Order Number 9431347

Periodization and decimation for FFT's and crystallographic FFT's

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City University of New York, 1994

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PERIODIZATION AND DECIMATION FOR FFT'S AND CRYSTALLOGRAPHIC FFT'S

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A dissertation submitted to the Graduate Faulty in Engineering in partial fulfillment of the requirements for the degree of Doctor of Philosophy,
The City University of New York

1994

This manuscript has been read and accepted for the Graduate Faculty in Engineering in satisfaction of the dissertation requirements for the degree of Doctor of Philosophy.

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ACKNOWLEDGMENT

I wish to express my deep gratitude to Professor Richard Tolimieri for his interest, encouragement and valuable guidance during the progress of this research.

I would like to thank the members of my doctoral committee: Professor T. Saadawi, Professor J. Barba, Professor M. Conner, and Dr M. An for the time and effort each has taken to read and constructively criticize this dissertation.

Special thanks to my family for their support and encouragement.

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1 THE DISCRETE FOURIER TRANSFORM

1.1. Introduction

The Discrete Fourier Transform (DFT) plays an important role in many applications of digital signal processing, including linear filtering, correlation analysis, and spectrum analysis. A major reason for its importance is the existence of efficient algorithms for computing the DFT. Historically, the first additive Fast Fourier Transform (FFT) algorithm is described in the fundamental work of J. W. Cooley and J. W. Tukey in 1965. Straightforward computation of N-point FFT requires a number of arithmetic operations proportional to N^2 . The Cooley-Tukey FFT algorithm significantly reduced the computational cost, for many transform sizes N, to an operational count proportional to $N \log N$ [1].

1.2. Tensor Product and Stride Permutation

Tensor product algebra is an important tool for presenting mathematical formulation of DSP algorithms so that these algorithms can be studied and analyzed in a unified format. We will define the tensor product of both vectors and matrices; then we will use it in the manipulation and factorization of the discrete Fourier transform matrices [15].

Consider vectors $\underline{a}$ *and* $\underline{b}$ of sizes M and N, respectively. We write $\underline{a}$ *and* $\underline{b}$ as column vectors:

$$\underline{a} = \begin{bmatrix} a_0 \\ a_1 \\ \cdot \\ \cdot \\ \cdot \\ a_{M-1} \end{bmatrix}, \qquad \underline{b} = \begin{bmatrix} b_0 \\ b_1 \\ \cdot \\ \cdot \\ \cdot \\ b_{N-1} \end{bmatrix} \tag{1}$$

The tensor product $\underline{a} \otimes \underline{b}$ is the vector of size MN defined by

$$\begin{bmatrix} a_0\underline{b} \\ a_1\underline{b} \\ \cdot \\ \cdot \\ \cdot \\ a_{M-1}\underline{b} \end{bmatrix} \tag{2}$$

The tensor product is bilinear in the following sense.

$$(\underline{a} + \underline{b}) \otimes \underline{c} = \underline{a} \otimes \underline{c} + \underline{b} \otimes \underline{c} \tag{3}$$

$$\underline{a} \otimes (\underline{b} + \underline{c}) = \underline{a} \otimes \underline{b} + \underline{a} \otimes \underline{c} \tag{4}$$

but it is not commutative. In general, $\underline{a} \otimes \underline{b} \neq \underline{b} \otimes \underline{a}$.

The tensor product of an MxM matrix A and an NxN matrix B is the MNxMN matrix

$$A \otimes B = \begin{bmatrix} a_{00}B & \cdots & a_{0,M-1}B \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{M-1,0}B & \cdots & a_{M-1,M-1}B \end{bmatrix} \tag{5}$$

In general a stride permutation, P(mn,n) reorders the coordinates at stride n into n consecutive segments of m elements. For example, let

$$X = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} \tag{6}$$

then

$$P\,(\,6{,}2\,)\,X = \begin{bmatrix} x_0 \\ x_2 \\ x_4 \\ x_1 \\ x_3 \\ x_5 \end{bmatrix} \qquad (7)$$

1.3. Properties of FFT Matrix

The FFT matrix of order N, denoted by F(N) is defined in [1] as

$$F(N) = [\, W_N^{jk} \,] \qquad W_N = \exp\,(\, 2\pi i/N \,) \qquad (8)$$

The conjugate of W_N , denoted by W_N^* is

$$(\, W_N^* \,) = \exp(\, -2\pi i/N \,) = W_N^{-1} \qquad (9)$$

Direct computation shows that

$$F(N)F(N)^* = N I_N \tag{10}$$

The inverse FFT matrix is

$$F(N)^{-1} = \frac{1}{N} F(N)^* \tag{11}$$

and F(N) is symmetric, i.e

$$F(N)^t = F(N) \tag{12}$$

1.4. Cooley-Tukey FFT for N=RS

Let N=RS and consider the N-point FFT

$$y_k = \sum_{n=0}^{N-1} w^{nk} x_n , \qquad 0 \le k < N \tag{13}$$

We will derive a Cooley-Tukey algorithm computing the N-point FFT [1]. Associate to the N-point vector x the SxR array

$$X = \begin{bmatrix} x_0 & x_S & \cdots & x_{(R-1)S} \\ x_1 & x_{S+1} & \cdots & x_{(R-1)S+1} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ x_{S-1} & x_{2S-1} & \cdots & x_{N-1} \end{bmatrix} \tag{14}$$

and set

$$X_1 = X^t = \begin{bmatrix} x_0 & x_1 & \cdots & x_{S-1} \\ x_S & x_{S+1} & \cdots & x_{2S-1} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ x_{(R-1)S} & x_{(R-1)S+1} & \cdots & x_{N-1} \end{bmatrix} \tag{15}$$

The corresponding N-tuple $\underline{x}_1$ is given by applying the N-point stride-S permutation P(N,S) to $\underline{x}$.

Associate to the output vector $\underline{y}$ the RxS array

$$Y = \begin{bmatrix} y_0 & y_R & \cdots & y_{(S-1)R} \\ y_1 & y_{R+1} & \cdots & y_{(S-1)R+1} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ y_{R-1} & y_{2R+1} & \cdots & y_{N-1} \end{bmatrix} \tag{16}$$

We can write

$$X_1(k_1,k_2) = x(k_2 + k_1 S) \qquad 0 \le k_1 < R,\ 0 \le k_2 < S \tag{17}$$

$$Y(l_1,l_2) = y(l_1 + l_2 R) \qquad 0 \le l_1 < R,\ 0 \le l_2 < S \tag{18}$$

Formula (13) can be written as

$$Y(l_1,l_2) = \sum_{k_1=0}^{S-1} \sum_{k_2=0}^{R-1} w^{(k_2 + k_1 S)(l_1 + l_2 R)} X_1(k_1,k_2) \tag{19}$$

now

$$(k_2 + k_1 S)(l_1 + l_2 R) = k_2 l_1 + k_1 l_1 S + k_2 l_2 R \qquad \text{mod } N \tag{20}$$

Set $u = w^S$ *and* $v = w^R$. since $w^N = 1$, we can rewrite (19) as

$$Y(l_1,l_2) = \sum_{k_2=0}^{S-1} \left(\sum_{k_1=0}^{R-1} X_1(k_1,k_2)\ u^{k_1 l_1} \right) w^{k_2 l_1}\ v^{k_2 l_2} \tag{21}$$

First observe that the inner sum

$$Y_1(l_1,k_2) = \sum_{k_1=0}^{R-1} X_1(k_1,k_2)\ u^{k_1 l_1} \tag{22}$$

computes, for each $0 \le k_2 < S$, the R-point FFT of the $k_2 - th$ column of X_1 and places the result in the $k_2 - th$ column of Y_1 . Let $\underline{y_1}$ be the vector formed by reading, in order, down the columns of Y_1 . Then

$$\underline{y_1} = (I_S \otimes F(R))\ \underline{x_1} \tag{23}$$

and

$$\underline{y_1} = (I_S \otimes F(R))\ P(N,S)\ \underline{x} \tag{24}$$

The next stage of the computation

$$Y_2(l_1,l_2) = Y_1(l_1,k_2)\, w^{k_2 l_1} \tag{25}$$

can be given by the diagonal matrix multiplication

$$\underline{y}_2 = T_R(N)\, \underline{y}_1 \tag{26}$$

where

$$T_R(N) = \sum_{S=0}^{S-1} \oplus\, D_R^S(N) = \begin{bmatrix} I_R & & & & \\ & D_R(N) & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \cdot \\ & & & & & D_R^S(N) \end{bmatrix}$$

and

$$D_R(N) = \begin{bmatrix} 1 & & & & \\ & w & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \cdot \\ & & & & & w^{R-1} \end{bmatrix} \tag{28}$$

The final computation

$$Y(l_1,l_2) = \sum_{k_2=0}^{S-1} Y_2(l_1,k_2)\ v^{k_2 l_2} \tag{29}$$

Therefore for N=RS

$$\underline{y} = F(N)\ \underline{x} = (\ F(S) \otimes I_R\ )\ T_R(N)\ (\ I_S \otimes F(R)\ )\ P(N,S)\ \underline{x} \tag{30}$$

2 PERIODIZATION AND DECIMATION

2.1. Introduction

This chapter provides the basic definitions of most of the mathematical ideas and tools used in the workout of the periodization and decimation algorithm. At this point the algorithm will be described on the function theoretic level. The Fourier transform will be redefined as a linear operator of the vector space L(Z/N), where L(Z/N) is the set of all complex-valued functions on the ring Z/N.

Rings:

Definition:

Let R be a set of elements a, b, c, ... for which the sum a + b and the product ab of any two elements a and b (distinct or not) of R are defined. The set R is called a **ring** if the following postulates hold [2] :

(1) Closure. If a and b are in R, then the sum a+b and the product ab are in R ;

(2) Uniqueness. If a=a' and b=b' in R, then a+b=a'+b' and ab=a'b' ;

(3) Associative Laws. For all a,b, and c in R ,

$a+(b+c) = (a+b)+c$, $a(bc) = (ab)c$;

(4) Distributive Law. for all a,b, and c in R ,

$a(b+c) = ab + ac$;

(5) Zero. R contains an element 0 such that

$a+0 = a$ for all a in R ;

(6) Unity. R contains an element $1 \neq 0$ such that

$a\,1 = a$, for all a in R ;

(7) Additive inverse. For each a in R, the equation

$a+x = 0$ has a solution in R .

R is called a **commutative ring** if

$a+b = b+a$, $ab = ba$ for all a,b in R .

2.2. The Ring of Integers

The set Z of all integers $\{ 0, \pm 1, \pm 2, \pm 3, \ldots \}$ satisfies the above postulates, it also has another property:

If $c \neq 0$ and $ca = cb$ in Z, then $a=b$.

The integers therefore constitute not only a commutative ring but an **integral domain.**

The ring of integers satisfies the following important condition [1] :

Divisibility condition. If a and b are integers with $b \neq 0$ then we can write

$$a \equiv bq + r\,, \qquad 0 \le r < b \tag{1}$$

where q and r are uniquely determined integers.

The integer q is called the quotient of the division of a by b, and it is the largest integer satisfying

$$bq \le a \tag{2}$$

The integer r is called the remainder of the division of a by b and is given by the formula

$$r = a - bq \tag{3}$$

If r = 0, then

$$a = bq \tag{4}$$

<u>Ideal</u>

Definition:

A subset C of a commutative ring R is called an **ideal** [2] when $a \in C \; and \; b \in C$ imply $(a \pm b) \in C$, and $a \in C\,,\, r \in R$ imply $ra \in C$.

The set nZ is an ideal of the ring Z where:

$$nZ = \{ nk \mid k \in Z \} \tag{5}$$

for a fixed integer n.

The Ring Z/n

Fix an integer n > 1. For any integer a, set **a mod n** , equal to the remainder of the division of n into a. Therefore [1] :

$$0 \le (a \bmod n) < n \tag{6}$$

Set

$$Z/n = \{ 0, 1, 2, \ldots , n-1 \} \tag{7}$$

Define addition in Z/n by

$$(a + b) \bmod n , \qquad a,b \in Z/n \tag{8}$$

and multiplication in Z/n by

$$(a{\cdot}b) \bmod n\,, \qquad a,b \in Z/n \tag{9}$$

2.3. Groups and Characters

<u>Group</u>

Definition:

A group G is a system of elements which is closed under a single-valued binary operation which is associative, and relative to which G contains an element satisfying the identity law, and with each element another element (called its inverse) satisfying the inverse law [3] .

Associative Law: a(bc) = (ab)c for all a,b,c ;

Identity Law: ae = ea = a for all a ;

Inverse Law: $a\,a^{-1} = a^{-1}a = e$ for each a and some a^{-1}

A group whose operation satisfies the commutative law is called a "**commutative**" or "**Abelian**" group.

Let G be a group. We shall say that G **is cyclic** if there exists an element a of G such that every element x of G can be written in the form a^n for some $n \in Z$. Such an element a of G is then called a **generator** of G.

Character

Definition:

Let G be a set and k a field. By a **character** of G in k we mean [3] a homomorphism

$$\chi : G \mapsto k^* \qquad (10)$$

of G into the multiplicative group of k. The **trivial character** is the homomorphism taking the constant value 1.

Where a **homomorphism** of G into G' is a mapping

$$f : G \mapsto G' \qquad (11)$$

such that

$$f(xy) = f(x)\, f(y) \qquad x,y \in G \qquad (12)$$

and mapping the unit element of G into that of G'.

The ring structure of Z/n plays an important role in algorithm design. Let n-point data be viewed as a complex valued function having the set Z/n as its domain of definition [1] . Denote by

$$L\ (\ Z/n\ ) \tag{13}$$

the set of all complex valued functions on Z/n and regard L(Z/n) as a complex vector space under the following rules of addition and scalar multiplication:

$$(\ f + g\ )\ (\ j\ ) = f\ (\ j\ ) + g\ (\ j\ ) \tag{14}$$

$$(\ a f\ )\ (\ j\ ) = a\ (\ f\ (\ j\ )\ ) \qquad f,g \in L(Z/n)\ ,\ 0 \le j < n \tag{15}$$

Denote by $C^{\times}$ the multiplicative group of non-zero complex numbers. A function

$$\chi\ :\ Z/n \mapsto C^{\times} \tag{16}$$

is called an **additive character** if the following condition holds

$$\chi(l + K) = \chi(l) + \chi(k) \qquad 0 \le l, k < n \tag{17}$$

Denote the subgroup of $C^{\times}$ consisting of all n-th roots of unity by U_n. The additive character on Z/n can be described as follows:

An additive character χ of Z/n is a homomorphism of the additive group Z/n into the multiplicative group U_n and is uniquely determined by $\chi(1)$, by the formula

$$\chi(j) = \chi(1)^j, \qquad 0 \le j < n \tag{18}$$

The group U_n is the cyclic group having the element

$$w = \exp(2\pi i/n) \tag{19}$$

as a generator.

For each k, $0 \le k < n$, we define the mapping

$$\chi_k : Z/n \mapsto U_n \tag{20}$$

by setting

$$\chi_k(j) = w^{kj} \qquad 0 \le j,k < n \tag{21}$$

Therefore the set

$$\{ \chi_k : 0 \le k < n \} \tag{22}$$

is the set of additive characters on Z/n.

2.4. Periodic and Decimated Data

A subset B of z/n is called an ideal if the following two conditions hold [1] :

(1) B is a subgroup of the additive group z/n.

(2) $BZ/n \subset B$

Theorem: Every ideal of Z has the form nZ, for some integer $n \ge 0$.

proof:

Let B be an ideal in Z. $B \ne Z \text{ and } \ne 0$. Let n be the smallest integer > 0 lying in B. If $d \in B$ then there exists integers q, r with $0 \le r < n$ such that

$$d = nq + r \tag{23}$$

since B is an ideal, it follows that r lies in B, hence r = 0 . Thus d = nq and B = nZ. Therefore every ideal B of Z/n has the form

$$B = r\, Z/n \tag{24}$$

where r is a divisor of n.

