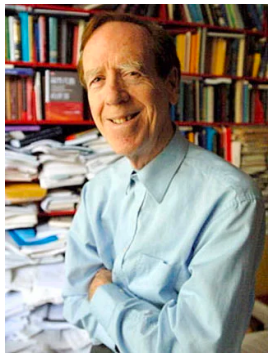
Fast Fourier Transforms (FFT algorithms)

"the most important numerical algorithm of our lifetime"
— Gil Strang, MIT

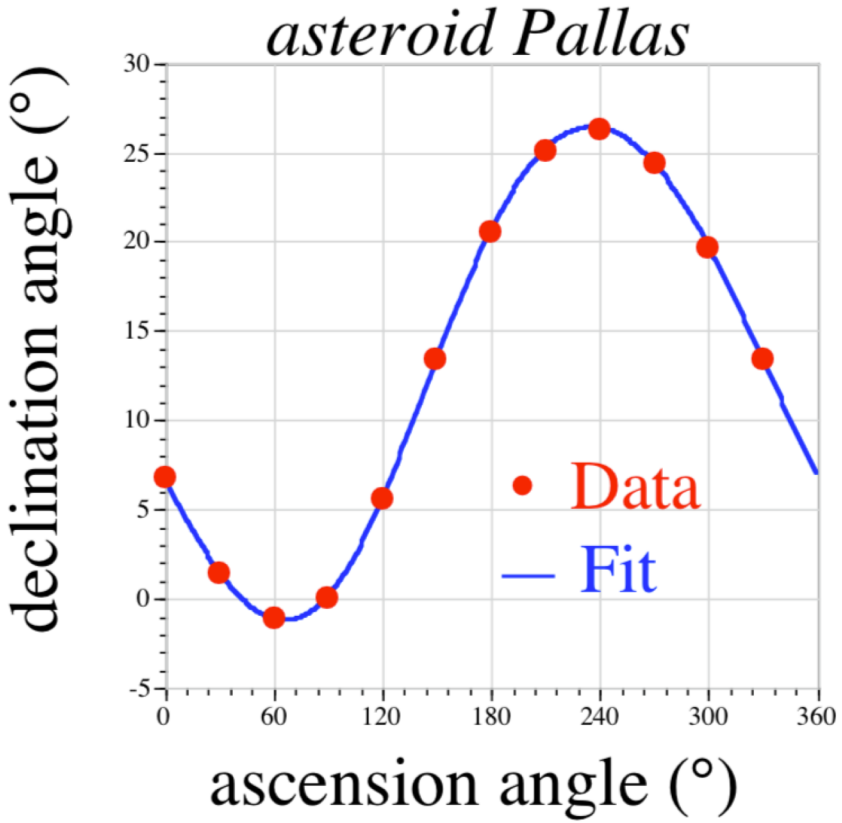


one of
"Top 10 Algorithms of 20th Century"

- Jack Dongarra & F. Sullivan, *Computing in Science and Engineering* (2000)

MIT course 18.335, spring 2021
Steven G. Johnson MIT Applied Math

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



trigonometric interpolation:

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

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' DFT notation:

From "*Theoria interpolationis methodo nova tractata*"

Quum haec formula indefinite pro valore quocunque ipsius t locum habeat, manifestum est, si producta sinuum in numeratoribus in cosinus sinusque arcuum multiplicium evolvantur, id quod provenit cum

$$\alpha + \alpha' \cos t + \alpha'' \cos 2t + \alpha''' \cos 3t + \text{ etc.}$$
$$+ \mathfrak{b}' \sin t + \mathfrak{b}'' \sin 2t + \mathfrak{b}''' \sin 3t + \text{ etc.}$$

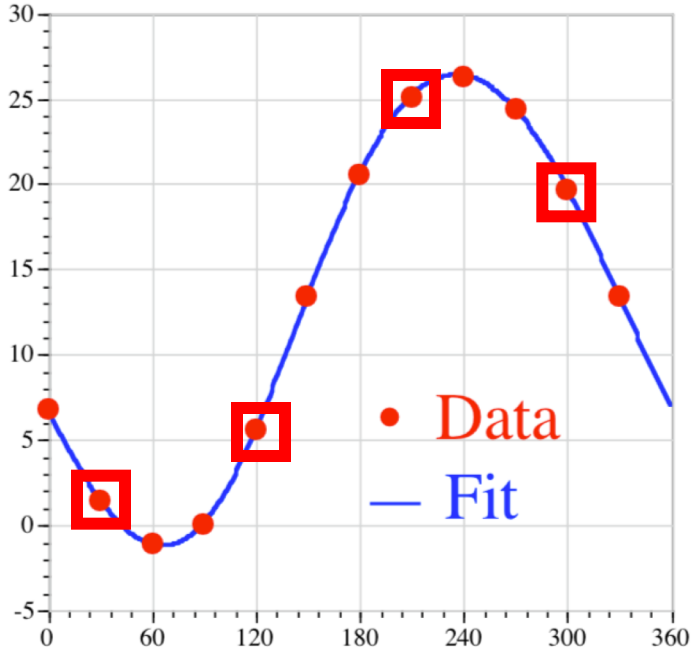
identicum esse debere, unde coëfficientes α, α', $\mathfrak{b}'$, α'', $\mathfrak{b}''$ etc. innotescent. Ceterum formula pro T, ut hic exhibita est, ita est comparata, ut sponte et sine calculo pateat, substitutis pro t resp. a, b, c, d etc. valoribus propositis A, B, C, D etc. probe satisfieri.

