

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

B is a diagonal matrix of multiplications,

C is a matrix with entries 0, ±1, ±i, defining the ‘post-additions’.

The elements on the diagonal of **B** can be shown to be either real or pure imaginary, by the same argument as in Section 1.3.3.2.3.1. Matrices **A** and **C** may be rectangular rather than square, so that intermediate results may require extra storage space.

1.3.3.3. *Multidimensional algorithms*

From an algorithmic point of view, the distinction between one-dimensional (1D) and multidimensional DFTs is somewhat blurred by the fact that some factoring techniques turn a 1D transform into a multidimensional one. The distinction made here, however, is a practical one and is based on the dimensionality of the indexing sets for data and results. This section will therefore be concerned with the problem of factoring the DFT when the *indexing sets* for the input data and output results are multidimensional.

1.3.3.3.1. *The method of successive one-dimensional transforms*

The DFT was defined in Section 1.3.2.7.4 in an *n*-dimensional setting and it was shown that when the decimation matrix **N** is diagonal, say $\mathbf{N} = \text{diag}(N^{(1)}, N^{(2)}, \dots, N^{(n)})$, then $\bar{F}(N)$ has a tensor product structure:

$$\bar{F}(\mathbf{N}) = \bar{F}(N^{(1)}) \otimes \bar{F}(N^{(2)}) \otimes \dots \otimes \bar{F}(N^{(n)}).$$

This may be rewritten as follows:

$$\begin{aligned} \bar{F}(\mathbf{N}) &= [\bar{F}(N^{(1)}) \otimes I_{N^{(2)}} \otimes \dots \otimes I_{N^{(n)}}] \\ &\quad \times [I_{N^{(1)}} \otimes \bar{F}(N^{(2)}) \otimes \dots \otimes I_{N^{(n)}}] \\ &\quad \times \dots \\ &\quad \times [I_{N^{(1)}} \otimes I_{N^{(2)}} \otimes \dots \otimes \bar{F}(N^{(n)})], \end{aligned}$$

where the *I*'s are identity matrices and × denotes ordinary matrix multiplication. The matrix within each bracket represents a one-dimensional DFT along one of the *n* dimensions, the other dimensions being left untransformed. As these matrices commute, the order in which the successive 1D DFTs are performed is immaterial.

This is the most straightforward method for building an *n*-dimensional algorithm from existing 1D algorithms. It is known in crystallography under the name of ‘Beavers–Lipson factorization’ (Section 1.3.4.3.1), and in signal processing as the ‘row–column method’.

1.3.3.3.2. *Multidimensional factorization*

Substantial reductions in the arithmetic cost, as well as gains in flexibility, can be obtained if the factoring of the DFT is carried out in several dimensions simultaneously. The presentation given here is a generalization of that of Mersereau & Speake (1981), using the abstract setting established independently by Auslander, Tolimieri & Winograd (1982).

Let us return to the general *n*-dimensional setting of Section 1.3.2.7.4, where the DFT was defined for an arbitrary decimation matrix **N** by the formulae (where |**N**| denotes |det **N**|):

$$\begin{aligned} F(\mathbf{N}) : \quad X(\mathbf{k}) &= \frac{1}{|\mathbf{N}|} \sum_{\mathbf{k}^*} X^*(\mathbf{k}^*) e[-\mathbf{k}^* \cdot (\mathbf{N}^{-1}\mathbf{k})] \\ \bar{F}(\mathbf{N}) : \quad X^*(\mathbf{k}^*) &= \sum_{\mathbf{k}} X(\mathbf{k}) e[\mathbf{k}^* \cdot (\mathbf{N}^{-1}\mathbf{k})] \end{aligned}$$

with

$$\mathbf{k} \in \mathbb{Z}^n / \mathbf{N}\mathbb{Z}^n, \quad \mathbf{k}^* \in \mathbb{Z}^n / \mathbf{N}^T \mathbb{Z}^n.$$