Hence

$$B = \{\, rk : 0 \le k < s \,\}\ ,\quad n = rs \tag{25}$$

The ring structure of Z/n gives rise to the bilinear paring [1]

$$< l,k > \; = w^{lk}\ ,\ w = \exp\,(2\pi i/n)\ ,\ 0 \le l,k < n \tag{26}$$

The product, lk, can be taken either mod n or in Z since $w^n = 1$. Direct computation shows that the bilinear paring (26) satisfies the following three properties:

$$(I)\quad < l + k , m > \; = w^{(l+k)m} = w^{lk + km} = w^{lk} \cdot w^{km} = < l,k > < k,m > \tag{27}$$

$$(II)\quad < lk , m > \; = w^{lkm} = (w^{lm})^{k} = < l , m >^{k} \tag{28}$$

$$(III)\quad < l , k > \; = \; < k , l > , \qquad 0 \le l,k,m < n \tag{29}$$

The dual $B^{\perp}$ of an ideal B of Z/n is defined by setting

$$B^{\perp} = \{ \, l \in Z/n : \; < l,k > \; = 1, \textit{for all } k \in B \, \} \tag{30}$$

the above conditions imply that $B^{\perp}$ is also an ideal.

Example 1 : Take n = 8 and B = 2 Z/8.

Z/8 = { 0,1,2,3,4,5,6,7 }

B = { 0,2,4,6 }

$B^{\perp}$ = 4 Z/8

= { 0,4 }

Example 2 : Take n = 9 and B = 3 Z/9

Z/9 = { 0,1,2,3,4,5,6,7,8 }

B = { 0,3,6 }

$B^{\perp}$ = { 0,3,6 }

= { 0,3,6 }

Then $B = B^{\perp}$.

Theorem : If B = r Z/n then $B^{\perp}$ = s Z/n, n = rs

proof: Since n = rs and $w^{n} = 1$, we have

$$B^{\perp} \supset s\ Z/n$$

conversely if $k \in B^{\perp}$ then, $w^{kr} = 1$ which implies that s divides k and

$$B^{\perp} \subset s\ Z/n$$

An immediate consequence of the above theorem is that

$$(B^{\perp})^{\perp} = B \tag{31}$$

Take B = r Z/n, n = rs. A function $f \in L(A)$ is called **B-periodic** if the following condition is satisfied [1] :

$$f(a+b)=f(a) \qquad a \in A,\ b \in B \tag{32}$$

The set of functions:

$$\{\ e_k : 0 \le k < n\ \} \tag{33}$$

where

$$e_k = \begin{cases} 0\ , & k = l \\ 1\ , & k \neq l \end{cases} \tag{34}$$

is a basis of L(Z/n) called the **standard basis.** Where, a basis of a vector space is a linearly independent subset which generates (spans) the whole space. If $f \in L(Z/n)$, we can write

$$f = \sum_{k=0}^{n-1} f(k)\ e_k \tag{35}$$

and we call the n-tuple of components

$$f = \begin{bmatrix} f(0) \\ f(1) \\ \cdot \\ \cdot \\ \cdot \\ f(n-1) \end{bmatrix} \tag{36}$$

the **standard representation** of f.

A B-periodic function f is uniquely determined by the vector values

$$g = \begin{bmatrix} f(0) \\ f(1) \\ \cdot \\ \cdot \\ \cdot \\ f(r-1) \end{bmatrix} \tag{37}$$

by the formula,

$$f(l + rk) = f(l), \quad 0 \le l < r, 0 \le k < s \tag{38}$$

In vector notation

$$f = 1_s \otimes g \tag{39}$$

where $\underline{f}$ is the standard representation of f, and $\otimes$ denotes the tensor-product notation.

A function $f \in L(Z/n)$ is called **B-decimated** if we have [1]

$$f(a) = 0, \qquad a \notin B \tag{40}$$

If f is B-decimated then

$$\underline{f} = \begin{bmatrix} f(0) \\ f(r) \\ \cdot \\ \cdot \\ \cdot \\ f(n-r) \end{bmatrix} \otimes \underline{d} \tag{41}$$

where $\underline{d}$ is the r-tuple

$$d = \begin{bmatrix} 1 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix} \qquad (42)$$

2.5. Fourier Transform of Periodic and Decimated Data

The Fourier transform computation of periodic and decimated functions will now be examined [1] . Take

$$B = r\, Z/n \,, \qquad n = r\, s \qquad (43)$$

suppose $f \in L(Z/n)$ is B-periodic and F(f) is its Fourier transform. By definition

$$F(f)(l) = \sum_{k=0}^{n-1} f(k) \, <k,l> \,, \qquad 0 \le l < n \qquad (44)$$

But since f is b-periodic, we see that every k, $0 \le k < n$, can be written uniquely in the form,

$$k = k' + b\,, \qquad 0 \le k' < r\,,\ b \in B \tag{45}$$

Example: Take n = 8 and B = 2 Z/8

$k \in Z/8 \;= \{\, 0,1,2,3,4,5,6,7 \,\}$

$b \in B \;= \{\, 0,2,4,6 \,\}$

$k' \in \{\, 0,1 \,\}$

k = k'+ b

= 0 + 0 = 0

= 1 + 0 = 1

= 0 + 2 = 2

= 1 + 2 = 3

= 0 + 4 = 4

= 1 + 4 = 5

= 0 + 6 = 6

= 1 + 6 = 7

It follows that

$$F(f)(l) = \sum_{k'=0}^{r-1} \sum_{b \in B} f(k'+b) <k',l> <b,l> \qquad (46)$$

f is B-periodic, hence

$$F(f)(l) = \sum_{k=0}^{r-1} f(k) <k,l> \cdot \sum_{b \in B} <b,l> \qquad (47)$$

Let

$$\gamma(l) = \sum_{b \in B} < b,l > \qquad (48)$$

There are two cases to consider. First suppose $l \in B^{\perp}$. Then, by definition

$$< b,l > = 1, \qquad b \in B \qquad (49)$$

Example : Continuing with the previous example

B = { 0,2,4,6 }

$B^{\perp}$ = { 0,4 }

$w = \exp(2\pi i/8)$

$$< b,l > = w^{bl}$$

$$w^0 = 1$$
$$w^8 = 1$$
$$w^{16} = 1$$
$$w^{24} = 1$$

and therefore we have that:

$$\gamma(l) = s , \quad l \in B^{\perp} \qquad (50)$$

Otherwise $l \notin B^{\perp}$ and there exists $c \in B$ such that

$$< c,l > \neq 1 \qquad (51)$$

Example: Continuing with the same example

$B = \{ 0,2,4,6 \}$

$B^{\perp} = \{ 0,2 \}$

Let: $l = 3$ $\quad l \notin B^{\perp}$

$c = 2$ $\quad c \in B$

then

$$< 2,3 > = \exp(12\pi i/8) = \exp(3\pi i/2) \neq 1$$

Then

$$\begin{aligned} < c,l > \gamma(l) &= < c,l > \sum_{b \in B} < b,l > \\ &= \sum_{b \in B} < c,l > < b,l > \\ &= \sum_{b \in B} < c + b,l > \\ &= \sum_{b \in B} < b,l > \\ &= \gamma(l) \end{aligned} \tag{52}$$

but if $< c,l > \neq 1$, then the above equation is only valid if

$$\gamma(l) = 0 , \qquad l \in B^{\perp} \tag{53}$$

Therefore:

$$F(f)(l) = 0 , \qquad l \notin B^{\perp} \tag{54}$$

$$F(f)(l) = s \sum_{k=0}^{r-1} f(k) < k,l > , \qquad l \in B^{\perp} \tag{55}$$

$B^{\perp} = s\, Z/n$ which implies that

$$F(f)(ls) = s \sum_{k=0}^{r-1} f(k) < k,l >^s , \quad 0 \le l < r \tag{56}$$

$$< k,l >^s = w^{kls} = (w^s)^{kl} \tag{57}$$

Let $v = w^s$, then

$$< k,l > = v^{lk} \tag{58}$$

where

$$v = w^s = \exp(2\pi i/n)^s = \exp(2\pi i/r) \tag{59}$$

Therefore

$$F(f)(ls) = s \sum_{k=0}^{r-1} f(k)\, v^{kl} \tag{60}$$

Theorem: Let B = r Z/n, n = rs. If f is B-periodic then F(f) is $B^{\perp}$ - *decimated* , and on $B^{\perp}$, is given by

$$\begin{bmatrix} F(f)(0) \\ F(f)(s) \\ \cdot \\ \cdot \\ \cdot \\ F(f)(n-s) \end{bmatrix} = s\,F(r) \begin{bmatrix} f(0) \\ f(1) \\ \cdot \\ \cdot \\ \cdot \\ f(r-1) \end{bmatrix} \tag{61}$$

Observe that computing the n-point FFT of B-decimated data can be carried out using one r-point FFT.

Example: Continuing with the same example

$Z/8 = \{ 0,1,2,3,4,5,6,7 \}$

$B = 2\,Z/8 = \{ 0,2,4,6 \}$

$B^{\perp} = 4\,Z/8 = \{ 0,4 \}$

$n = 8$

$r = 2$

$s = 4$

$$\begin{bmatrix} F(f)(0) \\ F(f)(4) \end{bmatrix} = 4\,F(2) \begin{bmatrix} f(0) \\ f(1) \end{bmatrix}$$

and the 8-point Fourier transform computation of f can be carried out using a

2-point FFT.

Suppose that a B-decimated function $g \in L(Z/n)$. Where B = r Z/n. The Fourier transform F(g) of g is given by the formula

$$F(g)(l) = \sum_{k \in B} g(k) < k,l > \qquad 0 \le l < n \tag{62}$$

If $l \in B^{\perp}$, then < k,l > = 1, for all $k \in B$. Replacing l by l+s in (62)

$$\begin{aligned} F(g)(l+s) &= \sum_{k \in B} g(k) < k,l+s > \\ &= \sum_{k \in B} g(k) < k,l > < k,s > \\ &= F(g)(l) \qquad 0 \le l < n \end{aligned} \tag{63}$$

and therefore F(g) is $B^{\perp}$ *- periodic* . Hence

$$F(g)(l) = \sum_{k=0}^{s-1} g(rk)\, v^{lk} \tag{64}$$

where

$$v = w^{r} = \exp(2\pi i/s) \qquad 0 \le l < s \tag{65}$$

Theorem: Let B = r Z/n, n = rs. If g is B-decimated then F(g) is $B^{\perp}$ - *periodic* and is given by the formula

$$\begin{bmatrix} F(g)(0) \\ F(g)(1) \\ \cdot \\ \cdot \\ \cdot \\ F(g)(s-1) \end{bmatrix} = F(s) \begin{bmatrix} g(0) \\ g(r) \\ \cdot \\ \cdot \\ \cdot \\ g(n-r) \end{bmatrix} \tag{66}$$

Observe that computing the n-point Fourier transform of B-decimated data can be carried out using an s-point FFT.

2.6. Fourier Transform of Finite Abelian Groups

Consider a finite Abelian group A of order M. A mapping

$$\chi : A \mapsto U \tag{67}$$

where U is the multiplicative group of M-th roots of unity, is called a character of A if

$$\chi(a + b) = \chi(a)\, \chi(b) \qquad a,b \in A \tag{68}$$

Denote the set of all characters of A by A^* , which is a group under the addition rule

$$(a^* + b^*)(c) = a^*(c)\, b^*(c) \tag{69}$$

The action of $a^* \in A^*$ *on* $a \in A$ will be denoted by $< a,a^* >$. The group addition on A^* is given by

$$< a,a^* + b^* > = < a,a^* > < a,b^* > \tag{70}$$

Denote the set of all complex valued functions on a set S by L(S). The Fourier transform of A is the linear isomorphism F from L(A) onto $L(A^*)$ defined by

$$F(f)(a^*) = \sum_{a \in A} f(a) < a,a^* > \qquad f \in L(A)\ ,\ a^* \in A^* \tag{71}$$

This definition depends solely on the group A and as given does not include coordinates or dimension. Any group isomorphism Φ *from* A *onto* A^* determines a representation F_Φ *of* F defined by

$$F_\Phi(f)(a) = F(f)\,(\Phi(a)) \qquad a \in A \tag{72}$$

Example: Let A = Z/nZ, for a natural number n. Define Θ_1 by

$$< b \, , \Theta_1(a) > \; = e^{\frac{2\pi i}{n} ab} \qquad a,b \in A$$

We obtain the following familiar expression as the FT.

$$F_{\Theta_1}(f)(b) = \sum_{a=0}^{n-1} f(a)\, e^{\frac{2\pi i}{n} ab}$$

Two group isomorphisms Φ_1 *and* Φ_2 determine representations which are related by data permutation by the formula

$$F_{\Phi_1}(f)(a_1) = F_{\Phi_2}(f)(a_2) \tag{73}$$

where $a_2 = \Phi_2^{-1} \, \Phi_1 \, a_1$

Definition:

By an **isomorphism** between two groups G and G' is meant a one-one correspondence $a \leftrightarrow a'$ between their elements which preserves group multiplication-i.e., which is such that if $a \leftrightarrow a'$ and $b \leftrightarrow b'$ *, then* $ab \leftrightarrow a'b'$ [2] .

Fix a group isomorphism Φ *from* A *onto* A^* . Consider any subgroup B of A. The dual. $B^\perp$ *of* B is defined by

$$B^\perp = \{ a \in A : < b, \Phi(a) > = 1, \forall b \in B \} \tag{74}$$

$B^\perp$ is the subgroup of A which corresponds under Φ to the subgroup of all characters $a^* \in A^*$ which act trivially on B.

Φ induces a group isomorphism Φ_1 form

$$B^\perp \mapsto (A/B)^* \tag{75}$$

If F_1 denotes the FFT of the group A/B, then a linear isomorphism F^1_Φ *from* $L(A/B)$ *onto* $L(B^\perp)$ is defined by

$$(F_\Phi, f) = F_1(f)\,(\Phi_1(b^\perp)) \qquad b^\perp \in B^\perp , f \in L(A/B) \tag{76}$$

A Cooley-Tukey Algorithm will be designed which decomposes the computation into parallel stages which compute the FFT of f on each of the cosets of $B^{\perp}$. Set

$$N = O(A)\ ,\ \ M = O(B)\ ,\ \ L = O(B^{\perp}) \tag{77}$$

where O(S) is the number of elements in the set S. Since $B^{\perp}$ is group isomorphic to A/B, we have N = LM.

A function $f \in L(A)$ is B-periodic if

$$f(a + b) = f(a)\ , \qquad a \in A\ , b \in B \tag{78}$$

The space of B-periodic functions in L(A), denoted by $L_B(A)$, can be identified with the space L(A/B). Consider coset representatives $a_0 = 0, a_1, \ldots, a_{L-1}$ for A/B. A is the disjoint union of cosets

$$B\ , a_1 + B\ , \ldots\ , a_{L-1} + B \tag{79}$$

and each $a \in A$ can be written uniquely as $a = a_l + b$, for some $0 \le l < L\ , b \in B$. If f is B-periodic, then

$$f(a_l) = f(a_l + b)\,, \qquad 0 \le l < L\,,\, b \in B \tag{80}$$

and f induces uniquely a function on A/B that assigns to the coset $a_l + B$ the value $f(a_l)$.

Consider $F_\Phi(f)$, for any B-periodic function f. Then

$$\begin{aligned} F_\Phi(f)\,(c) &= \sum_{a\in A} f(a) < a, \Phi(c) > \\ &= \sum_{l=0}^{L-1} f(a_l + b) < a_l + b, \Phi(c) > \end{aligned} \tag{81}$$

which by the B-periodicity of f can be rewritten as

$$F_\Phi\,(f)\,(c) = \sum_{l=0}^{L-1} f(a_l) < a_l, \Phi(c) > \sum_{b\in B} < b, \Phi(c) > \tag{82}$$

Take $c \notin B^\perp$, then, there is a $b_0 \in B$ such that $< b_0, \Phi(c) > \neq 1$.

From

$$\begin{aligned} \sum_{b\in B} < b, \Phi(c) > &= \sum_{b\in B} < b + b_0, \Phi(c) > \\ &= < b_0\,,\, \Phi(c) > \sum_{b\in B} < b, \Phi(c) > \end{aligned}$$

therefore

$$\sum_{b \in B} < b, \Phi(c) > = 0 \tag{84}$$

and

$$F_{\Phi}(f)(c) = 0 \qquad whenever\ c \notin B^{\perp} \tag{85}$$

Take $c \in B^{\perp}$, we now have

$$\sum_{b \in B} < b, \Phi(c) > = O(B) = M \tag{86}$$

therefore

$$F_{\Phi}(f)(c) = M \sum_{l=0}^{L-1} f(a_l) < a_l, \Phi(c) > \qquad c \in B^{\perp} \tag{87}$$

viewing f as a function in L(A/B), the summation on the right-hand side of (20) is

$$F_1(f)(c) \tag{88}$$

where F_1 is the Fourier transform of L(A/B) onto $L(B^{\perp})$ induced by Φ . We see that computing the FFT of f *on* $B^{\perp}$ is given by computing the smaller size FFT of the periodization of f viewed as a function on A/B. In this method each preprocessing step is a periodization requiring no complex twiddle factor multiplication. In general however, this method leads to redundant computations.

