Algorithms of Scientific Computing

Fast Fourier Transform (FFT)

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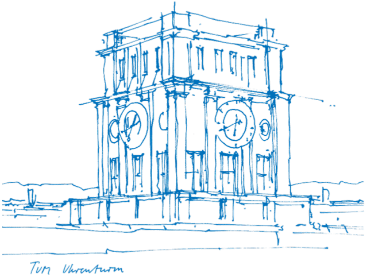


The Pair DFT/IDFT as Matrix-Vector Product

DFT and IDFT may be computed in the form

$$F_k = \frac{1}{N} \sum_{n=0}^{N-1} f_n \omega_N^{-nk} \qquad f_n = \sum_{k=0}^{N-1} F_k \omega_N^{nk}$$

or as matrix-vector products

$$\mathbf{F} = \frac{1}{N} \mathbf{W}^H \mathbf{f}\,, \qquad \mathbf{f} = \mathbf{W}\mathbf{F}\,,$$

with a **computational complexity of $\mathcal{O}(N^2)$**.

Note that

$$\mathrm{DFT}(f) = \frac{1}{N} \overline{\mathrm{IDFT}(\bar{f})}\,.$$

A fast computation is possible via the **divide-and-conquer** approach.

Fast Fourier Transform for $N = 2^p$

Basic idea: sum up even and odd indices separately in IDFT

$\rightarrow$ first for $n = 0, 1, \ldots, \frac{N}{2} - 1$:

$$x_n = \sum_{k=0}^{N-1} X_k \omega_N^{nk} = \sum_{k=0}^{\frac{N}{2}-1} X_{2k} \omega_N^{2nk} + \sum_{k=0}^{\frac{N}{2}-1} X_{2k+1} \omega_N^{(2k+1)n}$$

We set $Y_k := X_{2k}$ and $Z_k := X_{2k+1}$, use $\omega_N^{2nk} = \omega_{N/2}^{nk}$, and get a sum of two IDFT on $\frac{N}{2}$ coefficients:

$$x_n = \sum_{k=0}^{N-1} X_k \omega_N^{nk} = \underbrace{\sum_{k=0}^{\frac{N}{2}-1} Y_k \omega_{N/2}^{nk}}_{:= y_n} + \omega_N^n \underbrace{\sum_{k=0}^{\frac{N}{2}-1} Z_k \omega_{N/2}^{nk}}_{:= z_n} .$$

Note: this formula is actually valid for all $n = 0, \ldots, N-1$; however, the IDFTs of size $\frac{N}{2}$ will only deliver the y_n and z_n for $n = 0, \ldots, \frac{N}{2} - 1$ (but: y_n and z_n are periodic!)

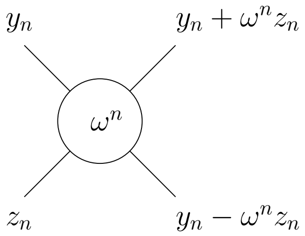
Fast Fourier Transform (FFT)

Consider the formular $x_n = y_n + \omega_N^n z_n$ for indices $\frac{N}{2}, \ldots, N-1$:

$$x_{n+\frac{N}{2}} = y_{n+\frac{N}{2}} + \omega_N^{\left(n+\frac{N}{2}\right)} z_{n+\frac{N}{2}} \qquad \text{for } n = 0, \ldots, \frac{N}{2} - 1$$

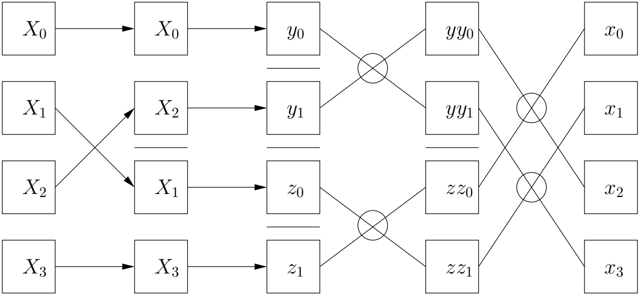
Since $\omega_N^{\left(n+\frac{N}{2}\right)} = -\omega_N^n$ and y_n and z_n have a period of $\frac{N}{2}$, we obtain the so-called **butterfly scheme**:

$$\begin{aligned} x_n &= y_n + \omega_N^n z_n \\ x_{n+\frac{N}{2}} &= y_n - \omega_N^n z_n \end{aligned}$$