1.3.3.3.2.1. *Multidimensional Cooley–Tukey factorization*

Let us now assume that this decimation can be factored into *d* successive decimations, *i.e.* that

$$\mathbf{N} = \mathbf{N}_1 \mathbf{N}_2 \dots \mathbf{N}_{d-1} \mathbf{N}_d$$

and hence

$$\mathbf{N}^T = \mathbf{N}_d^T \mathbf{N}_{d-1}^T \dots \mathbf{N}_2^T \mathbf{N}_1^T.$$

Then the coset decomposition formulae corresponding to these successive decimations (Section 1.3.2.7.1) can be combined as follows:

$$\begin{aligned} \mathbb{Z}^n &= \bigcup_{\mathbf{k}_1} (\mathbf{k}_1 + \mathbf{N}_1 \mathbb{Z}^n) \\ &= \bigcup_{\mathbf{k}_1} \left\{ \mathbf{k}_1 + \mathbf{N}_1 \left[\bigcup_{\mathbf{k}_2} (\mathbf{k}_2 + \mathbf{N}_2 \mathbb{Z}^n) \right] \right\} \\ &= \dots \\ &= \bigcup_{\mathbf{k}_1} \dots \bigcup_{\mathbf{k}_d} (\mathbf{k}_1 + \mathbf{N}_1 \mathbf{k}_2 + \dots + \mathbf{N}_1 \mathbf{N}_2 \times \dots \times \mathbf{N}_{d-1} \mathbf{k}_d + \mathbf{N} \mathbb{Z}^n) \end{aligned}$$

with $\mathbf{k}_j \in \mathbb{Z}^n / \mathbf{N}_j \mathbb{Z}^n$. Therefore, any $\mathbf{k} \in \mathbb{Z} / \mathbf{N} \mathbb{Z}^n$ may be written uniquely as

$$\mathbf{k} = \mathbf{k}_1 + \mathbf{N}_1 \mathbf{k}_2 + \dots + \mathbf{N}_1 \mathbf{N}_2 \times \dots \times \mathbf{N}_{d-1} \mathbf{k}_d.$$

Similarly:

$$\begin{aligned} \mathbb{Z}^n &= \bigcup_{\mathbf{k}_d^*} (\mathbf{k}_d^* + \mathbf{N}_d^T \mathbb{Z}^n) \\ &= \dots \\ &= \bigcup_{\mathbf{k}_d^*} \dots \bigcup_{\mathbf{k}_1^*} (\mathbf{k}_d^* + \mathbf{N}_d^T \mathbf{k}_{d-1}^* + \dots + \mathbf{N}_d^T \times \dots \times \mathbf{N}_2^T \mathbf{k}_1^* \\ &\quad + \mathbf{N}^T \mathbb{Z}^n) \end{aligned}$$

so that any $\mathbf{k}^* \in \mathbb{Z}^n / \mathbf{N}^T \mathbb{Z}^n$ may be written uniquely as

$$\mathbf{k}^* = \mathbf{k}_d^* + \mathbf{N}_d^T \mathbf{k}_{d-1}^* + \dots + \mathbf{N}_d^T \times \dots \times \mathbf{N}_2^T \mathbf{k}_1^*$$

with $\mathbf{k}_j^* \in \mathbb{Z}^n / \mathbf{N}_j^T \mathbb{Z}^n$. These decompositions are the vector analogues of the multi-radix number representation systems used in the Cooley–Tukey factorization.

We may then write the definition of $\bar{F}(\mathbf{N})$ with *d* = 2 factors as

$$\begin{aligned} X^*(\mathbf{k}_2^* + \mathbf{N}_2^T \mathbf{k}_1^*) &= \sum_{\mathbf{k}_1} \sum_{\mathbf{k}_2} X(\mathbf{k}_1 + \mathbf{N}_1 \mathbf{k}_2) \\ &\quad \times e[(\mathbf{k}_2^{*T} + \mathbf{k}_1^{*T} \mathbf{N}_2) \mathbf{N}_2^{-1} \mathbf{N}_1^{-1} (\mathbf{k}_1 + \mathbf{N}_1 \mathbf{k}_2)]. \end{aligned}$$

