

## 1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

(i) form the  $|\mathbf{N}_1|$  vectors  $\mathbf{Y}_{\mathbf{k}_1}$  of shape  $\mathbf{N}_2$  by

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

(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

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

(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

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

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:

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

*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  $2 \times 2$  factoring, and to  $15M/32$  by simultaneous  $4 \times 4$  factoring.

The use of a nondiagonal 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 nonrectangular than in a rectangular lattice (Mersereau, 1979). If, for instance, the support  $K$  of the spectrum  $\Phi$  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:

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

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  $\mu_i$  of these pseudo-dimensions is equal to the cardinality of the set:

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

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

We may now permute the  $\mu$  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

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

points [by convention, dimension  $i$  is not transformed if  $v(i,j) = 0$ ]. 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.

## 1. GENERAL RELATIONSHIPS AND TECHNIQUES

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  $\mu$ -dimensional DFT. For each  $\kappa = 1, \dots, \mu$  [ $\kappa$  runs over those pairs  $(i, j)$  such that  $v(i, j) > 0$ ], the Rader/Winograd procedure may be applied to put the matrix of the  $\kappa$ 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

$$\left( \bigotimes_{\gamma=1}^{\mu} \mathbf{C}_{\gamma} \right) \times \left( \bigotimes_{\beta=1}^{\mu} \mathbf{B}_{\beta} \right) \times \left( \bigotimes_{\alpha=1}^{\mu} \mathbf{A}_{\alpha} \right)$$

and thus to form a matrix in which the *combined* pre-addition, multiplication and post-addition matrices have been *precomputed*. This procedure, called *nesting*, can be shown to afford a reduction of the arithmetic operation count compared to the row–column method (Morris, 1978).

Clearly, the nesting rearrangement need not be applied to all  $\mu$  dimensions, but can be restricted to any desired subset of them.

### 1.3.3.3.2.4. The Nussbaumer–Quandalle algorithm

Nussbaumer’s approach views the DFT as the evaluation of certain polynomials constructed from the data (as in Section 1.3.3.2.4). For instance, putting  $\omega = e(1/N)$ , the 1D  $N$ -point DFT

$$X^*(k^*) = \sum_{k=0}^{N-1} X(k) \omega^{k^*k}$$

may be written

$$X^*(k^*) = Q(\omega^{k^*}),$$

where the polynomial  $Q$  is defined by

$$Q(z) = \sum_{k=0}^{N-1} X(k) z^k.$$

Let us consider (Nussbaumer & Quandalle, 1979) a 2D transform of size  $N \times N$ :

$$X^*(k_1^*, k_2^*) = \sum_{k_1=0}^{N-1} \sum_{k_2=0}^{N-1} X(k_1, k_2) \omega^{k_1^*k_1 + k_2^*k_2}.$$

By introduction of the polynomials

$$Q_{k_2}(z) = \sum_{k_1} X(k_1, k_2) z^{k_1}$$

$$R_{k_2^*}(z) = \sum_{k_2} \omega^{k_2^*k_2} Q_{k_2}(z),$$

this may be rewritten:

$$X^*(k_1^*, k_2^*) = R_{k_2^*}(\omega^{k_1^*}) = \sum_{k_2} \omega^{k_2^*k_2} Q_{k_2}(\omega^{k_1^*}).$$

Let us now suppose that  $k_1^*$  is coprime to  $N$ . Then  $k_1^*$  has a unique inverse modulo  $N$  (denoted by  $1/k_1^*$ ), so that multiplication by  $k_1^*$  simply permutes the elements of  $\mathbb{Z}/N\mathbb{Z}$  and hence

$$\sum_{k_2=0}^{N-1} f(k_2) = \sum_{k_2=0}^{N-1} f(k_1^*k_2)$$

for any function  $f$  over  $\mathbb{Z}/N\mathbb{Z}$ . We may thus write:

$$\begin{aligned} X^*(k_1^*, k_2^*) &= \sum_{k_2} \omega^{k_1^*k_2^*k_2} Q_{k_1^*k_2}(\omega^{k_1^*}) \\ &= S_{k_1^*k_2}(\omega^{k_1^*}) \end{aligned}$$

where

$$S_{k^*}(z) = \sum_{k_2} z^{k^*k_2} Q_{k_2}(z).$$

Since only the value of polynomial  $S_{k^*}(z)$  at  $z = \omega^{k_1^*}$  is involved in the result, the computation of  $S_{k^*}$  may be carried out modulo the unique cyclotomic polynomial  $P(z)$  such that  $P(\omega^{k_1^*}) = 0$ . Thus, if we define:

$$T_{k^*}(z) = \sum_{k_2} z^{k^*k_2} Q_{k_2}(z) \bmod P(z)$$

we may write:

$$X^*(k_1^*, k_2^*) = T_{k_1^*k_2^*}(\omega^{k_1^*})$$

or equivalently

$$X^* \left( k_1^*, \frac{k_2^*}{k_1^*} \right) = T_{k_2^*}(\omega^{k_1^*}).$$

For  $N$  an odd prime  $p$ , all nonzero values of  $k_1^*$  are coprime with  $p$  so that the  $p \times p$ -point DFT may be calculated as follows:  
(1) form the polynomials

$$T_{k_2^*}(z) = \sum_{k_1} \sum_{k_2} X(k_1, k_2) z^{k_1 + k_2^*k_2} \bmod P(z)$$

for  $k_2^* = 0, \dots, p-1$ ;

(2) evaluate  $T_{k_2^*}(\omega^{k_1^*})$  for  $k_1^* = 0, \dots, p-1$ ;

(3) put  $X^*(k_1^*, k_2^*/k_1^*) = T_{k_2^*}(\omega^{k_1^*})$ ;

(4) calculate the terms for  $k_1^* = 0$  separately by