Kids: don't try this at home!

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:

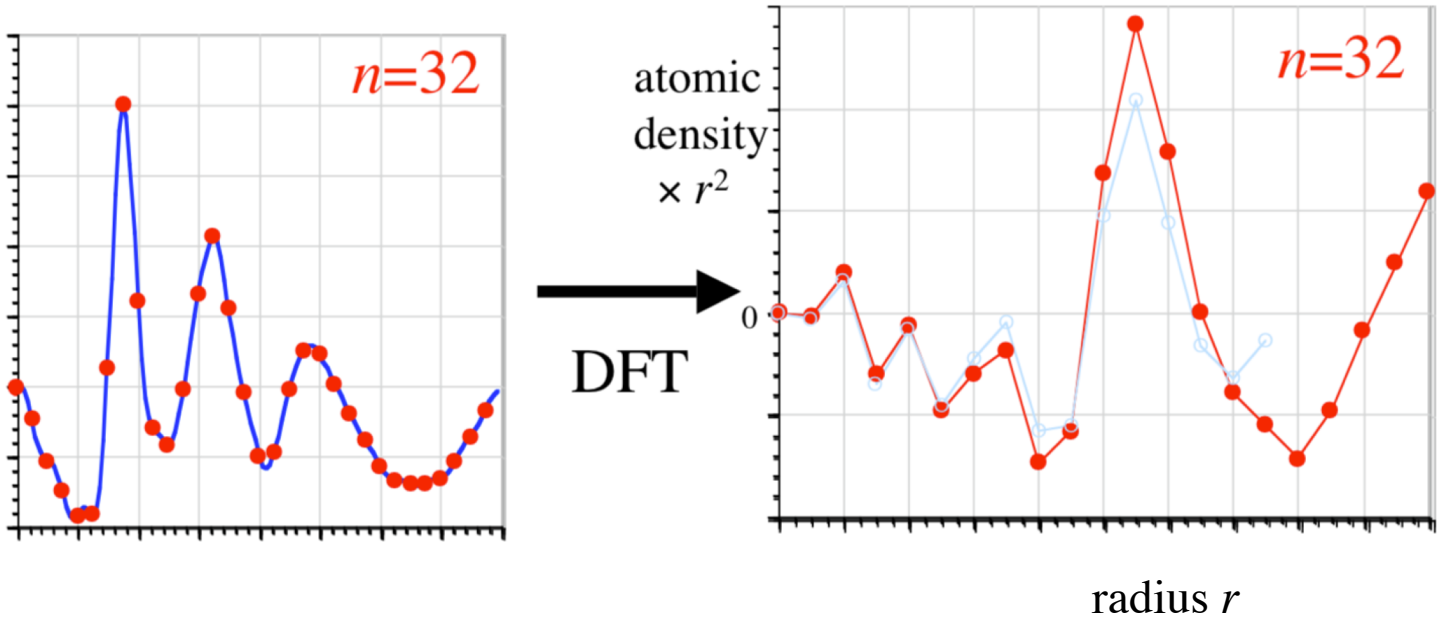
Danielson and Lanczos (1942)

[*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:

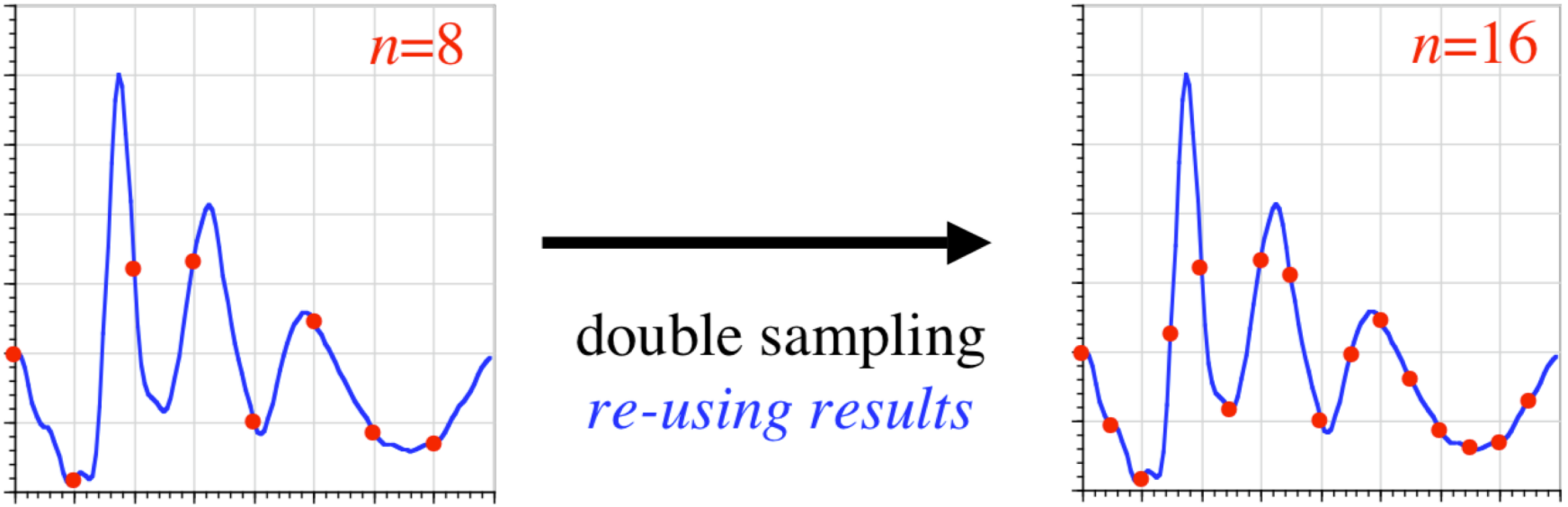


…double sampling until density (DFT) converges…

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 ???