The argument of *e*(–) may be expanded as

$$\mathbf{k}_2^* \cdot (\mathbf{N}_1^{-1} \mathbf{k}_1) + \mathbf{k}_1^* \cdot (\mathbf{N}_1^{-1} \mathbf{k}_1) + \mathbf{k}_2^* \cdot (\mathbf{N}_2^{-1} \mathbf{k}_2) + \mathbf{k}_1^* \cdot \mathbf{k}_2.$$

The first summand may be recognized as a twiddle factor, the second and third as the kernels of $\bar{F}(\mathbf{N}_1)$ and $\bar{F}(\mathbf{N}_2)$, respectively, while the fourth is an integer which may be dropped. We are thus led to a ‘vector-radix’ version of the Cooley–Tukey algorithm, in which the successive decimations may be introduced in all *n* dimensions simultaneously by general integer matrices. The computation may be decomposed into five stages analogous to those of the one-dimensional algorithm of Section 1.3.3.2.1:

(i) form the |**N**₁| vectors **Y**_{**k**₁} of shape **N**₂ by

$$Y_{\mathbf{k}_1}(\mathbf{k}_2) = X(\mathbf{k}_1 + \mathbf{N}_1 \mathbf{k}_2), \quad \mathbf{k}_1 \in \mathbb{Z}^n / \mathbf{N}_1 \mathbb{Z}^n, \quad \mathbf{k}_2 \in \mathbb{Z}^n / \mathbf{N}_2 \mathbb{Z}^n;$$

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(ii) calculate the $|\mathbf{N}_1|$ transforms $\mathbf{Y}_{\mathbf{k}_1}^*$ on $|\mathbf{N}_2|$ points:

$$Y_{\mathbf{k}_1}^*(\mathbf{k}_2^*) = \sum_{\mathbf{k}_2} e[\mathbf{k}_2^* \cdot (\mathbf{N}_2^{-1} \mathbf{k}_2)] Y_{\mathbf{k}_1}(\mathbf{k}_2), \quad \mathbf{k}_1 \in \mathbb{Z}^n / \mathbf{N}_1 \mathbb{Z}^n;$$

(iii) form the $|\mathbf{N}_2|$ vectors $\mathbf{Z}_{\mathbf{k}_2^*}$ of shape \mathbf{N}_1 by

$$\begin{aligned} Z_{\mathbf{k}_2^*}(\mathbf{k}_1) &= e[\mathbf{k}_2^* \cdot (\mathbf{N}_1^{-1} \mathbf{k}_1)] Y_{\mathbf{k}_1}^*(\mathbf{k}_2^*), \quad \mathbf{k}_1 \in \mathbb{Z}^n / \mathbf{N}_1 \mathbb{Z}^n, \\ \mathbf{k}_2^* &\in \mathbb{Z}^n / \mathbf{N}_2^T \mathbb{Z}^n; \end{aligned}$$

(iv) calculate the $|\mathbf{N}_2|$ transforms $\mathbf{Z}_{\mathbf{k}_2^*}$ on $|\mathbf{N}_1|$ points:

$$Z_{\mathbf{k}_2^*}^*(\mathbf{k}_1^*) = \sum_{\mathbf{k}_1} e[\mathbf{k}_1^* \cdot (\mathbf{N}_1^{-1} \mathbf{k}_1)] Z_{\mathbf{k}_2^*}(\mathbf{k}_1), \quad \mathbf{k}_2^* \in \mathbb{Z}^n / \mathbf{N}_2^T \mathbb{Z}^n;$$

(v) collect $X^*(\mathbf{k}_2^* + \mathbf{N}_2^T \mathbf{k}_1^*)$ as $Z_{\mathbf{k}_2^*}^*(\mathbf{k}_1^*)$.

