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D. R. Fitzwater
Iowa State University

T. R. Johnston
Iowa State University

D. H. Erbeck
Iowa State University

M. K. Rhyne
Iowa State University

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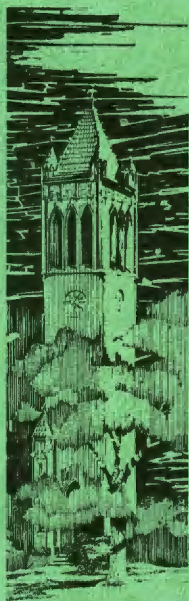

IOWA STATE UNIVERSITY

PATTERSON SUPERPOSITION SYSTEM FOR THE IBM 7074

by

D. R. Fitzwater, T. R. Johnston,
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AMES LABORATORY

RESEARCH AND DEVELOPMENT REPORT

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Research and Development Report

PATTERSON SUPERPOSITION SYSTEM FOR THE IBM 7074

by

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August 1964

Ames Laboratory
at
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ABSTRACT

A system is described which aids in resolving the N(N-1) peaks that appear on a PATTERSON MAP into the fundamental set of "N" vectors corresponding to the "N" atoms.

INTRODUCTION

A program (IS-876) was written by Mr. MADS LEDET to perform a two or three dimensional Crystallographic Fourier Summation on X-RAY reflection data. The output from this program comprises a PATTERSON MAP. It was desired to perform a superposition of this map utilizing a minimum function.

STATEMENT OF THE PROBLEM

The FOURIER SUMMATION PROGRAM has a limitation in that it can process a maximum block of 20 x 20 x 20 points per pass. Problems containing greater than this number of points must be run in successive partial passes.

The output block sequence, on magnetic tape, from the FOURIER SUMMATION PROGRAM of cells requiring more than one pass, is not the point sequence in which symmetry operations or a minimum function can be performed.

A merge program must rearrange the output form of the PATTERSON MAP into the form permitting these operations to take place.

The PATTERSON MAP which is the output from the FOURIER SUMMATION PROGRAM may comprise from half to an eighth of the unit cell. The remainder of the unit cell must be based upon the specified cell symmetry.

When the entire unit cell is constructed it must be shifted, using a three dimensional shift vector, to obtain a shifted PATTERSON MAP. This shifted map must be merged with another specified PATTERSON MAP of the same form, using a minimum function; in some cases a minimum map must be extracted from two PATTERSON MAPS without a shift.

The map that is the result of the two merged maps must be printed in a manner allowing easy interpretation of the PATTERSON peaks.

SOLUTION OF THE PROBLEM

Two modifications to the existing FOURIER SUMMATION PROGRAM were made. The first modification was the addition of a routine which would output the PATTERSON MAP onto a specified magnetic tape in internal notation. This was necessitated due to the original FOURIER program allowing output in printed form only, which does not permit further processing.

The second modification was made to speed up the input/output time of the PATTERSON SYSTEM, and to allow a greater volume of points to be contained on a single magnetic tape.

To satisfy the first modification requirement an alteration switch option was installed which works as follows:

ALTERATION SWITCH TWO ON: Printed PATTERSON MAP Only

ALTERATION SWITCH THREE ON: Internal Notation Output Only

ALTERATION SWITCH TWO and THREE ON: Both Printed and Internal Notation Output

Since the Fourier summation program is designed to contain the results of the summation in only the five high order digits of each memory word and the IBM 7074 has an instruction which will allow output to be written eliminating high order zeros of each memory word, the five high order digits are placed in the five low order digits of the memory word and the five high order digits are replaced by zeros. This allows twice as much data to be contained on magnetic tape or the same amount to be read, or written, in half the time.

A merge program was written which will rearrange the output blocks into the proper form for subsequent symmetry operations.

This program (PATTERSON MERGE) must be fed the number of blocks, and number of points per block, in all three directions (X, Y, Z) that were processed through the FOURIER program. The order of the PATTERSON MERGE is determined by multiplying the number of blocks in the "X" direction by the number of blocks in the "Y" direction. The PATTERSON MERGE program has the following merge order capability: 2, 4, 8, 16, 32. The number of blocks in the "Z" direction may range from one to eight.

The output blocks from the FOURIER program are arranged in layers of the unit cell in the "Z" direction (XY plane). Within each layer the points are row by row.

After the PATTERSON MERGE program has arranged the points in order, and they are stored on magnetic tape, an appropriate SYMMETRY BUILD program is called from the LIBRARY tape. The SYMMETRY BUILD set of programs, by performing various types of symmetry operations, constructs the remainder of the unit cell from the input one eight to one half unit cell. Six types of symmetry operations are possible.

1. TRICLINIC
2. MONOCLINIC TWOFOLD IN X
3. MONOCLINIC TWOFOLD IN Y
4. MONOCLINIC MIRROR IN X
5. MONOCLINIC MIRROR IN Y
6. ORTHORHOMBIC

For all symmetry operations the second half of the unit cell in the "Z" direction is constructed.