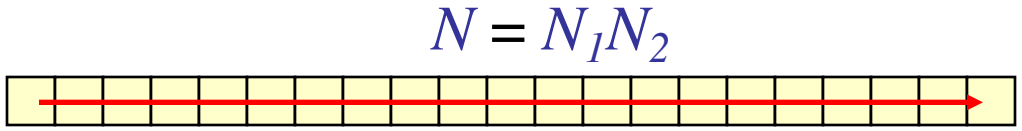
64-point DST in *only 140 minutes!*

re-inventing Gauss (for the last time)

Cooley and Tukey (1965)

[*Math. Comp.* **19**, 297–301]

1d DFT of size N:



= ~2d DFT of size $N_1 \times N_2$

(+ phase rotation by twiddle factors)

= Recursive DFTs of sizes N_1 and N_2

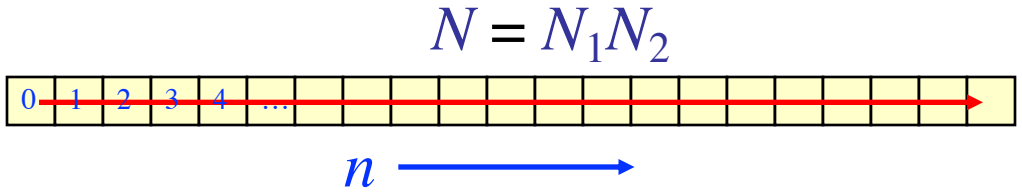
$O(N^2) \longrightarrow O(N \log N)$

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

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

The "Cooley-Tukey" FFT Algorithm

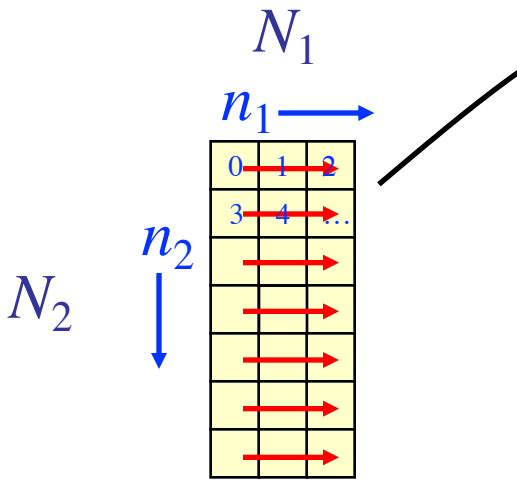
1d DFT of size N:



= ~2d DFT of size $N_1 \times N_2$

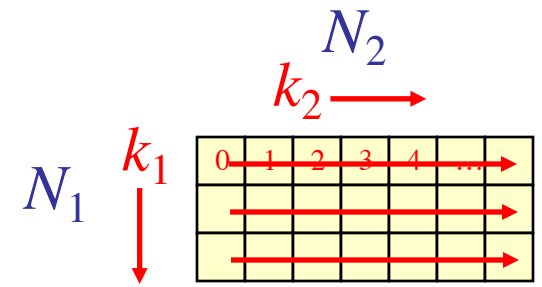
input re-indexing
$n = n_1 + N_1 n_2$

output re-indexing
$k = N_2 k_1 + k_2$



multiply by n
"twiddle factors"

transpose



→ = contiguous

first DFT columns, size N_2
(non-contiguous)

finally, DFT columns, size N_1
(non-contiguous)

"Cooley-Tukey" FFT, in math

Recall the definition of the DFT:

$$y_k = \sum_{n=0}^{N-1} \omega_N^{nk} x_n \quad \text{where} \quad \omega_N = e^{-\frac{2\pi i}{N}}$$

Trick: if $N = N_1 N_2$, re-index $n = n_1 + N_1 n_2$ and $k = N_2 k_1 + k_2$:

$$y_{N_2 k_1 + k_2} = \sum_{n_1=0}^{N_1-1} \sum_{n_2=0}^{N_2-1} \omega_N^{n_1 N_2 k_1} \omega_N^{n_1 k_2} \omega_N^{N_1 n_2 N_2 k_1} \omega_N^{N_1 n_2 k_2} x_{n_1 + N_1 n_2}$$

$$= \sum_{n_1=0}^{N_1-1} \omega_{N_1}^{n_1 k_1} \omega_N^{n_1 k_2} \left(\sum_{n_2=0}^{N_2-1} \omega_{N_2}^{n_2 k_2} x_{n_1 + N_1 n_2} \right)$$

size-N_1 DFTs twiddles size-N_2 DFTs

… repeat recursively.