The initial $|\mathbf{N}|$ -point transform $\bar{F}(\mathbf{N})$ can thus be performed as $|\mathbf{N}_1|$ transforms $\bar{F}(\mathbf{N}_2)$ on $|\mathbf{N}_2|$ points, followed by $|\mathbf{N}_2|$ transforms $\bar{F}(\mathbf{N}_1)$ on $|\mathbf{N}_1|$ points. This process can be applied successively to all d factors. The same decomposition applies to $F(\mathbf{N})$, up to the complex conjugation of twiddle factors, the normalization factor $1/|\mathbf{N}|$ being obtained as the product of the factors $1/|\mathbf{N}_j|$ in the successive partial transforms $F(\mathbf{N}_j)$.

The geometric interpretation of this factorization in terms of partial transforms on translates of sublattices applies in full to this n -dimensional setting; in particular, the twiddle factors are seen to be related to the residual translations which place the sublattices in register within the big lattice. If the intermediate transforms are performed *in place*, then the quantity

$$X^*(\mathbf{k}_d^* + \mathbf{N}_d^T \mathbf{k}_{d-1}^* + \dots + \mathbf{N}_d^T \mathbf{N}_{d-1}^T \times \dots \times \mathbf{N}_2^T \mathbf{k}_1^*)$$

will eventually be found at location

$$\mathbf{k}_1^* + \mathbf{N}_1 \mathbf{k}_2^* + \dots + \mathbf{N}_1 \mathbf{N}_2 \times \dots \times \mathbf{N}_{d-1} \mathbf{k}_d^*,$$

so that the final results will have to be *unscrambled* by a process which may be called ‘coset reversal’, the vector equivalent of digit reversal.

Factoring by 2 in all n dimensions simultaneously, *i.e.* taking $\mathbf{N} = 2\mathbf{M}$, leads to ‘ n -dimensional butterflies’. Decimation in time corresponds to the choice $\mathbf{N}_1 = 2\mathbf{I}$, $\mathbf{N}_2 = \mathbf{M}$, so that $\mathbf{k}_1 \in \mathbb{Z}^n / 2\mathbb{Z}^n$ is an n -dimensional parity class; the calculation then proceeds by

$$\begin{aligned} Y_{\mathbf{k}_1}(\mathbf{k}_2) &= X(\mathbf{k}_1 + 2\mathbf{k}_2), \quad \mathbf{k}_1 \in \mathbb{Z}^n / 2\mathbb{Z}^n, \quad \mathbf{k}_2 \in \mathbb{Z}^n / \mathbf{M}\mathbb{Z}^n, \\ Y_{\mathbf{k}_1}^* &= \bar{F}(\mathbf{M})[Y_{\mathbf{k}_1}], \quad \mathbf{k}_1 \in \mathbb{Z}^n / 2\mathbb{Z}^n; \\ X^*(\mathbf{k}_2^* + \mathbf{M}^T \mathbf{k}_1^*) &= \sum_{\mathbf{k}_1 \in \mathbb{Z}^n / 2\mathbb{Z}^n} (-1)^{\mathbf{k}_1^* \cdot \mathbf{k}_1} \\ &\quad \times e[\mathbf{k}_2^* \cdot (\mathbf{N}_1^{-1} \mathbf{k}_1)] Y_{\mathbf{k}_1}^*(\mathbf{k}_2^*). \end{aligned}$$

Decimation in frequency corresponds to the choice $\mathbf{N}_1 = \mathbf{M}$, $\mathbf{N}_2 = 2\mathbf{I}$, so that $\mathbf{k}_2 \in \mathbb{Z}^n / 2\mathbb{Z}^n$ labels ‘octant’ blocks of shape \mathbf{M} ; the calculation then proceeds through the following steps:

$$\begin{aligned} Z_{\mathbf{k}_2^*}(\mathbf{k}_1) &= \left[\sum_{\mathbf{k}_2 \in \mathbb{Z}^n / 2\mathbb{Z}^n} (-1)^{\mathbf{k}_2^* \cdot \mathbf{k}_2} X(\mathbf{k}_1 + \mathbf{M}\mathbf{k}_2) \right] \\ &\quad \times e[\mathbf{k}_2^* \cdot (\mathbf{N}_1^{-1} \mathbf{k}_1)], \\ Z_{\mathbf{k}_2^*}^* &= \bar{F}(\mathbf{M})[Z_{\mathbf{k}_2^*}], \\ X^*(\mathbf{k}_2^* + 2\mathbf{k}_1^*) &= Z_{\mathbf{k}_2^*}^*(\mathbf{k}_1^*), \end{aligned}$$

