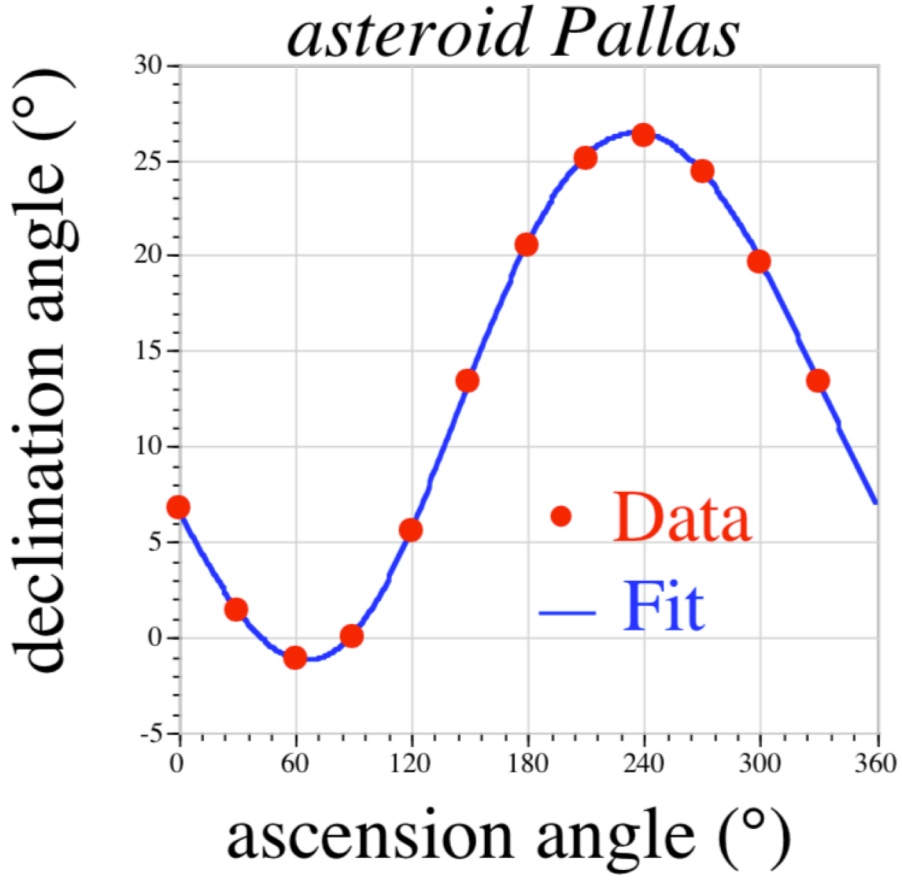
In the beginning (*c*. 1805):
Carl Friedrich Gauss



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):

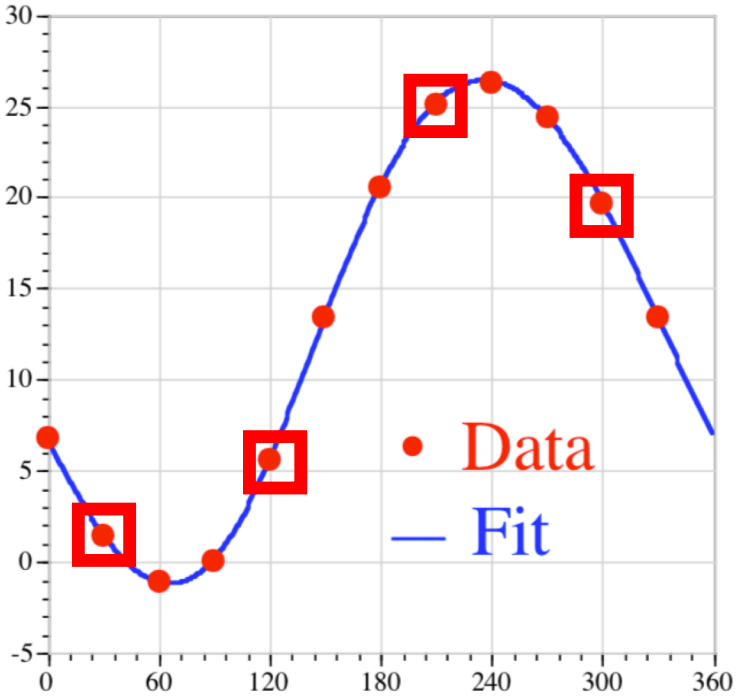
(before Fourier)

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

Gauss' 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.)

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!

two (of many) re-inventors:

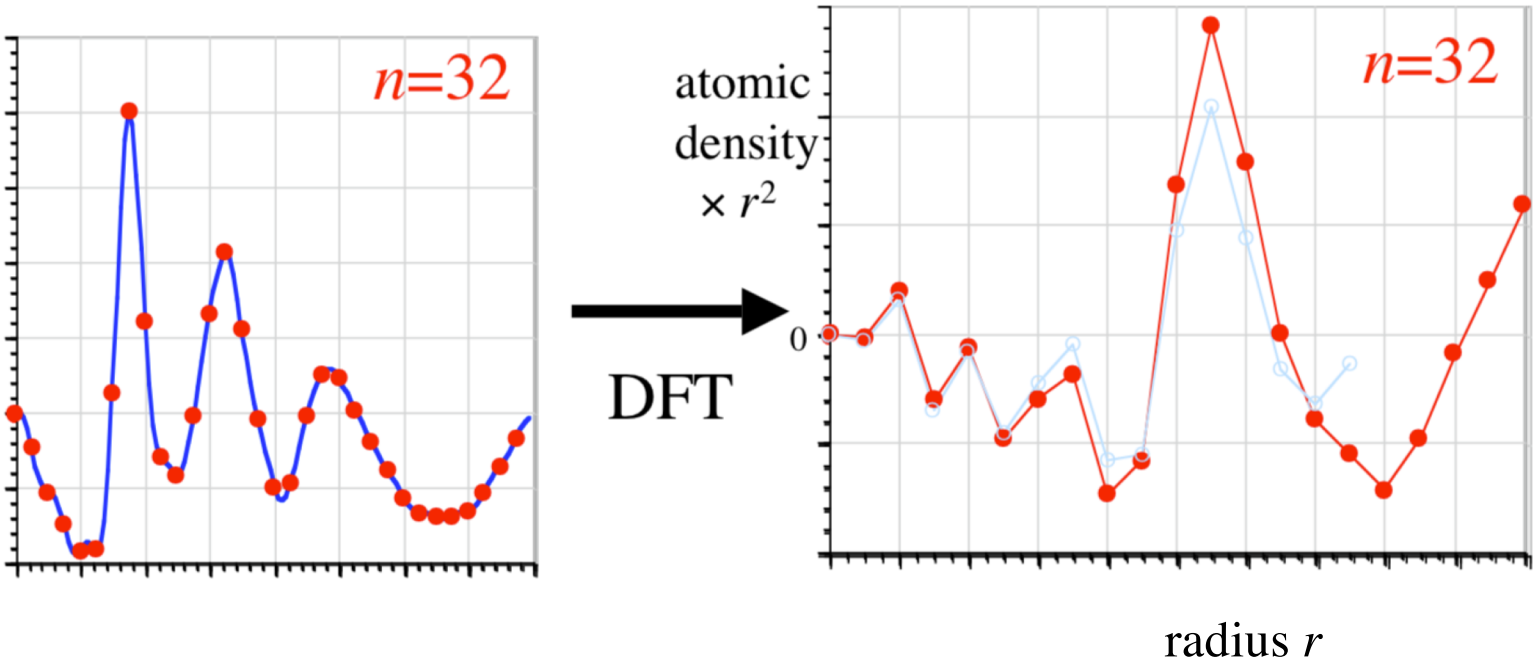
Danielson and Lanczos (1942)

[*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:

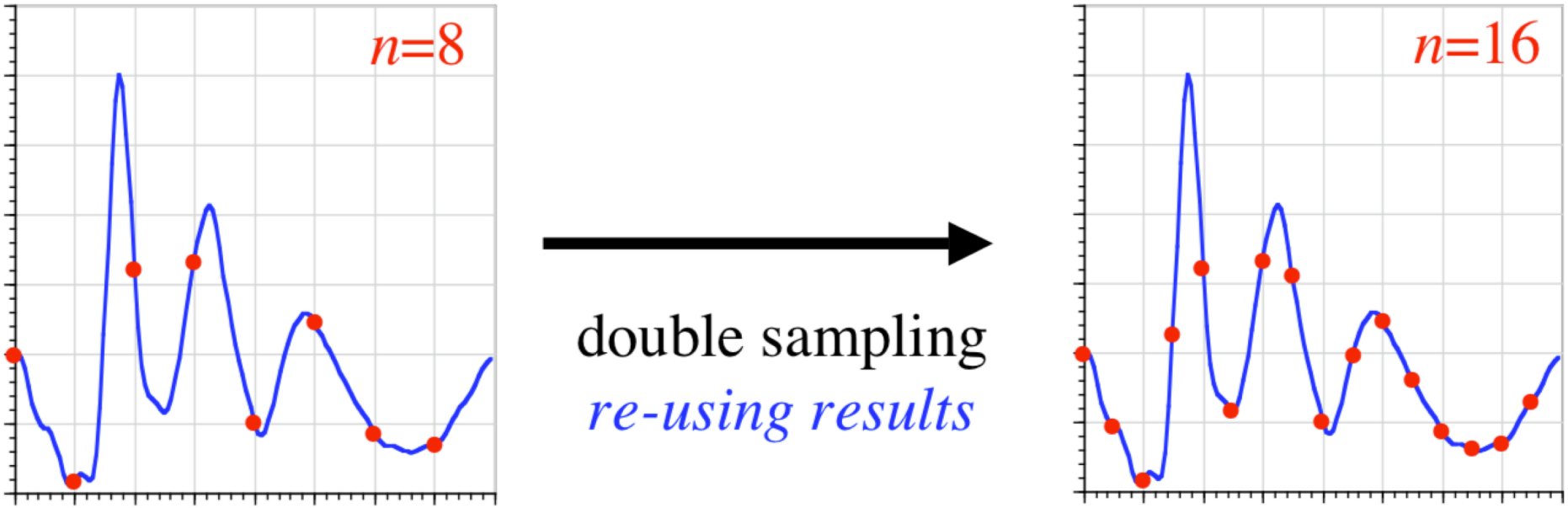


…double sampling until density (DFT) converges…

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!*

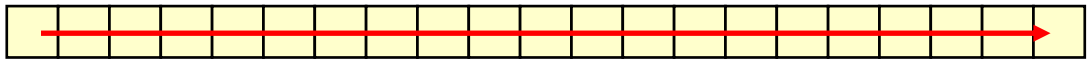
re-inventing Gauss (for the last time)

Cooley and Tukey (1965)

[*Math. Comp.* **19**, 297–301]

1d DFT of size N:

$N = N_1 N_2$



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

(+ phase rotation by twiddle factors)

= Recursive DFTs of sizes N_1 and N_2

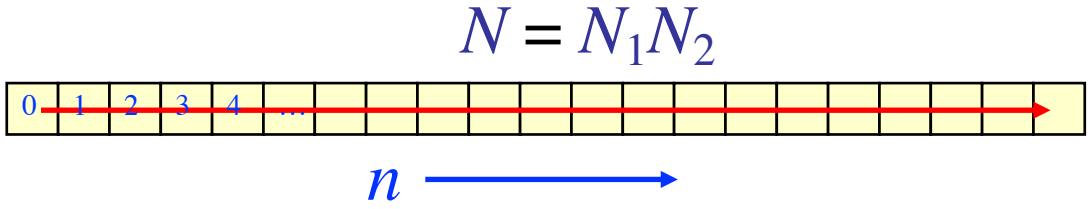
$O(N^2) \longrightarrow O(N \log N)$

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

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

The "Cooley-Tukey" FFT Algorithm

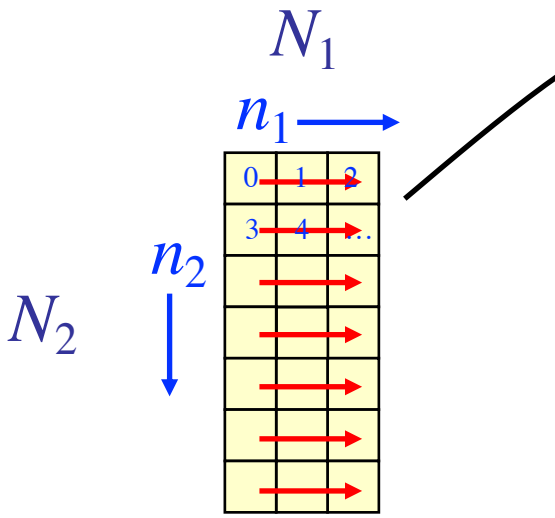
1d DFT of size N:



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

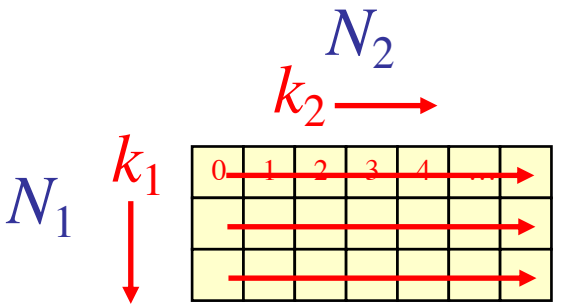
input re-indexing
$n = n_1 + N_1 n_2$

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 $k = N_2 k_1 + k_2$:

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

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

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)

…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…

Many other FFT algorithms

- Prime-factor algorithm: $N = N_1 N_2$ where N_1 and N_2 are co-prime: re-indexing based on Chinese Remainder Theorem with no twiddle factors.
- Rader's algorithm: for prime N, re-index using generator of multiplicative group to get a convolution of size N–1, do via FFTs.
- Bluestein's algorithm: re-index using $nk = -\frac{1}{2}(k-n)^2 + \frac{n^2}{2} + \frac{k^2}{2}$ to get convolution of size N, do via zero-padded FFTs.
- Many others…
- Specialized versions for real x_n, real-symmetric/antisymmetric x_n (DCTs and DSTs), etc.

The Next 30 Years…

Assume "time"

= # ~~multiplications~~

multiplications + # additions (= flops)

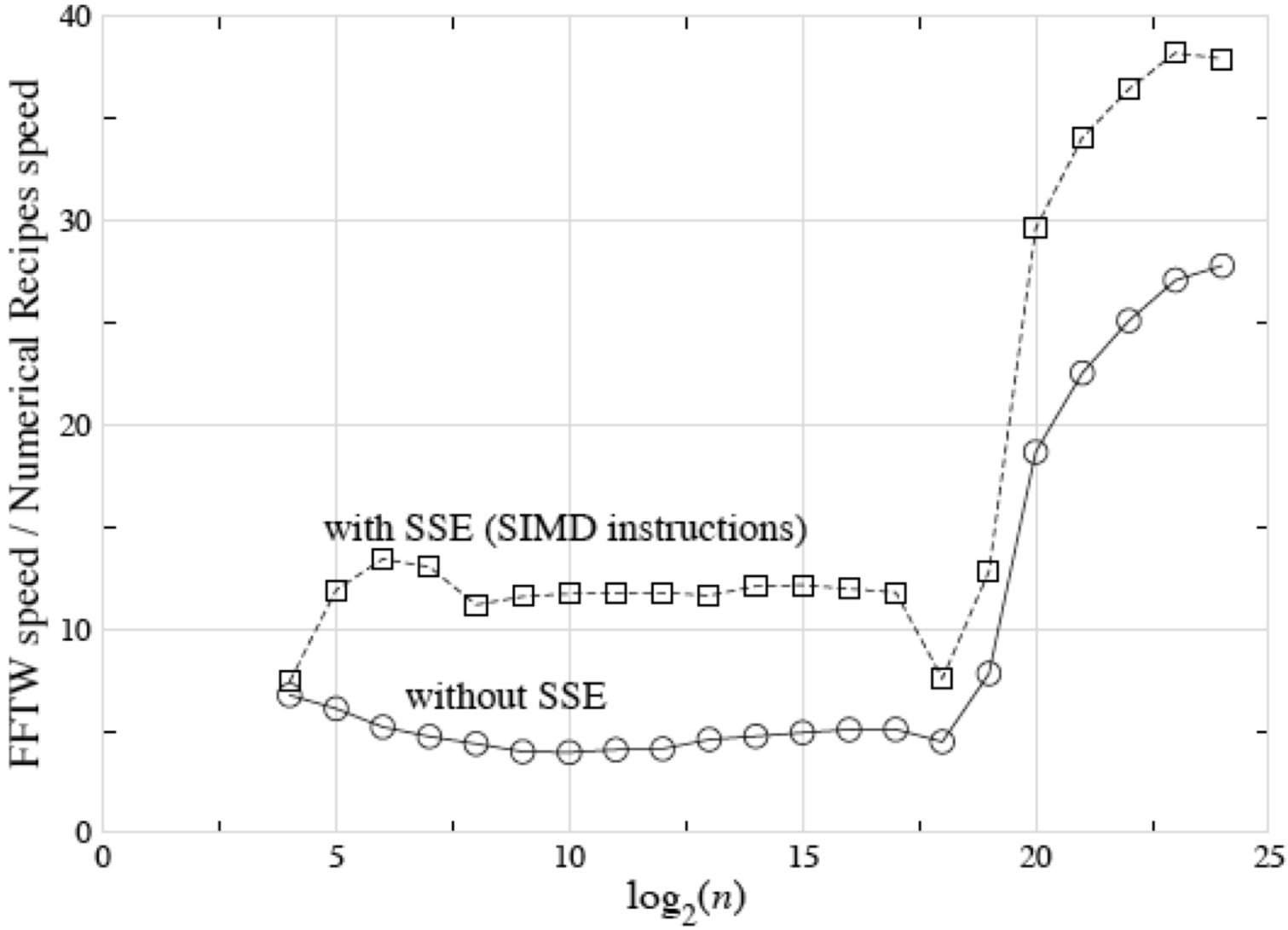
Winograd (1979): # multiplications = $\Theta(n)$

