сообщения
объединенного
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дубна

E10 - 12354

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C. The KATØK-F Auxiliary Modules

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Гаджоков В.

E10 - 12354

Обработка дискретных ядерных спектров на малых ЭВМ.
С. Вспомогательные модули КАТØК-Ф.

Эта работа - последняя в серии из трех, посвященных детальному описанию алгоритма программы КАТØК, которая после девятилетней эксплуатации на ЭВМ Минск-2 была усовершенствована и написана заново на ФОРТРАНЕ.

В работе дан полный текст 16-ти вспомогательных модулей программы и приведены данные о решенных тестовых задачах.

Работа выполнена в Лаборатории ядерных проблем ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1979

Gadjokov V.

E10 - 12354

Processing of Discrete Nuclear Spectra on Small Computers. C. The KATØK-F Auxiliary Modules

This paper is the last in a series of three dedicated to the detailed description of the KATØK-F algorithm. This code has recently been revised and re-written in FORTRAN after being run on Minsk-2 for nine years.

The full text of the remaining 16 auxiliary modules is reported and information on test problems solved is given.

The investigation has been performed at the Laboratory of Nuclear Problems, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1979

5.7. The KATØK-F Text (continued)

In two previous papers[1,2] we have described the mathematical foundations and the programmer's choices needed for the composition of the KATØK-F package as well as the texts of two chief modules. The full FORTRAN-IV text of the remaining auxiliary modules is reported here. For the sake of consistency, through-numbering of sections and formulae has been applied to the whole series of three reports.

The text reported is complete; in particular, a short dummy module (GRAPH) has also been included to allow for an immediate application of the entire package.

