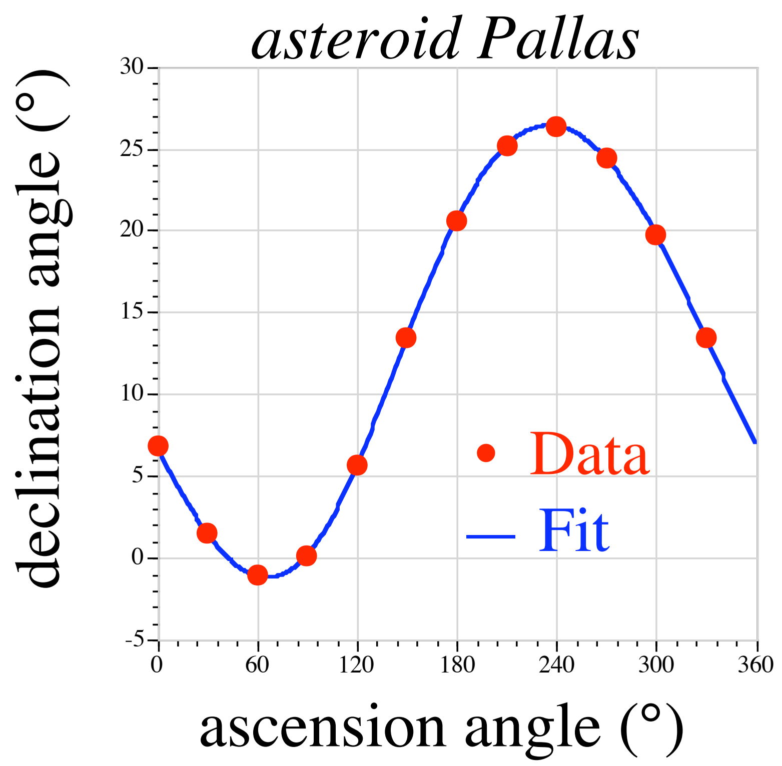
FFTW:

The “Fastest Fourier Transform in the West”

Steven G. Johnson, MIT Applied Mathematics

Matteo Frigo, Cilk Arts Inc.

In the beginning (*c*. 1805):
Carl Friedrich Gauss



trigonometric interpolation:

$$y_j = \sum_{k=0}^{n-1} c_k e^{i\frac{2\pi}{n}kj}$$

$$\Big\downarrow$$

generalizing work of Clairaut (1754) and Lagrange (1762)

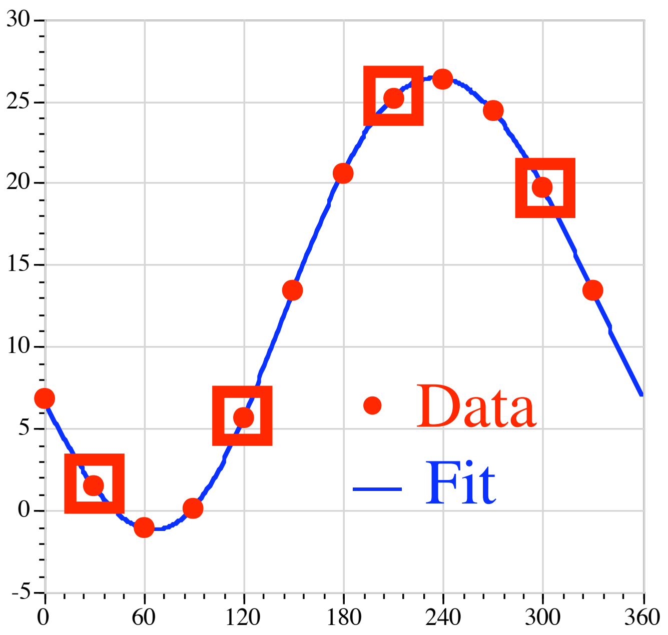
discrete Fourier transform (DFT):
(before Fourier)

$$c_k = \frac{1}{n}\sum_{k=0}^{n-1} y_j e^{-i\frac{2\pi}{n}kj}$$

Gauss' fast Fourier transform (FFT)

how do we compute: $c_k = \frac{1}{n}\sum_{k=0}^{n-1} y_j e^{-\frac{2\pi}{n}kj}$?

— not directly: O(n^2) operations … for Gauss, n=12



Gauss' insight: "*Distribuamus hanc periodum primo in tres periodos quaternorum terminorum.*"

= We first distribute this period [n=12] into 3 periods of length 4 …

Divide and conquer.

(any composite n)

But how fast was it?

“illam vero methodum calculi mechanici taedium magis minuere”

= “truly, this method greatly reduces
the tedium of mechanical calculation”

(For Gauss, being less boring was good enough.)

two (of many) re-inventors:

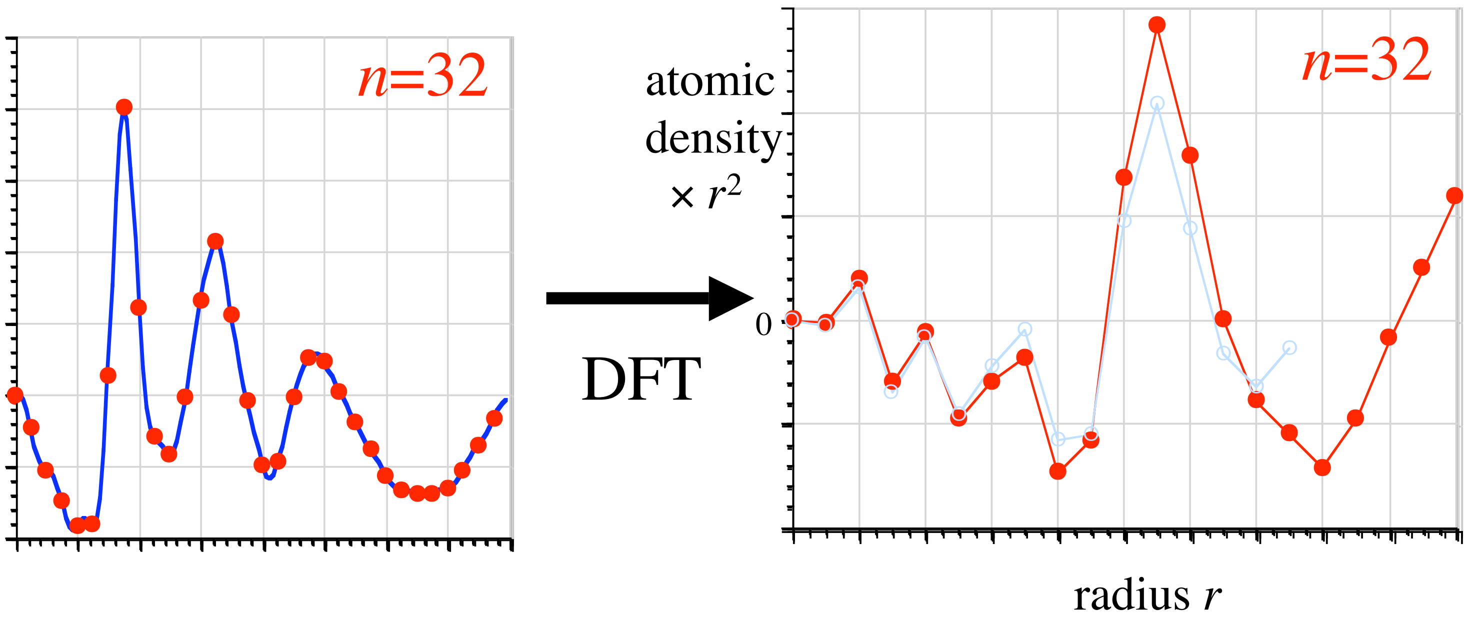
Danielson and Lanczos (1942)

[*J. Franklin Inst*. **233**, 365–380 and 435–452]

Given Fourier transform of density (X-ray scattering) find density:

discrete sine transform (DST-1) = DFT of real, odd-symmetry

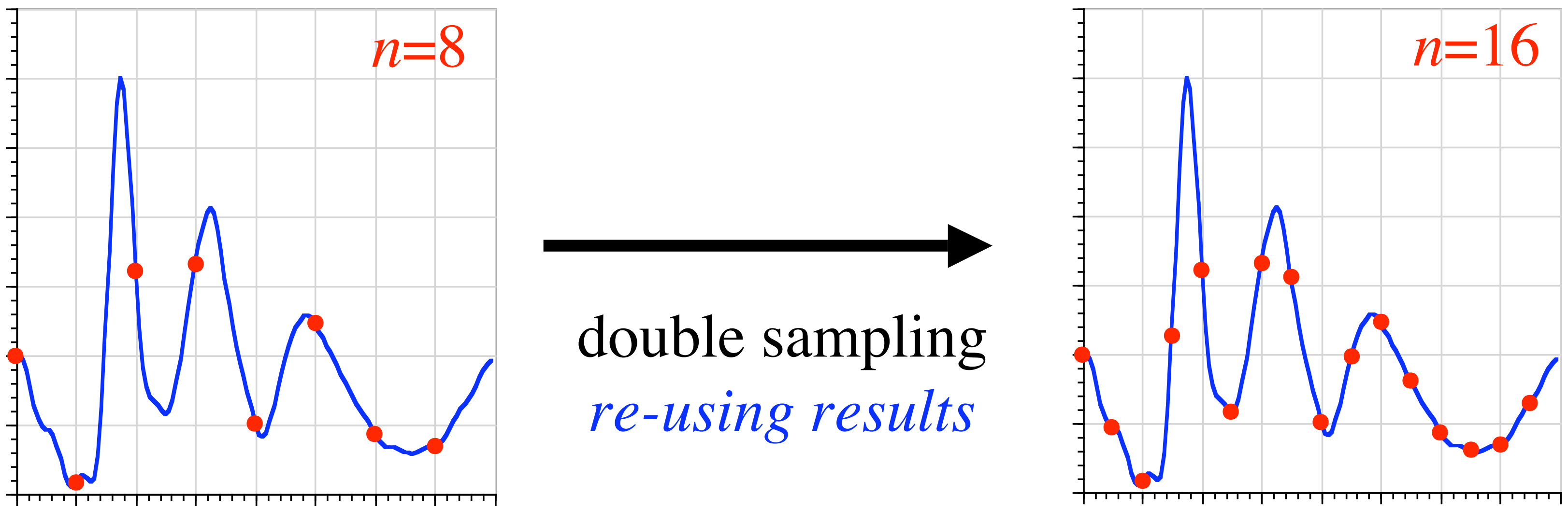
sample
the spectrum
at n points:



…double sampling until density (DFT) converges…

Gauss' FFT *in reverse*:
Danielson and Lanczos (1942)

[*J. Franklin Inst*. **233**, 365–380 and 435–452]



"By a certain transformation process, it is possible to double the number of ordinates with only slightly more than double the labor."

from
O(n^2) to ???