Cooley–Tukey terminology

- Usually N_1 or N_2 is small, called *radix r*
  - N_1 is radix: "decimation in time" (DIT)
  - N_2 is radix: "decimation in frequency" (DIF)
- Size-r DFTs of radix: "butterflies"
  - Cooley & Tukey *erroneously* claimed r=3 "optimal": they thought butterflies were $\Theta(r^2)$
  - In fact, $r \approx \sqrt{N}$ is optimal cache-oblivious
- "Mixed-radix" uses different radices at different stages (different factors of n)

Why is Cooley–Tukey $\Theta(N \log N)$?

Take the **radix-2 DIT** (N_1=2, N_2=N/2) case, and suppose $N=2^m$.

i.e., a size-N DFT is expressed as 2 size-N/2 DFTs + multiplication by $\Theta(N)$ twiddle factors + N/2 size-2 DFTs:

flop count for size-$N=2^m$ DFT:

$$T(N) = 2T\left(\frac{N}{2}\right) + \underbrace{\Theta(N) + \frac{N}{2}T(2)}_{\#N}$$

$$\approx 2T\left(\frac{N}{2}\right) + \#N$$

$$= 2\left[2T\left(\frac{N}{4}\right) + \#\frac{N}{2}\right] + \#N = 4T\left(\frac{N}{4}\right) + \#N(1+1)$$

$$= \cdots = NT(1) + \#N\underbrace{(1+1+\cdots+1)}_{m \text{ times}} = \boldsymbol{\#N\log_2 N}$$

…similarly for *any radices*, as long as the base cases (= the prime factors of N) are bounded.

Note that the radices do not need to be bounded!

It is a good exercise to show that radix-$\sqrt{N}$ also gives a $\Theta(N \log N)$ algorithm.

(this algorithm turns out to be the optimal cache-oblivious FFT, actually.)

Many other FFT algorithms

- Prime-factor algorithm (1958): $N = N_1 N_2$ where N_1 and N_2 are co-prime: re-indexing based on Chinese Remainder Theorem with no twiddle factors.
- Rader's (1968) algorithm: for prime N, re-index using generator of multiplicative group → convolution of size N–1 (not prime!), do via FFTs of size N–1.
- Bluestein's (1968) algorithm: re-index using $nk = -\frac{1}{2}(k-n)^2 + \frac{n^2}{2} + \frac{k^2}{2}$ to get size-N convolution, do via zero-padded FFTs.
- Many others…
- Specialized versions for real x_n, real-symmetric/antisymmetric x_n (DCTs and DSTs), etc.

…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

… can prove it only under restrictive assumptions,

e.g. linear algorithms with bounded multiplicative constants)

[unless we give up exactness]

We're left with the "constant" factor…

The Next 30 Years…

Assume "time"

= # ~~multiplications~~

multiplications + # additions (= flops)

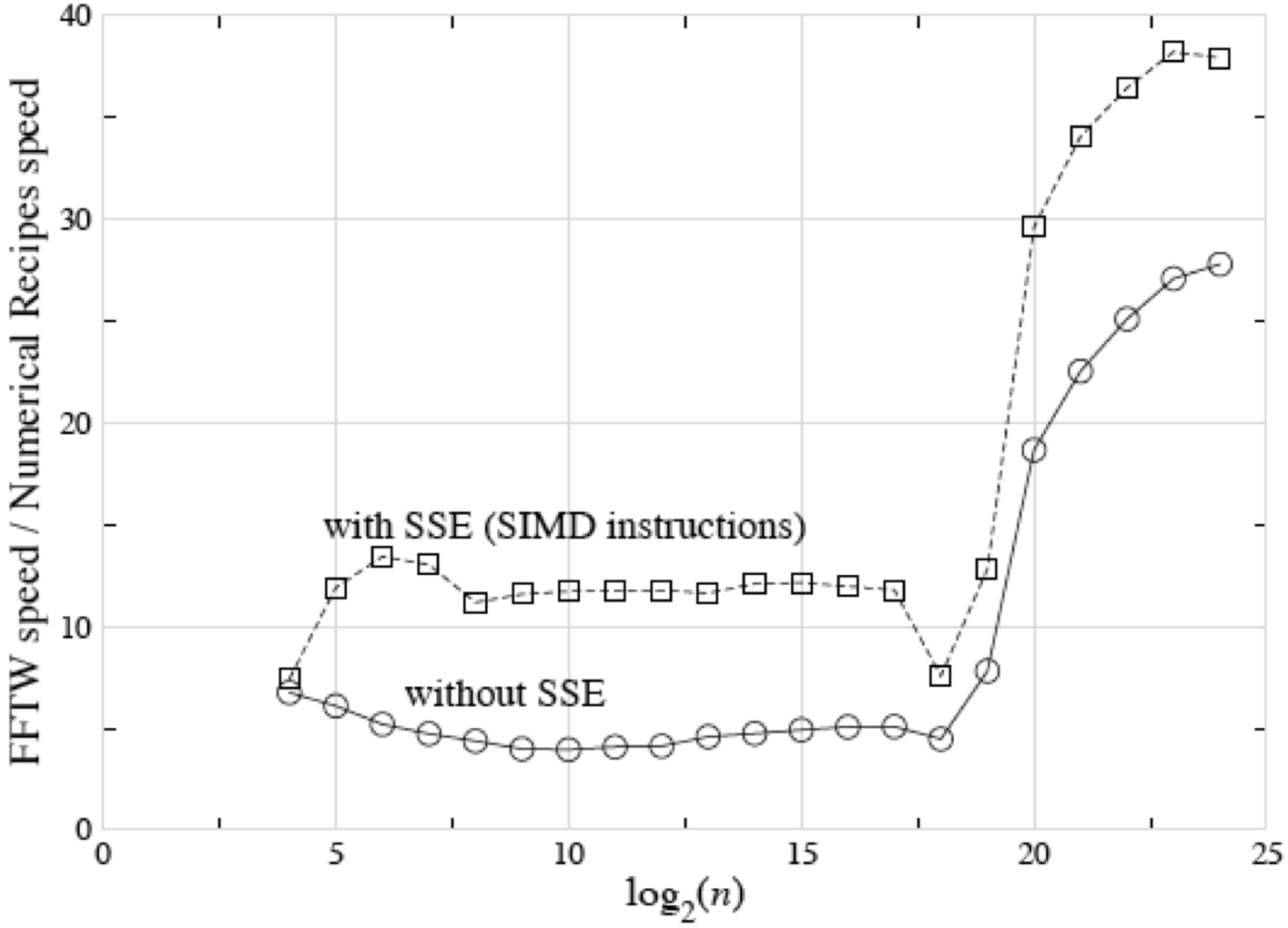
Winograd (1979): # multiplications = $\Theta(n)$