The program described has also been thoroughly tested. It solves, e.g., the Stachura's problem[3] with automatic reduction of superfluous peaks. Sample processing of real data shows full consistency with results of an earlier version[4] which is being used in the JINR since 1970 on,

```
      SUBROUTINE TITLE
      DIMENSION LBUF(80),LK(9,10),LA(9,10),LT(9,11),LO(9,10),LU(9,10),
     *                  LP(9,10)
      DATA LK/18*1HK,  6*1H ,2*1HK,1H ,    5*1H ,2*1HK,2*1H ,
     1              4*1H ,2*1HK,3*1H ,    3*1H ,3*1HK,3*1H ,
     2     2*1H ,2*1HK,1H ,2*1HK,2*1H ,    1H ,2*1HK,3*1H ,2*1HK,1H ,
     3              2*1HK,5*1H ,2*1HK,    1HK,7*1H ,1HK/
C
      DATA LA/                3*1H ,6*1HA,    2*1H ,7*1HA,
     1   1H ,2*1HA,2*1H ,2*1HA,2*1H ,    2*1HA,3*1H ,2*1HA,2*1H ,
     2        2*1HA,3*1H ,2*1HA,2*1H ,    2*1HA,3*1H ,2*1HA,2*1H ,
     3        2*1HA,3*1H ,2*1HA,2*1H ,    1H ,2*1HA,2*1H ,2*1HA,2*1H ,
     4                2*1H ,7*1HA,    3*1H ,6*1HA/
C
      DATA LT/2*1HT,7*1H ,   2*1HT,7*1H ,   2*1HT,7*1H ,   2*1HT,7*1H ,
     1 27*1HT,2*1HT,7*1H ,   2*1HT,7*1H ,   2*1HT,7*1H ,   2*1HT,7*1H /
C
      DATA LO/2*1H ,5*1HO,2*1H ,    1H ,7*1HO,1H ,
     1         2*1HO,5*1H ,2*1HO,    2*1HO,5*1H ,2*1HO,
     2         2*1HO,5*1H ,2*1HO,    2*1HO,5*1H ,2*1HO,
     3         2*1HO,5*1H ,2*1HO,    2*1HO,5*1H ,2*1HO,
     4             1H ,7*1HO,1H ,    2*1H ,5*1HO,2*1H /
C
```

```
C
      DATA LU/7*1HU,2*1H ,   8*1HU,1H ,     7*1H ,2*1HU,   7*1H ,2*1HU,
     1        7*1H ,2*1HU,   7*1H ,2*1HU,   7*1H ,2*1HU,   7*1H ,2*1HU,
     2        8*1HU,1H ,     7*1HU,2*1H /
C
      DATA LP/18*1HP, 2*1HP,3*1H ,2*1HP,2*1H , 2*1HP,3*1H ,2*1HP,2*1H ,
     1                2*1HP,3*1H ,2*1HP,2*1H , 2*1HP,3*1H ,2*1HP,2*1H ,
     2                2*1HP,3*1H ,2*1HP,2*1H , 2*1HP,3*1H ,2*1HP,2*1H ,
     3                          1H ,5*1HP,3*1H , 2*1H ,3*1HP,4*1H /
C
      DATA LSP/1H /
   99 FORMAT(    ///////////)
  100 FORMAT(1H ,70A1)
  101 FORMAT(  //  /)
  102 FORMAT(1H ,76A1)
C
      WRITE(1,99)
      DO 10 I=1,9
      DO 1 K=1,9
    1 LBUF(K)=LSP
      DO 2 K=1,10
      KB=K+9
    2 LBUF(KB)=LK(I,K)
      LBUF(20)=LSP
      LBUF(21)=LSP
      DO 3 K=1,10
      KB=K+21
    3 LBUF(KB)=LA(I,K)
      LBUF(32)=LSP
      LBUF(33)=LSP
      DO 4 K=1,11
      KB=K+33
    4 LBUF(KB)=LT(I,K)
      LBUF(45)=LSP
      LBUF(46)=LSP
      DO 5 K=1,10
      KB=K+46
    5 LBUF(KB)=LO(I,K)
      LBUF(57)=LSP
      LBUF(58)=LSP
      DO 6 K=1,10
      KB=K+58
    6 LBUF(KB)=LK(I,K)
   10 WRITE(1,100)(LBUF(KK),KK=1,68)
      WRITE(1,101)
C
C
C
      DO 20 I=1,9
      LBUF(1)=LSP
      LBUF(2)=LSP
      DO 11 K=1,10
      KB=K+2
   11 LBUF(KB)=LO(I,K)
      LBUF(13)=LSP
      LBUF(14)=LSP
      DO 12 K=1,10
      KB=K+14
```



```
   12 LBUF(KB)=LU(I,K)
      LBUF(25)=LSP
      LBUF(26)=LSP
      DO 13 K=1,11
      KB=K+26
   13 LBUF(KB)=LT(I,K)
      LBUF(38)=LSP
      LBUF(39)=LSP
      DO 14 K=1,10
      KB=K+39
   14 LBUF(KB)=LP(I,K)