64-point DST in *only 140 minutes!*

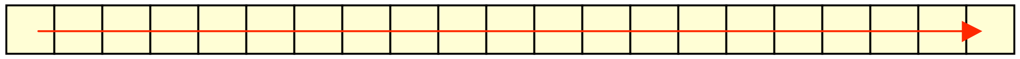
re-inventing Gauss (for the last time)

Cooley and Tukey (1965)

[*Math. Comp.* **19**, 297–301]

$n = pq$

1d DFT of size n:



= ~2d DFT of size p x q

(+ phase rotation by twiddle factors)

= Recursive DFTs of sizes p and q

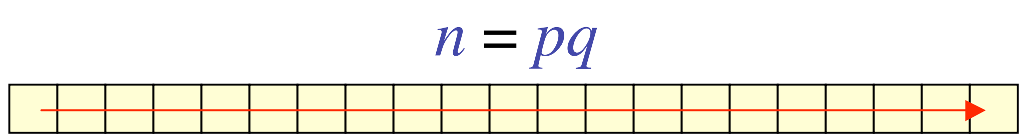
$$O(n^2) \longrightarrow O(n \log n)$$

n=2048, IBM 7094, 36-bit float: 1.2 seconds

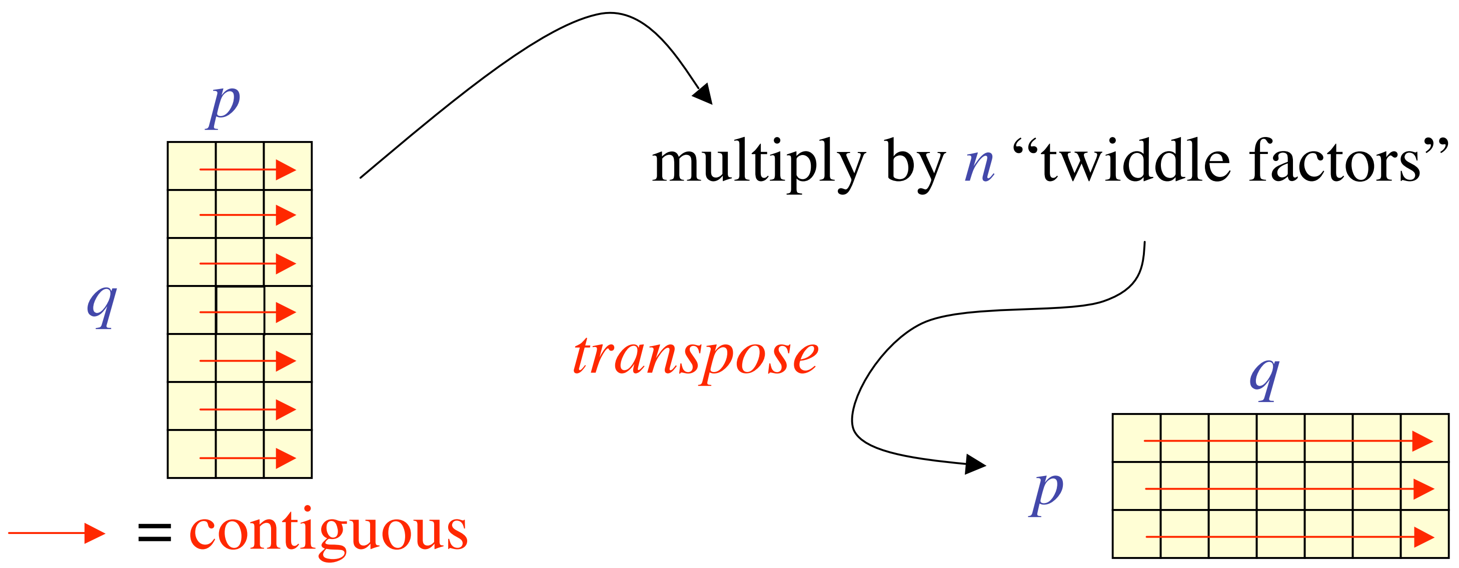
(~10^6 speedup vs. Dan./Lanc.)

The "Cooley-Tukey" FFT Algorithm

1d DFT of size n:



= ~2d DFT of size $p \times q$



first DFT columns, size q
(non-contiguous)

finally, DFT columns, size p
(non-contiguous)

“Cooley-Tukey” FFT, in math

Recall the definition of discrete Fourier transform:

$$y_k = \sum_{j=0}^{n-1} x_j \omega_n^{jk} \,, \qquad \text{where } \omega_n = e^{-2\pi\sqrt{-1}/n} \,.$$

Trick: If $n = pq$, write $j = pj_1 + j_2$ and $k = k_1 + qk_2$.

$$\begin{aligned} y_{k_1+qk_2} &= \sum_{j_2=0}^{p-1} \sum_{j_1=0}^{q-1} x_{pj_1+j_2} \omega_n^{pj_1k_1} \cdot \omega_n^{j_2k_1} \cdot \omega_n^{pqj_1k_2} \cdot \omega_n^{qj_2k_2} \\ &= \sum_{j_2=0}^{p-1} \left[\left(\sum_{j_1=0}^{q-1} x_{pj_1+j_2} \omega_q^{j_1k_1} \right) \omega_n^{j_2k_1} \right] \omega_p^{j_2k_2} \,. \end{aligned}$$

size-p DFTs   size-q DFTs   twiddles

…but how do we make it faster?

We (probably) cannot do better than $\Theta(n \log n)$.

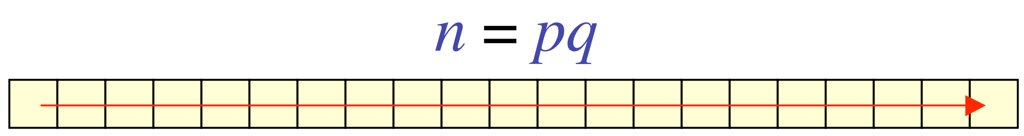
(the proof of this remains an open problem)

[unless we give up exactness]

We’re left with the “constant” factor…

Choice of factorizations: the "radix"

1d DFT of size n:



= ~2d DFT of size p x q

= p DFTs of size q,

… then q DFTs of size p

Usually, either p or q is small = "radix" r

e.g. p=2 is "radix-2 decimation in time"

Cooley & Tukey's error:

thought radix 3 was optimal (closest to e)

— they forgot that size-r DFTs can also use FFT

The Next 30 Years…

Assume "time"

= # ~~multiplications~~

# multiplications + # additions (= flops)

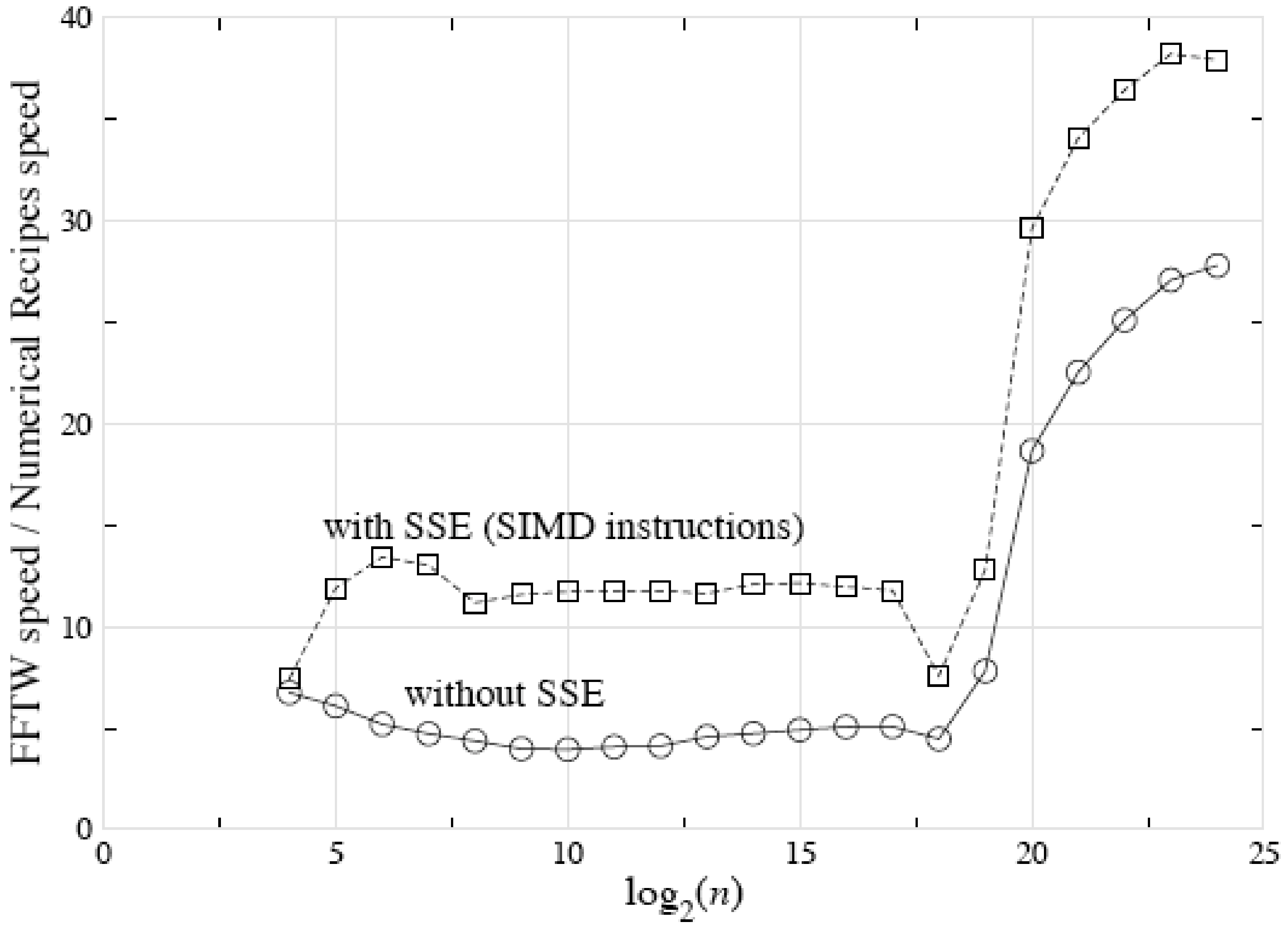
Winograd (1979): # multiplications = $\Theta(n)$

(…realizable bound! … but costs too many additions)

Yavne (1968): split-radix FFT, saves 20% over radix-2 flops

[unsurpassed until last 2007, another ~6% saved by Lundy/Van Buskirk and Johnson/Frigo]

Are arithmetic counts so important?