The SYMMETRY BUILD set of programs must also be fed the number of blocks and points per block in all directions. The entire unit cell is then written on magnetic tape. Two records (defining the data form) for use by the MINIMUM PLANE building program are also written on the tape. This tape now contains the PATTERSON MAP of the entire unit cell.

The MINIMUM PLANE building program extracts the fundamental vector set from the PATTERSON MAP using the SUPERPOSITION technique described by BUERGER in VECTOR SPACE. A peak from the PATTERSON MAP is chosen and shifted (by a shift vector) so as to superimpose on the origin of an identical PATTERSON MAP in the same orientation. All of the other PATTERSON peaks are shifted accordingly; under only the "N" peaks of the fundamental set and the "N" peaks of the inverse will there be peaks on the original (actually there may and probably will be accidental superpositions). The BUERGER minimum function is a very simple and efficient method of detecting the super-imposed peaks. The value of the PATTERSON function on the original map is compared to the value of the corresponding shifted map. The minimum of the two is retained. A positive result indicates the existence of a peak on both the shifted and non-shifted maps. Such a peak corresponds to a member of the fundamental set, a member of its inverse, or an accidental superposition. Subsequent superpositions will eliminate the inverse and the accidental superpositions.

A lister program will edit and print the MINIMUM PATTERSON layer by layer, twenty-one points per row in the "X" direction, on each page. The twenty-first point is identical to the first point on the second sheet (if there are more than twenty-one points in the "X" direction), giving one column of over lap.

One row will be printed directly beneath another ignoring overflow between pages. All negative points will be printed as positive zeros, thus only the peaks will contain numerical values.

One setup card is required for the LISTER program which specifies the input tape and the output tapes. One to three output tapes may be specified if it is felt the listing may more than fill a magnetic tape reel.

USAGE

The modified CRYSTALLOGRAPHIC FOURIER SUMMATION program is located on the AMES LABORATORY COMPUTER LIBRARY tape and is called "PATFOURIER".

The existing report (IS-876) is applicable except for the following changes.

CHANGE 1.

IS-876, PAGE 6, #3, Tape Options Card has been changed to read as follows.

CARD COLUMNS

1- 7	FOURIER
11-15	TAPES
21-22	1ST DATA INPUT TAPE
26-27	ALTERNATE DATA INPUT TAPE
31-32	X SUM OUTPUT TAPE
36-37	ALTERNATE X SUM OUTPUT TAPE
41-42	Y SUM OUTPUT TAPE
46-47	ALTERNATE Y SUM OUTPUT TAPE
51-52	FINAL OUTPUT TAPE (23 IS STANDARD)
56-57	ALTERNATE FINAL OUTPUT TAPE (23 IS STANDARD)
61-62	PATTERSON OUTPUT TAPE (11 IS STANDARD)
66-67	ALTERNATE PATTERSON OUTPUT TAPE (11 IS STANDARD)
74-75	T/2 APPROXIMATELY

CHANGE 2.

This change is in relation to the settings of the alteration switches and is explained previously.

Consider that we want to perform a summation on a cell containing eighty points in the "X" direction, 40 points in the "Y" direction, and 40 points in the "Z" direction. Figure 1 shows the number of passes necessary and the order in which they must be run to perform this calculation.

A setup card is required by the PATTERSON MERGE program telling it the number of blocks and the number of points per block in the "X", "Y", and "Z" directions (see example No. 1 for the PATTERSON MERGE setup card illustration). This card is in the numeric format.

It is evident from Fig. 1 that sixteen passes through the FOURIER SUMMATION program would be necessary to perform the summations for this cell containing 128, 000 input points. This may only comprise from an eighth to a half of the unit cell.

After the PATTERSON MERGE program has arranged the points in to "Z" layer by "Z" layer order the appropriate SYMMETRY BUILDER will be called from the LIBRARY tape. The remainder of the unit cell will be constructed based upon its symmetry specifications (see examples 2-7 for illustrations of the symmetry operations). The second half of the unit cell in the "Z" direction is constructed in all symmetry cases.

A set up card is required for the SYMMETRY BUILD programs which is identical to the setup card for the PATTERSON MERGE program except for an additional parameter specifying the desired symmetry operation (see example No. 8 for SYMMETRY BUILD setup card illustration).

The MINIMUM PLANE BUILDER is automatically called from the LIBRARY tape by the SYMMETRY BUILDER, but may be called separately if a tape has been saved for input. The PATTERSON MAP on the input tape is shifted the amount of the shift vector and is merged (using the minimum function) with the map on the merge tape. A shift and merge is performed for each parameter card. A zero shift may be specified, or a map may be merged with itself.

One or more parameter cards will be read from tape 14 with the last card followed by a TAPE MARK (see example No. 9 for setup card illustration). It is entirely possible to use the output tape from the first pass through the MINIMUM PLANE builder as the input or merge tape for the next pass. When the TAPE MARK following the last parameter card has been read, the LISTER program will be automatically called from the LIBRARY tape.

The LISTER program will edit and print the MINIMUM PATTERSON MAP. One setup card is required for the LISTER program. This card specifies the input tape and the output tapes (see example No. 10 for LISTER setup card illustration). Example No. 11 illustrates a running deck to process data completely through the PATTERSON SYSTEM.