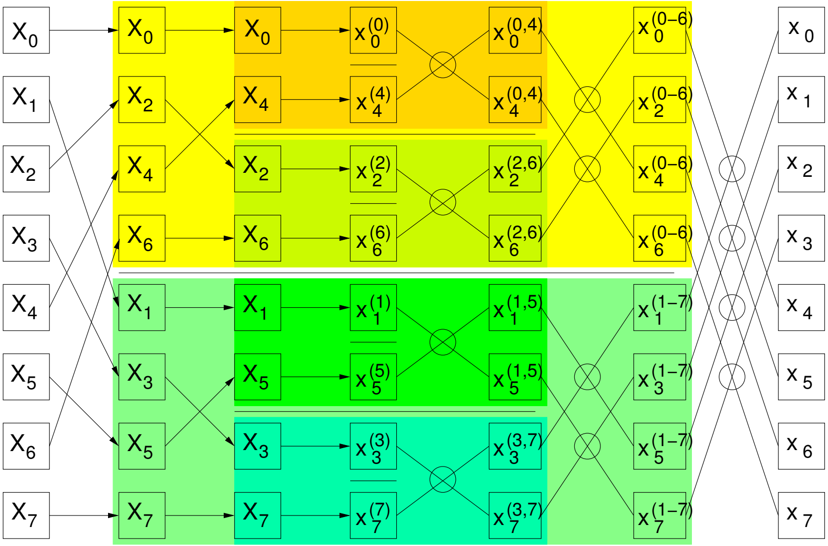


Fast Fourier Transform – Butterfly Scheme

$$\begin{aligned}(x_0, x_1, \ldots, \ldots, x_{N-1}) &= \mathrm{IDFT}(X_0, X_1, \ldots, \ldots, X_{N-1})\\ &\Downarrow\\ (y_0, y_1, \ldots, y_{\frac{N}{2}-1}) &= \mathrm{IDFT}(X_0, X_2, \ldots, X_{N-2})\\ (z_0, z_1, \ldots, z_{\frac{N}{2}-1}) &= \mathrm{IDFT}(X_1, X_3, \ldots, X_{N-1})\end{aligned}$$



Fast Fourier Transform – Butterfly Scheme (2)



Recursive Implementation of the FFT

$\texttt{rekFFT}(\mathbf{X}) \longrightarrow \mathbf{x}$

(1) Generate vectors **Y** and **Z**:

$$\text{for } n = 0, \ldots, \tfrac{N}{2} - 1: \qquad Y_n := X_{2n} \quad \text{und} \quad Z_n := X_{2n+1}$$

(2) compute 2 FFTs of half size:

$$\texttt{rekFFT}(\mathbf{Y}) \longrightarrow \mathbf{y} \qquad \text{and} \qquad \texttt{rekFFT}(\mathbf{Z}) \longrightarrow \mathbf{z}$$

(3) combine with “butterfly scheme”:

$$\text{for } k = 0, \ldots, \tfrac{N}{2} - 1: \quad \left\{ \begin{array}{rcl} x_k & = & y_k + \omega_N^k z_k \\ x_{k+\frac{N}{2}} & = & y_k - \omega_N^k z_k \end{array} \right.$$

Observations on the Recursive FFT

- Computational effort $C(N)$ ($N = 2^p$) given by recursion equation

$$C(N) = \begin{cases} \mathcal{O}(1) & \text{for} \quad N = 1 \\ \mathcal{O}(N) + 2C\left(\frac{N}{2}\right) & \text{for} \quad N > 1 \end{cases} \quad \Rightarrow \quad C(N) = \mathcal{O}(N \log N)$$

- Algorithm splits up in 2 phases:
  - resorting of input data
  - combination following the “butterfly scheme”

$\Rightarrow$ Anticipation of the resorting enables a simple, iterative algorithm without additional memory requirements.