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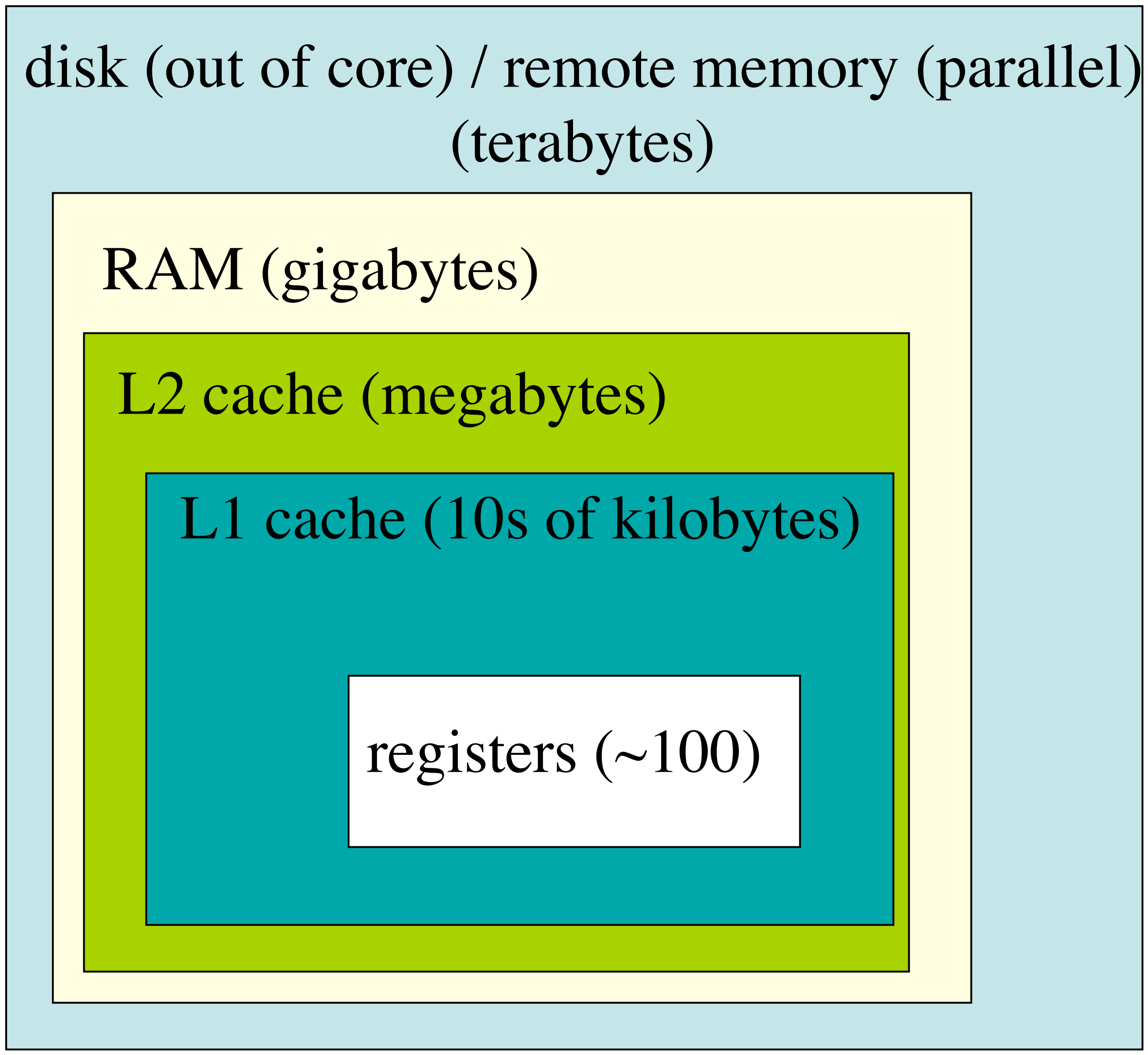
last 15+ years: flop count (varies by ~20%)

no longer determines speed (varies by factor of ~10+)

a basic question:

If arithmetic no longer dominates,
what does?

The Memory Hierarchy (not to scale)


disk (out of core) / remote memory (parallel) (terabytes)
RAM (gigabytes)
L2 cache (megabytes)
L1 cache (10s of kilobytes)
registers (~100)

…what matters is not how much work you do, but *when* and *where you do it*.

the name of the game:

- do as much work as possible before going out of cache

…difficult for FFTs
…many complications
…continually changing

What's the fastest algorithm for ______?

(computer science = math + time = math + $)

1 Find best asymptotic complexity

naïve DFT to FFT: $O(n^2)$ to $O(n \log n)$

~~2 Find best exact operation count?~~

3 Find variant/implementation that runs fastest

hardware-dependent — **unstable answer!**

Better to change the question…

A question with a more stable answer?

What's the smallest
set of "simple" algorithmic steps
whose compositions ~always
span the ~fastest algorithm?

FFTW the "Fastest Fourier Tranform in the West"

- C library for real & complex FFTs (arbitrary size/dimensionality)
  (+ parallel versions for threads & MPI)

- Computational kernels (80% of code) automatically generated

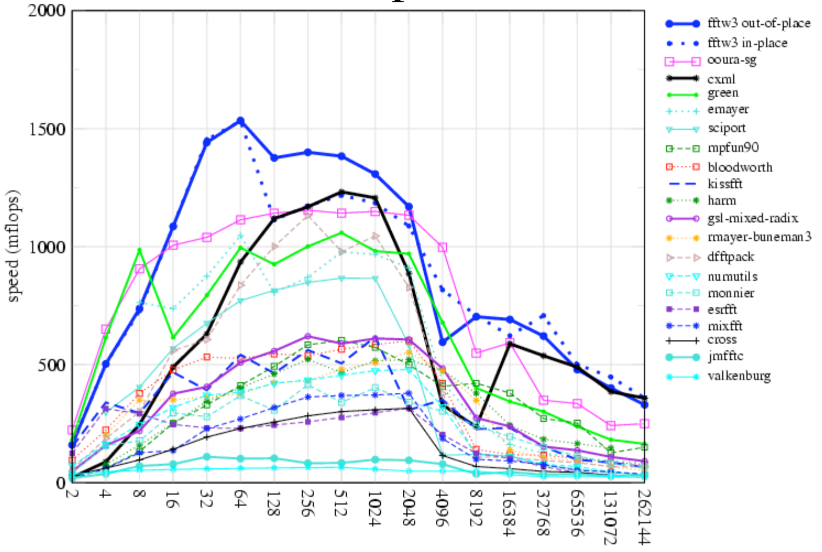
- Self-optimizes for your hardware (picks best composition of steps)
  = **portability + performance**