For our purpose in this work we will approach the problem in a more standard fashion by computing $F_{\Phi}(f)$ on each of the cosets if $B^{\perp}$ on A. The group isomorphism Φ induces an isomorphism Φ_2 from

$$\Phi_2 : A/B^{\perp} \mapsto B^{*} \tag{89}$$

Take a complete system of representatives c_k , $0 \le k < M$, for the cosets of $B^{\perp}$ in A and set $b_k^{*} = \Phi_2(k)$, $0 \le k < M$. We can compute F_{Φ} on the coset $c_k + B^{\perp}$ by the formula

$$\begin{aligned} F_{\Phi}(f)(c_k + b^{\perp}) &= \sum_{a \in A} f(a) <a, \Phi(c_k + b^{\perp})> \\ &= \sum_{l=0}^{L-1} \left(\sum_{b \in B} f(a_l + b) <a_l + b, \Phi(c_k)> \right) <a_l, \Phi(b^{\perp})> \end{aligned} \tag{90}$$

This computation can be organized as follows. For each $b^* \in B^*$, set

$$f_{b^*}(a) = \sum_{b \in B} <b,b^*> f(a + b) \tag{91}$$

and observe that f_{b^*} satisfies

$$f_{b^*}(a + b) = <b,b^*>^{-1} f_{b^*}(a) \tag{92}$$

The FFT of f_{b^*} is given by

$$\begin{aligned} F_{\Phi}(f_{b^*})(c) &= \sum_{a \in A} f_{b^*}(a) <a,\Phi(c)> \\ &= \sum_{l=0}^{L-1} \sum_{b \in B} f_{b^*}(a_l + b) <a_l + b,\Phi(c)> \\ &= \sum_{l=0}^{L-1} f_{b^*} <a_l,\Phi(c)> \sum_{b \in B} <b,\Phi(c) - b^* > \end{aligned} \tag{93}$$

If $b^* \neq \Phi_2(c)$ then

$$\sum_{b \in B} <b,\Phi(c) - b^*> = 0 \tag{94}$$

It follows that $F_{\Phi}(f_{b^*}(c))$ vanishes unless c is contained in the coset $\Phi_2^{-1}(b^*)$ *of* $B^{\perp}$ *in* A . Set $b^* = b_k^*$ *and* $c = c_k + b^{\perp}$. Then by (93)

$$\begin{aligned} F_{\Phi}(f_{b^*})(c_k + b^{\perp}) &= M \sum_{l=0}^{L-1} g_{b_k^*}(a_l) \langle a_l, \Phi(b^{\perp}) \rangle \\ &= M\, F_{\Phi_1}(g_{b_k^*})(b^{\perp}) \end{aligned} \tag{95}$$

where $g_{b_k^*} = \langle a, \Phi(c_k) \rangle f_{b_k^*}(a)$, is B-periodic. Comparing with (95) we have

$$F_{\Phi}(f)(c_k + b^{\perp}) = F_{\Phi_1}(g_{b_k^*}), \qquad b_k^* \in B^* \tag{96}$$

Three main stages can be distinguished in the computation of the FFT of f.

1. Form the M-functions

$$f_{b_k^*}(a) = \sum_{b \in B} \langle b, b^* \rangle f(a + b)$$

2. Twiddle the factors

$$g_{b_k^*}(a) = < a, \Phi(c_k) > f_{b_k^*}(a)$$

The functions $g_{b_k^*}$ are B-periodic and can be viewed as functions on A/B.

3. Compute the FFT's on A/B

$$F_{\Phi}(g_{b_k^*})(b^{\perp})$$

In the first two computations, we need to compute f and $g_{b_k^*}$ only at the points

$a = a_0 , a_1 , \dots , a_{L-1}$.

Example 1: Let A = Z/12Z. Define Θ_2 by

$$< a, \Theta_2(b) > = e^{\frac{2\pi i}{12} ab}$$

B_1 = {0, 6} is a subgroup of A. We have $B_1^{\perp} = \{ 0,2,4,6,8,10 \}$.

Choose the coset representatives $A / B_1^{\perp} = \{ 0,1 \}$, $A / B_1 = \{ 0,1,2,3,4,5 \}$.

Set $B^* = \{ \lambda_0, \lambda_1 \}$, where

	λ_0	λ_1
0	1	1
6	1	-1

1. For $a \in A/B_1$

$$f_{\lambda_0} = f(a) + f(a+6)$$

$$f_{\lambda_1} = f(a) - f(a+6)$$

2. $g_{\lambda_0}(a) = f_{\lambda_0}(a)$

$$g_{\lambda_1}(a) = e^{\frac{2\pi i}{12} a} f_{\lambda_1}(a)$$

3. for $b \in B_1^{\perp}$

$$F_{\Theta_2}(g_{\lambda_0})(b) = \sum_{a=0}^{5} g_{\lambda_0}(a)\, e^{\frac{2\pi i}{6} ab}$$

$$F_{\Theta_2}(g_{\lambda_1})(b+1) = \sum_{a=0}^{5} g_{\lambda_1}(a)\, e^{\frac{2\pi i}{6} ab}$$

Example 2: with a as above, let

$B_2 = \{0, 4, 8\}$. We have $B_2^{\perp} = \{ 0,3,6,9 \}$.

$A / B_2^{\perp} = \{ 0,1,2 \}$, $A / B_2 = \{ 0,1,2,3 \}$.

$B^* = \{ \gamma_0, \gamma_1, \gamma_2 \}$, where, with $w = e^{\frac{2\pi i}{3}}$

	γ_0	γ_1	γ_2
0	1	1	1
4	1	w	w^2
8	1	w^2	w

1. For $a \in A/B_2$

$$f_{\gamma_0} = f(a) + f(a+4) + f(a+8)$$

$$f_{\gamma_1} = f(a) + w f(a+4) + w^2 f(a+8)$$

$$f_{\gamma_2} = f(a) + w^2 f(a+4) + w f(a+8)$$

2. $g_{\gamma_0}(a) = f_{\gamma_0}(a)$

$$g_{\gamma_1}(a) = e^{\frac{2\pi i}{12} a} f_{\gamma_1}(a)$$

$$g_{\gamma_2}(a) = e^{\frac{2\pi i}{12} 2a} f_{\gamma_2}(a)$$

3. for $b \in B_2^{\perp}$

$$F_{\Theta_2}(g_{\gamma_0})(b) = \sum_{a=0}^{3} g_{\gamma_0}(a)\, e^{\frac{2\pi i}{4} ab}$$

$$F_{\Theta_2}(g_{\gamma_1})(b+1) = \sum_{a=0}^{3} g_{\gamma_1}(a)\, e^{\frac{2\pi i}{4} ab}$$

$$F_{\Theta_2}(g_{\gamma_2})(b+2) = \sum_{a=0}^{3} g_{\gamma_2}(a)\, e^{\frac{2\pi i}{4} ab}$$

3 PERIODIZATION AND DECIMATION ALGORITHM FOR CRYSTALLOGRAPHIC FFT

3.1. Introduction

3.1.1. Historical Background

X-rays were discovered by *Röntgen* in 1895. In 1912 the discovery of the diffraction of x-rays by crystals, constituted the beginning of one of the most remarkable developments in science. This lead to a sequence of experiments in one of which a pencil of x-rays fell on a copper sulfate crystal; and the hoped-for diffraction beams were photographically recorded. Noting the geometrical shapes of the spots, William Lawrence Bragg believed that this kind of diffraction could be regarded as cooperative reflections by the internal planes of the crystal, and accordingly reformulated diffraction by a crystal in these terms. In 1883, William Barlow published arrangements of atoms to be expected in certain symmetrical crystals such as alkali halids and zinc sulfides. Bragg tested these structures in an effort to explain the x-ray diffraction results. The success of these results lead to a new era in which the structure of crystals could be analyzed by x-ray diffraction. Bragg was able to set fourth the structures of NaCl, KCl, KBr and many more. This beginning set the stage for an increase in the detailed knowledge of the structure of matter. The earliest crystal-structure investigation proceeded without the formal use of symmetry information. Although space-group theory has been developed before the twentieth century, this information was not in use until after 1919, when a study contained not only graphical and analytical description of the space groups but pointed out how they could be determined by x-ray diffraction effects [4] .

The first successful x-ray analysis of a protein, that of myoglobin, occurred in 1960. It was followed by a sequence of experiments which yielded crucial information but also showed that dealing with x-ray analysis of proteins is much more difficult than inorganic crystallography. Since 1960, protein crystallography has emerged as an essential tool for protein engineering and other areas of advanced biotechnology.

3.1.2. The Fourier Transform in X-ray Crystallography

One of the most important theoretical tools for dealing with problems in crystal-structure analysis is the Fourier transform. This is a mathematical function which provides a direct relation between the crystal structure and the diffraction effects it produces.

In normalized coordinates, an infinite crystal can be described by an electron density map $\rho(\underline{x})$, $\underline{x} \in \mathbb{R}^3$ satisfying the periodicity condition [8,9]

$$\rho(\underline{x} + \underline{n}) = \rho(\underline{x}) \qquad \underline{x} \in \mathbf{R}^3 \,, \underline{n} \in Z^3$$

The period lattice Z^3 is assumed to be the finest for which this periodicity condition holds. in this way a basic pattern is established in the unit cube and is regularly repeated by integer translations along each component throughout all $\mathbf{R}^3$.

$\rho(\underline{x})$ can be expanded as a Fourier series

$$\rho(\underline{x}) = \sum_{\underline{x} \in Z^3} H(\underline{n})\, e^{-2\pi i \underline{n} \cdot \underline{x}}$$

where $\underline{n} \cdot \underline{x} = n_1 x_1 + n_2 x_2 + n_3 x_3$.

Mathematically, the "structure factors" $H(\underline{n})$, uniquely determine $\rho(\underline{x})$ but, in general, are not available after x-ray diffraction. As a result we can only compute the absolute values $|H(\underline{n})|$ for n within some sphere $|\underline{n}| \leq \Delta^{-1}$ decided upon by the desired resolution Δ . The problem of phase recovery is called the "phase problem" which greatly complicates the determination of crystal structures. Many methods have been introduced to solve the phase problem. However, a precise mathematical solution does not exist. Recently developed methods have moved the Fourier transform to the center stage as a fundamental computational tool. Typically these methods are iterative, requiring large numbers of information transfer between direct and reciprocal spaces. This makes the computation of the Fourier transform and its inverse a major part of the overall cost of the procedure.

Sampled crystallographic data one given as a finite three-dimensional array of numbers. computing the Fourier transform of sampled electron density is called the forward Fourier transform, while computing the (inverse) Fourier transform of periodized structure factors is called the backward Fourier transform [13,14].

The crystallographic group Γ of a crystal with electron density $\rho(\underline{x})$ is defined as the group of all Euclidean motions r of $\mathbb{R}^3$ under which $\rho(\underline{x})$ is invariant.

$$\rho(r\underline{x}) = \rho(\underline{x})$$

However, we will theoretically use crystallographic groups as sitting inside, group actions on $Z/N_1 \times Z/N_2 \times Z/N_3$, rather than the standard theory of Euclidean actions on $\mathbb{R}^3$.

3.1.3. The Role of symmetry

crystal symmetry is an important factor in computational complexity and algorithm design. We will study the effect of symmetry on finite Fourier transform computations. The feasibility and cost of computational procedures are highly influenced by the availability of algorithms and code capable of dealing efficiently with crystal symmetry. Crystals can be invariant under the action of space groups. If $\rho(x,y,z)$ represents an electron density map in normalized coordinates and if L represents a space group action, then ρ is L-invariant if $\rho(x,y,z) = \rho(x',y',z')$, where the points (x,y,z) *and* (x',y',z') are related by the action of some element in L. If a crystal is invariant under the action of some non-trivial space group, then the contents of the unit cell are redundant as well as the corresponding structure factors of the crystal. An asymmetric unit of the crystal or the space group L, is any subset of the unit cell which includes all crystal information and contains no redundant information. A symmetric FFT for such a crystal is one that computes the contents of an asymmetric unit only and computes a non-redundant set of structure factors only [14] .

3.2. Crystallographic FFT

Definition: An isomorphism of a group G with itself is called an automorphism of G. Thus an automorphism α of G is a one-one transformation of G onto itself such that

$$(xy)\alpha = (x\alpha)(y\alpha) \quad \textit{for all } x,y \in G$$

The automorphisms of any group G themselves form a group A.

Denote the automorphism group of A by Aut(A) and the group of translations of A by T(A). The affine group of A is the semi-direct product

$$Aff(A) = T(A) \lessdot Aut(A) \tag{1}$$

For $a \in A$, $T_a \in T(A)$ is defined by

$$T_a(c) = a + c\,, \quad c \in A \tag{2}$$

Consider any abelian group X of Aff(A). X is a finite abelian group. Denote the character group of X by X^* .

Take $f \in L(A)$. For each $x^* \in X^*$, define

$$F_{x^*}(a) = \sum_{x \in X} \langle x,x^* \rangle\, f(xa) \tag{3}$$

The function f_{x^*} has the following invariance property relative to the action of X

$$f_{x^*}(xa) = \langle x,x^*, \rangle^{-1} f_{x^*}(a) \tag{4}$$

Set R = O(X) and $T = O\,(T_X)$, where $T_X = X \cap T(A)$ is the subgroup of all translations in X. Then

$$f = \frac{1}{R} \sum_{x^* \in X^*} f_{x^*} \tag{5}$$

and

$$F_{\Phi}(f) = \frac{1}{R} \sum_{x^* \in X^*} F_{\Phi}(f_{x^*}) \tag{6}$$

In this approach the initial FFT computation is replaced by R FFT computations. The trade off is contained in the invariance condition (4) which in principle reduces by a factor of 1/R the number of required computations and memory space.

Suppose Y is a subgroup of X and $f \in L(A)$ is Y-invariant :

$$f(ya) = f(a) \tag{7}$$

Set $R' = O(X/Y)$. Choose a complete system of representatives x_j , $0 \leq j < R'$ *for* X/Y . Then

$$\begin{aligned} f_{x^*}(a) &= \sum_{j=0}^{R'-1} \sum_{y \in Y} f(x_j ya) \langle x_j y, x^* \rangle \\ &= \sum_{j=0}^{R'-1} \langle x_j, x^* \rangle f(x_j a) \sum_{y \in Y} \langle y, x^* \rangle \end{aligned} \tag{8}$$

If x^* does not restrict to the identity character on Y, then

$$\sum_{y \in Y} \langle y, x^* \rangle = 0 \tag{9}$$

and

$$f_{x^*} = 0 \qquad x^*/y \neq 1 \tag{10}$$

It follows that for Y-invariant data, we can restrict our attention to f_{x^*} such that $x^*/y = 1$. The invariance of data under Y disables a part of the algorithm based on the group X. In this way the code implementing the above algorithm can be used for any subgroup Y of X.

3.3. Symmetry Conditions

In this section we will describe the action of four crystallographic groups. These are groups of order two. For $x \in Z/N$, these groups act on x in one of the following ways [6,7]

1. $x \to x$, denoted by I (for identity).
2. $x \to -x$, denoted by R (for reflection).
3. $x \to \frac{1}{2} + x$, denoted by T (for translation).
4. $x \to \frac{1}{2} - x$, denoted by S (for screw motion).

We will use this notation throughout the rest of this chapter. although one dimensional actions are shown above, multidimensional cases will be used. for these cases the same letters will be used but the dimension will be indicated.

3.4. Symmetrized FFT's

Now we will discuss some properties of the finite Fourier transform in the presence of the group actions described in the previous section [6,13].

Lemma 1. If **f** respects R then so does $\hat{f}$.

Proof: By definition the FFT is given by the formula:

$$\hat{f}(y) = \sum_{x=0}^{N-1} f(x)\, e^{-2\pi i \left(\frac{xy}{N}\right)}$$

replace x by -x

$$\hat{f}(y) = \sum_{x=0}^{N-1} f(-x)\, e^{-2\pi i \left(\frac{-xy}{N}\right)}$$

Therefore

$$\hat{f}(y) = \hat{f}(-y)$$

Lemma 2. If **f** respects T then $\hat{f}(y) = (-1)^y \hat{f}(y)$.