Sorting Phase of the FFT – Bit Reversal

Observation:

- even indices are sorted into the upper half,
  odd indices into the lower half.
- distinction even/odd based on least significant bit
- distinction upper/lower based on most significant bit

$\Rightarrow$ An index in the sorted field has the **reversed** (i.e. mirrored) binary representation compared to the original index.

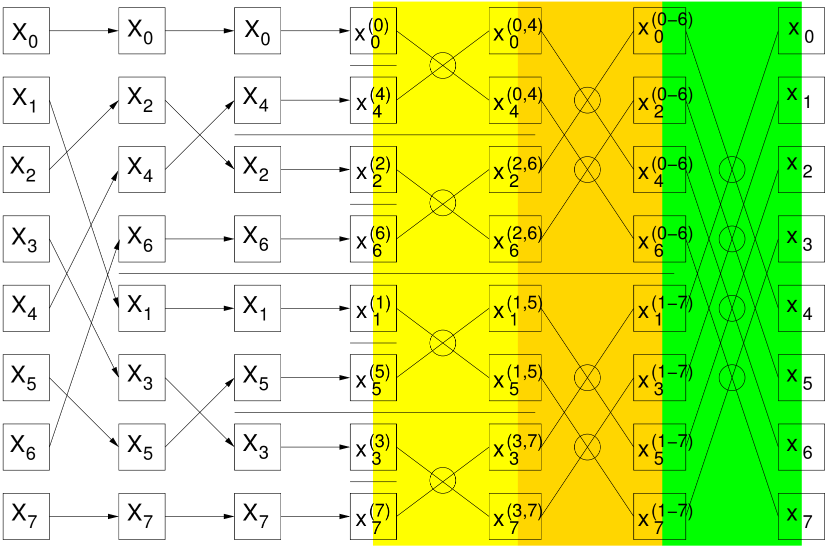
Sorting of a Vector ($N = 2^p$ Entries, Bit Reversal)

```
/** FFT sorting phase: reorder data in array X */
for(int n=0; n<N; n++) {
   // Compute p-bit bit reversal of n in j
   int j=0; int m=n;
   for(int i=0; i<p; i++) {
      j = 2*j + m%2; m = m/2;
   }
   // if j>n exchange X[j] and X[n]:
   if (j>n) { complex<double> h;
      h = X[j]; X[j] = X[n]; X[n] = h;
   }
}
```

Bit reversal needs $\mathcal{O}(p) = \mathcal{O}(\log N)$ operations

- $\Rightarrow$ Sorting results also in a complexity of $\mathcal{O}(N \log N)$
- $\Rightarrow$ Sorting may consume up to 10–30 % of the CPU time!

Iterative Implementation of the “Butterflies”



Iterative Implementation of the "Butterflies"

```
{Loop over the size of the IDFT}
for(int L=2; L<=N; L*=2)
   {Loop over the IDFT of one level}
   for(int k=0; k<N; k+=L)
      {perform all butterflies of one level}
      for(int j=0; j<L/2; j++) {
         {complex computation:}
         z ← ω_L^j * X[k+j+L/2]
         X[k+j+L/2] ← X[k+j] - z
         X[k+j] ← X[k+j] + z
      }
```

- k-loop und j-loop are "permutable"!
- How and when are the ω_L^j computed?