free software: `http://www.fftw.org/`

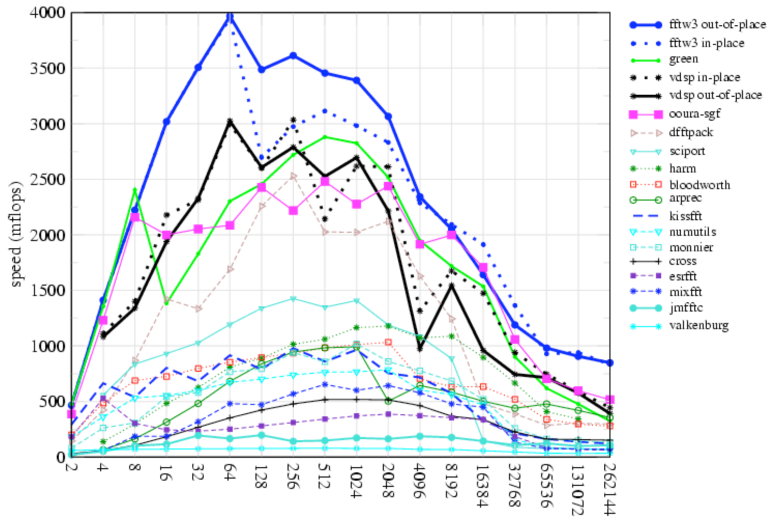
FFTW performance

power-of-two sizes, double precision

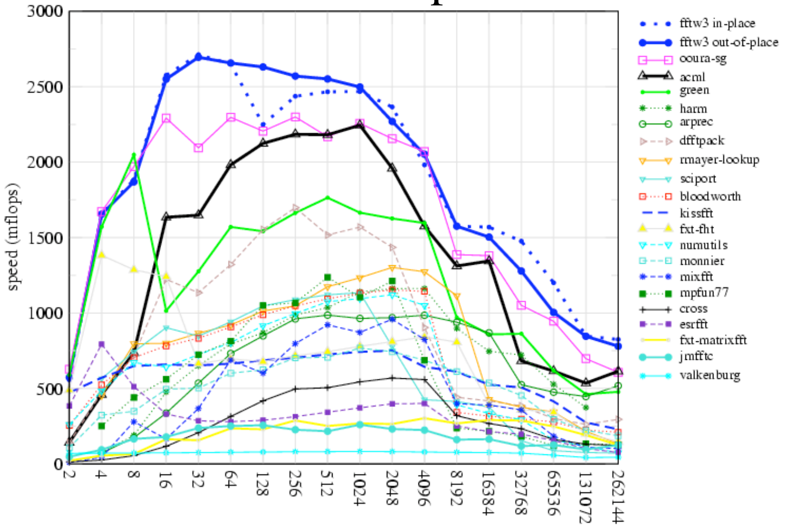
833 MHz Alpha EV6



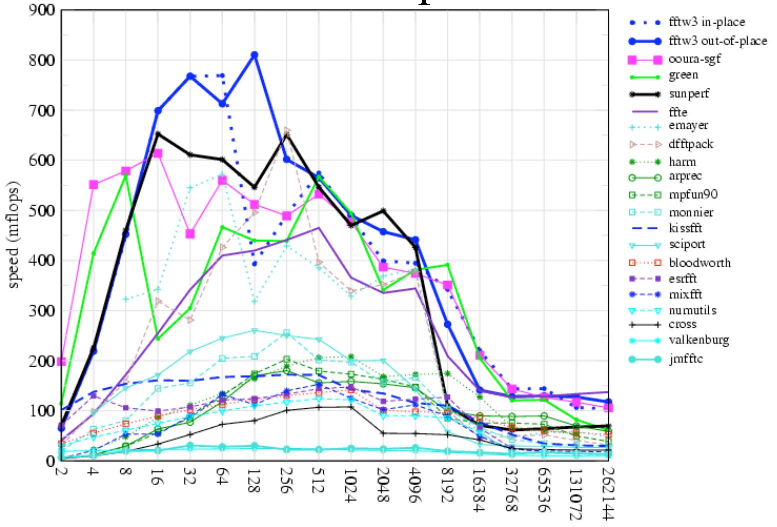
2 GHz PowerPC G5



2 GHz AMD Opteron



500 MHz Ultrasparc IIe

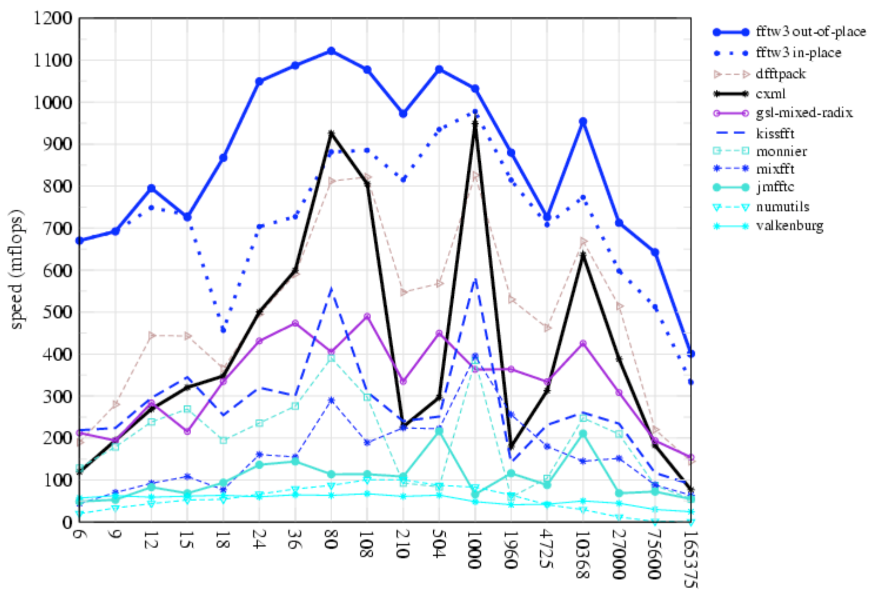


FFTW performance

non-power-of-two sizes, double precision

unusual: non-power-of-two sizes receive as much optimization as powers of two

833 MHz Alpha EV6



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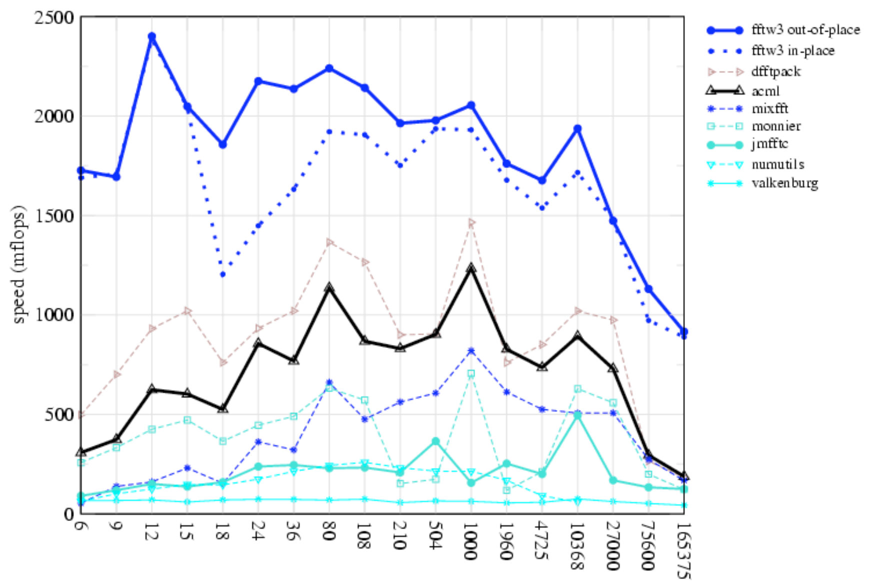
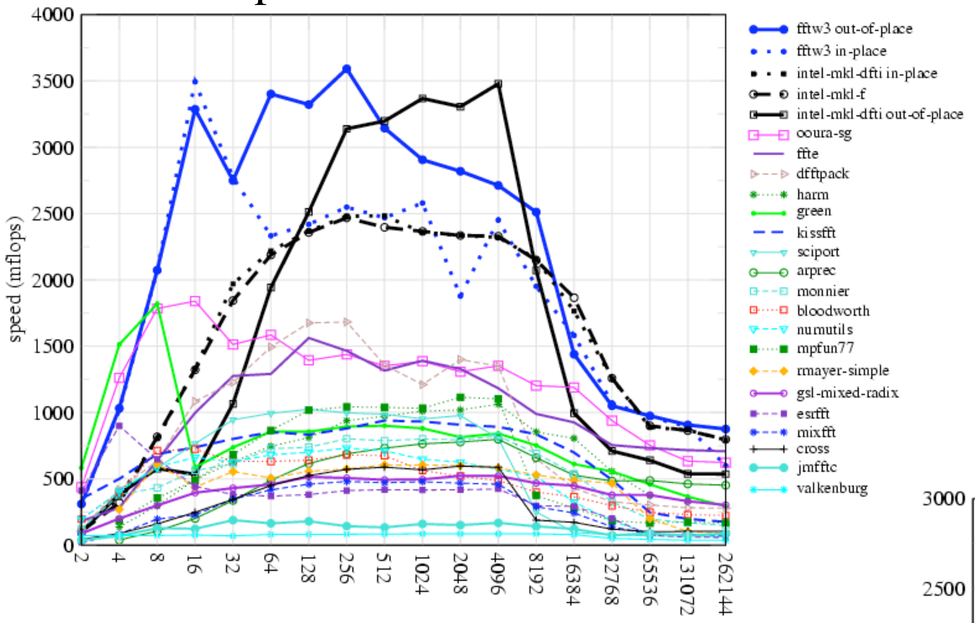


…because we let the code do the optimizing

FFTW performance

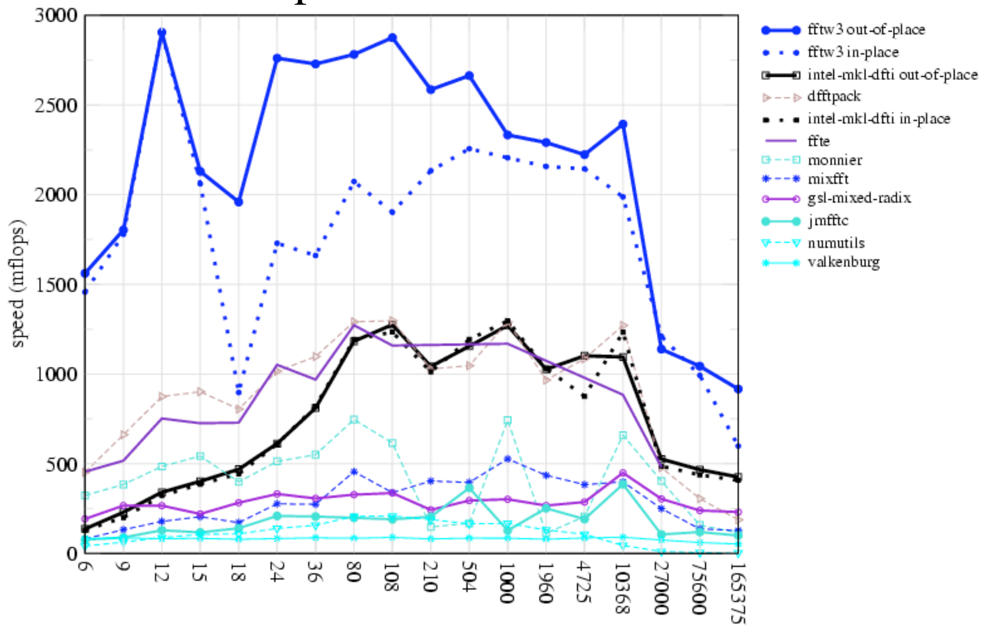
double precision, 2.8GHz Pentium IV: 2-way SIMD (SSE2)

powers of two



exploiting CPU-specific SIMD instructions (rewriting the code) is easy

non-powers-of-two



…because we let the code write itself

Why is FFTW fast?

FFTW implements many FFT algorithms:
A planner picks the best composition (*plan*)
by measuring the speed of different combinations.

Three ideas:

1. A recursive framework enhances locality.
2. Computational kernels (codelets) should be automatically generated.
3. Determining the unit of composition is critical.

FFTW is easy to use

```
{
     complex x[n];
     plan p;

     p = plan_dft_1d(n, x, x, FORWARD, MEASURE);
     ...
     execute(p); /* repeat as needed */
     ...
     destroy_plan(p);
}
```

Key fact: usually,
many transforms of same size
are required.

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Why is FFTW slow?