Proof :

$$\hat{f}(y) = \sum_{x=0}^{N-1} f(x)\, e^{-2\pi i \left(\frac{xy}{N}\right)}$$

replacing x by $\frac{N}{2} + x$

$$\begin{aligned} \hat{f}(y) &= \sum_{x=0}^{N-1} f\left(\frac{N}{2} + x\right) e^{-2\pi i \frac{\left(\frac{N}{2} + x\right) y}{N}} \\ &= \sum_{x=0}^{N-1} f(x)\, e^{-2\pi i \left(\frac{xy}{N}\right)} e^{-\pi i y} \end{aligned}$$

therefore

$$\hat{f}(y) = (-1)^y \hat{f}(y)$$

Lemma 3. If **f** respects S then $\hat{f}(y) = (-1)^y \hat{f}(-y)$

Proof: proof of this follows from 1 and 2, since S = RT.

Lemma 4. If f is a real-valued function then $\hat{f}$ is Hermitian.

Proof:

By definition

$$\hat{f}(y) = \sum_{x=0}^{N-1} f(x)\, e^{-2\pi i \frac{xy}{N}}$$

If f is real then

$$\hat{f}(y) = \sum_{x=0}^{N-1} f^*(x) \left(e^{2\pi i \frac{xy}{N}} \right)^*$$

therefore

$$\hat{f}(y) = \hat{f}^*(-y)$$

where the star denotes the complex conjugate.

Lemma 4.1. If f(x) is real-valued and f(x) = f(-x) then

$\hat{f}(y)$ is pure-real and

$\hat{f}(y) = \hat{f}(-y)$

Lemma 4.2. If f(x) is real-valued and f(x) = -f(-x) then

$\hat{f}(y)$ is pure-imaginary and

$$\hat{f}(y) = -\hat{f}(-y)$$

3.5. Periodization and Decimation Algorithm

3.5.1. Introduction

In this section we will show a direct application of the periodization and decimation algorithm to the crystallographic FFT. We will choose a super group X and periodize our data with respect to this group.

For a positive integer N, denote by L(N) the space of functions on $Z/N1 \times Z/N2 \times Z/N3$, where Z denotes the set of integers. Consider the finite function $f(x_1,x_2,x_3), f \in L(N), x_1,x_2,x_3 \in Z/N1 \times Z/N2 \times Z/N3$. Let

$$M1 = \frac{N1}{2} \ , \ M2 = \frac{N2}{2} \ , \ M3 = \frac{N3}{2}, \quad M1, M2, M3 \ \textit{are odd} \tag{11}$$

Using matrix notation for crystallographic group actions, let

$$t_1 = \begin{bmatrix} M1 \\ 0 \\ 0 \end{bmatrix} \ , \ t_2 = \begin{bmatrix} 0 \\ M2 \\ 0 \end{bmatrix} \ , \ t_3 = \begin{bmatrix} 0 \\ 0 \\ M3 \end{bmatrix} \tag{12}$$

where t_1 , t_2 , t_3 represent translational action in one dimension. Let

$$r_1 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & 1 \end{bmatrix}, r_2 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix}, r_3 = \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \end{bmatrix} \tag{13}$$

where r_1 , r_2 , r_3 represent rotational action in one dimension.

3.5.2. Periodization With Respect to The Super Group

Consider the finite abelian group X generated by

$$X \ : \ < I , t_1 , t_2 , t_3 , r_1 , r_2 , r_3 > \tag{14}$$

I is the identity element. This group contains 64 elements, therefore the order of the group X, O(X) = 64. Since $x \cdot x = I , x \in X$, each element in this group has order two.

The first step of the algorithm will be periodizing the function f with respect to the group X. Since each element in the group X has order two, the character group X^* of X is the set of all mappings from X onto the 2-th roots of unity (± 1) . Assign the binary values (0 to +1) and (1 to -1). The periodization with respect to X will lead to 64 functions, $\{ f_0 (x) , f_1 (x) , \ldots , f_{63} (x) \}$, where the index of each function represents the magnitude of the binary value of the six generators respectively. Hence

$$
\begin{aligned}
f_0(x) &= f(x) + f(t_1x) + \dots + f(r_3x) + \dots \\
f_1(x) &= f(x) + f(t_1x) + \dots - f(r_3x) \pm \dots \\
&\vdots \\
f_{63}(x) &= f(x) - f(t_1x) - \dots - f(r_3x) - \dots
\end{aligned}
\tag{15}
$$

where the sign of each of the remaining elements of the above functions is directly determined from the signs of the generators in a multiplicative fashion.

Direct addition of the above 64 functions leads to the following equation:

$$f(x) = \frac{1}{64}\{ f_0(x) + f_1(x) + \dots + f_{63}(x) \} \tag{16}$$

Moreover the above 64 functions are invariant under the action of X. Therefore

$$
\begin{aligned}
f_0(x) &= f_0(t_1x) = f_0(t_2x) = \dots \\
&\vdots \\
f_{63}(x) &= -f_{63}(t_1x) = -f_{63}(t_2x) = -\dots
\end{aligned}
\tag{17}
$$

Consider the bilinear form

$$< x,y > = x_1y_1 + x_2y_2 + x_3y_3 \tag{18}$$

set

$$\omega_N = e^{\left(\frac{-2\pi i}{N}\right)} \tag{19}$$

The three dimensional finite Fourier transform is defined by the formula

$$\hat{f}(y_1,y_2,y_3) = \sum_{x_3=0}^{N3-1} \sum_{x_2=0}^{N2-1} \sum_{x_1=0}^{N1-1} f(x_1,x_2,x_3)\, e^{-2\pi i\left(\frac{x_1 y_1}{N1} + \frac{x_2 y_2}{N2} + \frac{x_3 y_3}{N3}\right)} \tag{20}$$

or

$$\hat{f}(y) = \sum_{x_3=0}^{N3-1} \sum_{x_2=0}^{N2-1} \sum_{x_1=0}^{N1-1} f(x)\, \omega_N^{<x,y>} \tag{21}$$

It is clear from (16) that the Fourier transform of f(x) can be obtained by computing the Fourier transform of each of the 64 functions $f_0(x)$ *through* $f_{63}(x)$ by the following formula

$$\hat{f}(y) = \frac{1}{64}\{\hat{f}_0(y) + \hat{f}_1(y) + \dots + \hat{f}_{63}(y)\} \tag{22}$$

3.5.3. Twiddle Factors

We will now study the Fourier transform computation of $f_0(x)$ *through* $f_{63}(x)$, and we will show the effect of symmetry conditions on the FFT computation. In general this will lead to complex twiddle factors. We will divide these functions into eight sets where each set will contain functions in which the translational generators t_1, t_2, t_3 have the same sign. This will lead to the following eight sets

1. $S_1 = \{ f_0(x), f_1(x), \dots, f_7(x) \}$

2. $S_2 = \{ f_8(x), f_9(x), \dots, f_{15}(x) \}$

3. $S_3 = \{ f_{16}(x), f_{17}(x), \dots, f_{23}(x) \}$

4. $S_4 = \{ f_{24}(x), f_{25}(x), \dots, f_{31}(x) \}$

5. $S_5 = \{ f_{32}(x), f_{33}(x), \dots, f_{39}(x) \}$

6. $S_6 = \{ f_{40}(x), f_{41}(x), \dots, f_{47}(x) \}$

7. $S_7 = \{ f_{48}(x), f_{49}(x), \dots, f_{55}(x) \}$

8. $S_8 = \{ f_{56}(x), f_{57}(x), \dots, f_{63}(x) \}$

We will now group the above eight sets into four major groups based on the order of the twiddle factors.

1. No twiddle factor.
2. One dimensional twiddle factor.
3. Two dimensional twiddle factor.
4. Three dimensional twiddle factor.

3.5.3.1. No Twiddle Factor

The first group contains only the set S_1 . In this set the functions $\{ f(t_1 x), f(t_2 x), f(t_3 x) \}$ are all positive.

Therefore

$$f_i(x) = f_i(t_1 x) = f_i(t_2 x) = f_i(t_3 x) \qquad f_i(x) \in S_1 \tag{23}$$

Applying these symmetry conditions to (20) and using Lemma 2 section (3.4), leads to

$$\hat{f}_i(y_1,y_2,y_3) = (-1)^{y_1} \hat{f}_i(y_1,y_2,y_3) \tag{24}$$

$$\hat{f}_i(y_1,y_2,y_3) = (-1)^{y_2} \hat{f}_i(y_1,y_2,y_3) \tag{25}$$

$$\hat{f}_i(y_1,y_2,y_3) = (-1)^{y_3} \hat{f}_i(y_1,y_2,y_3) \tag{26}$$

Therefore $\hat{f}_i\,(y)$ is nonzero only when y_1 , y_2 , y_3 are all even.

Let:

$$
\begin{aligned}
y_1 &= 2u_1 & 0 &\le u_1 < M1 \\
y_2 &= 2u_2 & 0 &\le u_2 < M2 \\
y_3 &= 2u_3 & 0 &\le u_3 < M3
\end{aligned}
$$

Then applying these conditions to (20) leads to

$$
\begin{aligned}
\hat{f}_i\,(2u_1,2u_2,2u_3) &= \sum_{x_3=0}^{N3-1} \sum_{x_2=0}^{N2-1} \sum_{x_1=0}^{N1-1} f\,(x_1,x_2,x_3)\ \omega_N^{<x,2u>} \\
&= 8 \sum_{x_3=0}^{M3-1} \sum_{x_2=0}^{M2-1} \sum_{x_1=0}^{M1-1} f\,(x_1,x_2,x_3)\ \omega_M^{<x,u>}
\end{aligned}
\tag{27}
$$

Let $g_i\,(x_1,x_2,x_3) = f_i\,(x_1,x_2,x_3)$. Hence

$$
\hat{f}_i\,(2u_1,2u_2,2u_3) = 8 \sum_{x_3=0}^{M3-1} \sum_{x_2=0}^{M2-1} \sum_{x_1=0}^{M1-1} g_i\,(x_1,x_2,x_3)\ \omega_M^{<x,u>}
\tag{28}
$$

or

$$
\hat{f}_i\,(2u_1,2u_2,2u_3) = 8\,\hat{g}_i\,(u_1,u_2,u_3) \qquad 0 \le u_j < M_j
$$
$$
\textit{where } i = 0\ ,\ 1,\ \ldots\ ,\ 7 \ \textit{ and }\ j = 1\ ,\ 2\ ,\ 3
\tag{29}
$$

As a result the Fourier transform of each of the functions $f_0(x), \ldots, f_7(x)$ can be obtained directly from (28) using only 1/8 the original transform size. Note also that in this case there are no twiddle factors.

3.5.3.2. One Dimensional Twiddle Factor

This group contains sets S_2, S_3, S_5 . Set $S_2 = \{f_8(x), \ldots, f_{15}(x)\}$. In this set translational symmetries t_1 *and* t_2 are positive while t_3 is negative. Therefore

$$f_i(x) = f_i(t_1 x) = f_i(t_2 x) = -f_i(t_3 x) \qquad f_i(x) \in S_2 \tag{30}$$

Applying these symmetry conditions to (20) and using Lemma 2 section (3.4) leads to

$$\hat{f}_i(y_1,y_2,y_3) = (-1)^{y_1} \hat{f}_i(y_1,y_2,y_3) \tag{31}$$

$$\hat{f}_i(y_1,y_2,y_3) = (-1)^{y_2} \hat{f}_i(y_1,y_2,y_3) \tag{32}$$

$$\hat{f}_i(y_1,y_2,y_3) = (-1)^{y_3+1} \hat{f}_i(y_1,y_2,y_3) \tag{33}$$

Therefore $\hat{f}_i\,(y)$ is nonzero only when y_1 , y_2 , *are even,* y_3 *is odd* .

Let:

$$
\begin{aligned}
y_1 &= 2u_1 & 0 \le u_1 < M1 \\
y_2 &= 2u_2 & 0 \le u_2 < M2 \\
y_3 &= 2u_3 + 1 & 0 \le u_3 < M3
\end{aligned}
$$

Then applying these conditions to (20) leads to

$$
\begin{aligned}
\hat{f}_i\,(2u_1,2u_2,2u_3+1) &= \sum_{x_3=0}^{N3-1} \sum_{x_2=0}^{N2-1} \sum_{x_1=0}^{N1-1} f\,(x_1,x_2,x_3)\ \omega_N^{<x,(2u_1,2u_2,2u_3+1)>} \\
&= 8 \sum_{x_3=0}^{M3-1} \sum_{x_2=0}^{M2-1} \sum_{x_1=0}^{M1-1} f\,(x_1,x_2,x_3)\ \omega_M^{<x,u>}\ e^{-2\pi i\left(\frac{x_3}{N3}\right)}
\end{aligned} \tag{34}
$$

let

$$
g_i\,(x_1,x_2,x_3) = f_i\,(x_1,x_2,x_3)\ e^{-2\pi i\left(\frac{x_3}{N3}\right)} \tag{35}
$$

hence

$$
\hat{f}_i\,(2u_1,2u_2,2u_3+1) = 8 \sum_{x_3=0}^{M3-1} \sum_{x_2=0}^{M2-1} \sum_{x_1=0}^{M1-1} g_i\,(x_1,x_2,x_3)\ \omega_M^{<x,u>} \tag{36}
$$

or

$$\hat{f}_i\,(2u_1,2u_2,2u_3+1) = 8\,\hat{g}_i\,(u_1,u_2,u_3) \qquad 0 \le u_j < M_j \tag{37}$$
$$where\ i = 8\ ,\ 9,\ \dots\ ,\ 15\quad and\quad j = 1\ ,\ 2\ ,\ 3$$

In this case the function $g_i\,(x)$ is related to the initial data $f_i\,(x)$ by the complex twiddle factor $e^{-2\pi i\left(\frac{x_3}{N_3}\right)}$, which is one dimensional in the sense the it effects only the third variable (x_3). Note that the FT computation can be obtained using only 1/8 of the original data set.

Set $S_3 = \{f_{16}\,(x)\ ,\ \dots\ ,f_{23}\,(x)\}$. In this set translational symmetries t_1 *and* t_3 are positive while t_2 is negative. Therefore

$$f_i\,(x) = f_i\,(t_1x) = -\,f_i\,(t_2x) = f_i\,(t_3x) \qquad f_i\,(x) \in S_2 \tag{38}$$

Applying these symmetry conditions to (20) and using Lemma 2 section (3.4) leads to

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_1}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{39}$$

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_2+1}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{40}$$

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_3}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{41}$$

Therefore $\hat{f}_i\,(y)$ is nonzero only when y_1 , y_3 , *are even,* y_2 *is odd* .

Let:

$$\begin{array}{ll} y_1 = 2u_1 & 0 \le u_1 < M1 \\ y_2 = 2u_2+1 & 0 \le u_2 < M2 \\ y_3 = 2u_3 & 0 \le u_3 < M3 \end{array}$$

Then applying these conditions to (20) leads to

$$\begin{aligned} \hat{f}_i\,(2u_1,2u_2+1,2u_3) &= \sum_{x_3=0}^{N3-1}\sum_{x_2=0}^{N2-1}\sum_{x_1=0}^{N1-1} f\,(x_1,x_2,x_3)\,\omega_N^{<x,(2u_1,2u_2+1,2u_3)>} \\ &= 8\sum_{x_3=0}^{M3-1}\sum_{x_2=0}^{M2-1}\sum_{x_1=0}^{M1-1} f\,(x_1,x_2,x_3)\,\omega_M^{<x,u>}\,e^{-2\pi i\left(\frac{x_2}{N2}\right)} \end{aligned} \tag{42}$$

let

$$g_i\,(x_1,x_2,x_3) = f_i\,(x_1,x_2,x_3)\,e^{-2\pi i\left(\frac{x_2}{N2}\right)} \tag{43}$$

hence

$$\hat{f}_i\,(2u_1,2u_2+1,2u_3) = 8\sum_{x_3=0}^{M3-1}\sum_{x_2=0}^{M2-1}\sum_{x_1=0}^{M1-1} g_i\,(x_1,x_2,x_3)\,\omega_M^{<x,u>} \tag{44}$$

or

$$\hat{f}_i\,(2u_1,2u_2+1,2u_3) = 8\,\hat{g}_i\,(u_1,u_2,u_3) \qquad 0 \le u_j < M_j \qquad (45)$$

$$where\ i = 16\ ,\ 17,\ \dots\ ,\ 23\ \ and\ \ j = 1\ ,\ 2\ ,\ 3$$

In this case the function $g_i\,(x)$ is related to the original data $f_i\,(x)$ by the complex twiddle factor $e^{-2\pi i\left(\frac{x_2}{N2}\right)}$, which is one dimensional in the sense the it effects only the second variable (x_3) . Again note that only 1/8 of the initial data set is needed to compute the FT, and that the transform size is also 1/8 the original size.