After the data has been processed through the FOURIER SUMMATION program, the MERGE program and the SYMMETRY BUILD program, the output tape should be saved. This tape may be used with any number of different shift vectors without reprocessing completely through the system. Example No. 12 illustrates a running deck which will shift the original PATTERSON MAP, compute the minimum plane and print the results.

ASSIGNMENT OF TAPES

Tape assignments are made on the basis of the MERGE order being run. The method of determining this order has been described previously. If the PATTERSON output from the FOURIER SUMMATION program is to be run immediately through the PATTERSON SYSTEM the PATTERSON output tape number must be Autocoder 11 on the tape parameter card of the FOURIER program.

In all cases the input to the PATTERSON MERGE program must be on Autocoder tape unit 11. If the order of the MERGE is "2" the output from the SYMMETRY BUILDER is on Autocoder tape unit 22, thus 22 should be specified as the input tape to the MINIMUM PLANE BUILDER program. If the order is 4, 8, 16, or 32 the output from the SYMMETRY BUILDER is on Autocoder tape unit 11.

ONE PASS PATTERSON

If the order of the PATTERSON is one, only one block or pass through the FOURIER program, the MERGE phase is not required. The map from the FOURIER program becomes the input tape to the SYMMETRY BUILD ONE program (SYMBUILD1). The imput tape to SYMBUILD1 is Autocoder 11. Example 13 is an illustration of a running deck for a one block PATTERSON.