(…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?



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]

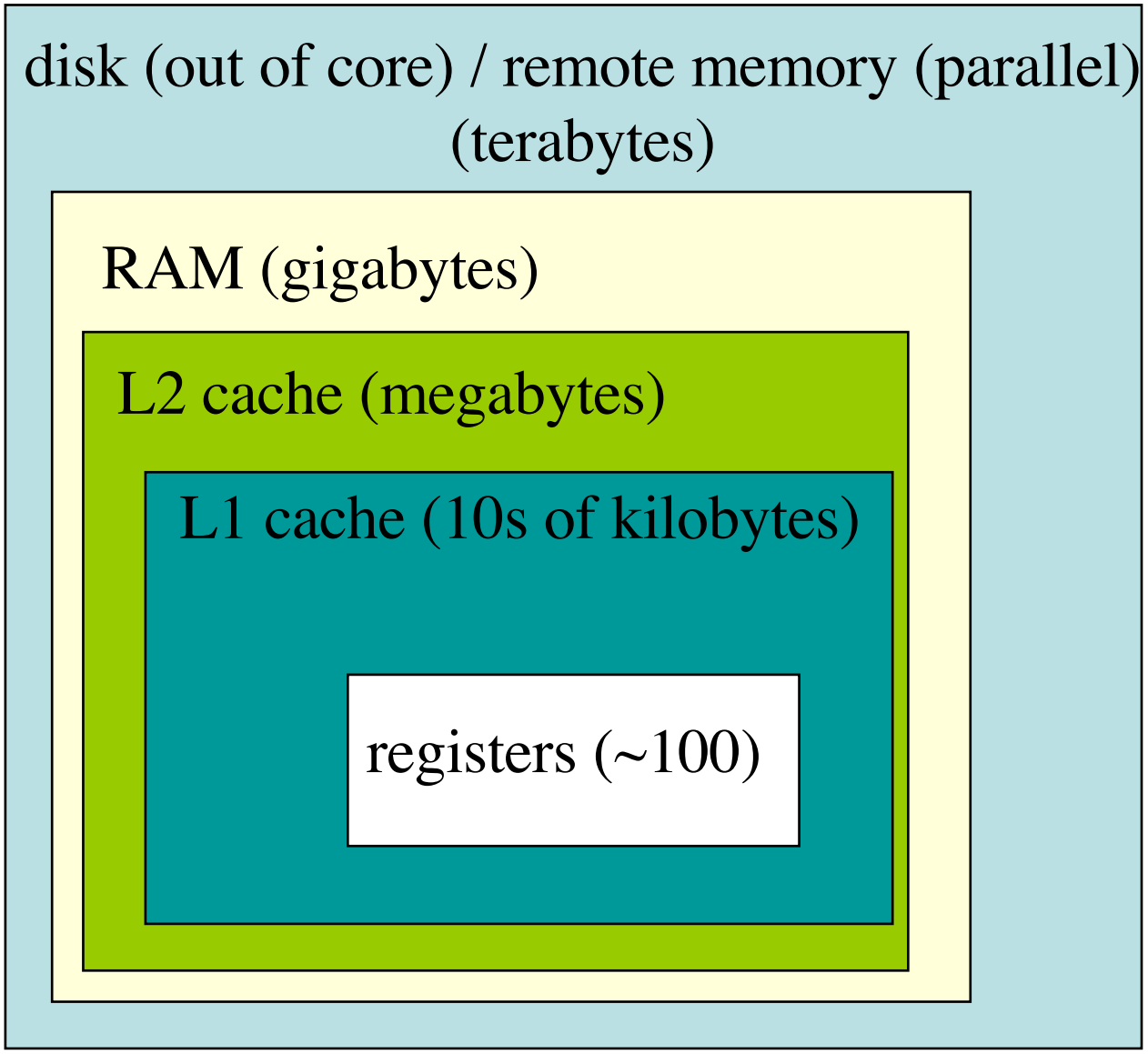
last 15+ years: flop count (varies by ~20%)

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

The “Fastest Fourier Transform in the West”

Steven G. Johnson, MIT Applied Mathematics

Matteo Frigo, Oracle; formerly MIT LCS (CSAIL)

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

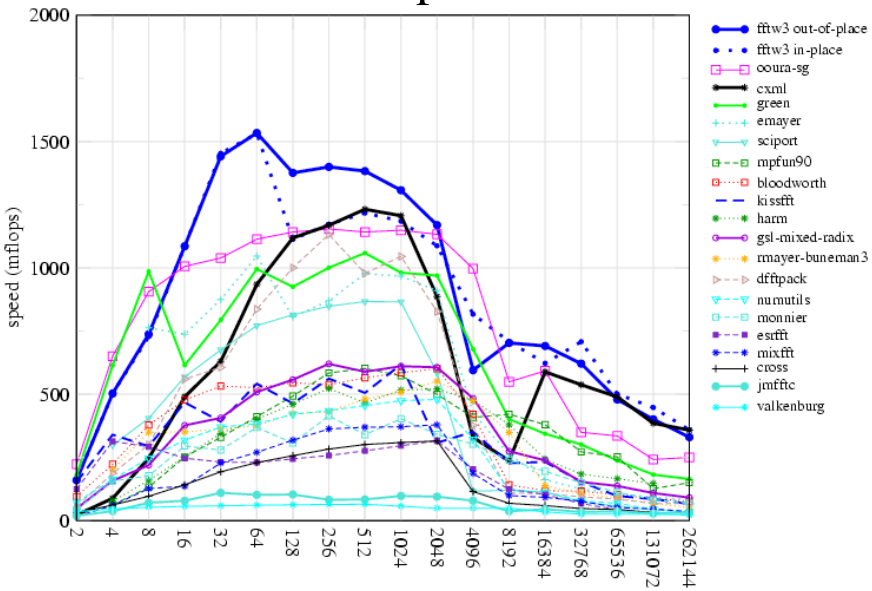
- Self-optimizes for your hardware (picks best composition of steps)
  = **portability + performance**