Set $S_5 = \{f_{32}\,(x)\ ,\ \dots\ ,f_{39}\,(x)\}$. In this set translational symmetries t_2 *and* t_3 are positive while t_1 is negative. Therefore

$$f_i\,(x) = -f_i\,(t_1x) = f_i\,(t_2x) = f_i\,(t_3x) \qquad f_i\,(x) \in S_2 \qquad (46)$$

Applying these symmetry conditions to (20) and using Lemma 2 section (3.4) leads to

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_1+1}\,\hat{f}_i\,(y_1,y_2,y_3) \qquad (47)$$

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_2}\,\hat{f}_i\,(y_1,y_2,y_3)$$

$$\hat{f}_i\ (y_1,y_2,y_3) = (-1)^{y_3}\,\hat{f}_i\ (y_1,y_2,y_3) \tag{49}$$

Therefore $\hat{f}_i\ (y)$ is nonzero only when y_2 , y_3 , *are even,* y_1 *is odd* .

Let:

$$\begin{array}{ll} y_1 = 2u_1+1 & 0 \le u_1 < M1 \\ y_2 = 2u_2 & 0 \le u_2 < M2 \\ y_3 = 2u_3 & 0 \le u_3 < M3 \end{array}$$

Then applying these conditions to (20) leads to

$$\begin{aligned} \hat{f}_i\ (2u_1+1,2u_2,2u_3) &= \sum_{x_3=0}^{N3-1} \sum_{x_2=0}^{N2-1} \sum_{x_1=0}^{N1-1} f\ (x_1,x_2,x_3)\ \omega_N^{<x,(2u_1+1,2u_2,2u_3)>} \\ &= 8 \sum_{x_3=0}^{M3-1} \sum_{x_2=0}^{M2-1} \sum_{x_1=0}^{M1-1} f\ (x_1,x_2,x_3)\ \omega_M^{<x,u>}\ e^{-2\pi i\left(\frac{x_1}{N1}\right)} \end{aligned} \tag{50}$$

let

$$g_i\ (x_1,x_2,x_3) = f_i\ (x_1,x_2,x_3)\ e^{-2\pi i\left(\frac{x_1}{N1}\right)} \tag{51}$$

hence

$$\hat{f}_i\ (2u_1+1,2u_2,2u_3) = 8 \sum_{x_3=0}^{M3-1} \sum_{x_2=0}^{M2-1} \sum_{x_1=0}^{M1-1} g_i\ (x_1,x_2,x_3)\ \omega_M^{<x,u>} \tag{52}$$

or

$$\hat{f}_i\,(2u_1+1,2u_2,2u_3) = 8\,\hat{g}_i\,(u_1,u_2,u_3) \qquad 0 \le u_j < M_j \tag{53}$$

$$\textit{where } i = 32\ ,\ 33,\ \dots\ ,\ 39 \ \ \textit{and} \ \ j = 1\ ,\ 2\ ,\ 3$$

In the same way $g_i\,(x)$ is related to the original function $f_i\,(x)$ from (51) by the complex twiddle factor multiplication, $e^{-2\pi i\left(\frac{x_1}{N1}\right)}$. Again note that only 1/8 of the initial data set is needed to compute the FT, and that the transform size is also 1/8 the original size.

3.5.3.3. Two Dimensional Twiddle Factor

This group contains the following sets S_4 , S_6 , S_7 . Set $S_4 = \{f_{24}\,(x)\ ,\ \dots\ ,f_{31}\,(x)\}$. In this set translational symmetries t_2 *and* t_3 are negative while t_1 is positive. Therefore

$$f_i\,(x) = f_i\,(t_1 x) = -\,f_i\,(t_2 x) = -\,f_i\,(t_3 x) \qquad f_i\,(x) \in S_2 \tag{54}$$

Applying these symmetry conditions to (20) and using Lemma 2 section (3.4) leads to

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_1}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{55}$$

$$\hat{f}_i\,(y_1,y_2,y_3) \;=\; (-1)^{y_2+1}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{56}$$

$$\hat{f}_i\,(y_1,y_2,y_3) \;=\; (-1)^{y_3+1}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{57}$$

Therefore $\hat{f}_i\,(y)$ is nonzero only when y_2 , y_3 , *are odd,* y_1 *is even* .

Let:

$$\begin{array}{ll} y_1 = 2u_1 & 0 \le u_1 < M1 \\ y_2 = 2u_2+1 & 0 \le u_2 < M2 \\ y_3 = 2u_3+1 & 0 \le u_3 < M3 \end{array}$$

Then applying these conditions to (20) leads to

$$\begin{aligned} \hat{f}_i\,(2u_1,2u_2+1,2u_3+1) &= \sum_{x_3=0}^{N3-1}\sum_{x_2=0}^{N2-1}\sum_{x_1=0}^{N1-1} f\,(x_1,x_2,x_3)\;\omega_N^{<x,(2u_1,2u_2+1,2u_3+1)>} \\ &= 8\sum_{x_3=0}^{M3-1}\sum_{x_2=0}^{M2-1}\sum_{x_1=0}^{M1-1} f\,(x_1,x_2,x_3)\;\omega_M^{<x,u>}\;e^{-2\pi i\left(\frac{x_2}{N2}+\frac{x_3}{N3}\right)} \end{aligned} \tag{58}$$

let

$$g_i\,(x_1,x_2,x_3) \;=\; f_i\,(x_1,x_2,x_3)\;e^{-2\pi i\left(\frac{x_2}{N2}+\frac{x_3}{N3}\right)} \tag{59}$$

hence

$$\hat{f}_i\,(2u_1,2u_2+1,2u_3+1) = 8 \sum_{x_3=0}^{M3-1} \sum_{x_2=0}^{M2-1} \sum_{x_1=0}^{M1-1} g_i\,(x_1,x_2,x_3)\ \omega_M^{<x,u>} \qquad (60)$$

or

$$\hat{f}_i\,(2u_1,2u_2+1,2u_3+1) = 8\ \hat{g}_i\,(u_1,u_2,u_3) \qquad 0 \le u_j < M_j \qquad (61)$$
$$\textit{where } i = 24\ ,\ 25,\ \dots\ ,\ 31 \ \textit{ and } \ j = 1\ ,\ 2\ ,\ 3$$

From (59) we can see that the function $g_i\,(x)$ is related to the original function $f_i\,(x)$ by the complex twiddle factor multiplication, $e^{-2\pi i\left(\frac{x_2}{N2}+\frac{x_3}{N3}\right)}$. This is a two dimensional twiddle factor since it effects two variables $x_2\ ,\ x_3$. It is clear from g(x) that a computational reduction to 1/8 of the original size is achieved once again.

Set $S_6 = \{f_{40}\,(x)\ ,\ \dots\ ,f_{47}\,(x)\}$. In this set translational symmetries t_1 *and* t_3 are negative while t_2 is positive. Therefore

$$f_i\,(x) = -f_i\,(t_1x) = f_i\,(t_2x) = -f_i\,(t_3x) \qquad f_i\,(x) \in S_2 \qquad (62)$$

Applying these symmetry conditions to (20) and using Lemma 2 section (3.4) leads to

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_1+1}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{63}$$

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_2}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{64}$$

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_3+1}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{65}$$

Therefore $\hat{f}_i\,(y)$ is nonzero only when y_1 , y_3 , *are odd,* y_2 *is even* .

Let:

$$\begin{array}{lll} y_1 = 2u_1+1 & 0 \le u_1 < M1 \\ y_2 = 2u_2 & 0 \le u_2 < M2 \\ y_3 = 2u_3+1 & 0 \le u_3 < M3 \end{array}$$

Then applying these conditions to (20) leads to

$$\begin{aligned} \hat{f}_i\,(2u_1+1,2u_2,2u_3+1) &= \sum_{x_3=0}^{N3-1}\sum_{x_2=0}^{N2-1}\sum_{x_1=0}^{N1-1} f\,(x_1,x_2,x_3)\;\omega_N^{<x,(2u_1+1,2u_2,2u_3+1)>} \\ &= 8\sum_{x_3=0}^{M3-1}\sum_{x_2=0}^{M2-1}\sum_{x_1=0}^{M1-1} f\,(x_1,x_2,x_3)\;\omega_M^{<x,u>}\; e^{-2\pi i\left(\frac{x_1}{N1}+\frac{x_3}{N3}\right)} \end{aligned} \tag{66}$$

let

$$g_i\,(x_1,x_2,x_3) = f_i\,(x_1,x_2,x_3)\;e^{-2\pi i\left(\frac{x_1}{N1}+\frac{x_3}{N3}\right)} \tag{67}$$

hence

$$\hat{f}_i\,(2u_1+1,2u_2,2u_3+1) = 8 \sum_{x_3=0}^{M3-1} \sum_{x_2=0}^{M2-1} \sum_{x_1=0}^{M1-1} g_i\,(x_1,x_2,x_3)\ \omega_M^{<x,u>} \qquad (68)$$

or

$$\hat{f}_i\,(2u_1+1,2u_2,2u_3+1) = 8\ \hat{g}_i\,(u_1,u_2,u_3) \qquad 0 \le u_j < M_j \qquad (69)$$
$$\textit{where } i = 40\,,\,41,\,\dots\,,\,47 \ \textit{ and } \ j = 1\,,\,2\,,\,3$$

From (67) we can see that the function $g_i\,(x)$ is related to the original function $f_i\,(x)$ by the complex twiddle factor multiplication, $e^{-2\pi i\left(\frac{x_1}{N1}+\frac{x_3}{N3}\right)}$. This is a two dimensional twiddle factor since it effects two variables. It is clear from g(x) that a computational reduction to 1/8 of the original size is achieved once again.

Set $S_7 = \{f_{48}\,(x)\ ,\ \dots\ ,f_{55}\,(x)\,\}$. In this set translational symmetries t_1 *and* t_2 are negative while t_3 is positive. Therefore

$$f_i\,(x) = -\,f_i\,(t_1x) = -\,f_i\,(t_2x) = f_i\,(t_3x) \qquad f_i\,(x) \in S_2 \qquad (70)$$

Applying these symmetry conditions to (20) and using Lemma 2 section (3.4) leads to

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_1+1}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{71}$$

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_2+1}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{72}$$

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_3}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{73}$$

Therefore $\hat{f}_i\,(y)$ is nonzero only when y_1 , y_2 , *are odd,* y_3 *is even* .

Let:

$$\begin{aligned} y_1 &= 2u_1+1 & 0 \le u_1 < M1 \\ y_2 &= 2u_2+1 & 0 \le u_2 < M2 \\ y_3 &= 2u_3 & 0 \le u_3 < M3 \end{aligned}$$

Then applying these conditions to (20) leads to

$$\begin{aligned} \hat{f}_i\,(2u_1+1,2u_2+1,2u_3) &= \sum_{x_3=0}^{N3-1} \sum_{x_2=0}^{N2-1} \sum_{x_1=0}^{N1-1} f\,(x_1,x_2,x_3)\ \omega_N^{<x,(2u_1+1,2u_2+1,2u_3)>} \\ &= 8 \sum_{x_3=0}^{M3-1} \sum_{x_2=0}^{M2-1} \sum_{x_1=0}^{M1-1} f\,(x_1,x_2,x_3)\ \omega_M^{<x,u>}\ e^{-2\pi i\left(\frac{x_1}{N1}+\frac{x_2}{N2}\right)} \end{aligned} \tag{74}$$

let

$$g_i\,(x_1,x_2,x_3) = f_i\,(x_1,x_2,x_3)\ e^{-2\pi i\left(\frac{x_1}{N1}+\frac{x_2}{N2}\right)} \tag{75}$$

hence

$$\hat{f}_i\,(2u_1+1,2u_2+1,2u_3) \;=\; 8 \sum_{x_3=0}^{M3-1} \sum_{x_2=0}^{M2-1} \sum_{x_1=0}^{M1-1} g_i\,(x_1,x_2,x_3)\;\omega_M^{<x,u>} \tag{76}$$

or

$$\hat{f}_i\,(2u_1+1,2u_2+1,2u_3) \;=\; 8\;\hat{g}_i\,(u_1,u_2,u_3) \qquad 0 \le u_j < M_j \tag{77}$$

$$\textit{where } i = 48\;,\;49,\;\ldots\;,\;55 \quad \textit{and} \quad j = 1\;,\;2\;,\;3$$

It is clear from (75) that the function $g_i\,(x)$ is related to the original function $f_i\,(x)$ by the complex twiddle factor multiplication, $e^{-2\pi i\left(\frac{x_1}{N1}+\frac{x_2}{N2}\right)}$. This is a two dimensional twiddle factor since it effects two variables. It is clear from g(x) that a computational reduction to 1/8 of the original size is achieved once again.

3.5.3.4. Three Dimensional Twiddle Factor

This group contains only the set S_8. In this set the functions $\{\,f\,(t_1x)\;,f\,(t_2x)\;,f\,(t_3x)\,\}$ are all negative. Therefore

$$f_i\,(x) \;=\; -\,f_i\,(t_1x) \;=\; -\,f_i\,(t_2x) \;=\; -\,f_i\,(t_3x) \qquad f_i\,(x) \in S_2 \tag{78}$$

Applying these symmetry conditions to (20) and using Lemma 2 section (3.4) leads to

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_1+1}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{79}$$

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_2+1}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{80}$$

$$\hat{f}_i\,(y_1,y_2,y_3) = (-1)^{y_3+1}\,\hat{f}_i\,(y_1,y_2,y_3) \tag{81}$$

Therefore $\hat{f}_i\,(y)$ is nonzero only when y_1 , y_2 , y_3 ***are all odd*** .

Let:

$$\begin{aligned} y_1 &= 2u_1+1 \quad 0 \le u_1 < M1 \\ y_2 &= 2u_2+1 \quad 0 \le u_2 < M2 \\ y_3 &= 2u_3+1 \quad 0 \le u_3 < M3 \end{aligned}$$

Then applying these conditions to (20) leads to

$$\begin{aligned} \hat{f}_i\,(2u_1+1,2u_2+1,2u_3+1) &= \sum_{x_3=0}^{N3-1}\sum_{x_2=0}^{N2-1}\sum_{x_1=0}^{N1-1} f\,(x_1,x_2,x_3)\;\omega_N^{<x,(2u_1+1,2u_2+1,2u_3+1)>} \\ &= 8\sum_{x_3=0}^{M3-1}\sum_{x_2=0}^{M2-1}\sum_{x_1=0}^{M1-1} f\,(x_1,x_2,x_3)\;\omega_M^{<x,u>}\;e^{-2\pi i\left(\frac{x_1}{N1}+\frac{x_2}{N2}+\frac{x_3}{N3}\right)} \end{aligned} \tag{82}$$

let

$$g_i\,(x_1,x_2,x_3) = f_i\,(x_1,x_2,x_3)\; e^{-2\pi i\left(\frac{x_1}{N1}+\frac{x_2}{N2}+\frac{x_3}{N3}\right)} \qquad (83)$$

hence

$$\hat{f}_i\,(2u_1+1,2u_2+1,2u_3+1) = 8 \sum_{x_3=0}^{M3-1}\sum_{x_2=0}^{M2-1}\sum_{x_1=0}^{M1-1} g_i\,(x_1,x_2,x_3)\;\omega_M^{<x,u>} \qquad (84)$$

or

$$\hat{f}_i\,(2u_1+1,2u_2+1,2u_3+1) = 8\;\hat{g}_i\,(u_1,u_2,u_3) \qquad 0 \le u_j < M_j$$
$$\text{where } i = 56\;,\,57,\,\ldots\,,\,63 \;\text{ and }\; j = 1\;,\,2\;,\,3 \qquad (85)$$

From (83) we can see that the function $g_i\,(x)$ is related to the original function $f_i\,(x)$ by the complex twiddle factor multiplication, $e^{-2\pi i\left(\frac{x_1}{N1}+\frac{x_2}{N2}+\frac{x_3}{N3}\right)}$. This is a three dimensional twiddle factor since it effects three variables. It is clear from g(x) that a computational reduction to 1/8 of the original size can be achieved.