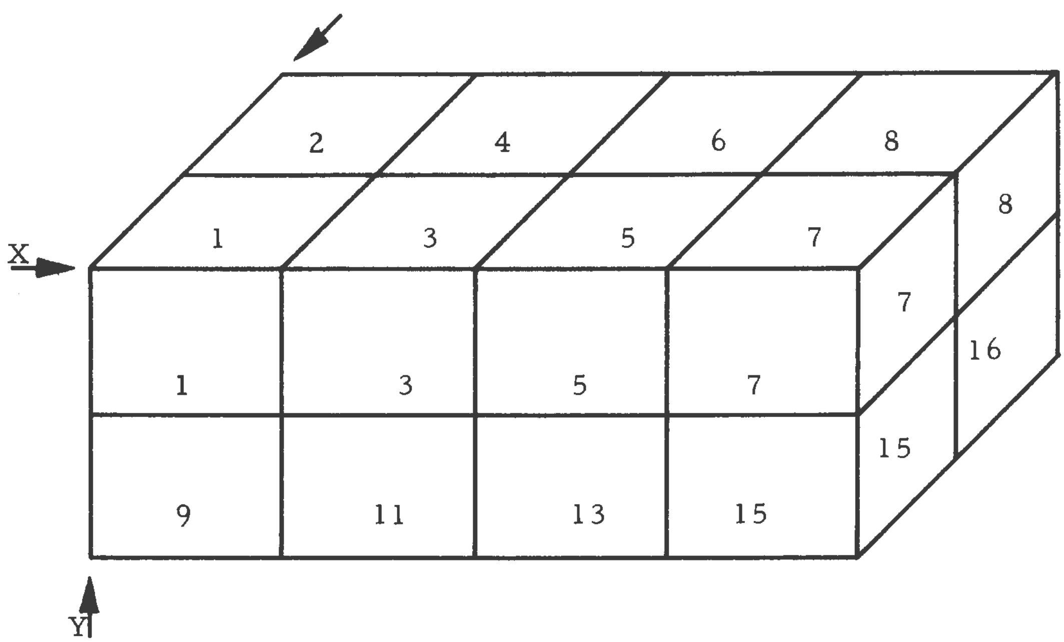


Fig. 1

X
AMES LABORATORY

80 COLUMN CONDENSED CARD PATCH SHEET

Program ______________________

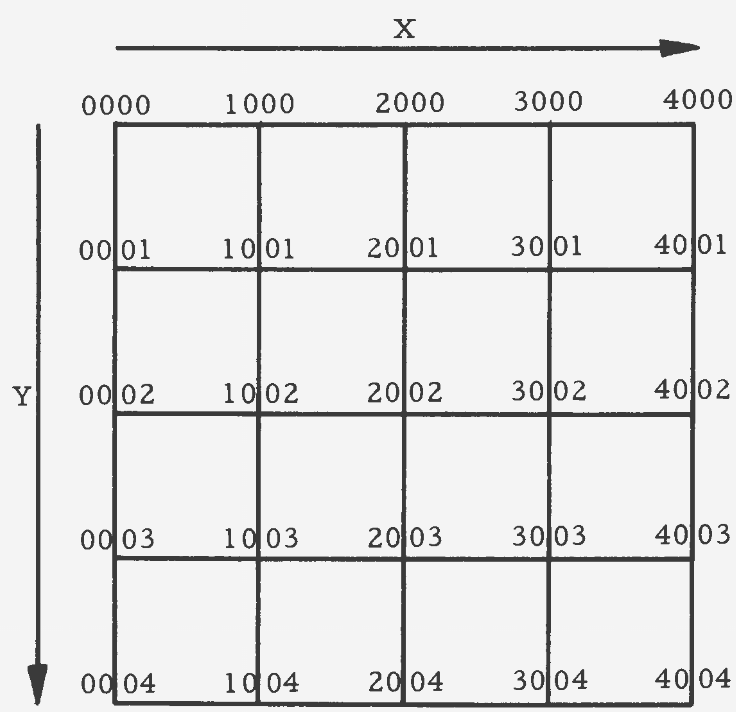
Programmed by ______________________

Date ______________________

WORD 1 (1–10)	WORD 2 (11–20)	WORD 3 (21–30)	WORD 4 (31–40)	WORD 5 (41–50)	LOAD INDICATORS 51	56 60	61	65	LOC. OF 1st inst. 70	CARD NO. 75	Ident. 80
EXAMPLE NO	.1 PATTE	RSON MERGE	SETUP CAR	D							
WORD 1 = N	O. OF BLOC	KS IN THE	X DIRECTIO	N							
WORD 2 = N	O. OF POIN	TS PER BLO	CK IN THE	X DIRECTIO	N						
WORD 3 = N	O. OF BLOC	KS IN THE	Y DIRECTIO	N							
WORD 4 = N	O. OF POIN	TS PER BLO	CK IN THE	Y DIRECTIO	N						
WORD 5 = N	O. OF BLOC	KS IN THE	Z DIRECTIO	N							
WORD 6 = N	O. OF POIN	TS PER BLO	CK IN THE	Z DIRECTIO	N						
+	+	+	+	+		+			+		+
0000000002	0000000020	0000000002	0000000020	0000000002	00000	00020	0000	0	00000	00000	00000