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

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

[$4N\log_2 N - 6N + 8$ flops, unsurpassed until 2007,
when another ~6% saved by Lundy/Van Buskirk and Johnson/Frigo]

Are arithmetic counts so important?



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[unsurpassed until last 2007, another ~6% saved]

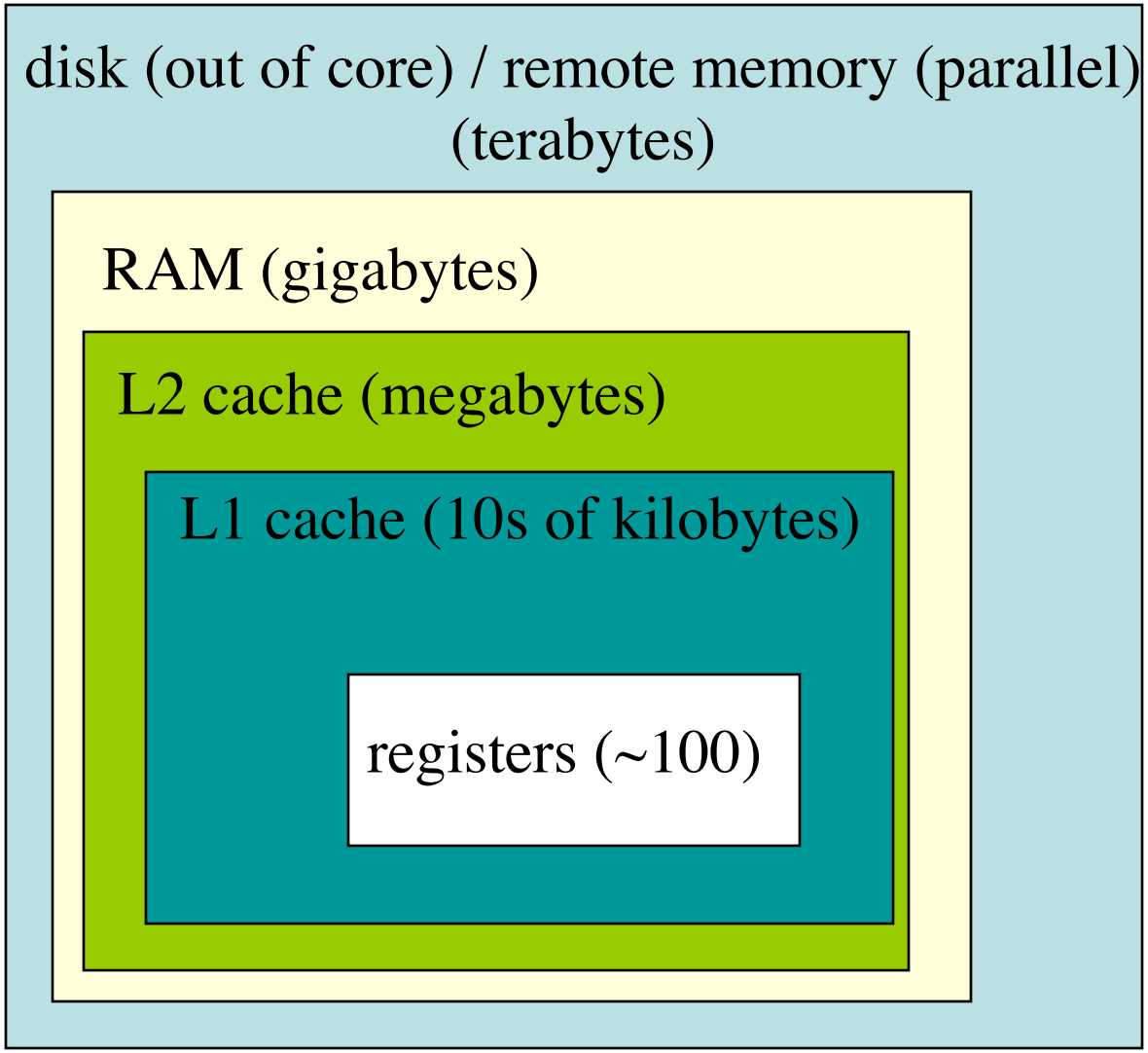
last 15+ years: flop count (varies by ~20%)

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)



…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?