      LBUF(50)=LSP
      LBUF(51)=LSP
      DO 15 K=1,10
      KB=K+51
   15 LBUF(KB)=LU(I,K)
      LBUF(62)=LSP
      LBUF(63)=LSP
      DO 16 K=1,11
      KB=K+63
   16 LBUF(KB)=LT(I,K)
   20 WRITE(1,102)(LBUF(KK),KK=1,74)
      WRITE(1,25)
   25 FORMAT(1H ////)
      RETURN
      END
C
      FUNCTION ALF0(THETA)
C CALCULATES INITIAL VALUE OF REGULARIZER
      DATA THEMAX,R0,R/24.0,0.125,3.0/
      DATA IFLAG/1/
      IF(IFLAG)20,10,20
   10 IFLAG=1
      WRITE(1,101)
      READ(1,102)IANSWR
      IF(IANSWR.NE.1HY)GO TO 20
      WRITE(1,103)
      READ(1,104)THEMAX,R0,R
   20 IF(THETA.GT.THEMAX)THETA=THEMAX
      ALF0=EXP(R0*THETA+R)
      RETURN
  101 FORMAT("WOULD YOU LIKE TO SET NEW VALUES OF: LIMITING DEFECT,"/
     1       "                                     ITS FACTOR,"/
     2       "                                     AND DECREMENT ?"/
     3       "IF YOU DON'T WANT OR DON'T KNOW HOW TO DO IT, ANSWER 'NO'")
  102 FORMAT(A1)
  103 FORMAT("ENTER THEM THEN IN '3F10.5'-FORMAT !")
  104 FORMAT(3F10.5)
      END
C
      FUNCTION ALPHA(ALPH0,ITER)
C CALCULATES VALUE OF REGULARIZER AT ITERATION NO. 'ITER'
      DATA R,ALINF/0.399952,0.02/
      DATA IFLAG/1/
      IF(IFLAG)20,10,20
   10 IFLAG=1
      WRITE(1,101)
      READ(1,102)IANSWR
      IF(IANSWR.NE.1HY)GO TO 20
      WRITE(1,103)
```

```
      READ(1,104)R,ALINF
   20 ALPHA=ALPH0*EXP(-R*FLOAT(ITER))+ALINF
      RETURN
  101 FORMAT("WOULD YOU LIKE TO SET NEW VALUES OF: DECREMENT"/
     1       "                                  AND LOWER LIMIT ?"/
     2       "IF YOU DON'T WANT OR DON'T KNOW HOW TO DO IT, ANSWER 'NO'")
  102 FORMAT(A1)
  103 FORMAT("ENTER THEM THEN IN '2F10.5'-FORMAT")
  104 FORMAT(2F10.5)
      END
C
      SUBROUTINE GRAPH(N,X,Y,Z,U)
      WRITE(1,10)
   10 FORMAT(   /"NO GRAPHIC PROVISION ON 80-COL.PRINT")
      RETURN
      END
C
      FUNCTION SERIN(X)
C THIS CODE CALCULATES THE INTEGRAL OF THE FUNCTION
C          (1/SQRT(3.14159))*EXP(-Z**2)
C OVER THE INTERVAL [-X,+X]. METHOD USED: POWER SE-
C RIES EXPANSION. BUILT-IN PRECISION: 0.00005.
      DIMENSION C(26)
      DATA C/.333333,.300000,.238095,.194444,.163636,
     1       .141026,.123810,.110294,.994152E-1,.904762E-1,
     2 .830040E-1,.766667E-1,.712251E-1,.665025E-1,.623656E-1,
     3 .587121E-1,.554622E-1,.525526E-1,.499325E-1,.475610E-1,
     4 .454042E-1,.434343E-1,.416281E-1,.399660E-1,.384314E-1,
     5 .370102E-1/
      IF(ABS(X)-2.82843)20,10,10
   10 SERIN=0.886227
      IF(X)11,12,12
   11 SERIN=-SERIN
   12 RETURN
   20 X2=X*X
      SERIN=X
      AN=X
      DO 30 L=1,26
      AN=-X2*AN*C(L)
      IF(ABS(AN)-.00005)40,25,25
   25 SERIN=SERIN+AN
   30 CONTINUE
   40 CONTINUE
      RETURN
      END
C
      SUBROUTINE INVKA(A,N,D,L,M)
      DIMENSION A(1),L(1),M(1)
C SEARCH FOR LARGEST ELEMENT
      D=1.0
      NK=-N
      DO 80 K=1,N
      NK=NK+N
      L(K)=K
      M(K)=K
      KK=NK+K
      BIGA=A(KK)
      DO 20 J=K,N
      IZ=N*(J-1)
      DO 20 I=K,N