Iterative Implementation – Variant 1

```
/** FFT butterfly phase: variant 1 */
for(int L=2; L<=N; L*=2)
   for(int k=0; k<N; k+=L)
      for(int j=0; j<L/2; j++) {
         complex<double> z = omega(L,j) * X[k+j+L/2];
         X[k+j+L/2] = X[k+j] - z;
         X[k+j] = X[k+j] + z;
      }
```

Advantage: consecutive (“stride-1”) access to data in array X

- ⇒ suitable for vectorisation
- ⇒ good cache performance due to prefetching (stream access) and usage of cache lines

Disadvantage: multiple computations of ω_L^j

Iterative Implementation – Variant 1 Vectorised

```
/** FFT butterfly phase: variant 1 vectorised*/
for(int L=2; L<=N; L*=2)
  for(int k=0; k<N; k+=L)
    for(int j=0; j<L/2; j+= SIMD_LENGTH) {
      kjStart = k+j;
      kjEnd = k+j + (SIMD_LENGTH-1);
      complex<double> z[0: SIMD_LENGTH-1];
      z[0: SIMD_LENGTH-1] = omega(L,j) * X[kjStart+L/2 : kjEnd+L/2];
      X[kjStart+L/2 : kjEnd+L/2] = X[kjStart:kjEnd] - z;
      X[kjStart:kjEnd] = X[kjStart:kjEnd] + z;
    }
```

Comments on the code:

- we assume that our CPU offers SIMD instructions that can add/multiply short vectors of SIMD_LENGTH complex numbers
- with the notation X[kjStart:kjEnd] we mean a subvector of SIMD_LENGTH consecutive complex numbers starting from element X[kjStart]
- Note: the term omega(L,j) has to be changed into such a short vector, as well

Iterative Implementation – Variant 2

```
/** FFT butterfly phase: variant 2 */
for(int L=2; L<=N; L*=2)
  for(int j=0; j<L/2; j++) {
    complex<double> w = omega(L,j);
    for(int k=0; k<N; k+=L) {
      complex<double> z = w * X[k+j+L/2];
      X[k+j+L/2] = X[k+j] - z;
      X[k+j] = X[k+j] + z;
  } }
```

Advantage: each ω_L^j only computed once

Disadvantage: "stride-L"-access to the array `X`

⇒ worse cache performance (inefficient use of cache lines)

⇒ not suitable for vectorisation

Separate Computation of $\omega_{\mathtt{L}}^{\mathtt{j}}$

- necessary: $N-1$ factors

$$\omega_2^0, \omega_4^0, \omega_4^1, \ldots, \omega_L^0, \ldots, \omega_L^{L/2-1}, \ldots, \omega_N^0, \ldots, \omega_N^{N/2-1}$$

- are computed in advance, and stored in an array `w`, e.g.:

```
for(int L=2; L<=N; L*=2)
   for(int j=0; j<L/2; j++)
      w[L/2+j] ← ω_L^j;
```

- Variant 2: access on `w` in sequential order
- Variant 1: access on `w` local (but repeated) and compatible with vectorisation
- Important: weight array w[:] needs to stay in cache!
  (as accesses to main memory can be slower than recomputation)

Cache Efficiency – Variant 1 Revisited

```
/** FFT butterfly phase: variant 1 */
for(int L=2; L<=N; L*=2)
  for(int k=0; k<N; k+=L)
    for(int j=0; j<L/2; j++) {
      complex<double> z = w[L/2+j] * X[k+j+L/2];
      X[k+j+L/2] = X[k+j] - z;
      X[k+j] = X[k+j] + z;
    }
```

Observation:

- each L-loop traverses entire array X
- in the ideal case $(N \log N)/B$ **cache line transfers** (N/B per L-loop, B the size of the cache line), unless all N elements fit into cache

Compare with recursive scheme:

- if $L < M_C$ (M_C the cache size), then the entire FFT fits into cache
- is it thus possible to require only $N \log N/(M_C B)$ cache line transfers?