1965 Cooley & Tukey, IBM 7094, 36-bit single precision:
size 2048 DFT in 1.2 seconds

2003 FFTW3+SIMD, 2GHz Pentium-IV 64-bit double precision:
size 2048 DFT in 50 microseconds (24,000x speedup)

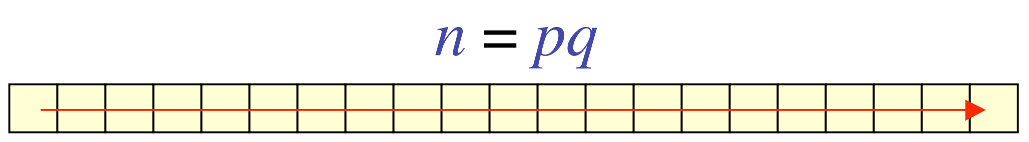
(= 30% improvement per year)

(Moore's prediction: 30 nanoseconds)

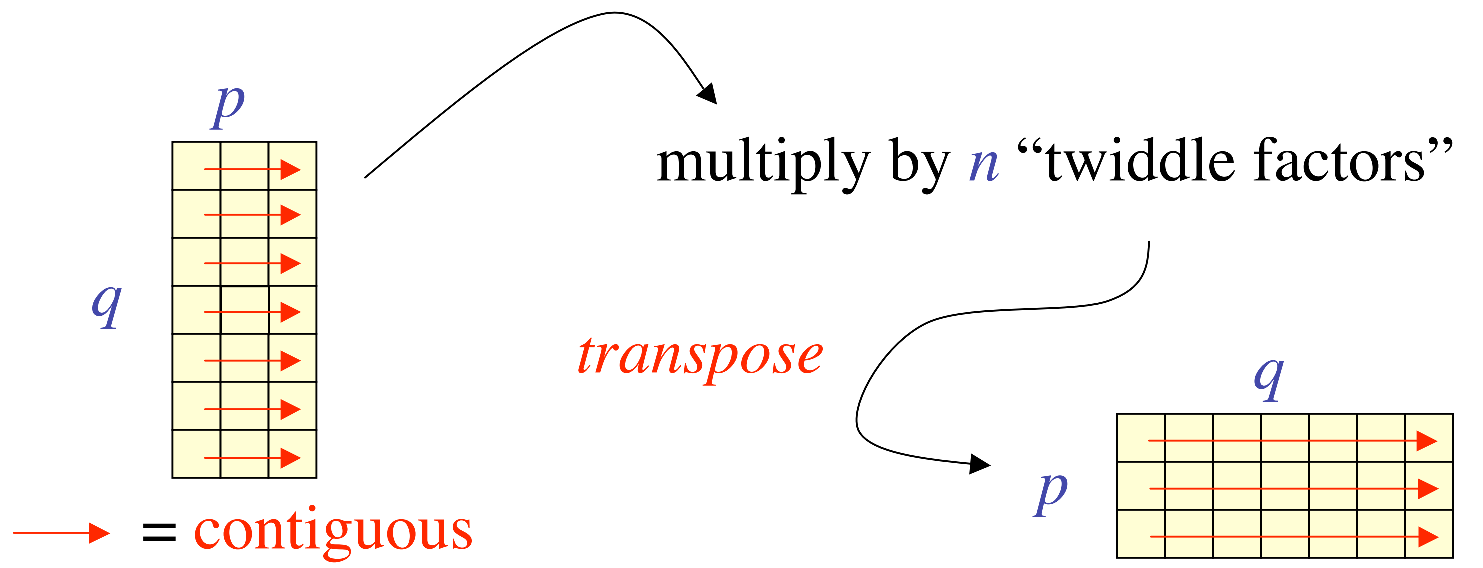
(= doubles every ~30 months)

FFTs are hard: don't get "peak" CPU speed
especially for large *n*,
unlike *e.g.* dense matrix multiply

Discontiguous Memory Access

1d DFT of size n: 

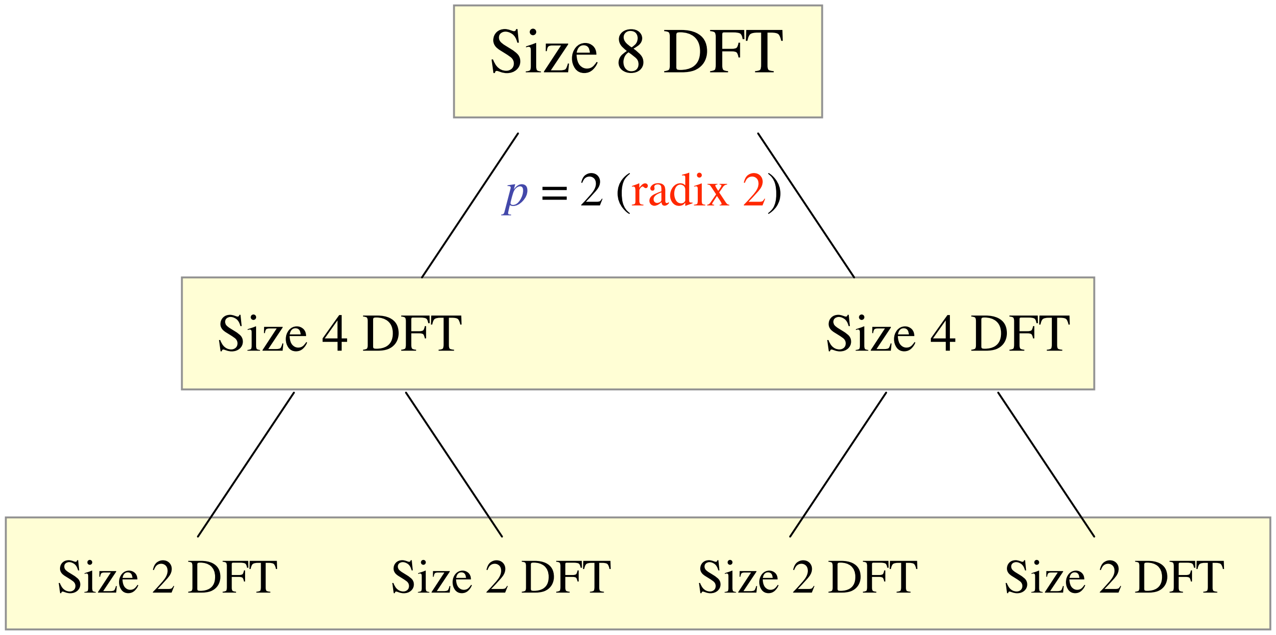
= ~2d DFT of size p x q



first DFT columns, size q
(non-contiguous)

finally, DFT columns, size p
(non-contiguous)

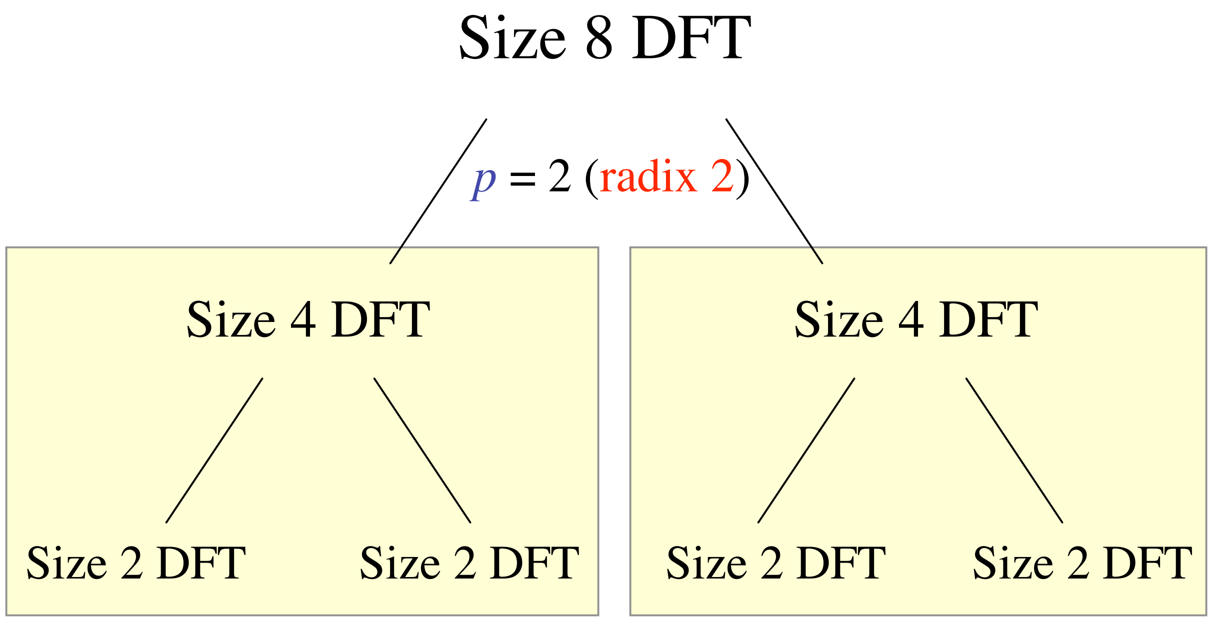
Cooley-Tukey is Naturally Recursive



But traditional implementation is non-recursive, breadth-first traversal:

$\log_2 n$ passes over whole array

Traditional cache solution: Blocking



breadth-first, but with *blocks* of size = cache

optimal choice: radix = cache size

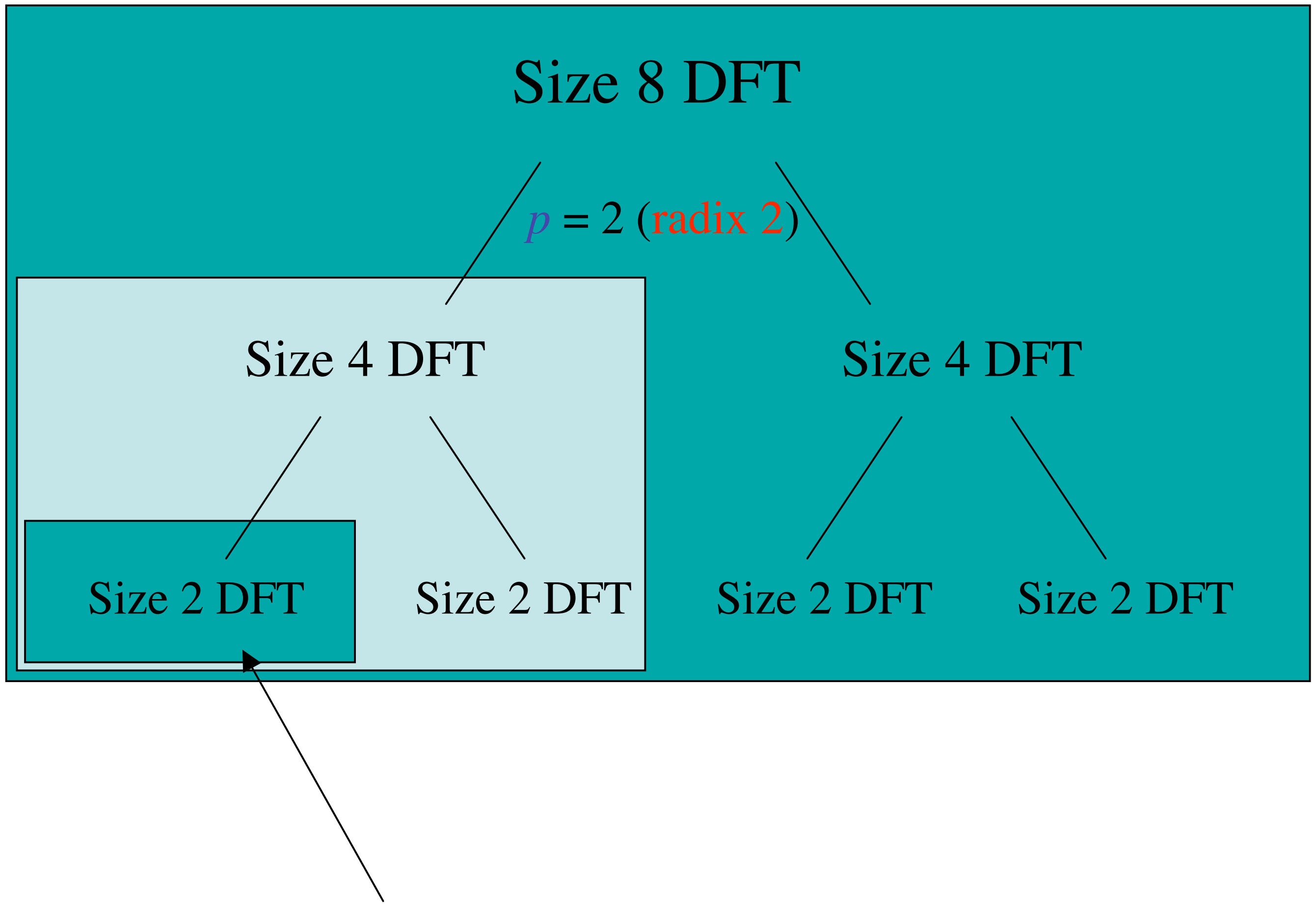
radix >> 2

…requires program specialized for cache size

…multiple levels of cache = multilevel blocking

Recursive Divide & Conquer is Good

(depth-first traversal) [Singleton, 1967]



eventually small enough to fit in cache

…no matter what size the cache is

Cache Obliviousness

- A cache-oblivious algorithm does not know the cache size
  - — for many algorithms [Frigo 1999], can be provably "big-O" optimal for any machine & for all levels of cache simultaneously

… but this ignores e.g. constant factors, associativity, …

cache-obliviousness is a good beginning,
but is not the end of optimization

we'll see: FFTW combines *both* styles
(breadth- and depth-first) with self-optimization

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The Codelet Generator

a domain-specific FFT “compiler”

- Generates fast hard-coded C for FFT of a given size

Necessary to give the planner a large space of codelets to experiment with (any factorization).

Exploits modern CPU deep pipelines & large register sets.

Allows easy experimentation with different optimizations & algorithms.

…CPU-specific hacks (SIMD) feasible

(& negates recursion overhead)

The Codelet Generator

written in Objective Caml [Leroy, 1998], an ML dialect

Abstract FFT algorithm

Cooley-Tukey: $n=pq$,
Prime-Factor: $\gcd(p,q) = 1$,
Rader: n prime, …

n

Symbolic graph (dag)

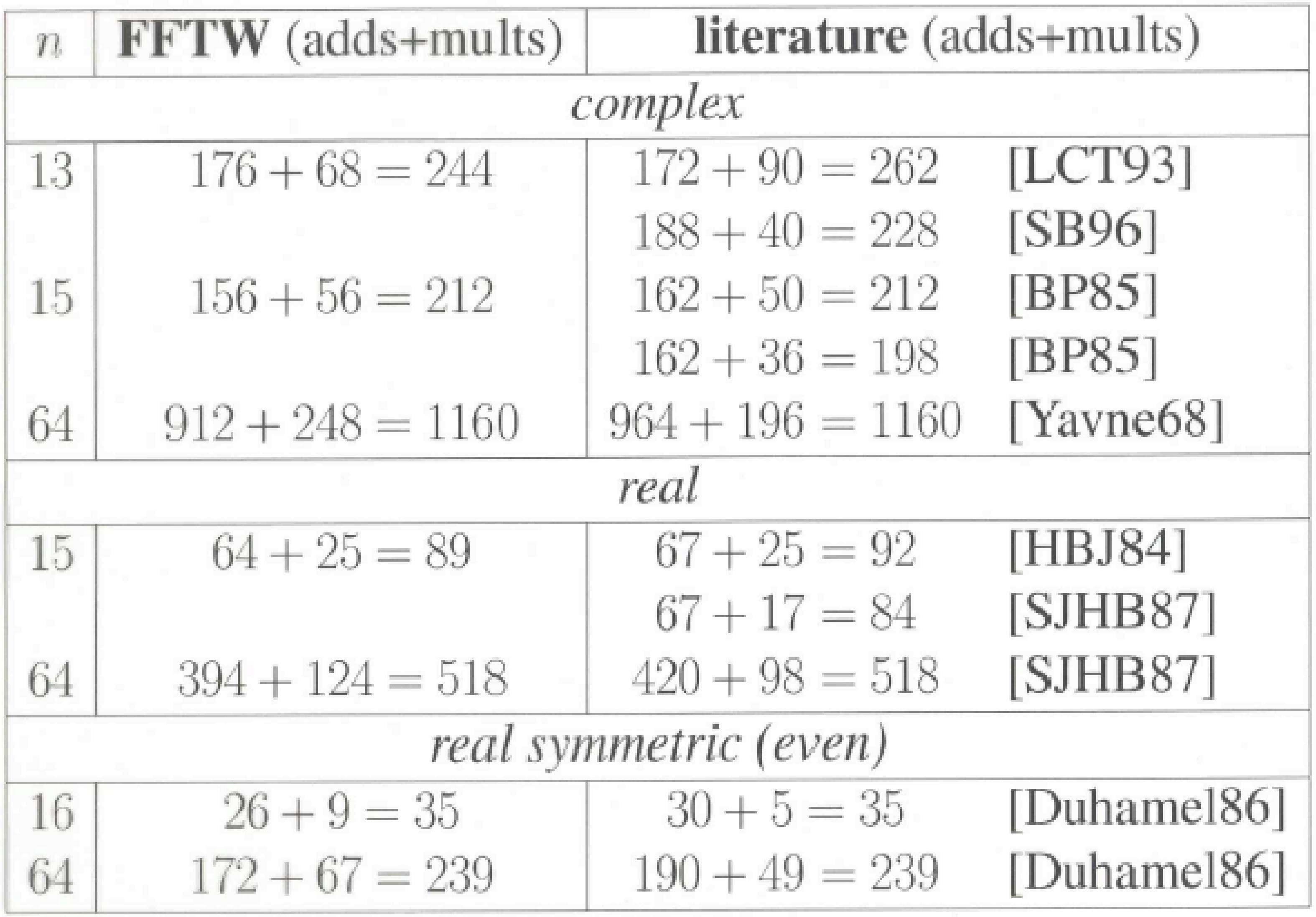
Simplifications

powerful enough
to *e.g.* derive real-input FFT
from complex FFT algorithm
and even find “new” algorithms

Optimal cache-oblivious
scheduling
(cache .EQ. registers)

Optimized C code (or other language)

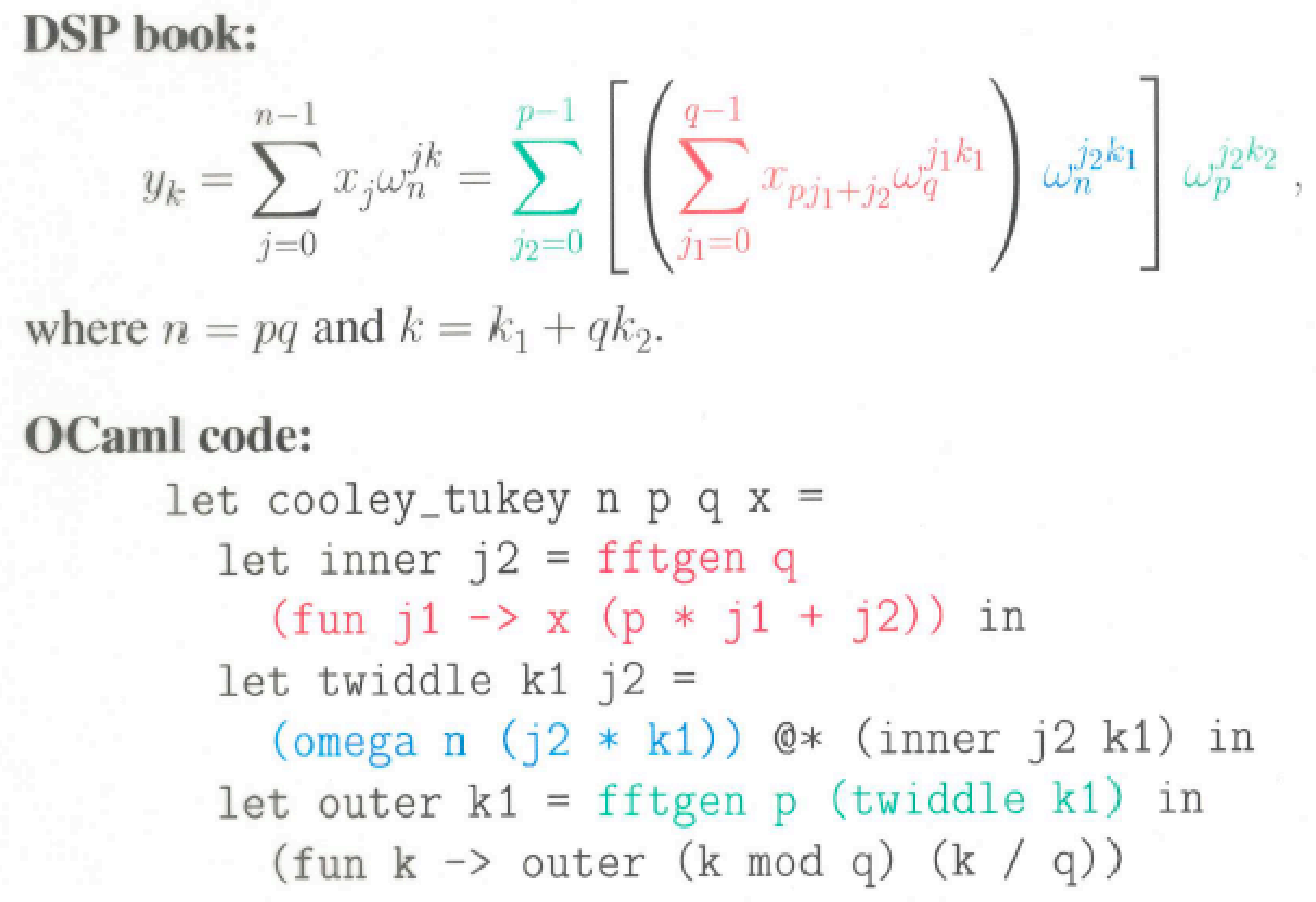
The Generator Finds Good/New FFTs



n	**FFTW** (adds+mults)	**literature** (adds+mults)	
		complex	
13	$176 + 68 = 244$	$172 + 90 = 262$	[LCT93]
		$188 + 40 = 228$	[SB96]
15	$156 + 56 = 212$	$162 + 50 = 212$	[BP85]
		$162 + 36 = 198$	[BP85]
64	$912 + 248 = 1160$	$964 + 196 = 1160$	[Yavne68]
		real	
15	$64 + 25 = 89$	$67 + 25 = 92$	[HBJ84]
		$67 + 17 = 84$	[SJHB87]
64	$394 + 124 = 518$	$420 + 98 = 518$	[SJHB87]
		real symmetric (even)	
16	$26 + 9 = 35$	$30 + 5 = 35$	[Duhamel86]
64	$172 + 67 = 239$	$190 + 49 = 239$	[Duhamel86]

