We "promise" the compiler that the loop is vectorizable
- No multi-thread parallelization there

OpenMP simd Directive

```
#pragma omp simd [clause[[,] clause],...]
for (int i = 0; i < n; i++)
    ...</pre>
```

Possible clauses (non-exhaustive list)

- reduction(+:v): already known
 - Breaks data dependency on accumulator variable
- simdlen(length): desired chunk size
- safelen(length): maximum allowed chunk size
 - E.g., beyond this a dependency problem could occur
- ▶ aligned(v[:k]): promise that v is aligned on k bytes
- linear(x[:step]): x is an affine function of i
 (x_i = x_init + i * step;)

Automatic Vectorization

- Fortran a has explicit vectors
 - Easy to vectorize
- ► In C, compiler detects **vectorizable loops**

C Code

```
for (int i = 0; i < n; i++)
    C[i] = lambda * A[i] + mu * B[i];</pre>
```

Assembler code produced by gcc

```
.loop:

vmulpd (%rsi,%rax), %ymm3, %ymm0

vmulpd (%rcx,%rax), %ymm2, %ymm1

vaddpd %ymm1, %ymm0, %ymm0

vmovapd %ymm0, (%rdx,%rax)

addq $32, %rax

cmpq %rcx, %rax

jne .loop
```

SIMD Instructions in gcc

- automatic vectorization is disabled by default
 - Without explicit options, "optimization level" = 0
 - automatic vectorization (and OpenMP) disabled
- Enable with option -ftree-vectorize
 - -03 activates this feature
- ▶ We're doing HPC: always compile with -02 or -03
 - ~\$ gcc -01 -ftree-vectorize vectorisation_auto.c
 - ~\$ gcc -01 -fopenmp vectorisation_omp.c
- gcc does not emit AVX2 (resp. FMA) instructions by default
 - Add -mavx2 (resp. -mfma) to the command-line
- Verbosity and diagnostics:
 - -fopt-info-vec, -fopt-info-vec-missed and -fopt-info-vec-all

Case Study

Discrete Fourier Transform (DFT)

▶ The DFT of an array *X* of *n* (complexes) numbers is

$$Y[k] = \sum_{j=0}^{n-1} X[j] \omega_n^{jk}, \quad \text{with} \quad \omega_n = e^{-\frac{2i\pi}{n}} \quad (0 \le k < n)$$

Optimized libraries (e.g. FFTW)

Rewriting the definition

When $n = n_1 \times n_2$, we set $j = j_1 n_2 + j_2$ and $k = k_1 + k_2 n_1$

$$Y[k_1 + k_2 n_1] = \sum_{j_2=0}^{n_2-1} \left[\left(\sum_{j_1=0}^{n_1-1} X[j_1 n_2 + j_2] \omega_{n_1}^{j_1 k_1} \right) \omega_n^{j_2 k_1} \right] \omega_{n_2}^{j_2 k_2}$$

$$n = n_1 \times n_2$$
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Algorithm to compute the DFT of size $n_1 \times n_2$

- 1. Do n_2 DFTs of size n_1 (internal sum)
- 2. Multiply by the *twiddle factors* $\omega_n^{j_2k_1}$
- 3. Do n_1 DFTs of size n_2 (external sum)

```
▶ Common choice : n_2 = 2
       "Radix-2 Decimation in Time"
 ▶ FFT of size 2 : (x,y) \rightarrow (x+y,x-y)
void FFT(const double * X, double *Y, int n, int s)
   if (n == 1) {
      Y[0] = X[0];
      return;
   double omega_n = exp(-2*I*pi / n);
   double omega = 1; // twiddle factor
   FFT(&X[0], &Y[0], n/2, 2*s);
   FFT(&X[s], &Y[n/2], n/2, 2*s);
   for (int i = 0; i < n/2; i++) {
       double p = Y[i];
       double q = Y[i + n/2] * omega;
       Y[i] = p + q;
       Y[i + n/2] = p - q;
       omega *= omega_n;
```