Lots of choices in FFT implementation

- What is the base case? N=1 is elegant but inefficient.
- What factorization of N ("radices")?
- Ordering of loops, memory layout?
- Other FFT algorithms besides Cooley–Tukey?
  - Cooley–Tukey is only for composite N (often just 2^m), but there are FFT algorithms even for prime N.

FFTW the "Fastest Fourier Transform in the West" — S. G. Johnson & Matteo Frigo (1997)

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

- Computational kernels (80% of code) automatically generated

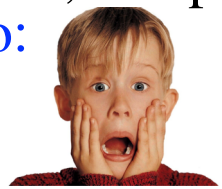
- Self-optimizes for your hardware (picks best composition of steps)
  = **portability + performance**

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

Julia interface: **FFTW** package
Matlab: it's the default `fft(...)`

Started (1997) with a practical need and a benchmark

- I was solving Maxwell's equations with FFTs and needed:
  3d, not just 2^m, parallel, portable.
- My friend Matteo suggested his Cilk FFT …
- I downloaded a bunch of other FFTs, benchmarked them, and put up a web page with results … no clear winner. Matteo:



- Could we do better? Key principles:
  - Benchmark against every competitor you can — otherwise you can't know if you did a good job.
  - Make it fast and portable, but…
  - Don't sacrifice generality / practicality.

(& I turned it in as final project in 18.337 taught by … … Alan Edelman)

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. Self-optimizes algorithm compositions …
   the unit of composition is critical.

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

What does the planner compose?

- The Cooley-Tukey algorithm presents many choices:
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Find simple steps that combine without restriction
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… steps to do WHAT?

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

Steps cannot solve problems that cannot be expressed.

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 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)}

Key component: 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 base cases ("codelets") to experiment with (any factorization).

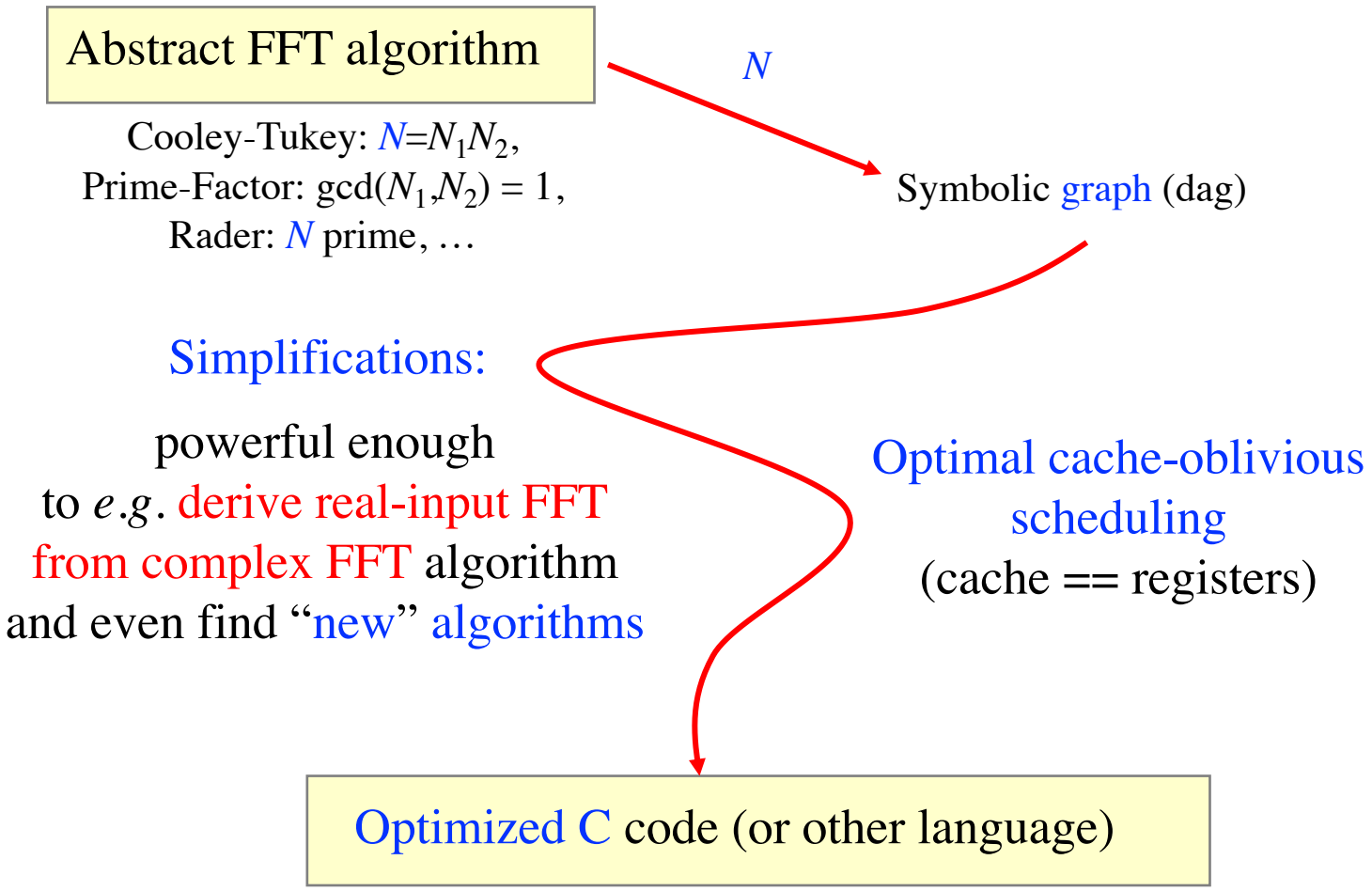
Exploits modern CPU deep pipelines & large register sets.