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

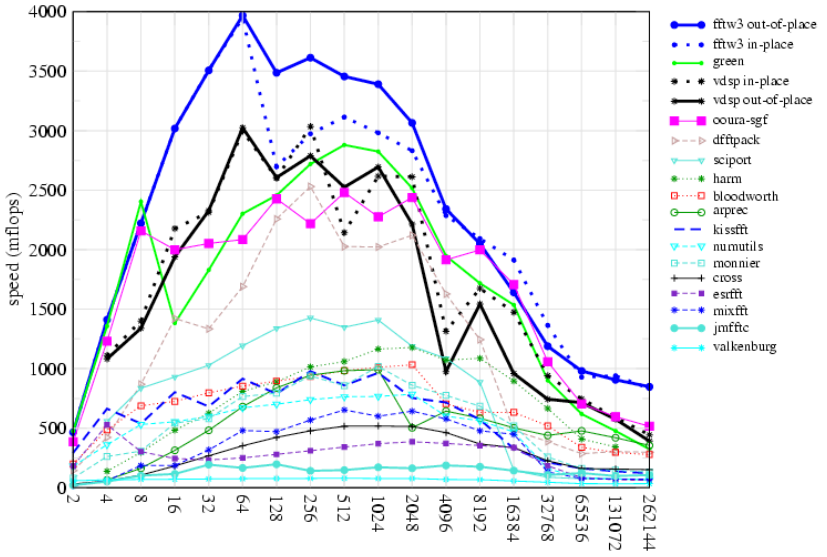
FFTW performance

power-of-two sizes, double precision

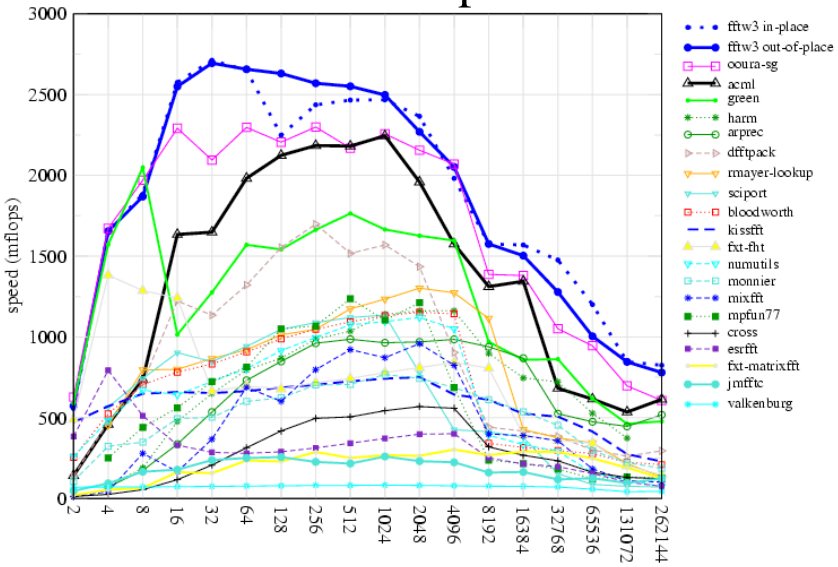
833 MHz Alpha EV6



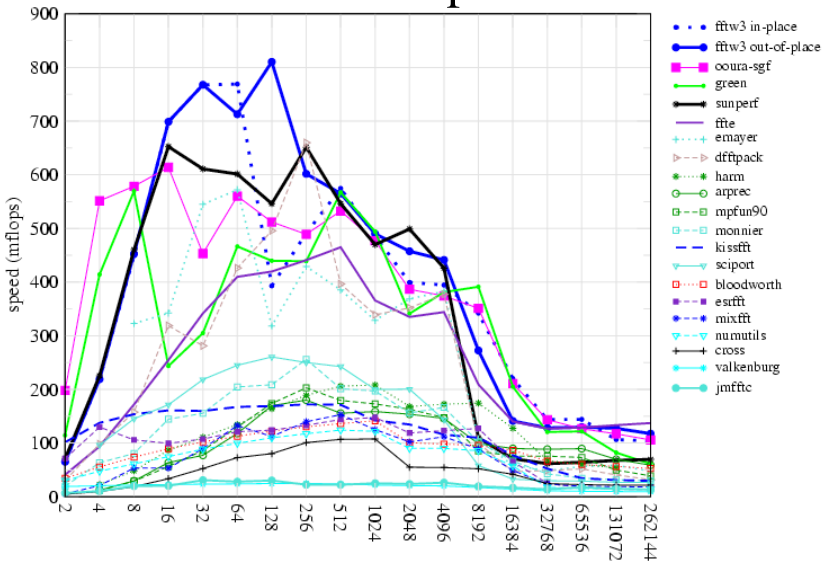
2 GHz PowerPC G5



2 GHz AMD Opteron



500 MHz Ultrasparc IIe

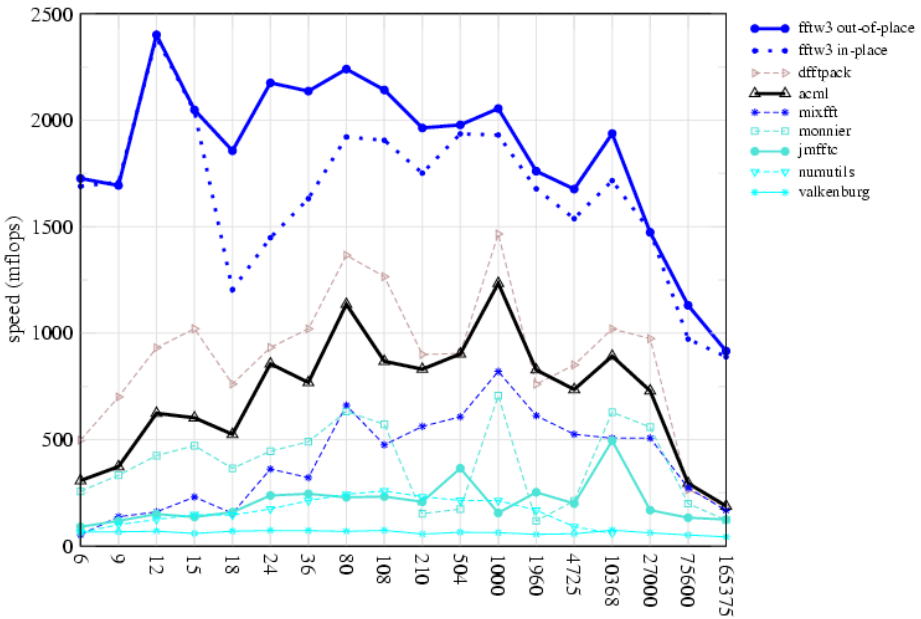


FFTW performance

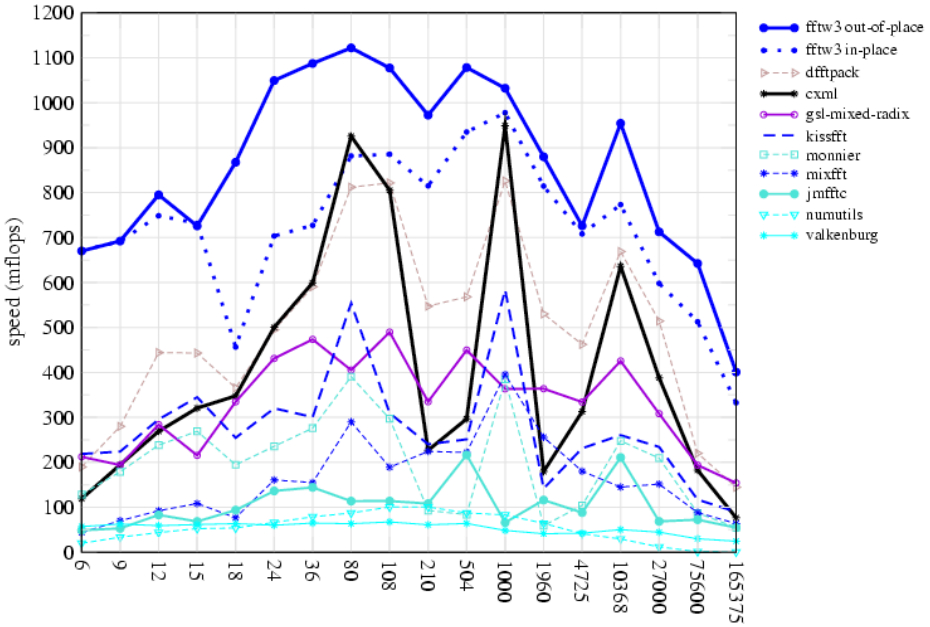
non-power-of-two sizes, double precision