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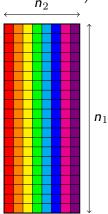
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       double p = Y[i];
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   double omega = 1; // twiddle factor
   FFT(&X[0], &Y[0], n/2, 2*s);
   FFT(&X[s], &Y[n/2], n/2, 2*s);
   for (int i = 0; i < n/2; i++) {
       double p = Y[i];
       double q = Y[i + n/2] * omega;
       Y[i] = p + q;
       Y[i + n/2] = p - q;
       omega *= omega_n;
```

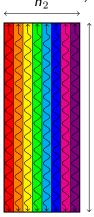
$$Y[k_1 + k_2 n_1] = \sum_{j_2=0}^{n_2-1} \left[\left(\sum_{j_1=0}^{n_1-1} X[j_1 n_2 + j_2] \omega_{n_1}^{j_1 k_1} \right) \omega_n^{j_2 k_1} \right] \omega_{n_2}^{j_2 k_2}$$

- $V[\star,j_2] \leftarrow FFT(X[\star,j_2])$
 - ▶ $0 \le j_2 < n_2$



$$Y[k_1 + k_2 n_1] = \sum_{j_2=0}^{n_2-1} \left[\left(\sum_{j_1=0}^{n_1-1} X[j_1 n_2 + j_2] \omega_{n_1}^{j_1 k_1} \right) \omega_n^{j_2 k_1} \right] \omega_{n_2}^{j_2 k_2}$$

- $V[\star,j_2] \leftarrow FFT(X[\star,j_2])$
 - ▶ $0 \le j_2 < n_2$



 n_1

$$Y[k_1 + k_2 n_1] = \sum_{j_2=0}^{n_2-1} \left(U[k_1 n_2 + j_2] \omega_n^{j_2 k_1} \right) \omega_{n_2}^{j_2 k_2}$$

- \triangleright $U[\star,j_2] \leftarrow FFT(X[\star,j_2])$
 - ▶ $0 \le j_2 < n_2$
- - ▶ $0 \le j_2 < n_2$
 - ▶ $0 \le k_1 < n_1$



 n_1

$$Y[k_1 + k_2 n_1] = \sum_{j_2=0}^{n_2-1} V[k_1 n_2 + j_2] \omega_{n_2}^{j_2 k_2}$$

$$ightharpoonup U[\star,j_2] \leftarrow FFT(X[\star,j_2])$$

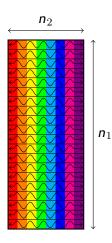
▶
$$0 \le j_2 < n_2$$

▶
$$0 \le j_2 < n_2$$

▶
$$0 \le k_1 < n_1$$

$$\blacktriangleright \ \ Y[k_1,\star] \leftarrow \textit{FFT}(\textit{V}[k_1,\star])$$

▶
$$0 \le k_1 < n_1$$



$$Y[k_1 + k_2 n_1] = \sum_{j_2=0}^{n_2-1} V[k_1 n_2 + j_2] \omega_{n_2}^{j_2 k_2}$$

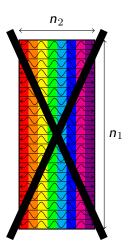
$$ightharpoonup U[\star,j_2] \leftarrow \textit{FFT}(X[\star,j_2])$$

▶
$$0 \le j_2 < n_2$$

▶
$$0 \le j_2 < n_2$$

▶
$$0 \le k_1 < n_1$$

- $\blacktriangleright \ \ Y[k_1,\star] \leftarrow \mathit{FFT}(V[k_1,\star])$
 - ▶ $0 \le k_1 < n_1$

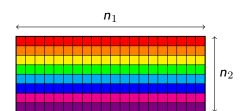


$$Y[k_1 + k_2 n_1] = \sum_{j_2=0}^{n_2-1} V[k_1 n_2 + j_2] \omega_{n_2}^{j_2 k_2}$$

$$\triangleright$$
 $U[\star,j_2] \leftarrow FFT(X[\star,j_2])$

▶
$$0 \le j_2 < n_2$$

- $V[k_1,j_2] \leftarrow U[k_1,j_2] \cdot \omega_n^{j_2k_1}$
 - ▶ $0 \le j_2 < n_2$
 - ▶ $0 \le k_1 < n_1$
- ► Transpose *V*
 - overhead from vectorization

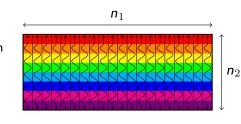


$$Y[k_1 + k_2 n_1] = \sum_{j_2=0}^{n_2-1} V[k_1 n_2 + j_2] \omega_{n_2}^{j_2 k_2}$$

$$V[\star,j_2] \leftarrow FFT(X[\star,j_2])$$

▶
$$0 \le j_2 < n_2$$

- $ightharpoonup V[k_1,j_2] \leftarrow U[k_1,j_2] \cdot \omega_n^{j_2k_1}$
 - ▶ $0 \le j_2 < n_2$
 - ▶ $0 \le k_1 < n_1$
- ► Transpose *V*
 - overhead from vectorization
- $Y[\star, k_1] \leftarrow \mathit{FFT}(V[\star, k_1])$
 - ▶ $0 \le k_1 < n_1$

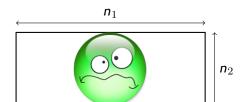


$$Y[k_1 + k_2 n_1] = \sum_{j_2=0}^{n_2-1} V[k_1 n_2 + j_2] \omega_{n_2}^{j_2 k_2}$$

$$V[\star,j_2] \leftarrow FFT(X[\star,j_2])$$

▶
$$0 \le j_2 < n_2$$

- $V[k_1,j_2] \leftarrow U[k_1,j_2] \cdot \omega_n^{j_2k_1}$
 - ▶ $0 \le j_2 < n_2$
 - ▶ $0 \le k_1 < n_1$
- ► Transpose *V*
 - overhead from vectorization
- $ightharpoonup Y[\star, k_1] \leftarrow \textit{FFT}(V[\star, k_1])$
 - ▶ $0 \le k_1 < n_1$



$$Y[k_1 + k_2 n_1] = \sum_{j_2=0}^{n_2-1} V[k_1 n_2 + j_2] \omega_{n_2}^{j_2 k_2}$$

$$V[\star,j_2] \leftarrow FFT(X[\star,j_2])$$

▶
$$0 \le j_2 < n_2$$

$$V[k_1,j_2] \leftarrow U[k_1,j_2] \cdot \omega_n^{j_2k_1}$$

▶
$$0 \le j_2 < n_2$$

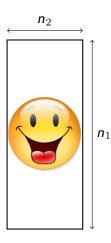
▶
$$0 \le k_1 < n_1$$

- ► Transpose *V*
 - overhead from vectorization

$$Y[\star, k_1] \leftarrow \mathit{FFT}(V[\star, k_1])$$

▶
$$0 \le k_1 < n_1$$

- Retranspose Y
 - overhead from vectorization



Addendum: Vectorized Transposition