EXAMPLE NO. 2

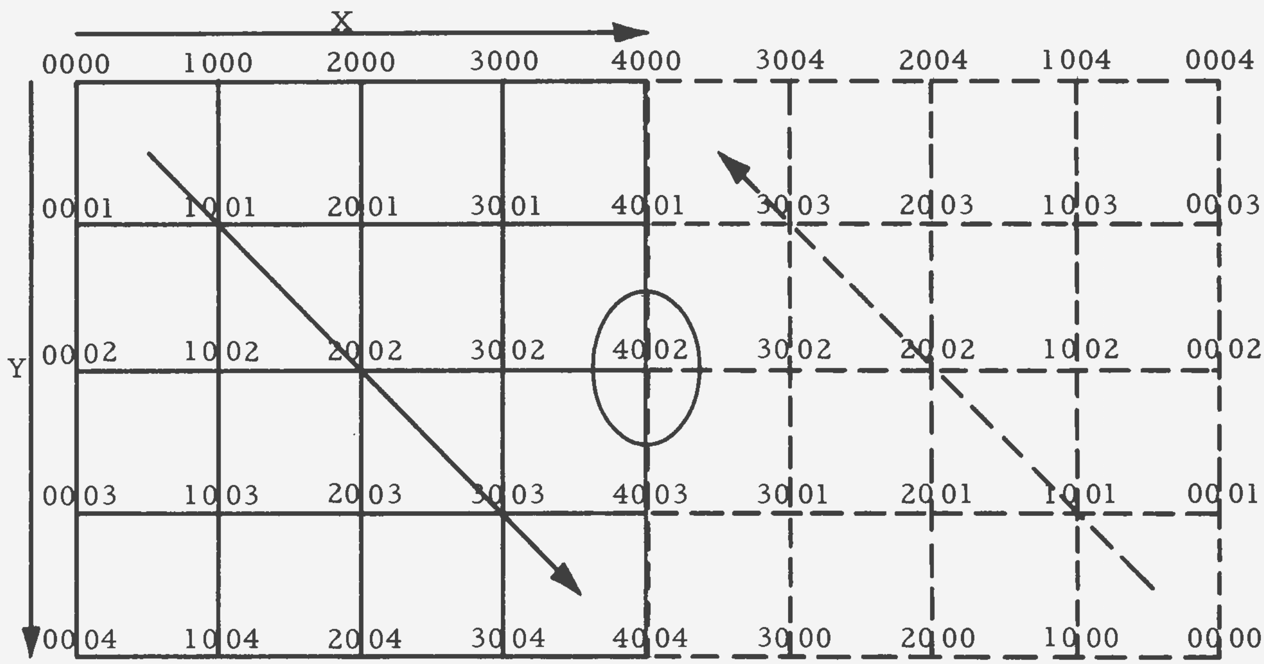
Triclinic Symmetry
Input Data Points



EXAMPLE NO. 3

Monoclinic Twofold Symmetry in X

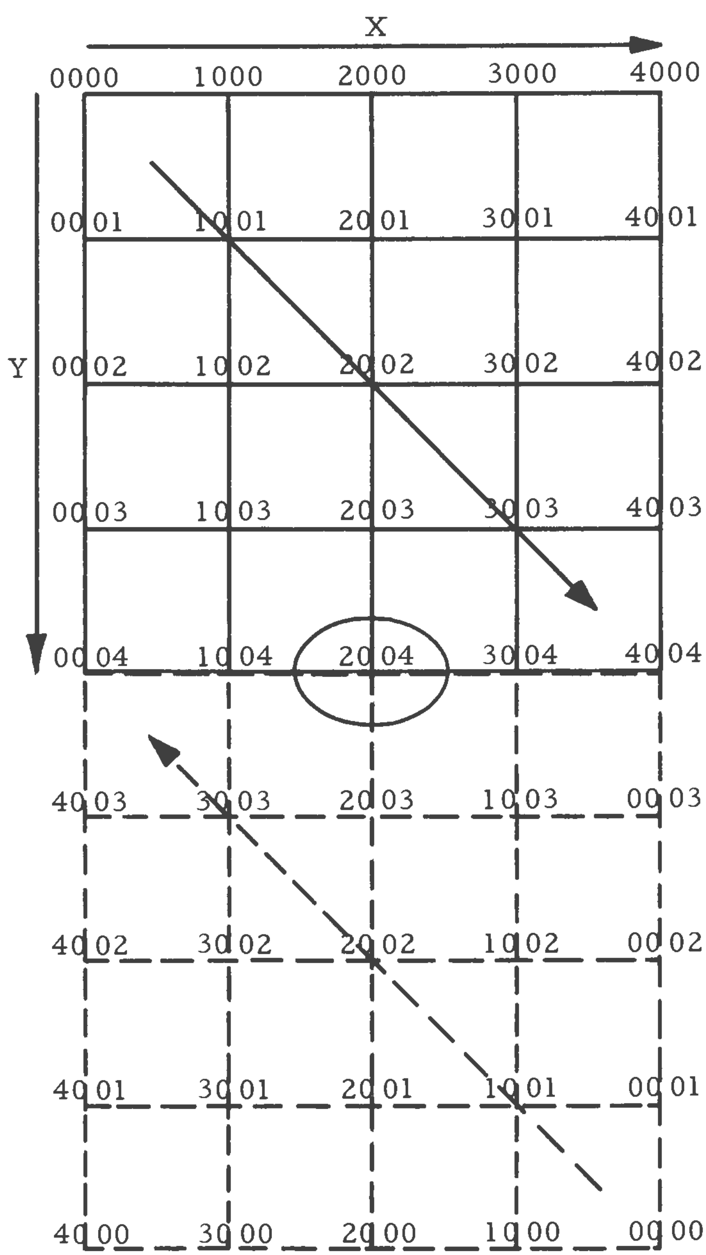
__________ Input Data Points
\- - - - - - - - - - Constructed Data Points



EXAMPLE NO. 4

Monoclinic Twofold Symmetry in Y

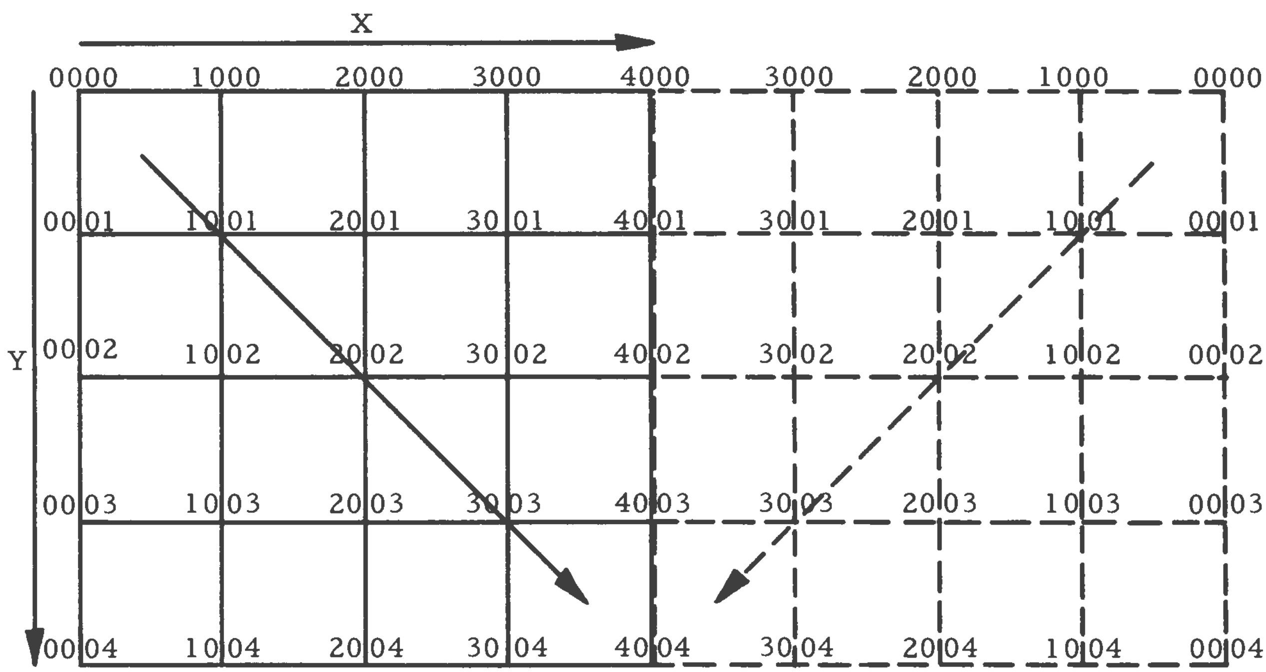
__________ Input Data Points
\- - - - - - - - - - Constructed Data Points