```



```
      IJ=IZ+I
      IF(ABS(BIGA)-ABS(A(IJ))) 15,20,20
   15 BIGA=A(IJ)
      L(K)=I
      M(K)=J
   20 CONTINUE
C
C INTERCHANGE ROWS
C
      J=L(K)
      IF(J-K)35,35,25
   25 KI=K-N
      DO 30 I=1,N
      KI=KI+N
      HOLD=-A(KI)
      JI=KI-K+J
      A(KI)=A(JI)
   30 A(JI)=HOLD
C
C INTERCHANGE COLUMNS
C
   35 I=M(K)
      IF(I-K)45,45,38
   38 JP=N*(I-1)
      DO 40 J=1,N
      JK=NK+J
      JI=JP+J
      HOLD=-A(JK)
      A(JK)=A(JI)
   40 A(JI)=HOLD
C
C DIVIDE COLUMN BY MINUS PIVOT (VALUE OF PIVOT ELEMENT
C                               IS CONTAINED IN BIGA)
C
   45 IF(BIGA)48,46,48
   46 D=0.0
      RETURN
   48 DO 55 I=1,N
      IF(I-K)50,55,50
   50 IK=NK+I
      A(IK)=A(IK)/(-BIGA)
   55 CONTINUE
C
C REDUCE MATRIX
C
      DO 65 I=1,N
      IK=NK+I
      HOLD=A(IK)
      IJ=I-N
      DO 65 J=1,N
      IJ=IJ+N
      IF(I-K)60,65,60
   60 IF(J-K)62,65,62
   62 KJ=IJ-I+K
      A(IJ)=HOLD*A(KJ)+A(IJ)
   65 CONTINUE
C
C DIVIDE ROW BY PIVOT
C
      KJ=K-N
```

```
      DO 75 J=1,N
      KJ=KJ+N
      IF(J-K)70,75,70
   70 A(KJ)=A(KJ)/BIGA
   75 CONTINUE
C
C PRODUCT OF PIVOTS
C
      D=D*BIGA
C
C REPLACE PIVOT BY RECIPROCAL
C
      A(KK)=1.0/BIGA
   80 CONTINUE
C
C FINAL ROW AND COLUMN INTERCHANGE
C
      K=N
  100 K=(K-1)
      IF(K)150,150,105
  105 I=L(K)
      IF(I-K)120,120,108
  108 JQ=N*(K-1)
      JR=N*(I-1)
      DO 110 J=1,N
      JK=JQ+J
      HOLD=A(JK)
      JI=JR+J
      A(JK)=-A(JI)
  110 A(JI)=HOLD
  120 J=M(K)
      IF(J-K)100,100,125
  125 KI=K-N
      DO 130 I=1,N
      KI=KI+N
      HOLD=A(KI)
      JI=KI-K+J
      A(KI)=-A(JI)
  130 A(JI)=HOLD
      GO TO 100
  150 RETURN
      END
C
C
C
C
C
C
C
C
      SUBROUTINE THETL(VALUE)
C COMPUTES 'VALUE' OF LONG SOLUTION DEFECT WITH LENGTH 'LENGTH'
C NOTE: MAX.LENGTH=5 (ENTERED VIA 'BLOCK DATA')
C
C
      LOGICAL PSV,OOV
      COMMON PSV(5)
      COMMON OOV(3)
      COMMON MM,M,K,L,N
      COMMON          Q(100),YQ(100),X0(40),IDENTF(36),NFC,NLC
```



```
      COMMON          W(100),FXT(100),F1XT(100,40),YQT(100),XT(40),
     1                ETOT(40),C(40),BGPC(6),WEIGHT(5),STACK(5),DUM(280),
     2                V(40,40),DELTXT(40),
     3                     MSWICH,NSECT,ITER,THETAT,THETIG,THETLT,REG,
     4                THECPS,THECPL,INTERR,DET
      COMMON          LENGTH
      COMMON          THETLM,TLIM,LMIN,LMAX,NMIN,NMAX,KMIN,KMAX,MMAX,
     1                MMDMAX,DEGER,ITRMAX,DEVMIN,SRCOEF
C
      VALUE=0.0
      DO 10 I=1,LENGTH
      VALUE=VALUE+WEIGHT(I)*STACK(I)
   10 CONTINUE
      RETURN
      END
C
C
      SUBROUTINE FLSTK(VALUE)
C FILS IN STACK OF SOLUTION DEFECT VALUES; DOES NOT DESTROY 'VALUE'
C
C
      LOGICAL PSV,OOV
      COMMON PSV(5)
      COMMON OOV(3)
      COMMON MM,M,K,L,N
      COMMON          Q(100),YQ(100),X0(40),IDENTF(36),NFC,NLC
      COMMON          W(100),FXT(100),F1XT(100,40),YQT(100),XT(40),
     1                ETOT(40),C(40),BGPC(6),WEIGHT(5),STACK(5),DUM(280),
