

1. GENERAL RELATIONSHIPS AND TECHNIQUES

which are different for each \mathbf{h}_2 . The vectors $\mathbf{Z}_{\mathbf{h}_2}$ of intermediate results after the twiddle-factor stage may then be multiplexed in pairs as

$$\mathbf{Z} = \mathbf{Z}_{\mathbf{h}_2} + \mathbf{Z}_{\mathbf{h}'_2}.$$

After transforming by $F(\mathbf{M})$, the results \mathbf{Z}^* may be demultiplexed by using the relations

$$\begin{aligned} Z_{\mathbf{h}_2}^*(\mathbf{h}_1) + Z_{\mathbf{h}'_2}^*(\mathbf{h}_1) &= Z^*(\mathbf{h}_1) \\ Z_{\mathbf{h}_2}^*(\mathbf{h}_1 - \mathbf{h}'_2) + Z_{\mathbf{h}'_2}^*(\mathbf{h}_1 - \mathbf{h}_2) &= \varepsilon Z^*[\mathbf{M}\zeta(\mathbf{h}_1) - \mathbf{h}_1] \end{aligned}$$

which can be solved recursively as in Section 1.3.4.3.5.1(b)(ii).

1.3.4.3.5.4. Real symmetric transforms

Conjugate symmetric (Section 1.3.2.4.2.3) implies that if the data \mathbf{X} are real and symmetric [*i.e.* $X(\mathbf{k}) = \overline{X(\mathbf{k})}$ and $X(-\mathbf{k}) = X(\mathbf{k})$], then so are the results \mathbf{X}^* . Thus if ρ contains a centre of symmetry, \mathbf{F} is real symmetric. There is no distinction (other than notation) between structure-factor and electron-density calculation; the algorithms will be described in terms of the former. It will be shown that if $\mathbf{N} = 2\mathbf{M}$, a real symmetric transform can be computed with only 2^{n-2} partial transforms $F(\mathbf{M})$ instead of 2^n .

(i) Decimation in time ($\mathbf{N}_1 = 2\mathbf{I}, \mathbf{N}_2 = \mathbf{M}$)

Since $\mathbf{m}_1 \in \mathbb{Z}^n/2\mathbb{Z}^n$ we have $-\mathbf{m}_1 = \mathbf{m}_1$ and $\zeta(\mathbf{m}_1) = \mathbf{m}_1 \bmod 2\mathbb{Z}^n$. The decimated vectors $\mathbf{Y}_{\mathbf{m}_1}$ are not only real, but have an internal symmetry expressed by

$$\mathbf{Y}_{\mathbf{m}_1}[\mathbf{M}\zeta(\mathbf{m}_2) - \mathbf{m}_2 - \mathbf{m}_1] = \varepsilon \mathbf{Y}_{\mathbf{m}_1}(\mathbf{m}_2).$$

This symmetry, however, is different for each \mathbf{m}_1 so that we may multiplex two such vectors $\mathbf{Y}_{\mathbf{m}'_1}$ and $\mathbf{Y}_{\mathbf{m}''_1}$ into a general real vector

$$\mathbf{Y} = \mathbf{Y}_{\mathbf{m}'_1} + \mathbf{Y}_{\mathbf{m}''_1},$$

for each of the 2^{n-1} pairs $(\mathbf{m}'_1, \mathbf{m}''_1)$. The 2^{n-1} Hermitian-symmetric transform vectors

$$\mathbf{Y}^* = \mathbf{Y}_{\mathbf{m}'_1}^* + \mathbf{Y}_{\mathbf{m}''_1}^*$$

can then be evaluated by the methods of Section 1.3.4.3.5.1(b) at the cost of only 2^{n-2} general complex $F(\mathbf{M})$.

The demultiplexing relations by which the separate vectors $\mathbf{Y}_{\mathbf{m}'_1}^*$ and $\mathbf{Y}_{\mathbf{m}''_1}^*$ may be recovered are most simply obtained by observing that the vectors \mathbf{Z} after the twiddle-factor stage are real-valued since $F(2\mathbf{I})$ has a real matrix. Thus, as in Section 1.3.4.3.5.1(c)(i),

$$\begin{aligned} \mathbf{Y}_{\mathbf{m}'_1}^* &= (c' - is')\mathbf{R}' \\ \mathbf{Y}_{\mathbf{m}''_1}^* &= (c'' - is'')\mathbf{R}'' \end{aligned}$$

where \mathbf{R}' and \mathbf{R}'' are real vectors and where the multipliers $(c' - is')$ and $(c'' - is'')$ are the inverse twiddle factors. Therefore,

$$\begin{aligned} \mathbf{Y}^* &= (c' - is')\mathbf{R}' + (c'' - is'')\mathbf{R}'' \\ &= (c'\mathbf{R}' + c''\mathbf{R}'') - i(s'\mathbf{R}' + s''\mathbf{R}'') \end{aligned}$$

and hence the demultiplexing relation for each \mathbf{h}_2 :

$$\begin{pmatrix} R' \\ R'' \end{pmatrix} = \frac{1}{c's'' - s'c''} \begin{pmatrix} s'' & -c'' \\ -s' & c' \end{pmatrix} \begin{pmatrix} \text{Re } Y^* \\ -\text{Im } Y^* \end{pmatrix}.$$