Symbolic Algorithms are Easy

Cooley-Tukey in OCaml



DSP book:

$$y_k = \sum_{j=0}^{n-1} x_j \omega_n^{jk} = \sum_{j_2=0}^{p-1}\left[\left(\sum_{j_1=0}^{q-1} x_{pj_1+j_2}\omega_q^{j_1k_1}\right)\omega_n^{j_2k_1}\right]\omega_p^{j_2k_2},$$

where $n = pq$ and $k = k_1 + qk_2$.

OCaml code:

```
let cooley_tukey n p q x =
  let inner j2 = fftgen q
    (fun j1 -> x (p * j1 + j2)) in
  let twiddle k1 j2 =
    (omega n (j2 * k1)) @* (inner j2 k1) in
  let outer k1 = fftgen p (twiddle k1) in
    (fun k -> outer (k mod q) (k / q))
```

Simple Simplifications

Well-known optimizations:

Algebraic simplification, $e.g.\ a + 0 = a$

Constant folding

Common-subexpression elimination

Symbolic Pattern Matching in OCaml

The following *actual code fragment* is
solely responsible for simplifying multiplications:

```
stimesM = function
    | (Uminus a, b) -> stimesM (a, b) >>= suminusM
    | (a, Uminus b) -> stimesM (a, b) >>= suminusM
    | (Num a, Num b) -> snumM (Number.mul a b)
    | (Num a, Times (Num b, c)) ->
        snumM (Number.mul a b) >>= fun x -> stimesM (x, c)
    | (Num a, b) when Number.is_zero a -> snumM Number.zero
    | (Num a, b) when Number.is_one a -> makeNode b
    | (Num a, b) when Number.is_mone a -> suminusM b
    | (a, b) when is_known_constant b && not (is_known_constant a) ->
        stimesM (b, a)
    | (a, b) -> makeNode (Times (a, b))
```

(Common-subexpression elimination is implicit
via “memoization” and monadic programming style.)

Simple Simplifications

Well-known optimizations:

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Common-subexpression elimination

FFT-specific optimizations:

Network transposition (transpose + simplify + transpose)

____________________ negative constants…

A Quiz: Is One Faster?

Both compute the same thing, and have the same number of arithmetic operations:

```
a = 0.5 * b;
c = 0.5 * d;
e = 1.0 + a;
f = 1.0 - c;
```

```
a = 0.5 * b;
c = -0.5 * d;
e = 1.0 + a;
f = 1.0 + c;
```

Faster because no separate load for `-0.5`

10–15% speedup

Non-obvious transformations require experimentation

Quiz 2: Which is Faster?

accessing strided array
inside codelet (amid dense numeric code), nonsequential

`array[stride * i]`

`array[strides[i]]`

using precomputed stride array:

`strides[i] = stride * i`

This is faster, of course!
Except on brain-dead architectures…

…namely, Intel Pentia:
integer multiplication
conflicts with floating-point

up to ~10–20% speedup

(even better to bloat:
pregenerate various constant strides)

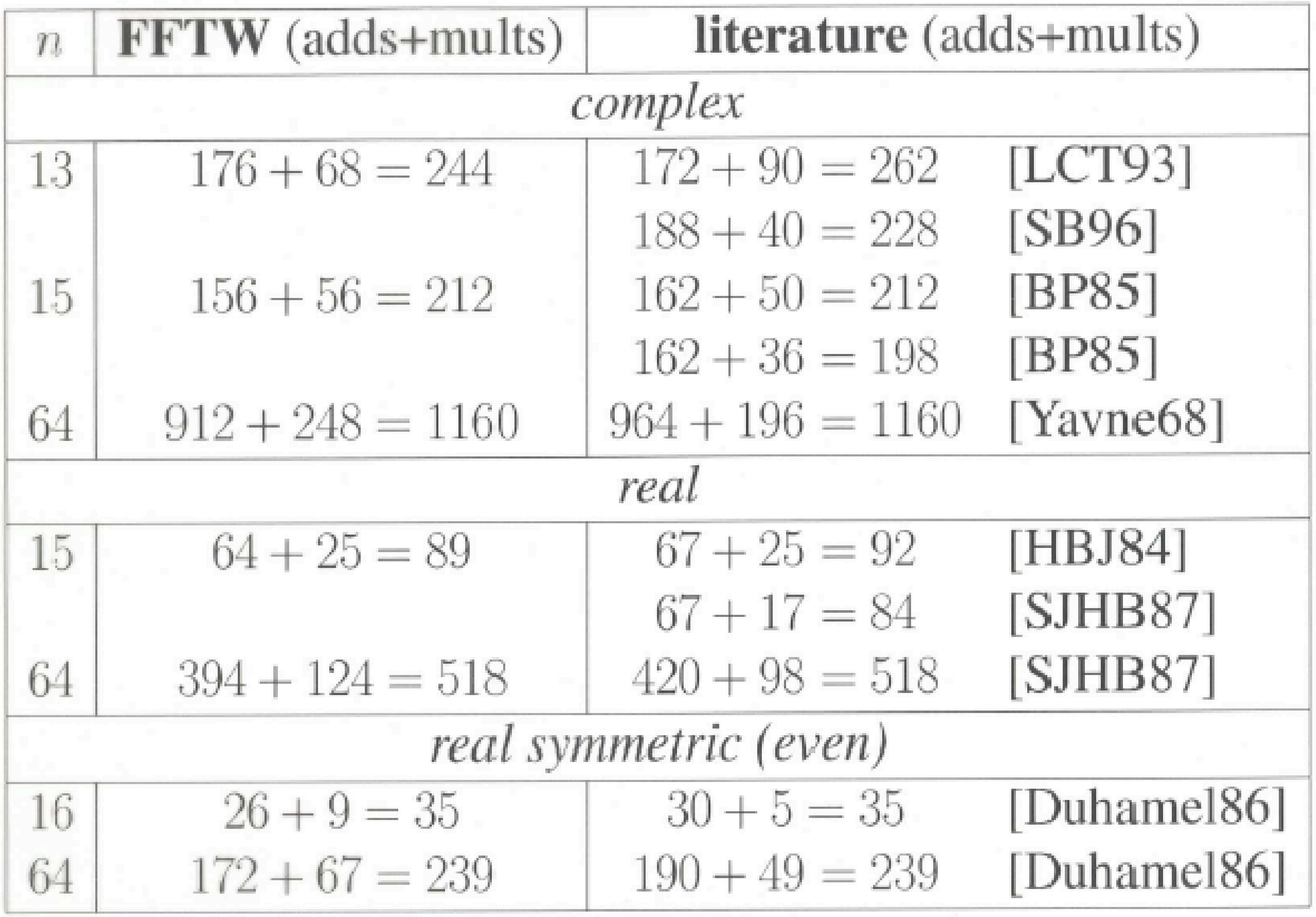
Machine-specific hacks are feasible if you just generate special code

stride precomputation

SIMD instructions (SSE, Altivec, 3dNow!)

fused multiply-add instructions…

The Generator Finds Good/New FFTs



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What does the planner compose?

- The Cooley-Tukey algorithm presents many choices:
  - — which factorization? what order? memory reshuffling?

Find simple steps that combine without restriction
to form many different algorithms.

… steps to do WHAT?

FFTW 1 (1997): steps solve out-of-place DFT of size n

"Composable" Steps in FFTW 1

SOLVE — Directly solve a small DFT by a codelet

CT-FACTOR[r] — Radix-r Cooley-Tukey step = execute loop of r sub-problems of size n/r

✗ Many algorithms difficult to express via simple steps.

— e.g. expresses only depth-first recursion (loop is *outside* of sub-problem)

— e.g. in-place without bit-reversal requires combining two CT steps (DIT + DIF) + transpose

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FFTW 1 (1997): steps solve out-of-place DFT of size n

Steps cannot solve problems that cannot be expressed.

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… steps to do WHAT?

