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# PROGRAM FOR CALCULATION OF AUGMENTED JACOBI POLYNOMIALS

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*Abstract:* The augmented Jacobi polynomials, designated $Z_{\ell mn}$ by Roe, or the closely related generalized Legendre functions, $P_{\ell}^{mn}(\cos \phi)$ of Bunge, are required for series expansions of the crystallite orientation distribution. The problem of publishing extensive tabular information has limited compilation of these functions to certain crystal and physical symmetries. This paper gives a brief description and listing of a computer program which permits calculation of Fourier sine (m-n odd) or cosine (m-n even) series expansions of $Z_{\ell mn}(\xi)$ for $\ell = 0, 1, \ldots, 32$; $m = 0, 1, \ldots, \ell$; $n = 0, 1, \ldots, \ell$.

## INTRODUCTION

The augmented Jacobi polynomials, designated $Z_{\ell mn}(\xi)$ by Roe,[1] or the closely related generalized Legendre functions, $P^{mn}(\cos \phi)$ of Bunge,[2] where

$$P_{\ell}^{mn}(\alpha) = \left(\frac{2}{2\ell + 1}\right)^{\frac{1}{2}} Z_{\ell mn}(\alpha),$$

are required for series expansions of the crystallite orientation distribution. The problem of publishing extensive tabular information has limited compilation of these functions to certain crystal and physical symmetries.[3-6] The computer program described briefly and listed in this paper permits calculation of Fourier sine (m-n odd) or cosine (m-n even) series expansions of $Z_{\ell mn}(\xi)$ for $\ell = 0, 1, \ldots, 32$; $m = 0, 1, \ldots, \ell$; $n = 0, 1, \ldots, \ell$.

The program was written in the course of developing a method for determining the crystallite orientation distribution of sheet steel samples from back reflection "sheet" pole figures, and has been run on a CDC-6600 computer using double precision (approximately 29 significant figures). Maximum detected error was $6 \times 10^{-20}$ at 16th order and $2 \times 10^{-8}$ at 32nd order. For single precision (approximately 15 significant figures) corresponding errors were $7 \times 10^{-6}$ and $2 \times 10^{8}$, respectively. The three loops DO 51 LG = 5, 23, 2; DO 51 NX = 1, NUP, 4; DO 51 MX = 1, MUP; where LG = $\ell + 1$, NX = $n + 1$, and MX = $m + 1$ together with MUP and NUP are used to specify lower and upper limits and symmetry conditions on $\ell$, n, and m. In the listing shown, $\ell$ is restricted to even values (a consequence of Friedel's law, see Roe[1]), from 4 to 22, and n to integral multiples of 4, including 0. Running time on the CDC-6600 for these conditions was 141 system seconds. Substitution of NUP = L2+1 and DO 51 NX = 1, NUP removes restriction on n, so that n = 0, 1, ..., $\ell$. The program should prove useful in the study of textures in geological materials, where low crystal and physical symmetries are common.