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

2 GHz AMD Opteron



833 MHz Alpha EV6

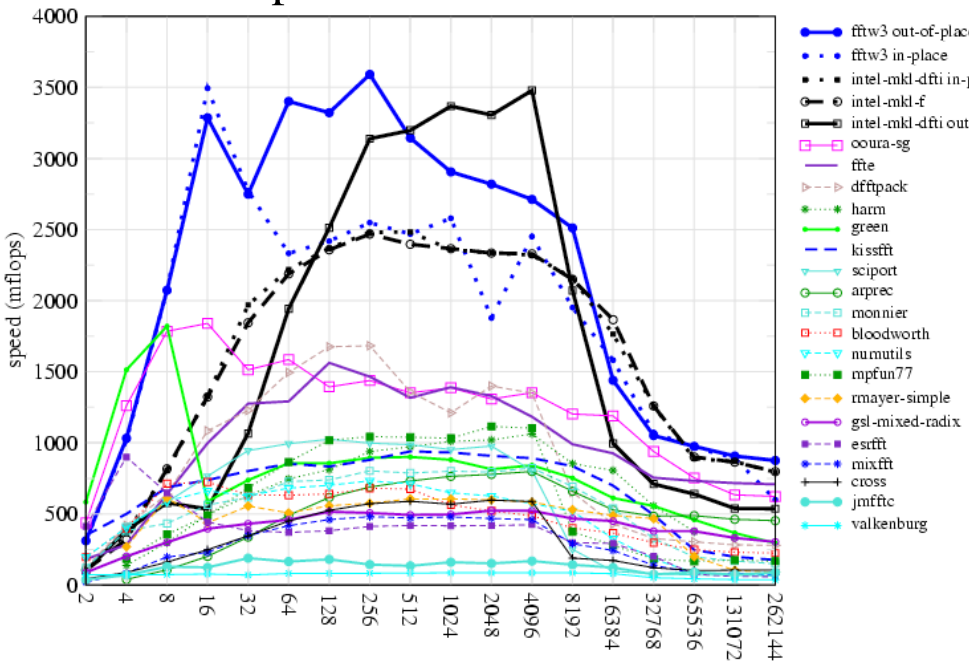


…because we let the code do the optimizing

FFTW performance

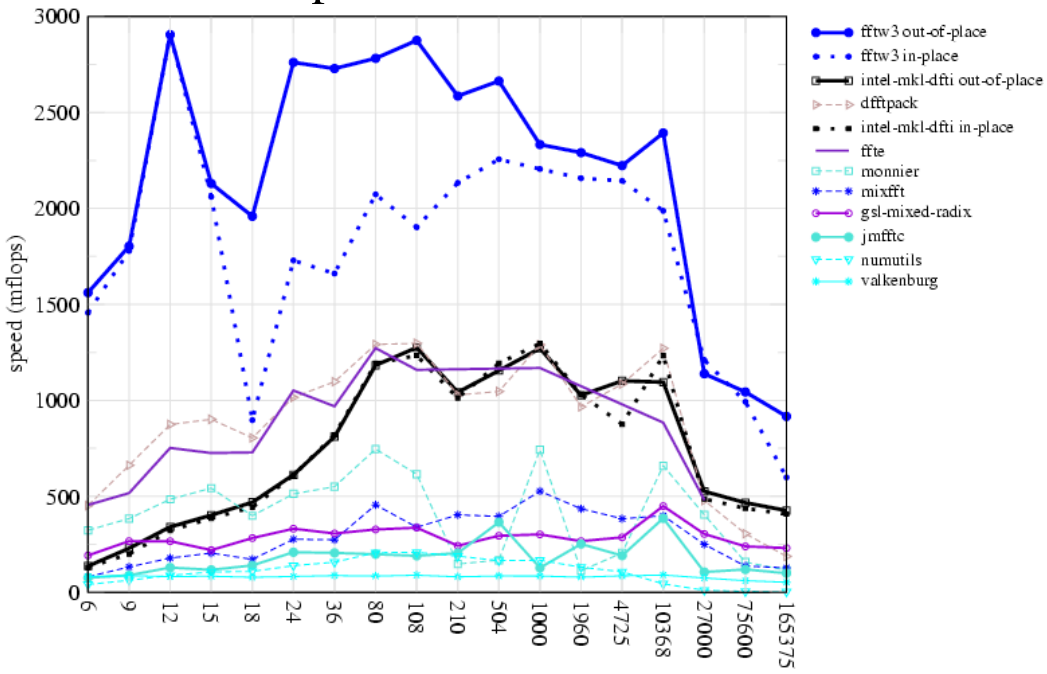
double precision, 2.8GHz Pentium IV: 2-way SIMD (SSE2)

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.

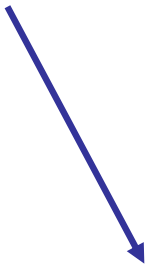
2. Computational kernels (codelets)
   should be automatically generated.

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.

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.

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)

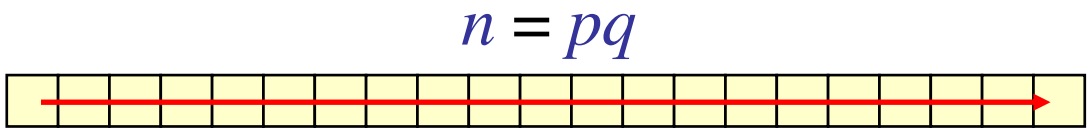
(Moore's prediction:
30 nanoseconds)

(= doubles every ~30 months)

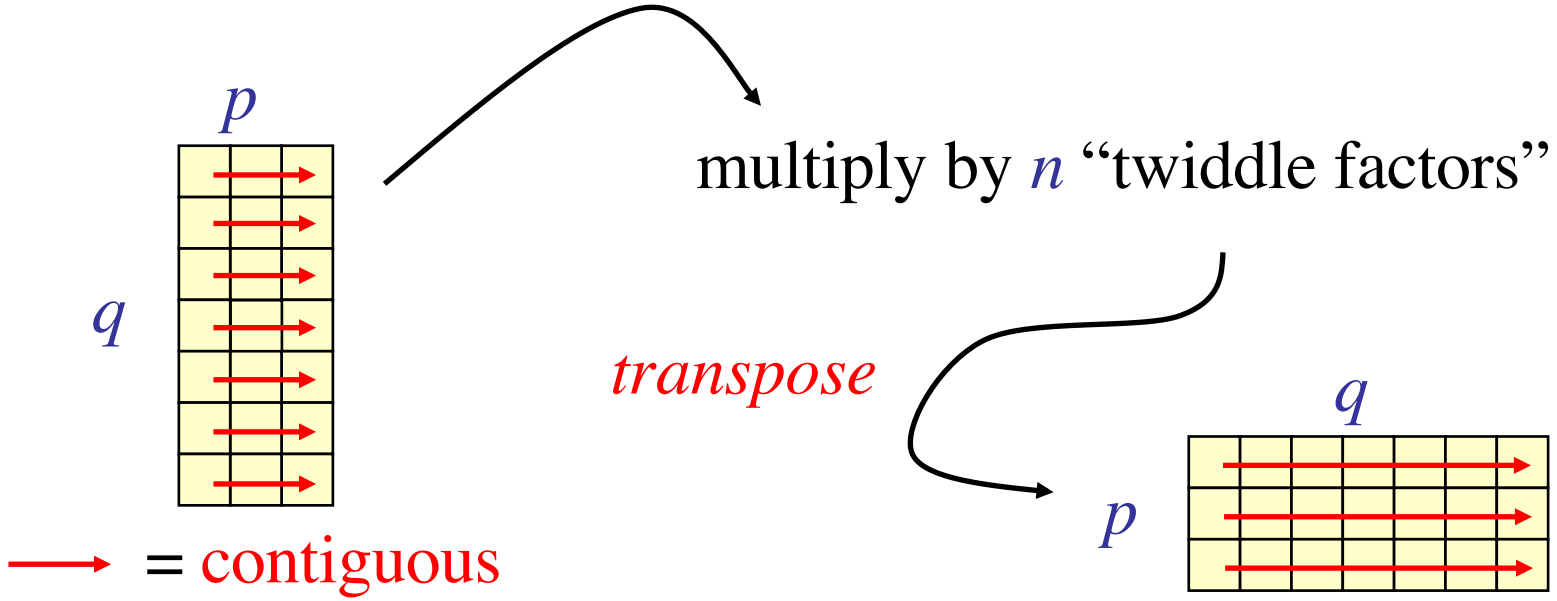
FFTs are hard: don't get "peak" CPU speed
especially for large n,
unlike *e.g.* dense matrix multiply