The values of $R'_{\mathbf{h}_2}$ and $R''_{\mathbf{h}_2}$ at those points \mathbf{h}_2 where $c's'' - s'c'' = 0$ can be evaluated directly while forming \mathbf{Y} . This demultiplexing and the final stage of the calculation, namely

$$F(\mathbf{h}_2 + \mathbf{M}\mathbf{h}_1) = \frac{1}{2^n} \sum_{\mathbf{m}_1 \in \mathbb{Z}^n/2\mathbb{Z}^n} (-1)^{\mathbf{h}_1 \cdot \mathbf{m}_1} R_{\mathbf{m}_1}(\mathbf{h}_2)$$

need only be carried out for the unique half of the range of \mathbf{h}_2 .

(ii) Decimation in frequency ($\mathbf{N}_1 = \mathbf{M}, \mathbf{N}_2 = 2\mathbf{I}$)

Similarly, the vectors $\mathbf{Z}_{\mathbf{h}_2}^*$ of decimated and scrambled results are real and obey internal symmetries

$$\tau_{\mathbf{h}_2} \mathbf{Z}_{\mathbf{h}_2}^* = \varepsilon \check{\mathbf{Z}}_{\mathbf{h}_2}^*$$

which are different for each \mathbf{h}_2 . For each of the 2^{n-1} pairs $(\mathbf{h}'_2, \mathbf{h}''_2)$ the multiplexed vector

$$\mathbf{Z} = \mathbf{Z}_{\mathbf{h}'_2} + \mathbf{Z}_{\mathbf{h}''_2}$$

is a Hermitian-symmetric vector without internal symmetry, and the 2^{n-1} real vectors

$$\mathbf{Z}^* = \mathbf{Z}_{\mathbf{h}'_2}^* + \mathbf{Z}_{\mathbf{h}''_2}^*$$

may be evaluated at the cost of only 2^{n-2} general complex $F(\mathbf{M})$ by the methods of Section 1.3.4.3.5.1(c). The individual transforms $\mathbf{Z}_{\mathbf{h}'_2}$ and $\mathbf{Z}_{\mathbf{h}''_2}$ may then be retrieved via the demultiplexing relations

$$\begin{aligned} Z_{\mathbf{h}'_2}(\mathbf{h}_1) + Z_{\mathbf{h}''_2}(\mathbf{h}_1) &= Z^*(\mathbf{h}_1) \\ Z_{\mathbf{h}'_2}(\mathbf{h}_1 - \mathbf{h}'_2) + Z_{\mathbf{h}''_2}(\mathbf{h}_1 - \mathbf{h}''_2) &= Z^*[\mathbf{M}\zeta(\mathbf{h}_1) - \mathbf{h}_1] \end{aligned}$$

which can be solved recursively as described in Section 1.3.4.3.5.1(b)(ii). This yields the unique half of the real symmetric results \mathbf{F} .

1.3.4.3.5.5. Real antisymmetric transforms

If \mathbf{X} is real antisymmetric, then its transform \mathbf{X}^* is purely imaginary and antisymmetric. The double-multiplexing techniques used for real symmetric transforms may therefore be adapted with only minor changes involving signs and factors of i .

1.3.4.3.5.6. Generalized multiplexing

So far the multiplexing technique has been applied to pairs of vectors with similar types of parity-related and/or conjugate symmetry properties, in particular the same value of ε .

It can be generalized so as to accommodate mixtures of vectors with different symmetry characteristics. For example if \mathbf{X}_1 is Hermitian-symmetric and \mathbf{X}_2 is Hermitian-antisymmetric, so that \mathbf{X}_1^* is real-valued while \mathbf{X}_2^* has purely imaginary values, the multiplexing process should obviously form $\mathbf{X} = \mathbf{X}_1 + \mathbf{X}_2$ (instead of $\mathbf{X} = \mathbf{X}_1 + i\mathbf{X}_2$ if both had the same type of symmetry), and demultiplexing consists in separating

$$\begin{aligned} \mathbf{X}_1^* &= \text{Re } \mathbf{X}^* \\ \mathbf{X}_2^* &= i \text{Im } \mathbf{X}^* \end{aligned}$$