## PROGRAM LISTING

```
      PROGRAM ZLMN(INPUT,OUTPUT,TAPE2=INPUT,TAPE3=OUTPUT,
         TAPE7)
C     P.R.MORRIS, ARMCO STEEL CORPORATION, SEPT.15,1975.
C
C     THIS PROGRAM CALCULATES FOURIER SINE (M-N ODD) OR
C     COSINE (M-N EVEN) SERIES EXPANSIONS OF THE AUG-
C     MENTED JACOBI POLYNOMIALS, Z SUB LMN, SEE RYONG-JOON
C     ROE, J. APPL. PHYS., VOL. 36, 1965, PP.2024-31,
C     EQS. (A1), (A2), (A3), (A4), (A5), (A6), (A8), (A11).

      INTEGER CDIN,HIG
      DOUBLE A,B,C,D,E,F,S,SN,SG
      DIMENSION I1(35,18),J2(4),I2(19),A(35),I3(18),D(35),
     1E(35),I4(18),1Z(35)
      CDIN=2
      LST=3
      I2(1)=2
      I2(2)=3
      I2(3)=5
      I2(4)=7
      I2(5)=11
      I2(6)=13
      I2(7)=17
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      I2(8)=19
      I2(9)=23
      I2(10)=29
      I2(11)=31
      I2(12)=37
      I2(13)=41
      I2(14)=43
      I2(15)=47
      I2(16)=53
      I2(17)=59
      I2(18)=61
      I2(19)=67
      IPG=0
      DO 51 LG=5,23,2
      L2=LG-1
      KUP=((LG+4)/5)*5
      LIM=2*L2+1
      I=1
      JUP=1
    1 I=I+1
      IF(I2(I)-LIM)2,3,54
    2 JUP=JUP+1
      GO TO 1
    3 JUP=JUP+1
   54 MUP=L2+1
      NUP=(L2/4)*4+1
      DO 51 NX=1,NUP,4
      N1=NX-1
      DO 51 MX=1,LG
      M1=MX-1
      DO 4 I=1,KUP
      A(I)=0.
      Z(I)=0.
      DO 4 J=1,JUP
    4 I1(I,J)=0
      IF(M1-N1)5,6,6
    5 M2=N1
      N2=M1
      K3=M2-N2
C
C     SIGN CHANGE ACCOMPANYING INTERCHANGE OF M,N FOR M+N
C     ODD, SEE ROE
C     EQ. (A11).
      S=(K3/2)*4-K3*2+1
      GO TO 7
    6 M2=M1
      N2=N1
      S=1.
      K3=M2-N2
C
```

```
C     SET UP LIMIT FOR 2F1 SERIES, SEE ROE EQ. (A6).
    7 LIM=L2-M2+1
      IF(LIM-1)8,8,9
    8 GO TO 16
    9 LIX=LIM-1
      DO 15 I=1,LIX
      IF(I-1)12,12,10
   10 DO 11 L=1,JUP
   11 I1(I+1,L)=I1(I,L)
C
C     J2(1)=GAMMA, GAMMA+1,---.
   12 J2(1)=M2-N2+I
C
C     J2(2)=MINUS ALPHA, MINUS(ALPHA+1),---,1.
      J2(2)=L2-M2+1-I
C
C
C     J2(3)=1,2,---.
      J2(3)=I
C
C     J2(4)=BETA, BETA+1,---.
      J2(4)=L2+M2+I
      DO 14 J=1,4
      K2=J2(J)
C
C     REDUCE PRODUCTS, QUOTIENTS OF TERMS IN EQ. (A6) TO
C     LOWEST TERMS.
      CALL RED(J,K2,I2,I3,JUP)
      DO 13 K=1,JUP
   13 I1(I+1,K)=I3(K)+I1(I+1,K)
   14 CONTINUE
   15 CONTINUE
   16 DO 17 I=1,LIM
      A(I)=2*I-(I/2)*4-1
      A(I)=S*A(I)
      DO 17 J=1,JUP
      B=I2(J)
   17 A(I)=A(I)*B**I1(I,J)
C
C     HAVE CALCULATED 2F1(-L+M,L+M+1;M-N+1;T), SEE ROE
C     EQ. (A5).
C
C     EXPRESS 2F1 IN TERMS OF XI, SEE ROE EQ. (A2).
      CALL TTX(LIM,A,M,N,J,K2,I2,I3,C,JUP)
C
C     EXPAND (1+XI)**N IN POWERS OF XI.