Discontiguous Memory Access

1d DFT of size n:



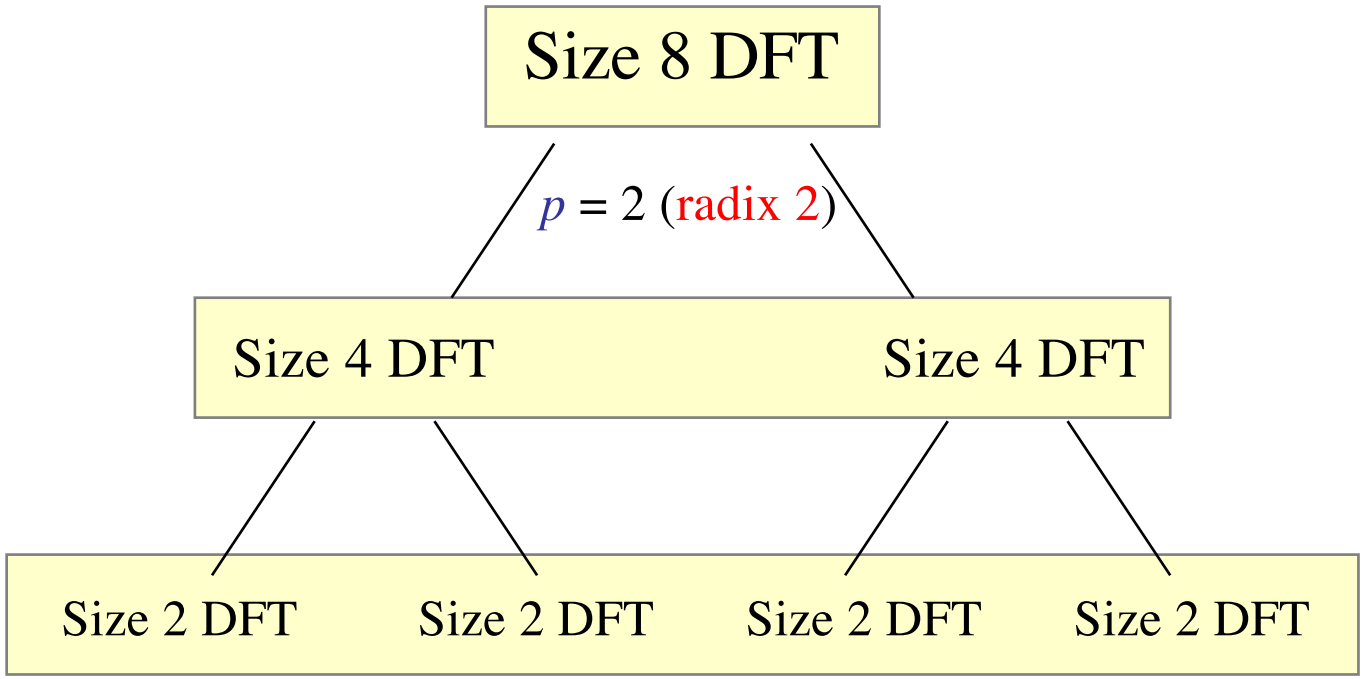
= ~2d DFT of size p x q



first DFT columns, size q
(non-contiguous)

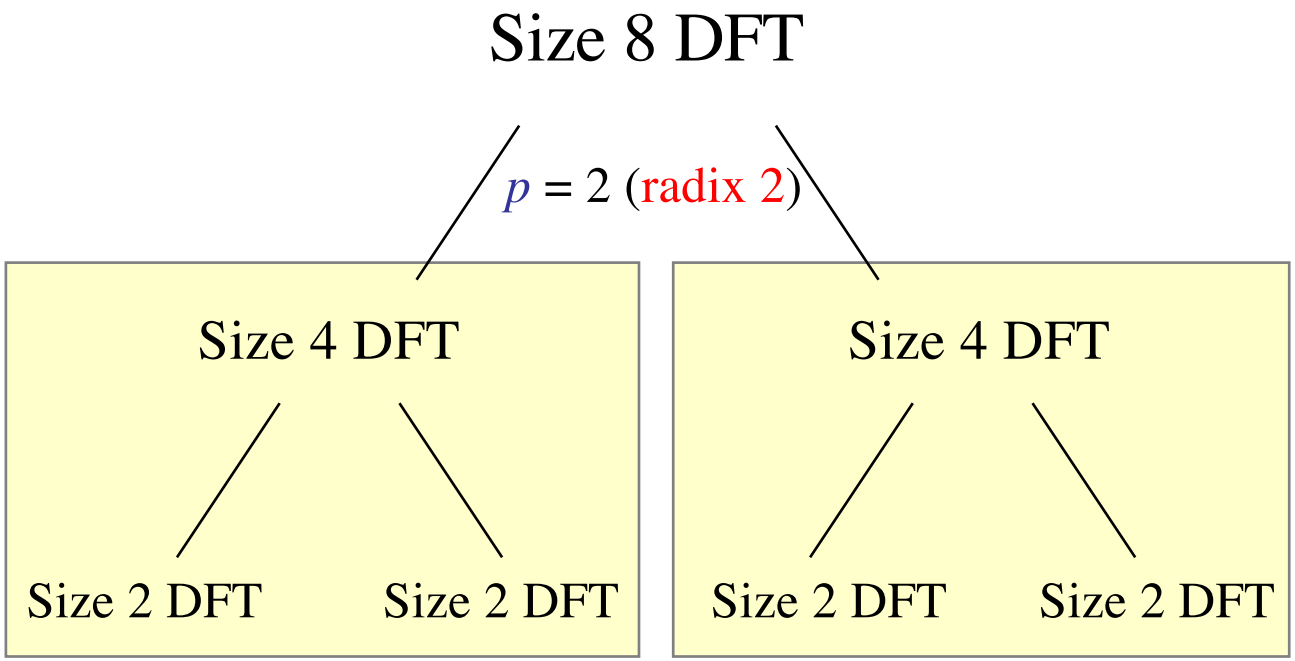
finally, DFT columns, size p
(non-contiguous)