i.e. the 2^n parity classes of results, corresponding to the different $\mathbf{k}_2^* \in \mathbb{Z}^n / 2\mathbb{Z}^n$, are obtained separately. When the dimension n is 2 and the decimating matrix is diagonal, this analysis reduces to the ‘vector radix FFT’ algorithms proposed by Rivard (1977) and Harris *et al.* (1977). These lead to substantial reductions in the number M of multiplications compared to the row–column method:

M is reduced to $3M/4$ by simultaneous 2×2 factoring, and to $15M/32$ by simultaneous 4×4 factoring.

The use of a non-diagonal decimating matrix may bring savings in computing time if the spectrum of the band-limited function under study is of such a shape as to pack more compactly in a non-rectangular than in a rectangular lattice (Mersereau, 1979). If, for instance, the support K of the spectrum Φ is contained in a sphere, then a decimation matrix producing a close packing of these spheres will yield an aliasing-free DFT algorithm with fewer sample points than the standard algorithm using a rectangular lattice.

1.3.3.3.2.2. Multidimensional prime factor algorithm

Suppose that the decimation matrix \mathbf{N} is diagonal

$$\mathbf{N} = \text{diag} (N^{(1)}, N^{(2)}, \dots, N^{(n)})$$

and let each diagonal element be written in terms of its prime factors:

$$N^{(i)} = \prod_{j=1}^m p_j^{\nu(i,j)},$$

where m is the total number of distinct prime factors present in the $N^{(i)}$.

The CRT may be used to turn each 1D transform along dimension i ($i = 1, \dots, n$) into a multidimensional transform with a separate ‘pseudo-dimension’ for each distinct prime factor of $N^{(i)}$; the number μ_i of these pseudo-dimensions is equal to the cardinality of the set:

$$\{j \in \{1, \dots, m\} | \nu(i,j) > 0 \text{ for some } i\}.$$

The full n -dimensional transform thus becomes μ -dimensional, with $\mu = \sum_{i=1}^n \mu_i$.

We may now permute the μ pseudo-dimensions so as to bring into contiguous position those corresponding to the same prime factor p_j ; the m resulting groups of pseudo-dimensions are said to define ‘ p -primary’ blocks. The initial transform is now written as a tensor product of m p -primary transforms, where transform j is on

$$p_j^{\nu(1,j)} \times p_j^{\nu(2,j)} \times \dots \times p_j^{\nu(n,j)}$$

points [by convention, dimension i is not transformed if $\nu(i,j) = 0$]. These p -primary transforms may be computed, for instance, by multidimensional Cooley–Tukey factorization (Section 1.3.3.3.1), which is faster than the straightforward row–column method. The final results may then be obtained by reversing all the permutations used.

The extra gain with respect to the multidimensional Cooley–Tukey method is that *there are no twiddle factors between p -primary pieces corresponding to different primes p .*

The case where \mathbf{N} is not diagonal has been examined by Guessoum & Mersereau (1986).

1.3.3.3.2.3. Nesting of Winograd small FFTs

Suppose that the CRT has been used as above to map an n -dimensional DFT to a μ -dimensional DFT. For each $\kappa = 1, \dots, \mu$ [κ runs over those pairs (i, j) such that $\nu(i, j) > 0$], the Rader/Winograd procedure may be applied to put the matrix of the κ th 1D DFT in the **CBA** normal form of a Winograd small FFT. The full DFT matrix may then be written, up to permutation of data and results, as

$$\bigotimes_{\kappa=1}^{\mu} (\mathbf{C}_{\kappa} \mathbf{B}_{\kappa} \mathbf{A}_{\kappa}).$$

A well known property of the tensor product of matrices allows this to be rewritten as