      N3=N2+1
      IF(N2)19,18,19
   18 D(1)=1.
      GO TO 21
```

```
   19 DO 20 I=1,N3
      N=I-1
      CALL CBN(N2,N,J,K2,I2,I3,C,JUP)
   20 D(I)=C
C
C     EXPAND PRODUCT OF 2F1*(1+XI)**N IN POWERS OF XI.
   21 DO 22 I=1,LG
   22 E(I)=0.
      DO 23 I=1,LIM
      DO 23 L=1,N3
   23 E(I+L-1)=A(I)*D(L)+3(I+L-1)
      LIM=LIM+N2
      DO 24 I=1,LG
      A(I)=0.
   24 D(I)=0.
C
C     EXPRESS 2F1*(1+XI)**N AS A COSINE SERIES.
      B=4.
      DO 29 I=1,LIM
      B=B/2.
      IF(I-2)25,25,26
   25 A(I)=E(I)
      GO TO 29
   26 M=I-1
      K=M/2.
      LM1=I/2
      DO 27 L=1,LM1
      N=L-1
      CALL CBN(M,N,J,K2,I2,I3,C,JUP)
      LL=M-2*L+3
   27 A(LL)=B*C*E(I)+A(LL)
      IF(M-(M/2)*2)28,28,29
   28 CALL CBN(M,K,J,K2,I2,I3,C,JUP)
      A(1)=0.5*B*C*E(I)+A(1)
   29 CONTINUE
C
C     EXPRESS (1-XI**2)**(M-N)/2 = (SIN THETA)**(M-N) AS
C     A SINE (M-N ODD) OR COSINE (M-N EVEN) SERIES.
      M=M2-N2
      K=M/2
      IF(M)31,30,31
   30 D(1)=1.
      GO TO 34
   31 LM2=(M2-N2+1)/2
      DO 32 L=1,LM2
      N=L-1
      CALL CBN(M,N,J,K2,I2,I3,C,JUP)
      LL=M-2*L+3
      MM=K-L+1
      F=4*(MM/2)-2*MM+1
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```
   32 D(LL)=C*F
      IF(M-2*K)34,33,34
   33 CALL CBN(M,K,J,K2,I2,I3,C,JUP)
      D(1)=0.5*C
   34 CONTINUE
C
C     HAVE EXPRESSED (SIN THETA)**(M-N) AS SINE OR COSINE
C     SERIES.
C
C     COMBINE (1-XI**2)**(M-N)/2 EXPRESSED AS A SINE (M-N
C     ODD) OR COSINE (M-N EVEN) SERIES WITH 2F1**(1+XI)**N
C     EXPRESSED AS A COSINE SERIES, EXPRESS PRODUCT AS
C     SINE (M-N ODD) OR COSINE (M-N EVEN) SERIES.
      DO 35 I=1,KUP
   35 E(I)=0.
      LL=M-2*K+1
      SN=4*K-2*M+1
      M3=M+1
      DO 38 I=LL,M3,2
      DO 38 L=1,LIM
      L3=I+L-1
      E(L3)=0.5*D(I)*A(L)+E(L3)
      L3=I-L
      SG=1.
      IF(L3)36,37,37
   36 L3=-L3
      SG=SN
   37 L3=L3+1
   38 E(L3)=0.5*SG*D(I)*A(L)+E(L3)
      S=(K3/2)*2-K3+1
C
C     SETS COEFFICIENT OF SIN 0 THETA = 0 FOR M-N ODD.
      E(1)=S*E(1)
C
C     CALCULATE (N SUB LMN) SQUARED.
      LIX=M3+LIM-1
      B=2*L2+1
      B=B/2.
      DO 39 I=1,JUP
   39 I4(I)=0
      J=2
      K2=L2+M2
      CALL FAC(J,K2,I2,I3,I4,JUP)
      J=1
      K2=L2-M2
      CALL FAC(J,K2,I2,I3,I4,JUP)
      J=2
      K2=L2-N2
      CALL FAC(J,K2,I2,I3,I4,JUP)
      J=1
```

```
      K2=L2+N2
      CALL FAC(J,K2,I2,I3,I4,JUP)
      DO 40 L=1,2
      J=1
      K2=M2-N2
   40 CALL FAC(J,K2,I2,I3,I4,JUP)
      DO 41 I=1,JUP
      C=I2(I)
   41 B=B*C**I4(I)
      B=SQRT(B)
C
C     HAVE CALCULATED N SUB LMN.
C
C     (1/2)**M, SEE ROE, EQS. (A2), (A3).