EXAMPLE NO. 5

Monoclinic Mirror Symmetry in X

__________ Input Data Points
\- - - - - - - - - - Constructed Data Points

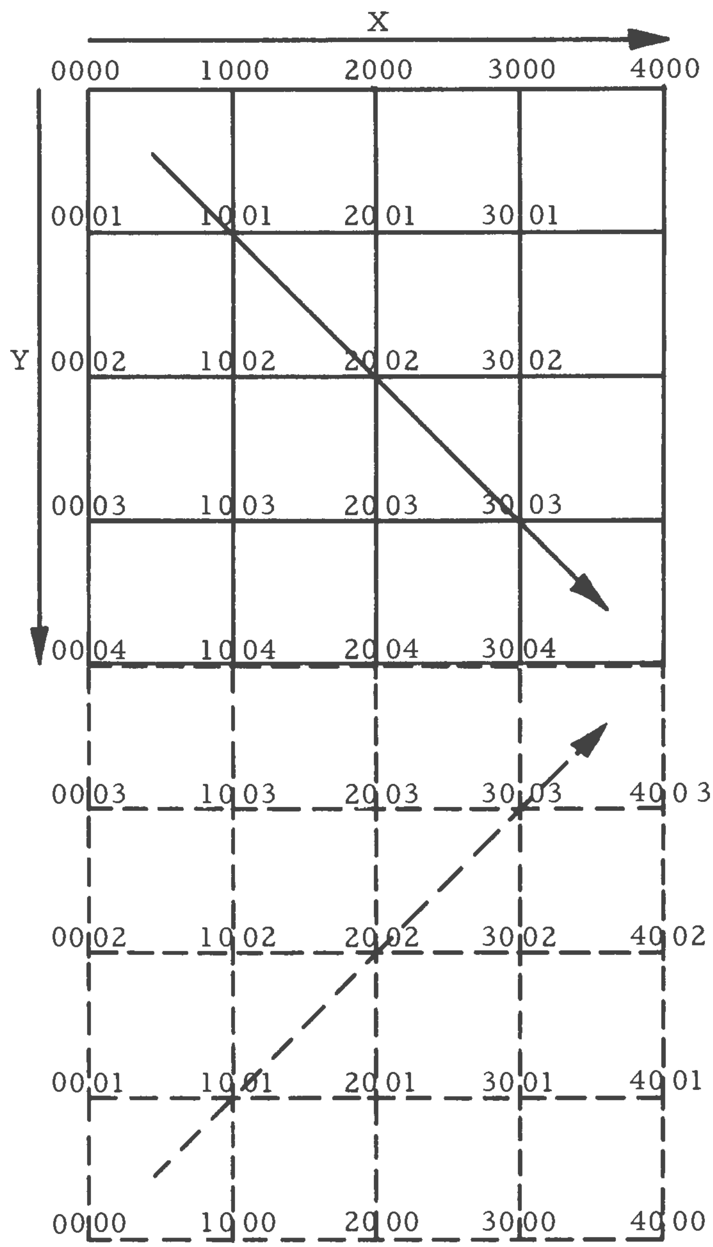


EXAMPLE NO. 6

Monoclinic Mirror Symmetry in Y

___________ Input Data Points

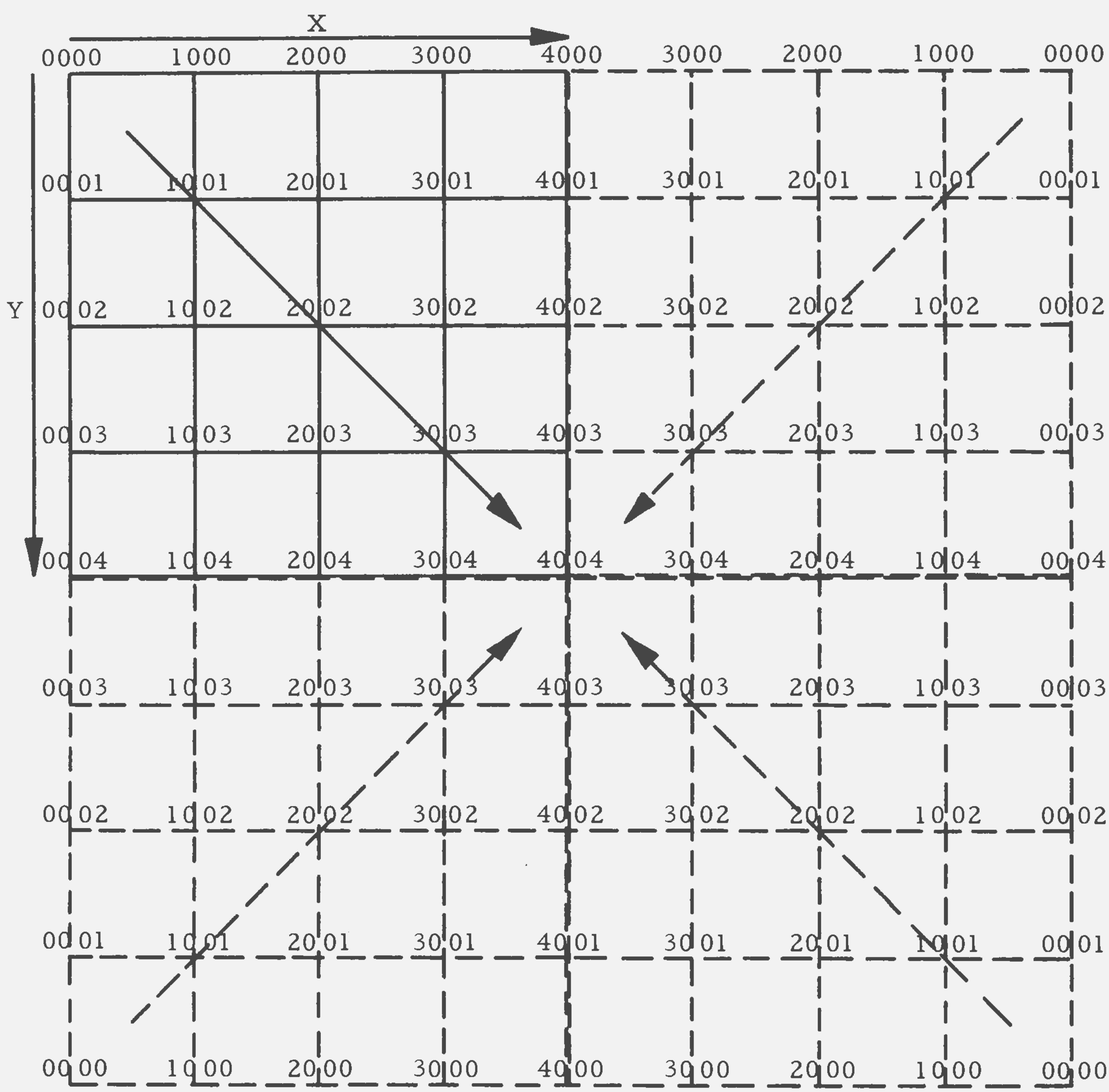
\- - - - - - - - - - Constructed Data Points



EXAMPLE NO. 7

Orthorhombic Symmetry

Input Data Points
Constructed Data Points



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Program

Programmed by

Date

EXAMPLE NO. 8 SYMMETRY BUILD SET UP CARD

WORD 1 = NO. OF BLOCKS IN THE X DIRECTION

WORD 2 = NO. OF POINTS PER BLOCK IN THE X DIRECTION

WORD 3 = NO. OF BLOCKS IN THE Y DIRECTION

WORD 4 = NO. OF POINTS PER BLOCK IN THE Y DIRECTION

WORD 5 = NO. OF BLOCKS IN THE Z DIRECTION

WORD 6 = NO. OF POINTS PER BLOCK IN THE Z DIRECTION

WORD 7 = SYMMETRY OPERATION DESIRED(ORTHORHOMBIC SHOWN IN EXAMPLE

WORD 1 (1–10)	WORD 2 (11–20)	WORD 3 (21–30)	WORD 4 (31–40)	WORD 5 (41–50)	LOAD INDICATORS 51	56–60	61–65	LOC. OF 1st inst. 70	CARD NO. 75	Ident. 80
+	+	+	+	+		+		+		+
0000000002	0000000020	0000000002	0000000020	0000000002	00000	00020	00000	00006	00000	00000

EXAMPLE NO. 9 MINIMUM PLANE BUILDER(PATTERSON 1) SET UP CARD