3.5.4. Real Twiddle Factors

The previous section clearly shows that the periodization and decimation algorithm, in general, introduces complex twiddle factors into the Fourier transform computation. In this section we will show that in special cases the twiddle factor can be reduced into a real factor, requiring real multiplications only. Consider the finite function $f(x_1,x_2,x_3)$, $f \in L(N)$, $x_1,x_2,x_3, \in Z/N1 \times Z/N2 \times Z/N3$. Let

$$M1 = \frac{N1}{2} , M2 = \frac{N2}{2} , M3 = \frac{N3}{2} , \qquad M1 , M2 , M3 , \text{ are odd} \tag{86}$$

From section (3.5.5) we sow that the Fourier transform computation of f can be obtained by computing the FT of the 64 periodic functions f_0 , *through* , f_{63} , which we divided into eight sets. We then used the translational symmetries and were able to reduce the FT computation to be that of the 64 functions g_0 *through* , g_{63} , which are defined on $M1 \times M2 \times M3$ or 1/8 the original function f(x).

(1) $g_i(x) = f_i(x) \quad i=0,...,7$

(2) $g_i(x) = f_i(x)\, e^{-2\pi i \left(\frac{x_3}{N3}\right)} \quad i=8,...,15$

(3) $g_i(x) = f_i(x)\, e^{-2\pi i \left(\frac{x_2}{N2}\right)} \quad i=16,...,23$

(4) $g_i(x) = f_i(x)\, e^{-2\pi i \left(\frac{x_2}{N2}+\frac{x_3}{N3}\right)} \quad i=24,...,31$

(5) $g_i(x) = f_i(x)\, e^{-2\pi i \left(\frac{x_1}{N1}\right)} \quad i=32,...,39$

(6) $g_i(x) = f_i(x)\, e^{-2\pi i\left(\frac{x_1}{N1}+\frac{x_3}{N3}\right)}$ i=40,...,47

(7) $g_i(x) = f_i(x)\, e^{-2\pi i\left(\frac{x_1}{N1}+\frac{x_2}{N2}\right)}$ i=48,...,55

(8) $g_i(x) = f_i(x)\, e^{-2\pi i\left(\frac{x_1}{N1}+\frac{x_2}{N2}+\frac{x_3}{N3}\right)}$ i=56,...,63

Let

$$M1' = \frac{M1-1}{2} \tag{87}$$

$$M2' = \frac{M2-1}{2} \tag{88}$$

$$M3' = \frac{M3-1}{2} \tag{89}$$

In the first set there are no twiddle factors. Let

$$h_i(x_1,x_2,x_3) = g_i(x_1,x_2,x_3) \tag{90}$$

then

$$h_i\ (x_1,x_2,x_3)\ = f_i\ (x_1,x_2,x_3) \qquad i = 0\ , \ldots ,\ 7 \tag{91}$$

In the second set there is a one dimensional twiddle factor. Let

$$h_i\ (x_1,x_2,x_3)\ = g_i\ (x_1,x_2,x_3)\ e^{-2\pi i \left(\frac{M3'}{M3} x_3\right)} \tag{92}$$

then from equation (35), section (3.5) we get

$$h_i\ (x_1,x_2,x_3)\ = f_i\ (x_1,x_2,x_3)\ (-1)^{x_3} \qquad i = 8\ , \ldots ,\ 15 \tag{93}$$

In the third set there is a one dimensional twiddle factor. Let

$$h_i\ (x_1,x_2,x_3)\ = g_i\ (x_1,x_2,x_3)\ e^{-2\pi i \left(\frac{M2'}{M2} x_2\right)} \tag{94}$$

then from equation (43), section (3.5) we get

$$h_i\ (x_1,x_2,x_3)\ = f_i\ (x_1,x_2,x_3)\ (-1)^{x_2} \qquad i = 16\ , \ldots ,\ 23 \tag{93}$$

In the fourth set there is a two dimensional twiddle factor. Let

$$h_i\ (x_1,x_2,x_3)\ = g_i\ (x_1,x_2,x_3)\ e^{-2\pi i \left(\frac{M2'}{M2} x_2 + \frac{M3'}{M3} x_3\right)} \tag{94}$$

then from equation (59), section (3.5) we get

$$h_i(x_1,x_2,x_3) = f_i(x_1,x_2,x_3)\,(-1)^{x_2+x_3} \qquad i = 24, \ldots, 31 \tag{95}$$

In the fifth set there is a one dimensional twiddle factor. Let

$$h_i(x_1,x_2,x_3) = g_i(x_1,x_2,x_3)\, e^{-2\pi i\left(\frac{M1'}{M1}x_1\right)} \tag{96}$$

then from equation (51), section (3.5) we get

$$h_i(x_1,x_2,x_3) = f_i(x_1,x_2,x_3)\,(-1)^{x_1} \qquad i = 32, \ldots, 39 \tag{97}$$

In the sixth set there is a two dimensional twiddle factor. Let

$$h_i(x_1,x_2,x_3) = g_i(x_1,x_2,x_3)\, e^{-2\pi i\left(\frac{M1'}{M1}x_1 + \frac{M3'}{M3}x_3\right)} \tag{98}$$

then from equation (67), section (3.5) we get

$$h_i(x_1,x_2,x_3) = f_i(x_1,x_2,x_3)\,(-1)^{x_1+x_3} \qquad i = 40, \ldots, 47 \tag{99}$$

In the seventh set there is a two dimensional twiddle factor. Let

$$h_i(x_1,x_2,x_3) = g_i(x_1,x_2,x_3)\, e^{-2\pi i\left(\frac{M1'}{M1}x_1 + \frac{M2'}{M2}x_2\right)} \tag{100}$$

then from equation (75), section (3.5) we get

$$h_i\,(x_1,x_2,x_3) = f_i\,(x_1,x_2,x_3)\,(-1)^{x_1+x_2} \qquad i = 48\,,\,\ldots\,,\,55 \tag{101}$$

In the eighth set there is a three dimensional twiddle factor. Let

$$h_i\,(x_1,x_2,x_3) = g_i\,(x_1,x_2,x_3)\,e^{-2\pi i\left(\frac{M1'}{M1}x_1+\frac{M2'}{M2}x_2+\frac{M3'}{M3}x_3\right)}$$

then from equation (83), section (3.5) we get

$$h_i\,(x_1,x_2,x_3) = f_i\,(x_1,x_2,x_3)\,(-1)^{x_1+x_2+x_3} \qquad i = 56\,,\,\ldots\,,\,63 \tag{103}$$

3.5.5. Fourier Transform Computation

In this section we will examine the Fourier transform computation of the 64 functions that we obtained from the periodization and decimation algorithm. We will continue to use the same eight sets established before. The results of the pervious sections lead to the following equations

1. $\hat{f}_i\,(2y_1,2y_2,2y_3) = 8\,\hat{h}_i\,(y_1,y_2,y_3) \qquad i = 0,\ldots,7$

2. $\hat{f}_i\,(2y_1,2y_2,2y_3+1) = 8\,\hat{h}_i\,(y_1,y_2,y_3-M3') \qquad i = 8,\ldots,15$

3. $\hat{f}_i\,(2y_1, 2y_2+1, 2y_3) = 8\,\hat{h}_i\,(y_1, y_2-M2', y_3)$
$i = 16,\ldots,23$

4. $\hat{f}_i\,(2y_1, 2y_2+1, 2y_3+1) = 8\,\hat{h}_i\,(y_1, y_2-M2', y_3-M3')$
$i = 24,\ldots,31$

5. $\hat{f}_i\,(2y_1+1, 2y_2, 2y_3) = 8\,\hat{h}_i\,(y_1-M1', y_2, y_3)$
$i = 32,\ldots,39$

6. $\hat{f}_i\,(2y_1+1, 2y_2, 2y_3+1) = 8\,\hat{h}_i\,(y_1-M1', y_2, y_3-M3')$
$i = 40,\ldots,47$

7. $\hat{f}_i\,(2y_1+1, 2y_2+1, 2y_3) = 8\,\hat{h}_i\,(y_1-M1', y_2-M2', y_3)$
$i = 48,\ldots,55$

8. $\hat{f}_i\,(2y_1+1, 2y_2+1, 2y_3+1) = 8\,\hat{h}_i\,(y_1-M1', y_2-M2', y_3-M3')$
$i = 56,\ldots,63$

The Fourier transform of the original data can now be obtained by computing the FT of the 64 functions $h_0\,(x)$, *through* $h_{63}\,(x)$. If the input data is real which is the case in crystallography, then from the above equations it is clear that the functions $h_0\,(x)$, *through* $h_{63}\,(x)$ are also real. Moreover these functions respect the rotational symmetries. Using Lemmas 4, 4.1, 4.2 and from the fact these functions are real and either symmetric or antisymmetric, we conclude that the Fourier transformed functions

$\hat{h}_0\ (y)$, *through* $\hat{h}_{63}\ (y)$ are either pure-real or pure-imaginary and also respect the same rotational symmetries. As a result a reduction of the computational complexity by 3/4, compared to complex data, is obtained. Note that the above 64 computations are completely independent and can be carried out in parallel once the initial input data is periodized with the respect to the super group X.

4 IMPLEMENTATION

4.1. Introduction

The periodization and decimation algorithm was designed in the previous chapter. In designing the algorithm several important issues were considered, such as computational complexity, data flow, memory space and management, efficiency, speed and programming ease. In this chapter we will discuss several implementation examples and show the advantages gained by using the algorithm. An important step in the algorithm design is choosing the super group X. In chapter 3, the group X was chosen for two reasons. First the G-invariant computations immediately reduce to a small collection of simple, nonredundant one dimensional routines. Second it is large enough to contain a significant number of crystallographic groups. The periodization and decimation algorithm of chapter 3 using the super group X provides algorithms for 80 crystallographic FFT's, which include both the Monoclinic and the Orthorhomblic groups. The first step in the algorithm is to periodize the input data with respect to the super group X. This is a preprocessing step which has to be computed only one time, at the beginning of the code. This step will lead to 64 totally independent computations which can be executed in parallel. The second step in the algorithm is to compute the twiddle factors. Coupled with the fact that the input data is real this step reduces the computational complexity, of each of the 64 invariant functions, to 1/64 that of the initial data. Moreover the Fourier transform computation of these functions remain real at all times. For crystallographic data which is invariant under the action of a given group Y, if Y is a subgroup of X , then the invariance of the data under Y disables a part of the based on the group X. Several key computational and implementation advantages are gained by using the algorithm, such as

1. **Computational complexity** : The algorithm leads to 64 computations each is 1/64 the original data complexity. Hence the complexity is reserved, and no additional arithmetic cost is required.

2. **Memory space and management** : In crystallographic applications, the computation of the Fourier transform and its inverse is a major part of the over all cost of the procedure. Typically, these procedures are iterative, requiring thousands of three dimensional FFT computations on data sets containing millions of points. The reduction of the FT computation to 1/64 that of the input data significantly reduces the memory requirements. Not only does it result in high savings of memory space but also it significantly reduces page defaults, leading to high gains in speed and performance.

3. **Data flow** : It is evident from the algorithm that once the preprocessing step is completed no inertprocessor communication is required. Moreover the big reduction in page defaults and memory allocation, lead to a simple and highly efficient data flow.

4. **Efficiency and speed** : The G-invariant computations immediately reduce to simple and highly efficient one dimensional routines. The elimination of all nonredundant calculations, the improvement in memory requirements and data flow performance, along with the ability to run all of these computations in parallel; lead to optimal results in speed and efficiency.

5. **Programming ease** : The periodization and decimation algorithm described in chapter 3 provides algorithms for 80 crystallographic FFT's. Previously this effort required 80 different programs. In this case only one program covers 80 crystallographic groups, the invariance of data under each group disables a part of the program. This means that only a subset of the 64 computations have to be carried out, while the rest will be idle.

4.2. $P2$

In this section will show implementation of a particular crystallographic group $P2$ using the periodization and decimation algorithm. We will use the notation of International Tables for X-ray Crystallography, volume I, 1952 for space groups. $P2$ respects the following symmetry conditions :

1. $f(x) = f(Ax) = f(N1 - x_1, x_2, N3 - x_3)$

This symmetry condition can be expressed in the matrix form

$$A = R\,x + T \tag{1}$$

where

$$A = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x \tag{2}$$

This group has a two-fold symmetry therefore it has order 2 and since the super group X has order 64, therefore the dual of this group has order 32. Denote $p2$ by Y and its dual by $Y^{\perp}$. Then from the preceding chapter, we need only to compute the FFT of these functions that belong to $Y^{\perp}$, the rest of the functions will vanish. In this example only the following 32 functions belong to $Y^{\perp}$:

1. From $S_1 : \{ f_0 , f_2 , f_5 , f_7 \}$
2. From $S_2 : \{ f_8 , f_{10} , f_{13} , f_{15} \}$
3. From $S_3 : \{ f_{16} , f_{18} , f_{21} , f_{23} \}$
4. From $S_4 : \{ f_{24} , f_{26} , f_{29} , f_{31} \}$
5. From $S_5 : \{ f_{32} , f_{34} , f_{37} , f_{39} \}$
6. From $S_6 : \{ f_{40} , f_{42} , f_{45} , f_{47} \}$

7. From S_7 : { f_{48} , f_{50} , f_{53} , f_{55} }

8. From S_8 : { f_{56} , f_{58} , f_{61} , f_{63} }

4.3. $P2_1$

$P2_1$ respects the following symmetry conditions :

1. $f(x) = f(Ax) = f(N1 - x_1 , M2 + x_2 , N3 - x_3)$

This symmetry condition can be expressed in the matrix form

$$A = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} 0 \\ M2 \\ 0 \end{bmatrix} \qquad (3)$$

This group has a two-fold symmetry therefore it has order 2 and since the super group X has order 64, therefore the dual of this group has order 32. Denote $P2_1$ by Y and its dual by $Y^{\perp}$. Then from the preceding chapter, we need only to compute the FFT of these functions that belong to $Y^{\perp}$, the rest of the functions will vanish. In this example only the following 32 functions belong to $Y^{\perp}$:

1. From S_1 : $\{ f_0 , f_2 , f_5 , f_7 \}$

2. From S_2 : $\{ f_8 , f_{10} , f_{13} , f_{15} \}$

3. From S_3 : $\{ f_{17} , f_{19} , f_{20} , f_{22} \}$

4. From S_4 : $\{ f_{25} , f_{27} , f_{28} , f_{30} \}$

5. From S_5 : $\{ f_{32} , f_{34} , f_{37} , f_{39} \}$

6. From S_6 : $\{ f_{40} , f_{42} , f_{45} , f_{47} \}$

7. From S_7 : $\{ f_{49} , f_{51} , f_{52} , f_{54} \}$

8. From S_8 : $\{ f_{57} , f_{59} , f_{60} , f_{62} \}$

4.4. *B2*

B2 respects the following symmetry conditions :

1. $f(x) = f(Ax) = f(N1 - x_1 , N2 - x_2 , x_3)$

This symmetry condition can be expressed in the matrix form

$$A = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x \qquad (4)$$

This group has a two-fold symmetry therefore it has order 2 and since the super group X has order 64, therefore the dual of this group has order 32. Denote $B2$ by Y and its dual by $Y^{\perp}$. Then from the preceding chapter, we need only to compute the FFT of these functions that belong to $Y^{\perp}$, the rest of the functions will vanish. In this example only the following 32 functions belong to $Y^{\perp}$:

1. From S_1 : $\{ f_0 , f_1 , f_6 , f_7 \}$
2. From S_2 : $\{ f_8 , f_9 , f_{14} , f_{15} \}$
3. From S_3 : $\{ f_{16} , f_{17} , f_{22} , f_{23} \}$
4. From S_4 : $\{ f_{24} , f_{25} , f_{30} , f_{31} \}$
5. From S_5 : $\{ f_{32} , f_{33} , f_{38} , f_{39} \}$
6. From S_6 : $\{ f_{40} , f_{41} , f_{46} , f_{47} \}$
7. From S_7 : $\{ f_{48} , f_{49} , f_{54} , f_{55} \}$
8. From S_8 : $\{ f_{56} , f_{57} , f_{62} , f_{63} \}$

4.5. $C2$

$C2$ respects the following symmetry conditions :