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

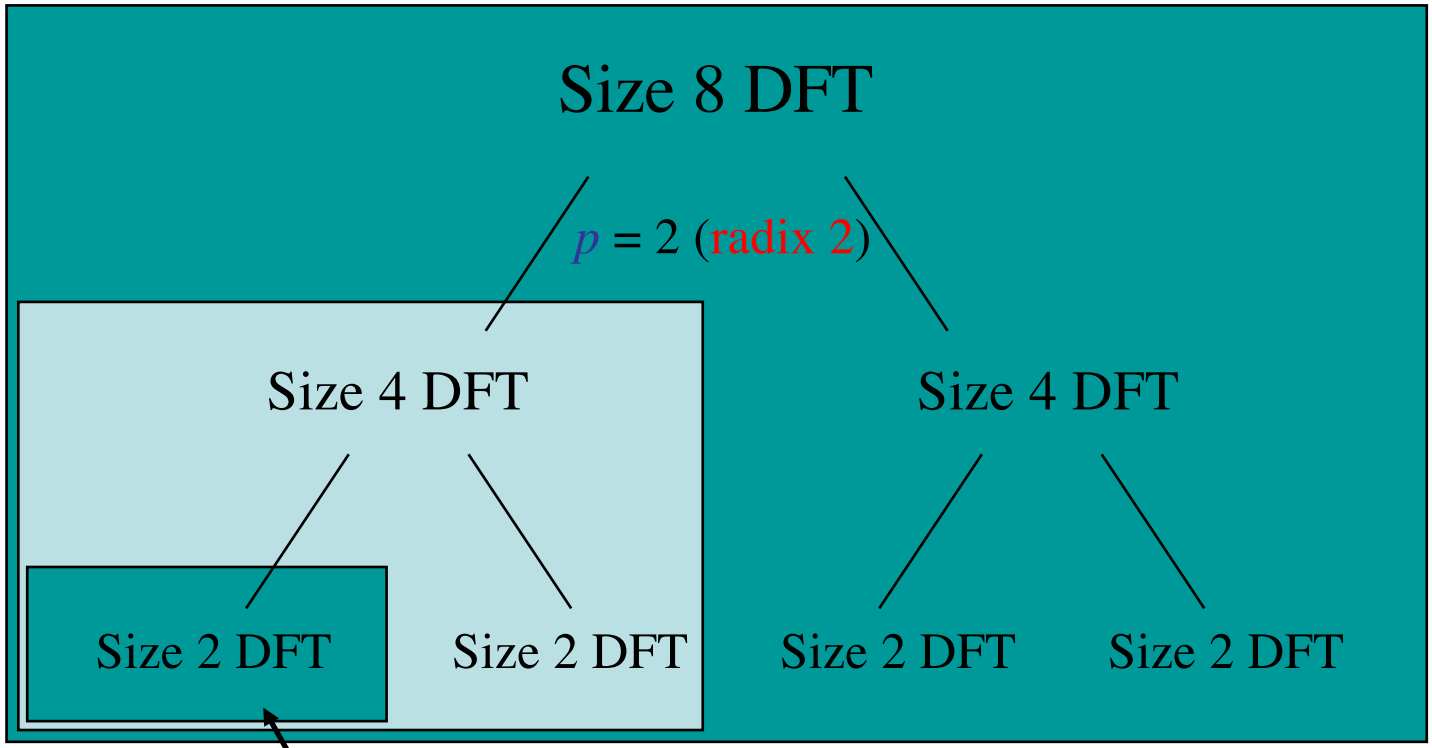
radix >> 2

…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

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.

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.

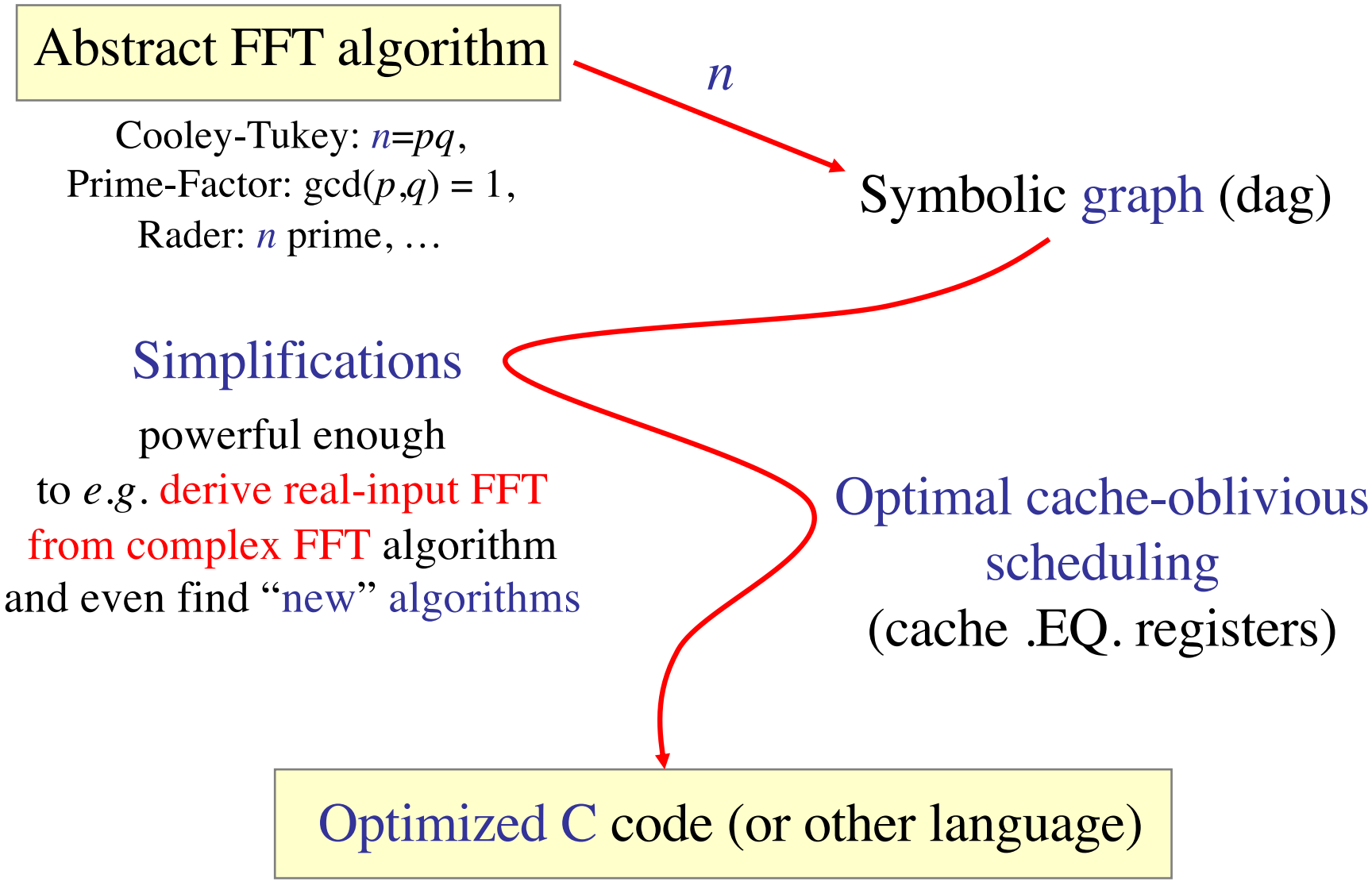
Allows easy experimentation with different optimizations & algorithms.

…CPU-specific hacks (SIMD) feasible

(& negates recursion overhead)

The Codelet Generator

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



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:

$$y_k = \sum_{j=0}^{n-1} x_j \omega_n^{jk} = \sum_{j_2=0}^{p-1} \left[\left(\sum_{j_1=0}^{q-1} x_{pj_1+j_2} \omega_q^{j_1 k_1} \right) \omega_n^{j_2 k_1} \right] \omega_p^{j_2 k_2},$$

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:

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

Constant folding

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]`

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

`array[strides[i]]`

using precomputed stride array:
`strides[i] = stride * i`

…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

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]

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.

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:
  — 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

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)}

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

Many Resulting "Algorithms"

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

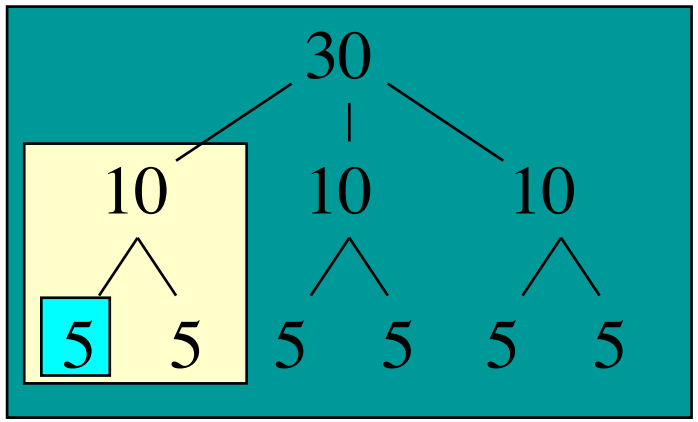
- VECLOOP can push topmost loop to "leaves"
  - "vector" FFT algorithm [Swarztrauber (1987)]

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

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

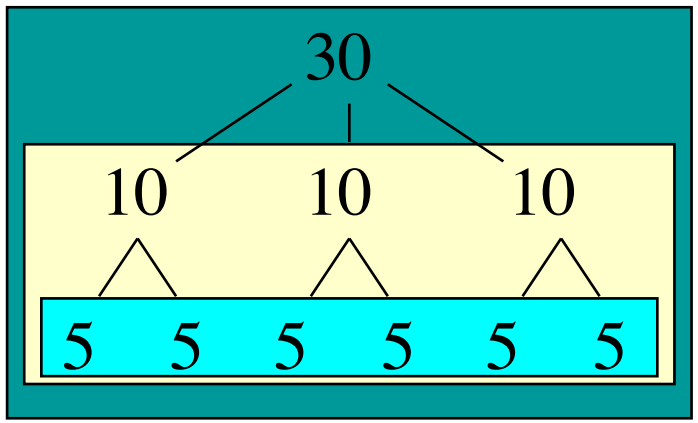
A "depth-first" plan:

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.)