WORD 1 = INPUT TAPE NO.(AUTOCODER)

WORD 2 = OUTPUT TAPE NO.(AUTOCODER)

WORD 3 = WORK TAPE 1 NO.(AUTOCODER)

WORD 4 = WORK TAPE 2 NO.(AUTOCODER)

WORD 5 = X SHIFT VALUE (21.3)

WORD 6 = Y SHIFT VALUE (5.1)

WORD 7 = Z SHIFT VALUE (9 LAYERS)

WORD 8 = MERGE TAPE NO.(AUTOCODER)

WORD 1 (1–10)	WORD 2 (11–20)	WORD 3 (21–30)	WORD 4 (31–40)	WORD 5 (41–50)	LOAD INDICATORS 51	56–60	61–65	LOC. OF 1st inst. 70	CARD NO. 75	Ident. 80
+	+	+	+	+		+		+		+
0000000022	0000000021	0000000011	0000000013	0000000213	00000	00051	00000	00009	00000	00012

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80 COLUMN CONDENSED CARD PATCH SHEET

Program ______________________

Programmed by ______________________

Date ______________________

WORD 1 (1–10)	WORD 2 (11–20)	WORD 3 (21–30)	WORD 4 (31–40)	WORD 5 (41–50)	LOAD INDICATORS (51)	(56 – 60)	(61 – 65)	LOC. OF 1st inst. (70)	CARD NO. (75)	Ident. (80)
EXAMPLE NO. 10 LISTER SET UP CARD										
WORD 1 = INPUT TAPE NO. (AUTOCODER)										
WORD 2 = OUTPUT TAPE 1 (AUTOCODER)										
WORD 3 = OUTPUT TAPE 2 (AUTOCODER)										
WORD 4 = OUTPUT TAPE 3 (AUTOCODER)										
+	+	+	+	+		+		+		
0000000021	0000000023	0000000000	0000000000	0000000000	00000	00000	00000	00000	00000	00000