FFTW 3 (2003):

steps solve a problem, specified as a DFT(input/output, **v**,**n**):
multi-dimensional "vector loops" **v** of multi-dimensional transforms **n**

{sets of (size, input/output strides)}

Some Composable Steps (out of ~16)

SOLVE — Directly solve a small DFT by a codelet

CT-FACTOR[r] — Radix-r Cooley-Tukey step = r (loop) sub-problems of size n/r (& recombine with size-r twiddle codelet)

VECLOOP — Perform one vector loop (can choose any loop, i.e. loop reordering)

INDIRECT — DFT = copy + in-place DFT (separates copy/reordering from DFT)

TRANSPOSE — solve in-place $m \times n$ transpose

Many Resulting "Algorithms"

- INDIRECT + TRANSPOSE gives in-place DFTs,
  - — bit-reversal = product of transpositions
    - … no separate bit-reversal "pass"
      - [Johnson (unrelated) & Burrus (1984)]

- VECLOOP can push topmost loop to "leaves"
  - — "vector" FFT algorithm [Swarztrauber (1987)]

- CT-FACTOR *then* VECLOOP(s) gives "breadth-first" FFT,
  - — erases iterative/recursive distinction

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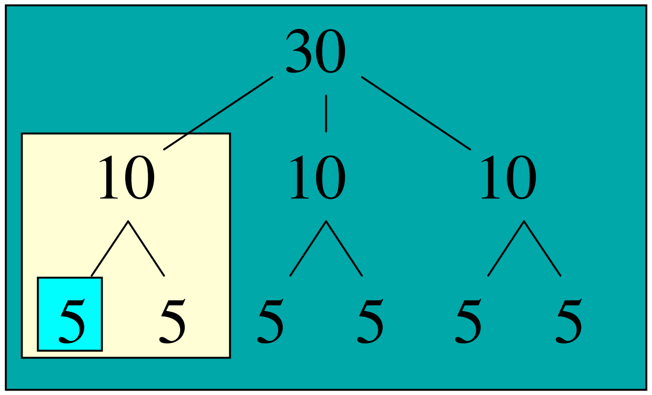
Depth- vs. Breadth- First for size $n = 30 = 3 \times 5 \times 2$

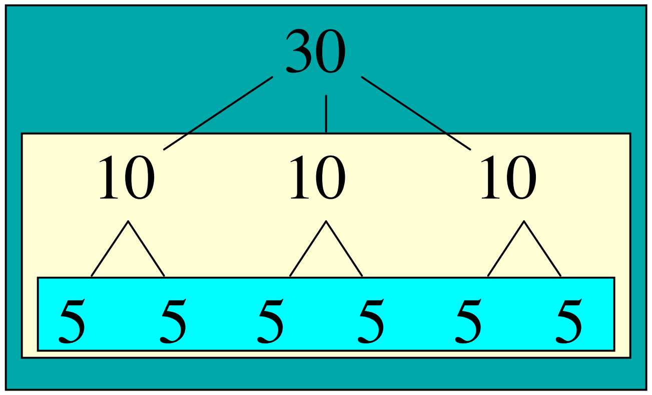
A "depth-first" plan:

```
CT-FACTOR[3]
    VECLOOP x3
        CT-FACTOR[2]
            SOLVE[2, 5]
```



A "breadth-first" plan:

```
CT-FACTOR[3]
    CT-FACTOR[2]
        VECLOOP x3
            SOLVE[2, 5]
```



(Note: *both* are executed by explicit recursion.)

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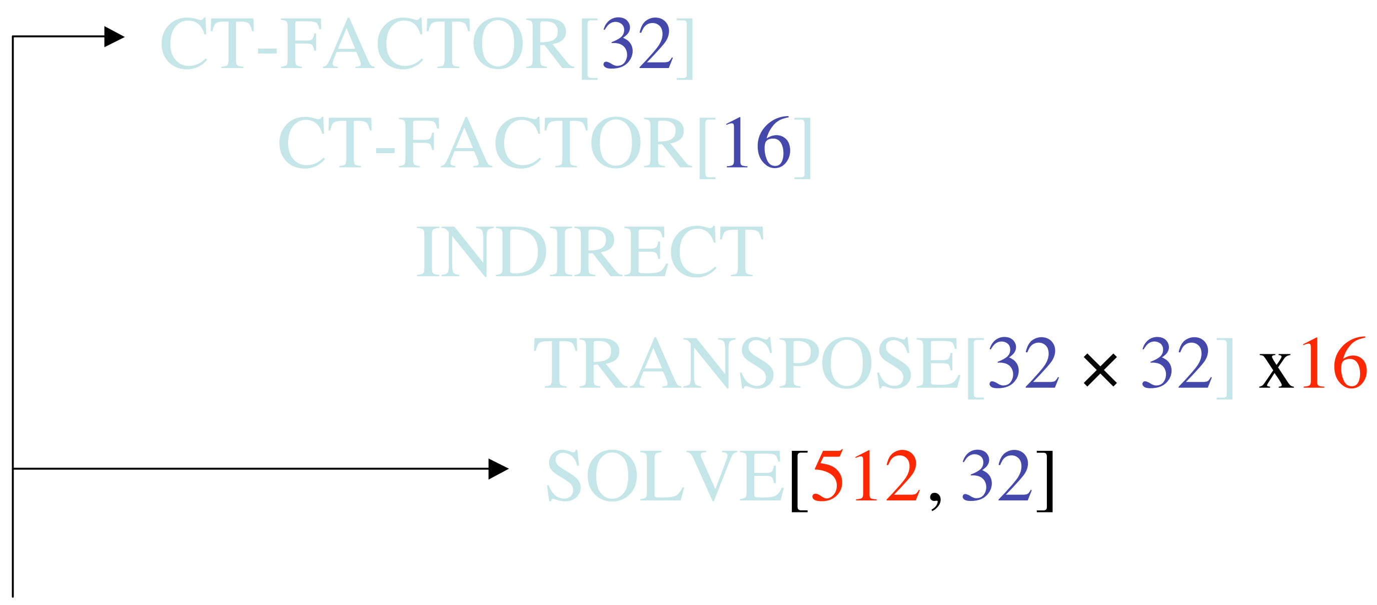
In-place plan for size $2^{14} = 16384$

(2 GHz PowerPC G5, double precision)



Radix-32 DIT + Radix-32 DIF = 2 loops = transpose

… where leaf SOLVE ~ “radix” 32 x 1

Out-of-place plan for size 2^{19}=524288

(2GHz Pentium IV, double precision)

```
CT-FACTOR[4] (buffered variant)
  CT-FACTOR[32] (buffered variant)
    VECLOOP (reorder) x32
      CT-FACTOR[64]
        INDIRECT
          VECLOOP (reorder) x64
            VECLOOP x4
              COPY[64]
          VECLOOP x4
            SOLVE[64, 64]
```

~2000 lines hard-coded C!

INDIRECT
+
VECLOOP (reorder)
(+ …)
=
huge improvements
for large 1d sizes

Unpredictable: (automated) experimentation is the only solution.

Dynamic Programming

the assumption of "optimal substructure"

Try all applicable steps:

DFT(16) = fastest of:

- CT-FACTOR[2]: 2 DFT(8)
- CT-FACTOR[4]: 4 DFT(4)

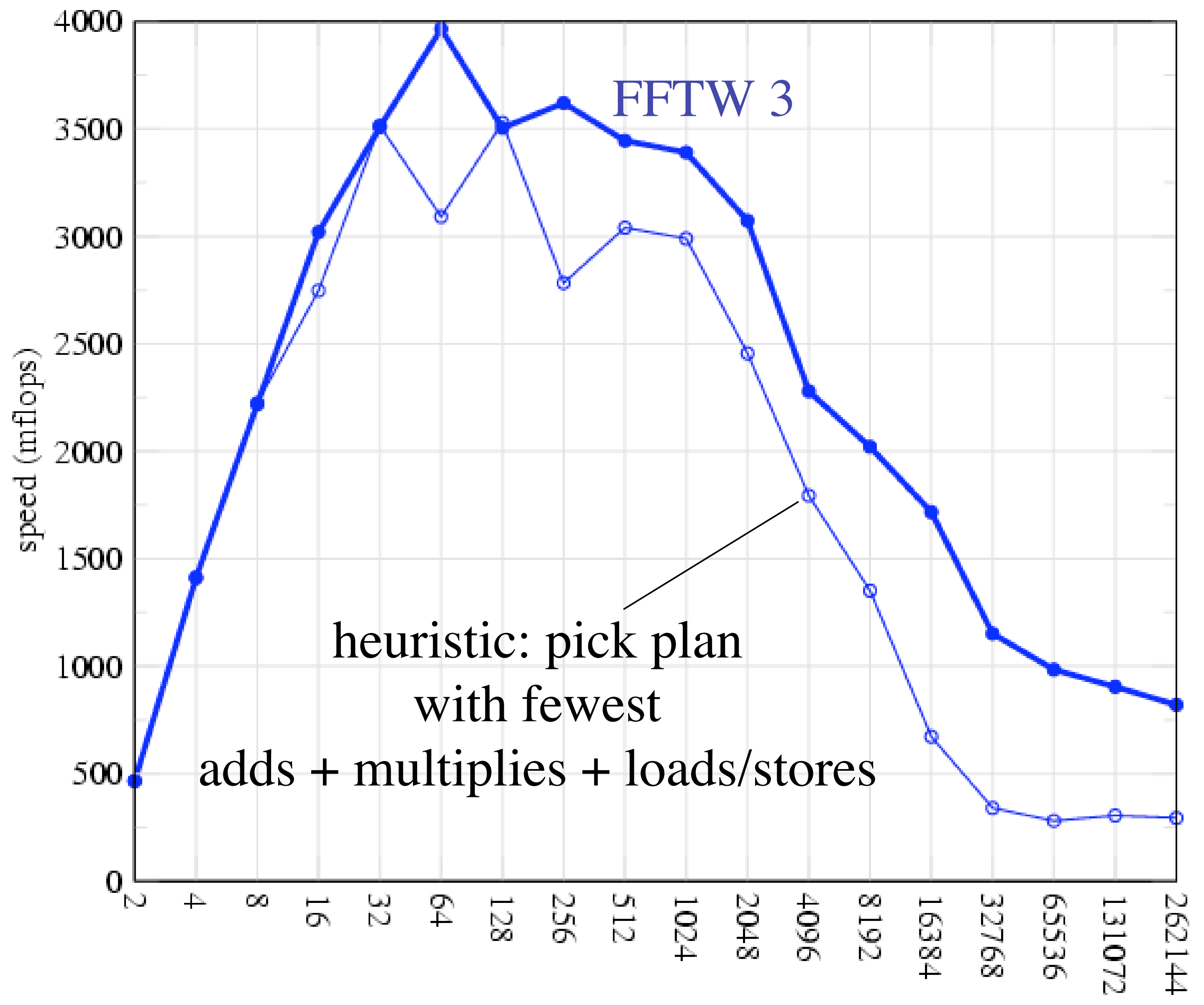
DFT(8) = fastest of:

- CT-FACTOR[2]: 2 DFT(4)
- CT-FACTOR[4]: 4 DFT(2)
- SOLVE[1,8]

If exactly the same problem appears twice,
assume that we can re-use the plan.
— i.e. *ordering* of plan speeds is assumed independent of context

Planner Unpredictability

double-precision, power-of-two sizes, 2GHz PowerPC G5



heuristic: pick plan
with fewest
adds + multiplies + loads/stores

Classic strategy:
minimize op's
fails badly

another test:
Use plan from:
another machine?
e.g. Pentium-IV?
… lose 20–40%

We've Come a Long Way?

- In the name of performance, computers have become complex & unpredictable.

- Optimization is hard: simple heuristics (*e.g.* fewest flops) no longer work.

- One solution is to avoid the details, not embrace them:

  (Recursive) composition of simple modules
  + feedback (self-optimization)

  High-level languages (not C) & code generation
  are a powerful tool for high performance.