Butterfly Phase with Loop Blocking

```
/** FFT butterfly phase: loop blocking for k */
for(int L=2; L<=N; L*=2)
  for(int kb=0; kb<N; kb+=M)
    for(int k=kb; k<kb+M; k+=L)
      for(int j=0; j<L/2; j++) {
          complex<double> z = w[L/2+j] * X[k+j+L/2];
          X[k+j+L/2] = X[k+j] - z;
          X[k+j] = X[k+j] + z;
      }
```

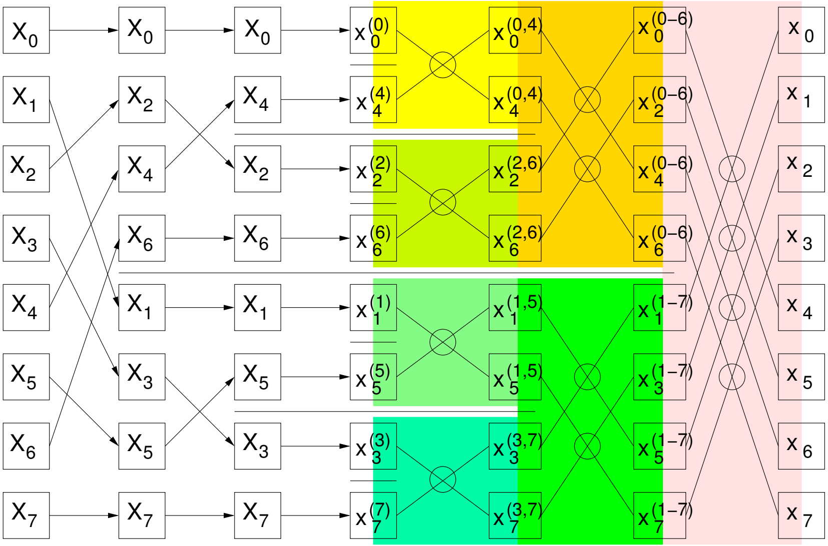
Question: can we make the L-loop an inner loop?

- kb-loop and L-loop may be swapped, if $M > L$
- however, we assumed $N > M_C$ (“data does not fit into cache”)
- we thus need to split the L-loop into a phase L=2..M (in cache) and a phase L=2∗M..N (out of cache)

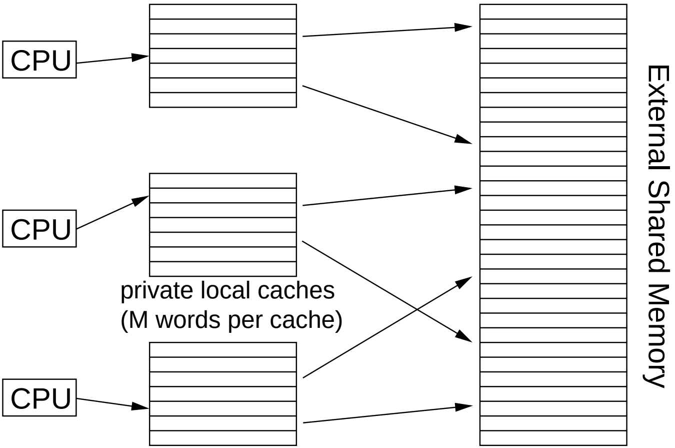
Butterfly Phase with Loop Blocking (2)

```
/** perform all butterfly phases of size M */
for(int kb=0; kb<N; kb+=M)
  for(int L=2; L<=M; L*=2)
    for(int k=kb; k<kb+M; k+=L)
      for(int j=0; j<L/2; j++) {
         complex<double> z = w[L/2+j] * X[k+j+L/2];
         X[k+j+L/2] = X[k+j] - z;
         X[k+j] = X[k+j] + z;
      }
/** perform remaining butterfly levels of size L>M */
for(int L=2*M; L<=N; L*=2)
   for(int k=0; k<N; k+=L)
      for(int j=0; j<L/2; j++) {
         complex<double> z = w[L/2+j] * X[k+j+L/2];
         X[k+j+L/2] = X[k+j] - z;
         X[k+j] = X[k+j] + z;
      }
```

Loop Blocking and Recursion – Illustration



Outlook: Parallel External Memory and I/O Model



[Arge, Goodrich, Nelson, Sitchinava, 2008]

Outlook: Parallel External Memory

Classical I/O model:

- large, global memory (main memory, hard disk, etc.)
- CPU can only access smaller working memory (cache, main memory, etc.) of M_C words each
- both organised as cache lines of size B words
- algorithmic complexity determined by memory transfers

Extended by Parallel External Memory Model:

- multiple CPUs access private caches
- caches fetch data from external memory
- exclusive/concurrent read/write classification (similar to PRAM model)

Outlook: FFT and Parallel External Memory

Consider Loop-Blocking Implementation:

```
/** perform all butterfly phases of size M */
for(int kb=0; kb<N; kb+=M)
  for(int L=2; L<=M; L*=2)
    for(int k=kb; k<kb+M; k+=L)
      for(int j=0; j<L/2; j++) {
        /* ... */
```

- choose M such that one kb-Block (M elements) fit into cache
- then: L-loop and inner loops access only cached data
- number of cache line transfers therefore:
  $\approx$ N divided by words per cache line (ideal case)

Outlook: FFT and Parallel External Memory (2)

Consider Non-Blocking Implementation:

```
/** perform remaining butterfly levels of size L>M */
for(int L=2*M; L<=N; L*=2)
   for(int k=0; k<N; k+=L)
      for(int j=0; j<L/2; j++) {
            /* ... */
```

- assume: N too large to fit all elements into cache
- then: each L-loop will need to reload all elements X into cache
- number of cache line transfers therefore:
  $\approx$ N divided by words per cache line (ideal case) **per L-iteration**

Compute-Bound vs. Memory-Bound Performance

Consider a memory-bandwidth intensive algorithm:

- you can do a lot more flops than can be read from memory
- **computational intensity** of a code:
  number of performed flops per accessed byte

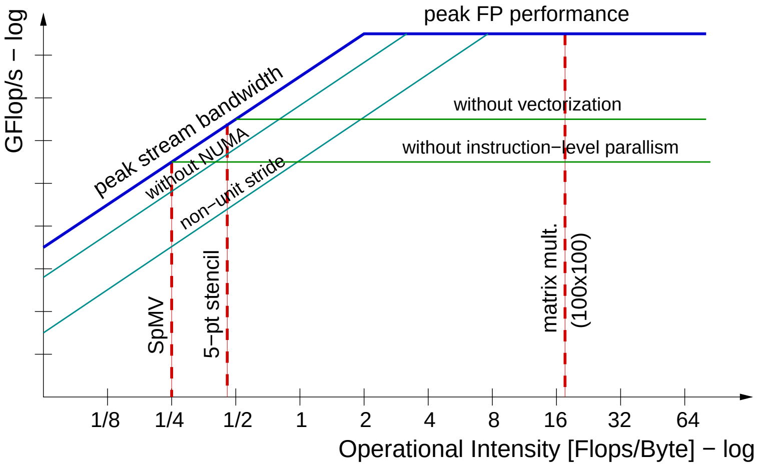
Memory-Bound Performance:

- computational intensity smaller than critical ratio
- you could execute additional flops “for free”
- speedup only possible by reducing memory accesses

Compute-Bound Performance:

- enough computational work to “hide” memory latency
- speedup only possible by reducing operations

Outlook: The Roofline Model



[Williams, Waterman, Patterson, 2008]

Outlook: The Roofline Model

Memory-Bound Performance:

- available bandwidth of a bytes per second
- computational intensity small: x flops per byte
- CPU thus executes $a \cdot x$ flops per second
- linear increase of the Flop/s with variable $x \rightsquigarrow$ linear part of "roofline"
- **"ceilings":** memory bandwidth limited due to "bad" memory access (strided access, non-uniform memory access, etc.) $\rightsquigarrow$ smaller a

Compute-Bound Performance:

- computational intensity large
- CPU executes highest possible Flop/s $\rightsquigarrow$ flat/constant "rooftop"
- **"ceilings":** fewer Flop/s due to "bad" instruction mix (no vectorization, bad branch prediction, no multi-add instructions, etc.)