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Program

Programmed by

Date

80 COLUMN CODING SHEET

EXAMPLE NO. 11

RUNNING DECK FOR COMPLETE PATTERSON

Pg. 1 2	Line 3 5	Label 6 15	Operation 16 20	OPERAND 21 — Basic Autocoder → 60	Autocoder → 65 70 75	Ident.	80
		START	ACCNT	A0000@ JOHNSTON@ 10MIN		POGO	
		TYPE	REM	@MOUNT AL150 ON UNIT 22@ AND HALT		POGO	
		ZX	LOAD	TAPE 14		POGO	
						FORN	
		(CONDENCED	DECK"	DATA PREPARATION PROGRAM FOR FOURIER SUM	MATION PROGRAM		
						FORF	
			DUMP	325 TO 19975		POGO	Z
			TAPE	TRW(OUTPUT TAPE)		POGO	
			ALTSW	2ON3ON(BOTH LISTING AND PATTERSON OUTPUT		POGO	
		Z	LLOAD	@PATFOURIER@		POGO	
		(FOUIER SU	MMATI	ON PROGRAM CONTROL CARDS)			
						WTM	
			DUMP	325 TO 19975		POGO	Z
			ALTSW	2 OFF 3 OFF		POGO	
		Z	LLOAD	@PATMERGEBB@		POGO	
						FORN	
		(PATTERSO	N MERGE SETUP CARD)				
		(SYMMETRY	BUILD SETUP CARD)				
		(MININ	IMUM PLANE BUILDER "PATTERSON1" SETUP CARD)				
						WTM	
		Z	LLOAD	@LISTER BBBB@		POGO	Y
						FORN	
		(LIS	TER SETUP CARD)				
						FORN	
			DUMP	325 TO 19975		POGO	
		TYPE	REM	@REMOVE AL 150 FROM UINT 22 AND SAVE@ AND HALT		POGO	
		END	ACCT	@JOHNSTON@		POGO	

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Program ____________________

Programmed by ____________________

Date ____________________

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EXAMPLE NO. 12

RUNNING DECK FOR PARTIAL PATTERSON RUN

Pg. 1 2	Line 3 5	Label 6 15	Operation 16 20	OPERAND 21 ... 60 (Basic Autocoder →)	65 ... 75 (Autocoder →)	Ident.	80
		START	ACCNT	A0000, @JOHNSTON@ 5MIN		POGO	
		TYPE	REM	@MOUNT AL 150 ON UNIT 22@ AND HALT		POGO	
		Z	LLOAD	@PATTERSON1@		POGO	
						FORN	
		(SETUP CARDS FOR "PATTERSON1")					
						WTM	
		Z	LLOAD	@LISTER BBBB@		POGO	Y
						FORN	
		(LISTER SETUP CARD)					
						FORF	
			DUMP	325 TO 19975		POGO	Z
		TYPE	REM	@REMOV AL 150 FROM UNIT 22 AND SAVE AND	HALT	POGO	
		END	ACCT	@JOHNSTON@			

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Program ______________________

Programmed by ______________________

Date ______________________

80 COLUMN CODING SHEET

EXAMPLE NO. 13
ONE BLOCK PATTERSON RUN

Pg. 1 2	Line 3 5	Label 6 15	Operation 16 20	OPERAND 21 … Basic Autocoder → 60	Autocoder → 75	Ident.	80
		START	ACCNT	A0000 @JOHNSTON@ 10MIN		POGO	
		TYPE	REM	@MOUNT AL 150 ON UNIT 22@ AND HALT		POGO	
		ZX	LOAD	TAPE 14		POGO	
						FORN	
		(CONDENSED DECK "DATA PREPARATION PROGRAM FOR FOURIER PROGRAM")					
						FORF	
			DUMP	325 TO 19975		POGO	Z
			TAPE	TRW (OUTPUT TAPE)		POGO	
			ALTSW	2ON, 3ON, (BOTH LISTING AND PATTERSON OUTPUT)		POGO	
		Z	LLOAD	@PATFOURIER@		POGO	
		(FOURIER SUMMATION PROGRAM CONTROL CARDS					
						WTM	
			ALTSW	2OFF, 3OFF		POGO	
		Z	LLOAD	@SYMBUILD1b		POGO	
						FORN	
		(SYMMETRY BUILD SETUP CARD)					
		(MINIMUM PLANE BUILDER "PATTERSON1" SETUP CARDS)					
						WTM	
		Z	LLOAD	@LISTERbbbb@		POGO	Y
						FORN	
		(LISTER SETUP CARD					
						FORF	
			DUMP	325 TO 19975		POGO	Z
		TYPE	REM	@REMOVE AL 150 FROM UNIT 22 AND SAVE, AND HALT		POGO	
		END	ACCNT	@JOHNSTON@		POGO	