Allows easy experimentation with different optimizations & algorithms. + CPU-specific hacks (SIMD)…

(& large base case negates recursion overhead: "recursion coarsening")

The Codelet Generator

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



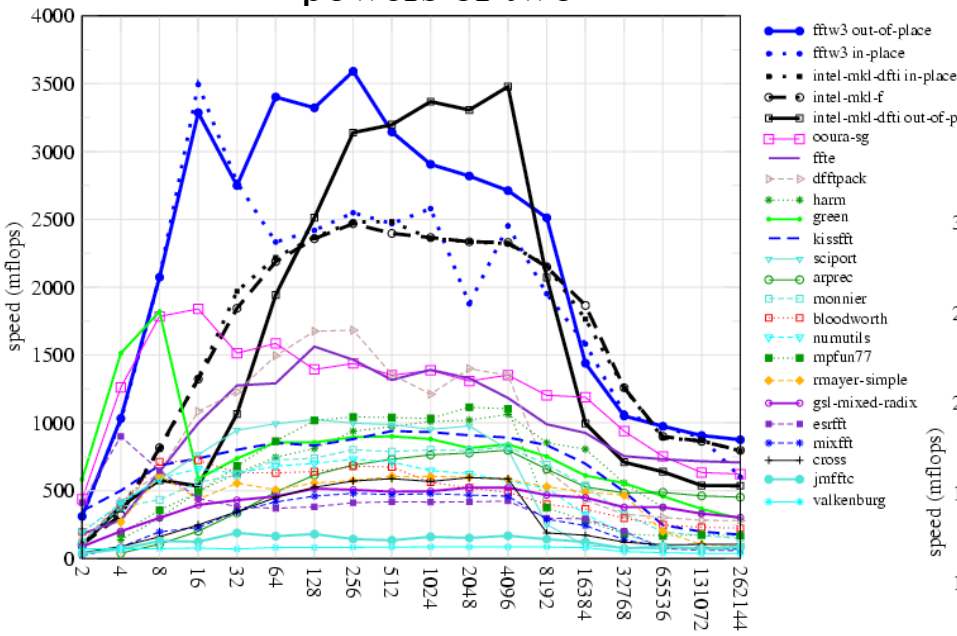
FFTW performance

double precision, most recent benchmarks on fftw.org

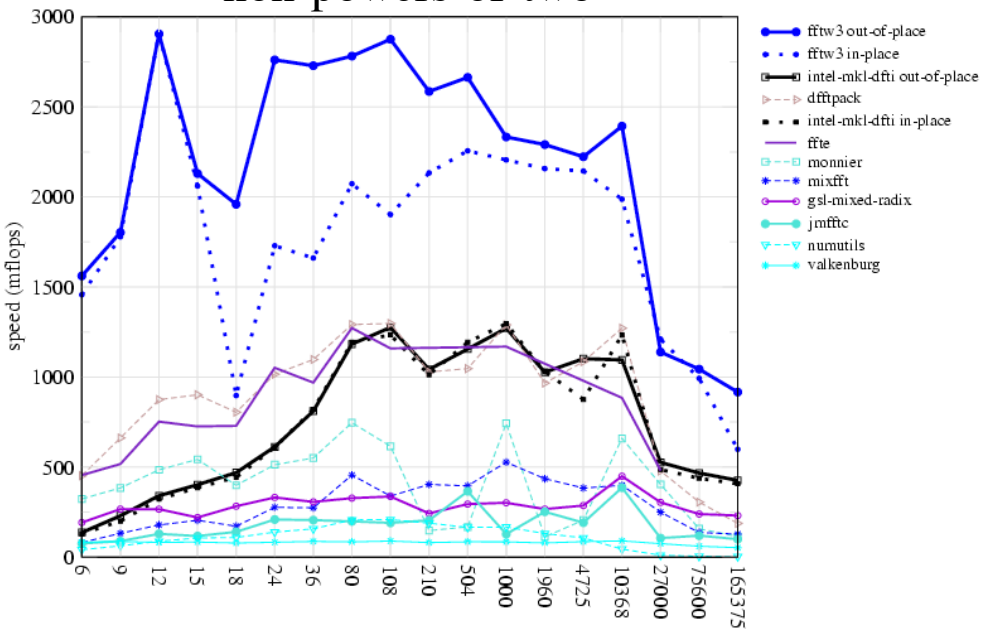
… a 2.8GHz Pentium IV Prescott (2004)

Maybe I need to re-run the benchmark?