      B=B*0.5**M2
      IF(M2-N2)43,43,42
C
C     (1/2)**(M-N-1) ARISING IN CONVERSION OF (SIN THETA)**
C     (M-N) TO SINE OR COSINE SERIES.
   42 B=B*0.5**(M2-N2-1)
   43 DO 44 I=1,LIX
      J=(L2-(L2/2)*2)-(I-(I/2)*2)
      IF(M1*M1*N1*N1+J*J)52,52,53
   52 E(I)=0.
   53 E(I)=B*E(I)
   44 Z(I)=E(I)
      IJJ=1
      LOW=1
   45 HIG=LOW+4
      IF(IPG)48,46,48
   46 WRITE(LST,47)
   47 FORMAT(1H1)
      IPG=60
   48 WRITE(LST,49)(Z(I),I=LOW,HIG),L2,M1,N1,IJJ
   49 FORMAT(1X5E14.7,2X,4I2)
      WRITE(7,50)(Z(I),I=LOW,HIG),L2,M1,N1,IJJ
   50 FORMAT(5E14.7,2X,4I2)
      IPG=IPG-1
      LOW=LOW+5
      IJJ=IJJ+1
      IF(LOW-LIX)45,45,51
   51 CONTINUE
      ENDFILE 7
      REWIND 7
      CALL EXIT
      END
      SUBROUTINE RED(J,K2,I2,I3,JUP)
      DIMENSION I2(19),I3(18)
      K=1
      DO 1 L=1,JUP
```

```
  1 I3(L)=0
  2 IF(K2-1)3,7,3
  3 K3=I2(K)
    K4=K2/K3
    K5=K3*K4
    IF(K2-K5)5,4,5
  4 I3(K)=(-1)**J+I3(K)
    K2=K4
    GO TO 2
  5 IF(K-JUP)6,7,7
  6 K=K+1
    GO TO 2
  7 CONTINUE
    RETURN
    END
    SUBROUTINE CBN(M,N,J,K2,I2,I3,C,JUP)
    DOUBLE B,C
    DIMENSION I2(19),I3(18),I4(18)
    LST=3
    K=IABS(M)-M
    L=IABS(N)-N
    IF(K*K+L*L)2,1,2
  1 IF(M-N)2,4,4
  2 WRITE(LIST,3)
  3 FORMAT(36H M OR N NEGATIVE OR N GREATER THAN M)
    GO TO 13
  4 C=1.
    DO 5 I=1,JUP
  5 I4(I)=0
    IF(M*N)7,6,7
  6 GO TO 13
  7 DO 11 K=1,N
    J=2
    K2=M-K+1
  8 CALL RED(J,K2,I2,I3,JUP)
    DO 9 I=1,JUP
  9 I4(I)=I3(I)+I4(I)
    GO TO(11,10),J
 10 J=1
    K2=K
    GO TO 8
 11 CONTINUE
    DO 12 L=1,JUP
    B=I2(L)
 12 C=C*B**I4(L)
 13 CONTINUE
    RETURN
    END
    SUBROUTINE TTX(LIM,A,M,N,J,K2,I2,I3,C,JUP)
    DOUBLE A,B,C,D
```

```
      DIMENSION A(35),I2(19),I3(18)
      B=2.
      DO 3 I=1,LIM
      M=I-1
      B=B/2.
      DO 3 L=1,I
      N=L-1
      CALL CBN(M,N,J,K2,I2,I3,C,JUP)
      D=2*L-(L/2)*4-1
      IF(I-L)2,1,2
    1 A(L)=B*C*D*A(I)
      GO TO 3
    2 A(L)=B*C*D*A(I)+A(L)
    3 CONTINUE
      RETURN
      END
      SUBROUTINE FAC(J,K2,I2,I3,I4,JUP)
      DIMENSION I2(19),I3(18),I4(18)
      IF(K2-1)3,3,1
    1 DO 3 I=2,K2
      K5=I
      CALL RED(J,K5,I2,I3,JUP)
      DO 2 K=1,JUP
    2 I4(K)=I3(K)+I4(K)
    3 CONTINUE
      RETURN
      END
```

*NOTE:* Since submission of this paper for publication, Dr. Jan Pospiech has called to my attention a paper[7] written in cooperation with Dr. Jerzy Jura. Their paper contains the listing of a FORTRAN IV program in which the Fourier coefficients of the generalized spherical functions are directly calculated.

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