Many Resulting "Algorithms"

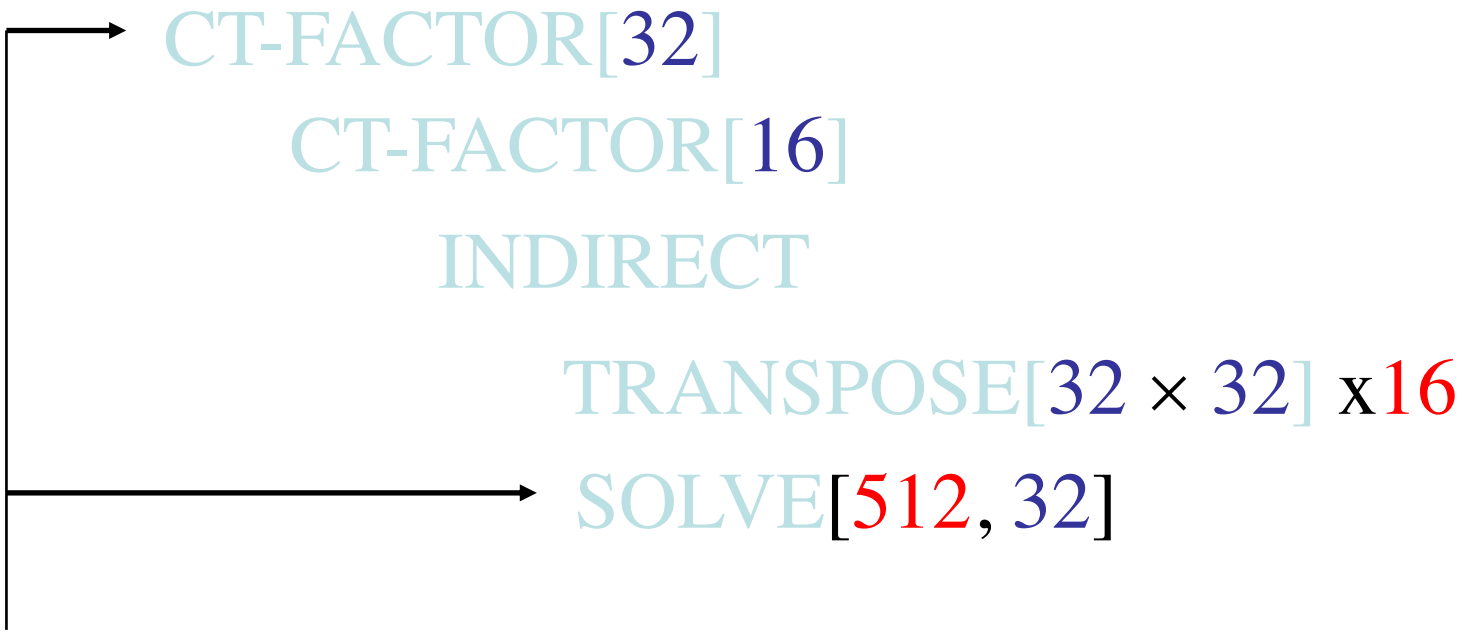
- INDIRECT + TRANSPOSE gives in-place DFTs,
  - bit-reversal = product of transpositions
    - … no separate bit-reversal "pass"
      - [Johnson (unrelated) & Burrus (1984)]

- 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

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)

(+ …)

=

huge improvements

for large 1d sizes

~2000 lines hard-coded C!

INDIRECT

VECLOOP (reorder) x64

VECLOOP x4

COPY[64]

VECLOOP x4

SOLVE[64, 64]

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)

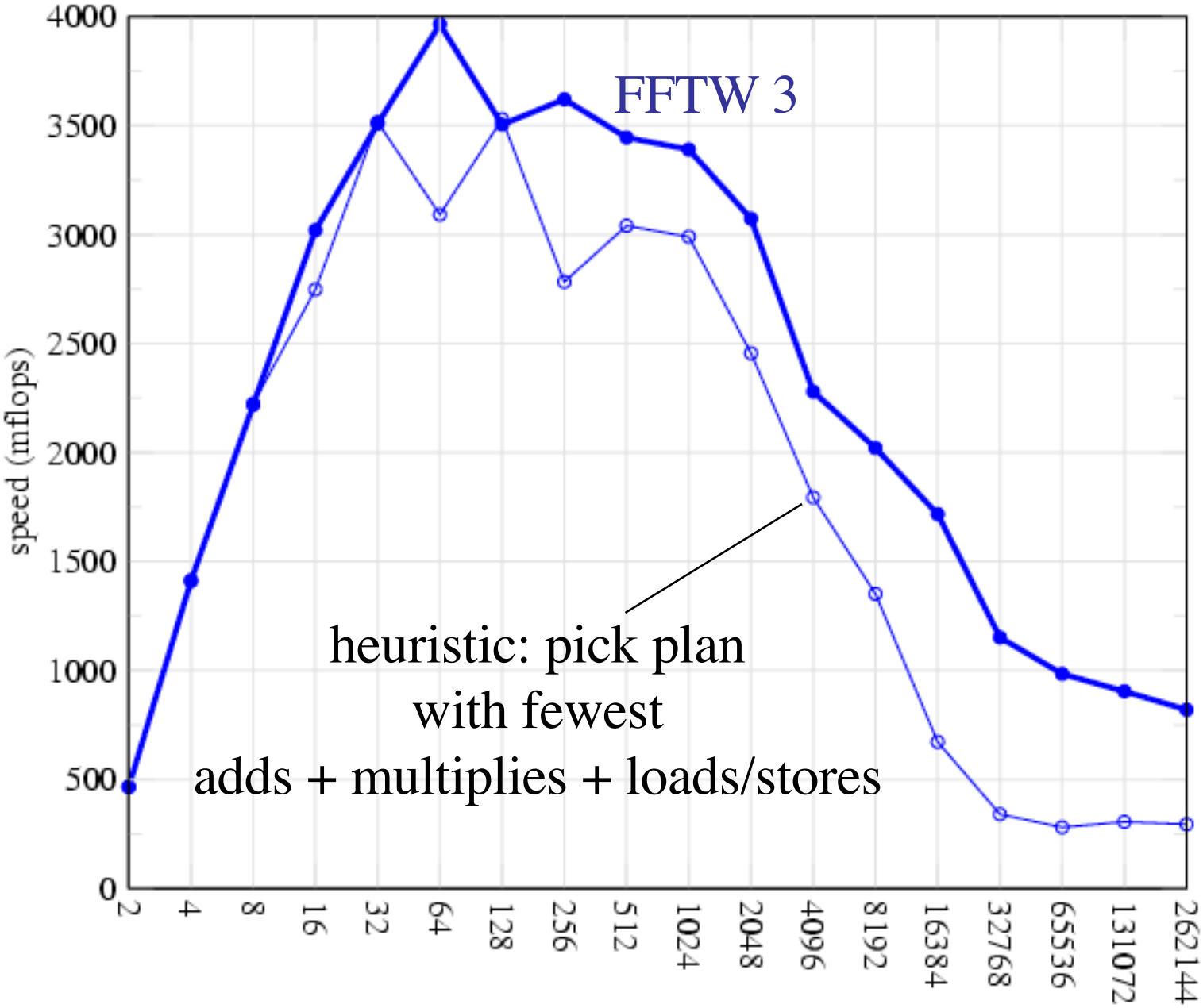
DFT(8) = fastest of:
- CT-FACTOR[2]: 2 DFT(4)
- CT-FACTOR[4]: 4 DFT(2)
- SOLVE[1,8]

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



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.