1. $f(x) = f(Ax) = f(N1 - x_1, x_2, N3 - x_3)$

This symmetry condition can be expressed in the matrix form

$$A = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x$$

This group has a two-fold symmetry therefore it has order 2 and since the super group X has order 64, therefore the dual of this group has order 32. Denote $C2$ by Y and its dual by $Y^{\perp}$. Then from the preceding chapter, we need only to compute the FFT of these functions that belong to $Y^{\perp}$, the rest of the functions will vanish. In this example only the following 32 functions belong to $Y^{\perp}$:

1. From S_1 : { f_0 , f_2 , f_5 , f_7 }
2. From S_2 : { f_8 , f_{10} , f_{13} , f_{15} }
3. From S_3 : { f_{16} , f_{18} , f_{21} , f_{23} }

4. From S_4 : { f_{24} , f_{26} , f_{29} , f_{31} }

5. From S_5 : { f_{32} , f_{34} , f_{37} , f_{39} }

6. From S_6 : { f_{40} , f_{42} , f_{45} , f_{47} }

7. From S_7 : { f_{48} , f_{50} , f_{53} , f_{55} }

8. From S_8 : { f_{56} , f_{58} , f_{61} , f_{63} }

4.6. *Pm*

Pm respects the following symmetry conditions :

1. $f(x) = f(Ax) = f(x_1 , N2 - x_2 , x_3)$

This symmetry condition can be expressed in the matrix form

$$A = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x \qquad (6)$$

This group has a two-fold symmetry therefore it has order 2 and since the super group X has order 64, therefore the dual of this group has order 32. Denote *Pm* by Y and its dual by $Y^{\perp}$. Then from the preceding chapter, we need only to compute the FFT of these functions that belong to $Y^{\perp}$, the rest of the functions will vanish. In this example only the following 32 functions belong to $Y^{\perp}$:

1. From S_1 : $\{ f_0 , f_1 , f_4 , f_5 \}$
2. From S_2 : $\{ f_8 , f_9 , f_{12} , f_{13} \}$
3. From S_3 : $\{ f_{16} , f_{17} , f_{20} , f_{21} \}$
4. From S_4 : $\{ f_{24} , f_{25} , f_{28} , f_{29} \}$
5. From S_5 : $\{ f_{32} , f_{33} , f_{36} , f_{37} \}$
6. From S_6 : $\{ f_{40} , f_{41} , f_{44} , f_{45} \}$
7. From S_7 : $\{ f_{48} , f_{49} , f_{52} , f_{53} \}$
8. From S_8 : $\{ f_{56} , f_{57} , f_{60} , f_{61} \}$

4.7. *Pb*

Pb respects the following symmetry conditions :

1. $f(x) = f(Ax) = f(x_1 , M2 + x_2 , N3 - x_3)$

This symmetry condition can be expressed in the matrix form

$$A = \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} 0 \\ M2 \\ 0 \end{bmatrix} \qquad (7)$$

This group has a two-fold symmetry therefore it has order 2 and since the super group X has order 64, therefore the dual of this group has order 32. Denote Pb by Y and its dual by $Y^{\perp}$. Then from the preceding chapter, we need only to compute the FFT of these functions that belong to $Y^{\perp}$, the rest of the functions will vanish. In this example only the following 32 functions belong to $Y^{\perp}$:

1. From S_1 : $\{ f_0 , f_2 , f_4 , f_6 \}$
2. From S_2 : $\{ f_8 , f_{10} , f_{12} , f_{14} \}$
3. From S_3 : $\{ f_{17} , f_{19} , f_{21} , f_{23} \}$
4. From S_4 : $\{ f_{25} , f_{27} , f_{29} , f_{31} \}$
5. From S_5 : $\{ f_{32} , f_{34} , f_{36} , f_{38} \}$
6. From S_6 : $\{ f_{40} , f_{42} , f_{44} , f_{46} \}$
7. From S_7 : $\{ f_{49} , f_{51} , f_{53} , f_{55} \}$
8. From S_8 : $\{ f_{57} , f_{59} , f_{61} , f_{63} \}$

4.8. *Pc*

Pc respects the following symmetry conditions :

1. $f(x) = f(Ax) = f(x_1, N2 - x_2, M3 + x_3)$

This symmetry condition can be expressed in the matrix form

$$A = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} 0 \\ 0 \\ M3 \end{bmatrix} \qquad (8)$$

This group has a two-fold symmetry therefore it has order 2 and since the super group X has order 64, therefore the dual of this group has order 32. Denote *Pc* by Y and its dual by $Y^{\perp}$. Then from the preceding chapter, we need only to compute the FFT of these functions that belong to $Y^{\perp}$, the rest of the functions will vanish. In this example only the following 32 functions belong to $Y^{\perp}$:

1. From S_1 : { f_0 , f_1 , f_4 , f_5 }

2. From S_2 : { f_{10} , f_{11} , f_{14} , f_{15} }

3. From S_3 : { f_{16} , f_{17} , f_{20} , f_{21} }

4. From S_4 : { f_{26} , f_{27} , f_{30} , f_{31} }

5. From S_5 : { f_{32} , f_{33} , f_{36} , f_{37} }

6. From S_6 : { f_{42} , f_{43} , f_{46} , f_{47} }

7. From S_7 : { f_{48} , f_{49} , f_{52} , f_{53} }

8. From S_8 : { f_{58} , f_{59} , f_{62} , f_{63} }

In addition there are four more monoclinic crystallographic groups of order two which the above algorithm includes. These groups are Bm, Cm, Bb, Cc.

4.9. $P2/m$

$P2/m$ respects the following symmetry conditions :

1. $f(x) = f(A1\,x) = f(x_1\,,\, N2 - x_2\,,\, x_3)$
2. $f(x) = f(A2\,x) = f(N1 - x_1\,,\, x_2\,,\, N3 - x_3)$
3. $f(x) = f(A3\,x) = f(N1 - x_1\,,\, N2 - x_2\,,\, N3 - x_3)$

This group has a 4-fold symmetry, therefore the order of this group is 4. These conditions can be expressed in the matrix form

$$A1 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x \tag{9}$$

$$A2 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x \tag{10}$$

$$A3 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \tag{11}$$

This group has order 4, and since $P2/m \subset X$ which has order 64, therefore the dual of $P2/m$ has order 16. Denote $P2/m$ by Y and its dual by $Y^{\perp}$. From the results of the preceding chapter, we need only to compute the FFT of these functions which belong to $Y^{\perp}$, the rest of the functions will vanish. In this case only the following 16 functions are in $Y^{\perp}$:

1. From S_1 : $\{ f_0(x), f_5(x) \}$
2. From S_2 : $\{ f_8(x), f_{13}(x) \}$
3. From S_3 : $\{ f_{16}(x), f_{21}(x) \}$

4. From S_4 : { $f_{24}(x)$, $f_{29}(x)$ }

5. From S_5 : { $f_{32}(x)$, $f_{37}(x)$ }

6. From S_6 : { $f_{40}(x)$, $f_{45}(x)$ }

7. From S_7 : { $f_{48}(x)$, $f_{53}(x)$ }

8. From S_8 : { $f_{56}(x)$, $f_{61}(x)$ }

4.10. $C2/c$

$C2/c$ respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(N1 - x_1, N2 - x_2, N3 - x_3)$

2. $f(x) = f(A2x) = f(N1 - x_1, x_2, M3 - x_3)$

3. $f(x) = f(A3x) = f(x_1, N2 - x_2, M3 + x_3)$

This group has a 4-fold symmetry, therefore the order of this group is 4. These conditions can be expressed in the matrix form

$$A1 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \tag{12}$$

$$A2 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} 0 \\ 0 \\ M3 \end{bmatrix} \tag{13}$$

$$A3 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} 0 \\ 0 \\ M3 \end{bmatrix} \tag{14}$$

This group has order 4, and since $C2/c \subset X$ which has order 64, therefore the dual of $C2/c$ has order 16. Denote $C2/c$ by Y and its dual by $Y^{\perp}$. From the results of the preceding chapter, we need only to compute the FFT of these functions which belong to $Y^{\perp}$, the rest of the functions will vanish. In this case only the following 16 functions are in $Y^{\perp}$:

1. From S_1 : $\{ f_0(x), f_5(x) \}$
2. From S_2 : $\{ f_{11}(x), f_{14}(x) \}$
3. From S_3 : $\{ f_{16}(x), f_{21}(x) \}$
4. From S_4 : $\{ f_{27}(x), f_{30}(x) \}$
5. From S_5 : $\{ f_{32}(x), f_{37}(x) \}$

6. From S_6 : { $f_{43}(x)$, $f_{46}(x)$ }

7. From S_7 : { $f_{48}(x)$, $f_{53}(x)$ }

8. From S_8 : { $f_{59}(x)$, $f_{62}(x)$ }

4.11. $B2/m$

$B2/m$ respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(x_1, x_2, N3 - x_3)$

2. $f(x) = f(A2x) = f(N1 - x_1, N2 - x_2, x_3)$

3. $f(x) = f(A3x) = f(N1 - x_1, N2 - x_2, N3 - x_3)$

This group has a 4-fold symmetry, therefore the order of this group is 4. These conditions can be expressed in the matrix form

$$A1 = \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x \tag{15}$$

$$A2 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x \qquad (16)$$

$$A3 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \qquad (17)$$

This group has order 4, and since $B2/m \subset X$ which has order 64, therefore the dual of $B2/m$ has order 16. Denote $B2/m$ by Y and its dual by $Y^{\perp}$. From the results of the preceding chapter, we need only to compute the FFT of these functions which belong to $Y^{\perp}$, the rest of the functions will vanish. In this case only the following 16 functions are in $Y^{\perp}$:

1. From S_1 : $\{ f_0(x), f_6(x) \}$

2. From S_2 : $\{ f_8(x), f_{14}(x) \}$

3. From S_3 : $\{ f_{16}(x), f_{22}(x) \}$

4. From S_4 : $\{ f_{24}(x), f_{30}(x) \}$

5. From S_5 : $\{ f_{32}(x), f_{38}(x) \}$

6. From S_6 : $\{ f_{40}(x), f_{46}(x) \}$

7. From S_7 : $\{ f_{48}(x), f_{54}(x) \}$

8. From S_8 : { $f_{56}(x)$, $f_{62}(x)$ }

4.12. *P2/b*

P2/b respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(N1 - x_1, N2 - x_2, N3 - x_3)$

2. $f(x) = f(A2x) = f(N1 - x_1, M2 - x_2, x_3)$

3. $f(x) = f(A3x) = f(x_1, M2 + x_2, N3 - x_3)$

This group has a 4-fold symmetry, therefore the order of this group is 4. These conditions can be expressed in the matrix form

$$A1 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \tag{18}$$

$$A2 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} 0 \\ M2 \\ 0 \end{bmatrix} \tag{19}$$

$$A3 = \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} 0 \\ M2 \\ 0 \end{bmatrix} \tag{20}$$

This group has order 4, and since $P2/b \subset X$ which has order 64, therefore the dual of $P2/b$ has order 16. Denote $P2/b$ by Y and its dual by $Y^{\perp}$. From the results of the preceding chapter, we need only to compute the FFT of these functions which belong to $Y^{\perp}$, the rest of the functions will vanish. In this case only the following 16 functions are in $Y^{\perp}$:

1. From S_1 : { $f_0(x)$, $f_6(x)$ }
2. From S_2 : { $f_8(x)$, $f_{14}(x)$ }
3. From S_3 : { $f_{19}(x)$, $f_{21}(x)$ }
4. From S_4 : { $f_{27}(x)$, $f_{29}(x)$ }
5. From S_5 : { $f_{32}(x)$, $f_{38}(x)$ }
6. From S_6 : { $f_{40}(x)$, $f_{46}(x)$ }
7. From S_7 : { $f_{51}(x)$, $f_{53}(x)$ }
8. From S_8 : { $f_{59}(x)$, $f_{61}(x)$ }

In addition there are six more monoclinic crystallographic groups of order four which the above algorithm includes. These groups are $P2_1/m$, C2/m, P2/c, $P2_1/b$, $P2_1/c$, B2/b, C2/c. Therefore there is a total of 22 monoclinic groups included.

4.13. $P2_12_12_1$

$P2_12_12_1$ respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(M1 + x_1, M2 - x_2, N3 - x_3)$
2. $f(x) = f(A2x) = f(M1 - x_1, N2 - x_2, M3 + x_3)$
3. $f(x) = f(A3x) = f(N1 - x_1, M2 + x_2, M3 - x_3)$

This group has a 4-fold symmetry, therefore the order of this group is 4. These conditions can be expressed in the matrix form

$$A1 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} M1 \\ M2 \\ 0 \end{bmatrix} \qquad (21)$$

$$A2 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} M1 \\ 0 \\ M3 \end{bmatrix} \qquad (22)$$

$$A3 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} 0 \\ M2 \\ M3 \end{bmatrix} \qquad (23)$$

This group has order 4, and since $P2_12_12_1 \subset X$ which has order 64, therefore the dual of $P2_12_12_1$ has order 16. Denote $P2_12_12_1$ by Y and its dual by $Y^\perp$. From the results of the preceding chapter, we need only to compute the FFT of these functions which belong to $Y^\perp$, the rest of the functions will vanish. In this case only the following 16 functions are in $Y^\perp$:

1. From S_1 : $\{ f_0(x), f_7(x) \}$
2. From S_2 : $\{ f_{11}(x), f_{12}(x) \}$
3. From S_3 : $\{ f_{17}(x), f_{22}(x) \}$
4. From S_4 : $\{ f_{26}(x), f_{29}(x) \}$
5. From S_5 : $\{ f_{34}(x), f_{37}(x) \}$
6. From S_6 : $\{ f_{41}(x), f_{46}(x) \}$

7. From S_7 : { $f_{51}(x)$, $f_{52}(x)$ }

8. From S_8 : { $f_{56}(x)$, $f_{63}(x)$ }

4.14. $F222$

$F222$ respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(N1 - x_1, N2 - x_2, x_3)$

2. $f(x) = f(A2x) = f(x_1, N2 - x_2, N3 - x_3)$

3. $f(x) = f(A3x) = f(N1 - x_1, x_2, N3 - x_3)$

This group has a 4-fold symmetry, therefore the order of this group is 4. These conditions can be expressed in the matrix form

$$A1 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x \tag{24}$$

$$A2 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \tag{25}$$

$$A3 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x \tag{26}$$

This group has order 4, and since $F222 \subset X$ which has order 64, therefore the dual of $F222$ has order 16. Denote $F222$ by Y and its dual by $Y^{\perp}$. From the results of the preceding chapter, we need only to compute the FFT of these functions which belong to $Y^{\perp}$, the rest of the functions will vanish. In this case only the following 16 functions are in $Y^{\perp}$:

1. From S_1 : $\{ f_0(x), f_7(x) \}$
2. From S_2 : $\{ f_8(x), f_{15}(x) \}$
3. From S_3 : $\{ f_{16}(x), f_{23}(x) \}$
4. From S_4 : $\{ f_{24}(x), f_{31}(x) \}$
5. From S_5 : $\{ f_{32}(x), f_{39}(x) \}$
6. From S_6 : $\{ f_{40}(x), f_{47}(x) \}$
7. From S_7 : $\{ f_{48}(x), f_{55}(x) \}$

8. From S_8 : { $f_{56}(x)$, $f_{63}(x)$ }

4.15. $Pna2_1$

$Pna2_1$ respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(N1 - x_1, N2 - x_2, M3 + x_3)$

2. $f(x) = f(A2x) = f(M1 - x_1, M2 + x_2, M3 + x_3)$

3. $f(x) = f(A3x) = f(M1 + x_1, M2 - x_2, x_3)$

This group has a 4-fold symmetry, therefore the order of this group is 4. These conditions can be expressed in the matrix form

$$A1 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} 0 \\ 0 \\ M3 \end{bmatrix} \qquad (27)$$

$$A2 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} M1 \\ M2 \\ M3 \end{bmatrix} \qquad (28)$$

$$A3 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} M1 \\ M2 \\ 0 \end{bmatrix} \tag{29}$$

This group has order 4, and since $Pna2_1 \subset X$ which has order 64, therefore the dual of $Pna2_1$ has order 16. Denote $Pna2_1$ by Y and its dual by $Y^{\perp}$. From the results of the preceding chapter, we need only to compute the FFT of these functions which belong to $Y^{\perp}$, the rest of the functions will vanish. In this case only the following 16 functions are in $Y^{\perp}$:

1. From S_1 : { $f_0(x)$, $f_1(x)$ }
2. From S_2 : { $f_{12}(x)$, $f_{13}(x)$ }
3. From S_3 : { $f_{22}(x)$, $f_{23}(x)$ }
4. From S_4 : { $f_{26}(x)$, $f_{27}(x)$ }
5. From S_5 : { $f_{38}(x)$, $f_{39}(x)$ }
6. From S_6 : { $f_{42}(x)$, $f_{43}(x)$ }
7. From S_7 : { $f_{48}(x)$, $f_{49}(x)$ }
8. From S_8 : { $f_{60}(x)$, $f_{61}(x)$ }

4.16. *Amm2*

Amm2 respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(N1 - x_1, N2 - x_2, x_3)$

2. $f(x) = f(A2x) = f(N1 - x_1, x_2, x_3)$

3. $f(x) = f(A3x) = f(x_1, N2 - x_2, x_3)$

This group has a 4-fold symmetry, therefore the order of this group is 4. These conditions can be expressed in the matrix form

$$A1 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x \tag{30}$$

$$A2 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & 1 \end{bmatrix} x \tag{31}$$

$$A3 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x \tag{32}$$

This group has order 4, and since $Amm2 \subset X$ which has order 64, therefore the dual of $Amm2$ has order 16. Denote $Amm2$ by Y and its dual by $Y^{\perp}$. From the results of the preceding chapter, we need only to compute the FFT of these functions which belong to $Y^{\perp}$, the rest of the functions will vanish. In this case only the following 16 functions are in $Y^{\perp}$:

1. From S_1 : $\{ f_0(x), f_1(x) \}$
2. From S_2 : $\{ f_8(x), f_9(x) \}$
3. From S_3 : $\{ f_{16}(x), f_{17}(x) \}$
4. From S_4 : $\{ f_{24}(x), f_{25}(x) \}$
5. From S_5 : $\{ f_{32}(x), f_{33}(x) \}$
6. From S_6 : $\{ f_{40}(x), f_{41}(x) \}$
7. From S_7 : $\{ f_{48}(x), f_{49}(x) \}$
8. From S_8 : $\{ f_{56}(x), f_{57}(x) \}$

In addition there are 26 more Orthorhombic crystallographic groups of order four which the above algorithm includes. These groups are P222, P222$_1$, P2$_1$2$_1$2, C222$_1$, C222, I222,

$I2_12_12_1$, Pmm2, $Pmc2_1$, Pcc2, Pma2, $Pca2_1$, Pnc2, $Pmn2_1$, Pba2, $Pna2_1$, Pnn2, Cmm2, $Cmc2_1$, Ccc2, Abm2, Ama2, Aba2, Fmm2, Imm2, Iba2, Ima2.

4.17. *Pmmm*

Pmmm respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(N1 - x_1, N2 - x_2, x_3)$

2. $f(x) = f(A2x) = f(x_1, N2 - x_2, N3 - x_3)$

3. $f(x) = f(A3x) = f(N1 - x_1, x_2, N3 - x_3)$

4. $f(x) = f(A4x) = f(N1 - x_1, N2 - x_2, N3 - x_3)$

5. $f(x) = f(A5x) = f(x_1, x_2, N3 - x_3)$

6. $f(x) = f(A6x) = f(N1 - x_1, x_2, x_3)$

7. $f(x) = f(A7x) = f(x_1, N2 - x_2, x_3)$

These conditions can be expressed in the matrix form by the following equations:

$$A1 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x \tag{33}$$

$$A2 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \tag{34}$$

$$A3 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x \tag{35}$$

$$A4 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \tag{36}$$

$$A5 = \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x \tag{37}$$

$$A6 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & 1 \end{bmatrix} x \tag{38}$$

$$A7 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x \qquad (39)$$

This group has an eight-fold symmetry, therefore the order of the group is 8. Since this is a subgroup of the super group X, then its dual has order 8. Denote $Pmmm$ by Y and its dual by $Y^{\perp}$. From the results of the periodization and decimation algorithm we need to compute the FFT of these functions that belong to $Y^{\perp}$. In this case only the following 8 functions are in $Y^{\perp}$:

1. From S_1 : { $f_0(x)$ }
2. From S_2 : { $f_8(x)$ }
3. From S_3 : { $f_{16}(x)$ }
4. From S_4 : { $f_{24}(x)$ }
5. From S_5 : { $f_{32}(x)$ }
6. From S_6 : { $f_{40}(x)$ }
7. From S_7 : { $f_{48}(x)$ }
8. From S_8 : { $f_{56}(x)$ }

4.18. *Pmma*

Pmma respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(N1 - x_1, x_2, N3 - x_3)$

2. $f(x) = f(A2x) = f(M1 - x_1, x_2, x_3)$

3. $f(x) = f(A3x) = f(M1 + x_1, x_2, N3 - x_3)$

4. $f(x) = f(A4x) = f(N1 - x_1, N2 - x_2, N3 - x_3)$

5. $f(x) = f(A5x) = f(x_1, N2 - x_2, x_3)$

6. $f(x) = f(A6x) = f(M1 + x_1, N2 - x_2, N3 - x_3)$

7. $f(x) = f(A7x) = f(M1 - x_1, N2 - x_2, x_3)$

These conditions can be expressed in the matrix form by the following equations:

$$A1 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x \tag{40}$$

$$A2 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} M1 \\ 0 \\ 0 \end{bmatrix} \tag{41}$$

$$A3 = \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} M1 \\ 0 \\ 0 \end{bmatrix} \tag{42}$$

$$A4 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \tag{43}$$

$$A5 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x \tag{44}$$

$$A6 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} M1 \\ 0 \\ 0 \end{bmatrix} \tag{45}$$

$$A7 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} M1 \\ 0 \\ 0 \end{bmatrix} \tag{46}$$

This group has an eight-fold symmetry, therefore the order of the group is 8. Since this is a subgroup of the super group X, then its dual has order 8. Denote $Pmma$ by Y and its dual by $Y^{\perp}$. From the results of the periodization and decimation algorithm we need to compute the FFT of these functions that belong to $Y^{\perp}$. In this case only the following 8 functions are in $Y^{\perp}$:

1. From S_1 : { $f_0(x)$ }

2. From S_2 : { $f_8(x)$ }

3. From S_3 : { $f_{16}(x)$ }

4. From S_4 : { $f_{24}(x)$ }

5. From S_5 : { $f_{37}(x)$ }

6. From S_6 : { $f_{45}(x)$ }

7. From S_7 : { $f_{53}(x)$ }

8. From S_8 : { $f_{61}(x)$ }

4.19. *Pbam*

Pbam respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(N1 - x_1, N2 - x_2, x_3)$

2. $f(x) = f(A2x) = f(M1 + x_1, N2 - x_2, N3 - x_3)$

3. $f(x) = f(A3x) = f(M1 - x_1, M2 + x_2, N3 - x_3)$

4. $f(x) = f(A4x) = f(NI - x_1, N2 - x_2, N3 - x_3)$

5. $f(x) = f(A5x) = f(x_1, x_2, N3 - x_3)$

6. $f(x) = f(A6x) = f(MI - x_1, M2 + x_2, x_3)$

7. $f(x) = f(A7x) = f(MI + x_1, M2 - x_2, x_3)$

These conditions can be expressed in the matrix form by the following equations:

$$A1 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x \qquad (47)$$

$$A2 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} MI \\ M2 \\ 0 \end{bmatrix} \qquad (48)$$

$$A3 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} MI \\ M2 \\ 0 \end{bmatrix} \qquad (49)$$

$$A4 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \qquad (50)$$

$$A5 = \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x \tag{51}$$

$$A6 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} M1 \\ M2 \\ 0 \end{bmatrix} \tag{52}$$

$$A7 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} M1 \\ M2 \\ 0 \end{bmatrix} \tag{53}$$

This group has an eight-fold symmetry, therefore the order of the group is 8. Since this is a subgroup of the super group X, then its dual has order 8. Denote $Pbam$ by Y and its dual by $Y^{\perp}$. From the results of the periodization and decimation algorithm we need to compute the FFT of these functions that belong to $Y^{\perp}$. In this case only the following 8 functions are in $Y^{\perp}$:

1. From S_1 : { $f_0(x)$ }

2. From S_2 : { $f_8(x)$ }

3. From S_3 : { $f_{22}(x)$ }

4. From S_4 : { $f_{30}(x)$ }

5. From S_5 : { $f_{38}(x)$ }

6. From S_6 : { $f_{46}(x)$ }

7. From S_7 : { $f_{48}(x)$ }

8. From S_8 : { $f_{56}(x)$ }

4.20. *Pbcn*

Pbcn respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(M1 - x_1, M2 - x_2, M3 + x_3)$
2. $f(x) = f(A2x) = f(M1 + x_1, M2 - x_2, N3 - x_3)$
3. $f(x) = f(A3x) = f(N1 - x_1, x_2, M3 - x_3)$
4. $f(x) = f(A4x) = f(N1 - x_1, N2 - x_2, N3 - x_3)$
5. $f(x) = f(A5x) = f(M1 + x_1, M2 + x_2, M3 - x_3)$
6. $f(x) = f(A6x) = f(M1 - x_1, M2 + x_2, x_3)$
7. $f(x) = f(A7x) = f(x_1, N2 - x_2, M3 + x_3)$

These conditions can be expressed in the matrix form by the following equations:

$$A1 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} M1 \\ M2 \\ M3 \end{bmatrix} \quad (54)$$

$$A2 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} M1 \\ M2 \\ 0 \end{bmatrix} \quad (55)$$

$$A3 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} 0 \\ 0 \\ M3 \end{bmatrix} \quad (56)$$

$$A4 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \quad (57)$$

$$A5 = \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} M1 \\ M2 \\ M3 \end{bmatrix} \tag{58}$$

$$A6 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} M1 \\ M2 \\ 0 \end{bmatrix} \tag{59}$$

$$A7 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} 0 \\ 0 \\ M3 \end{bmatrix} \tag{60}$$

This group has an eight-fold symmetry, therefore the order of the group is 8. Since this is a subgroup of the super group X, then its dual has order 8. Denote $Pbcn$ by Y and its dual by $Y^{\perp}$. From the results of the periodization and decimation algorithm we need to compute the FFT of these functions that belong to $Y^{\perp}$. In this case only the following 8 functions are in $Y^{\perp}$:

1. From S_1 : $\{ f_0 (x) \}$

2. From S_2 : $\{ f_{11} (x) \}$

3. From S_3 : $\{ f_{21} (x) \}$

4. From S_4 : { $f_{27}(x)$ }

5. From S_5 : { $f_{37}(x)$ }

6. From S_6 : { $f_{46}(x)$ }

7. From S_7 : { $f_{53}(x)$ }

8. From S_8 : { $f_{59}(x)$ }

4.21. *Ccca*

Ccca respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(N1 - x_1, N2 - x_2, x_3)$
2. $f(x) = f(A2x) = f(N1 - x_1, N2 - x_2, M3 - x_3)$
3. $f(x) = f(A3x) = f(x_1, M2 - x_2, M3 + x_3)$
4. $f(x) = f(A4x) = f(N1 - x_1, N2 - x_2, N3 - x_3)$
5. $f(x) = f(A5x) = f(N1 - x_1, x_2, N3 - x_3)$
6. $f(x) = f(A6x) = f(N1 - x_1, M2 + x_2, M3 + x_3)$
7. $f(x) = f(A7x) = f(x_1, M2 + x_2, M3 - x_3)$

These conditions can be expressed in the matrix form by the following equations:

$$A1 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x \tag{61}$$

$$A2 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} 0 \\ M2 \\ M3 \end{bmatrix} \tag{62}$$

$$A3 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} 0 \\ M2 \\ M3 \end{bmatrix} \tag{63}$$

$$A4 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \tag{64}$$

$$A5 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x \tag{65}$$

$$A6 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} 0 \\ M2 \\ M3 \end{bmatrix} \tag{66}$$

$$A7 = \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} 0 \\ M2 \\ M3 \end{bmatrix} \tag{67}$$

This group has an eight-fold symmetry, therefore the order of the group is 8. Since this is a subgroup of the super group X, then its dual has order 8. Denote $Ccca$ by Y and its dual by $Y^{\perp}$. From the results of the periodization and decimation algorithm we need to compute the FFT of these functions that belong to $Y^{\perp}$. In this case only the following 8 functions are in $Y^{\perp}$:

1. From S_1 : { $f_0\,(x)$ }
2. From S_2 : { $f_{15}\,(x)$ }
3. From S_3 : { $f_{23}\,(x)$ }

4. From S_4 : { $f_{24}(x)$ }

5. From S_5 : { $f_{32}(x)$ }

6. From S_6 : { $f_{47}(x)$ }

7. From S_7 : { $f_{55}(x)$ }

8. From S_8 : { $f_{56}(x)$ }

4.22. *Cmcm*

Cmcm respects the following symmetry conditions :

1. $f(x) = f(A1x) = f(x_1, N2 - x_2, N3 - x_3)$
2. $f(x) = f(A2x) = f(x_1, x_2, M3 - x_3)$
3. $f(x) = f(A3x) = f(x_1, N2 - x_2, M3 + x_3)$
4. $f(x) = f(A4x) = f(N1 - x_1, N2 - x_2, N3 - x_3)$
5. $f(x) = f(A5x) = f(N1 - x_1, x_2, x_3)$
6. $f(x) = f(A6x) = f(N1 - x_1, N2 - x_2, M3 + x_3)$
7. $f(x) = f(A7x) = f(N1 - x_1, x_2, M3 - x_3)$

These conditions can be expressed in the matrix form by the following equations:

$$A1 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \tag{68}$$

$$A2 = \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} 0 \\ 0 \\ M3 \end{bmatrix} \tag{69}$$

$$A3 = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} 0 \\ 0 \\ M3 \end{bmatrix} \tag{70}$$

$$A4 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & -1 \end{bmatrix} x \tag{71}$$

$$A5 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & 1 \end{bmatrix} x \tag{72}$$

$$A6 = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix} x + \begin{bmatrix} 0 \\ 0 \\ M3 \end{bmatrix} \tag{73}$$

$$A7 = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix} x + \begin{bmatrix} 0 \\ 0 \\ M3 \end{bmatrix} \tag{74}$$

This group has an eight-fold symmetry, therefore the order of the group is 8. Since this is a subgroup of the super group X, then its dual has order 8. Denote $Cmcm$ by Y and its dual by $Y^{\perp}$. From the results of the periodization and decimation algorithm we need to compute the FFT of these functions that belong to $Y^{\perp}$. In this case only the following 8 functions are in $Y^{\perp}$:

1. From S_1 : { $f_0\ (x)$ }
2. From S_2 : { $f_{11}\ (x)$ }
3. From S_3 : { $f_{19}\ (x)$ }

4. From S_4 : { f_{27} (x) }

5. From S_5 : { f_{35} (x) }

6. From S_6 : { f_{43} (x) }

7. From S_7 : { f_{51} (x) }

8. From S_8 : { f_{59} (x) }

In addition there are 22 more Orthorhombic crystallographic groups of order eight which the above algorithm includes. These groups are Pnnn, Pccm , Pbam, Pban , Pnna, Pmna, Pcca, Pccn, Pbcm, Pnnm, Pmmn, Pbca, Pnma, Cmca, Cmmm, Cccm, Cmma, Ccca, Fmmm, Immm, Ibam, Ibca, Imma.

Therefore the periodization and decimation algorithm is capable of solving 12 Monoclinic groups of order 2, 10 Monoclinic groups of order 4, 30 Orthohombic groups of order 4, and 28 Orthohombic groups of order 8, for a total of 80 crystallographic groups .

5 SOFTWARE IMPLEMENTATION

The periodization and decimation algorithm designed in chapters 3 and 4 has been successfully programmed. Once the right crystallographic data is entered, the program will immediately periodize it into the proper number of functions. These functions are totally independent and can be executed in parallel. The program then computes the three dimensional Fourier transform of each one of these functions, and adds up the results to generate the final answer. The inverse Fourier transform is also calculated in a similar fashion.

In our case Fortran-77 code was implemented on both Sun and Titan systems. Three dimensional real data of size [26 x 26 x 26] was used as an example and the following timing results were obtained:

1. On Sun system, the user time

   usrt = 1.8 seconds

2. On Titan system, t user time

   urst = 1.05 seconds

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