powers of two



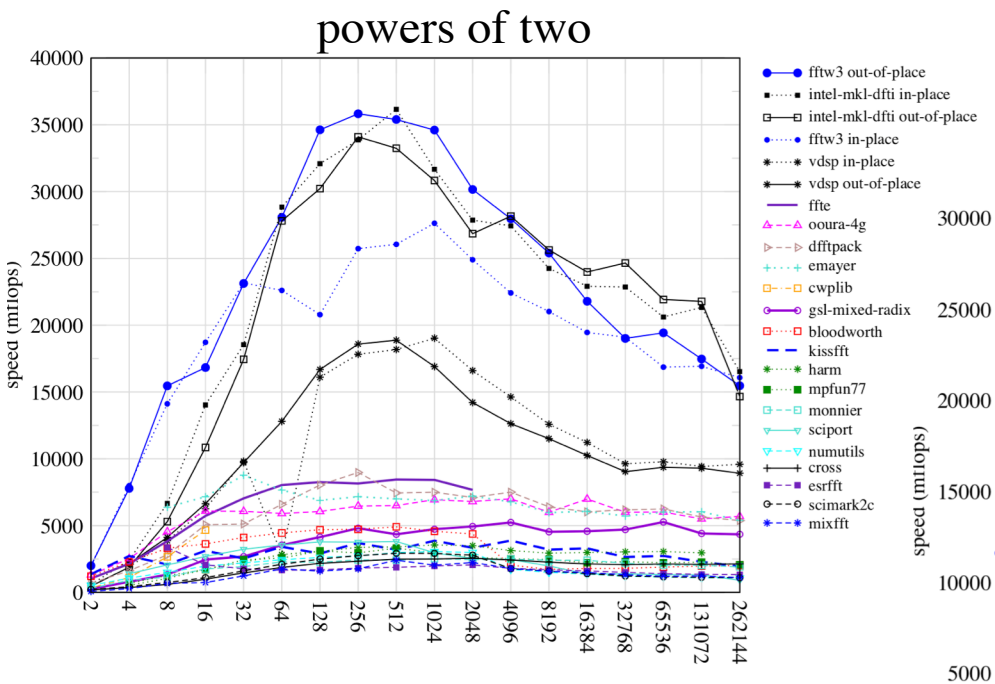
non-powers-of-two

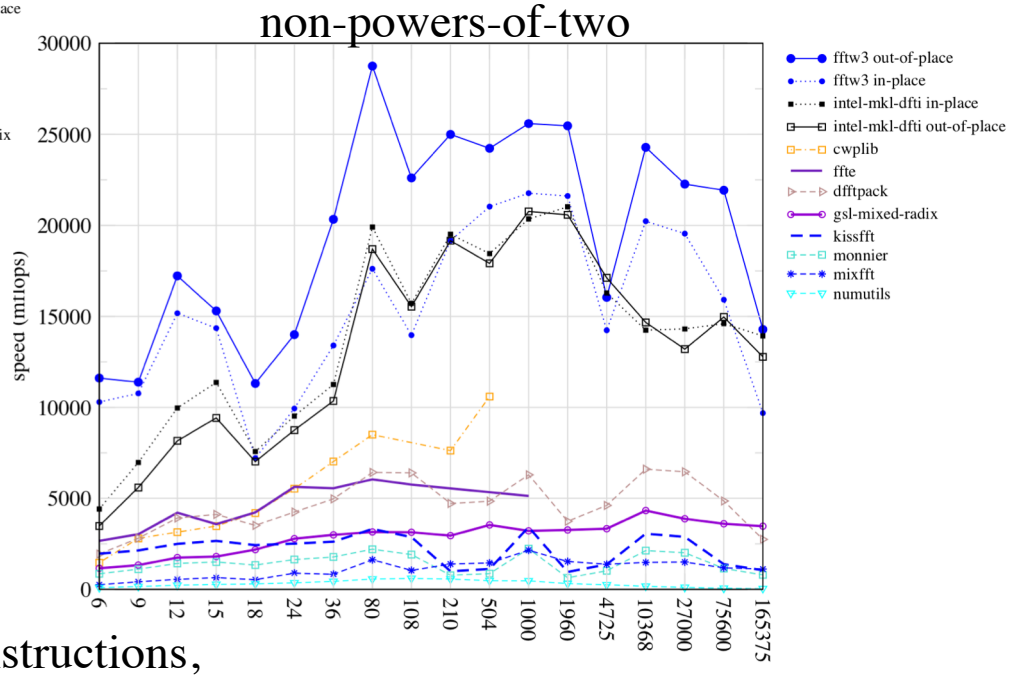


(If you don't hand code or generate SIMD instructions,
you lose … compilers won't save you for FFTs.)

Updated FFTW performance

double precision, 3GHz Intel Core i5 (2018 Mac mini)





(If you don't hand code or generate SIMD instructions,
you really lose … AVX2 etc. getting really wide.)

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.

A closing suggestion for numerical software

- Performance gets people's attention.

  … they don't take you seriously without it.

  … the "last factor of 2" is *really* hard to get, & not worth it for most problems.

- Usability & generality *keeps* the attention.

FFTW was the first widely available FFT library that supported arbitrary (even prime) sizes, arbitrary dimensions, strides, real/complex data, DCTs/DSTs, & parallelism … without that, it would have just been a hack for benchmark bragging.