     2                V(40,40),DELTXT(40),
     3                     MSWICH,NSECT,ITER,THETAT,THETIG,THETLT,REG,
     4                THECPS,THECPL,INTERR,DET
      COMMON          LENGTH
      COMMON          THETLM,TLIM,LMIN,LMAX,NMIN,NMAX,KMIN,KMAX,MMAX,
     1                MMDMAX,DEGER,ITRMAX,DEVMIN,SRCOEF
C
      DO 10 I=1,4
      STACK(I+1)=STACK(I)
      IF((I+1).GT.LENGTH)STACK(I+1)=0.0
   10 CONTINUE
      STACK(1)=VALUE
      RETURN
      END
C
C
C CALCULATE APPROXIMATING VALUE OF SPECTRUM AND JACOBI-MATRIX
C        (ISOLATED PEAKS SUPPOSED SYMMETRIC GAUSSIANS)
C
C DESCRIPTION OF ARGUMENTS:
C    IC - REGIME SWITCH
C         WHEN:   1    CALCULATE ACTUAL NUMBER OF UNKNOWNS N
C                 2    COMPUTE SPECTRUM VALUE IN V(1)
C                 3    CALCULATE N VALUES OF DERIVATIVES IN V(1) TO V(N)
C                 4    CALCULATE PURE SPECTRUM
C                 5    COMPUTE PURE BACKGROUND
C    X  - VALUE OF ARGUMENT (CHANNEL NUMBER)
C    V  - ARRAY OF RESULTS
C
      SUBROUTINE SYMGA(IC,X,V)
C
C
```

```
C
      LOGICAL PSV,OOV
      COMMON PSV(5)
      COMMON OOV(3)
      COMMON MM,M,K,L,N
      COMMON          Q(100),YQ(100),X0(40),IDENTF(36),NFC,NLC
      COMMON          W(100),FXT(100),F1XT(100,40),YQT(100),XT(40),
     1                ETOT(40),C(40),BGPC(6),WEIGHT(5),STACK(5),DUM(280),
     2                VA(40,40),DELTXT(40),
     3                      MSWICH,NSECT,ITER,THETAT,THETIG,THETLT,REG,
     4                THECPS,THECPL,INTERR,DET
      COMMON          LENGTH
      COMMON          THETLM,TLIM,LMIN,LMAX,NMIN,NMAX,KMIN,KMAX,MMAX,
     1                MMDMAX,DEGER,ITRMAX,DEVMIN,SRCOEF
C
C
C
      DIMENSION V(1)
      DATA ROOT2,ROOTPI/1.41421,1.77245/
C
C
C REGIME SWITCH
C
      GO TO(100,200,300,400,500),IC
C
C NUMBER OF UNKNOWNS
C
  100 N=2*K+L+2
      RETURN
C
C
C COMPUTE APPROXIMATING VALUE OF SPECTRUM FOR GIVEN PARAMETER SET
C
  200 GO TO 400
  210 GO TO 500
  220 V(1)=SPECTR+BGR
      RETURN
C
C COMPUTE DERIVATIVES (JACOBI MATRIX)
C
C          A. PREPARATORY STAGE
  300 V(1)=0.0
      SIGRT2=XT(1)*ROOT2
      SIGR2P=SIGRT2*ROOTPI
      SIGRPI=XT(1)*ROOTPI
      IINBGR=2*K+2
      XSHIFT=Q(1)+FLOAT(M-1)/2.0
C
C          B. DERIVATIVES ON SPECTRUM PARAMETERS
      DO 310 I=1,K
      IPOS=2*I
      IAREA=IPOS+1
      TI=(X-XT(IPOS))/SIGRT2
      PI=TI-1.0/SIGRT2
      SI=XT(IAREA)*C(IAREA)
      DIFF=SERIN(TI)-SERIN(PI)
      EXPI2=EXP(-(PI**2))
      EXTI2=EXP(-(TI**2))
      V(1)=V(1)+SI*(PI*EXPI2-TI*EXTI2)
      V(IPOS)=SI*(EXPI2-EXTI2)/SIGR2P
```



```
  310 V(IAREA)=C(IAREA)*DIFF/ROOTPI
      V(1)=V(1)/SIGRPI
C
C          C. DERIVATIVES ON BACKGROUND PARAMETERS
      IF(L)350,330,330
  330 DO 340 I=IINBGR,N
      IDEG=I-IINBGR
      IF(IDEG)334,332,334
  332 V(I)=C(I)
      GO TO 340
  334 V(I)=C(I)*(X-XSHIFT)**IDEG
  340 CONTINUE
  350 RETURN
C
C COMPUTE PURE SPECTRUM
C
C          A. PREPARATORY STAGE
  400 SPECTR=0.0
      SIGRT2=XT(1)*ROOT2
C
C          B. PILE UP PEAK CONTRIBUTION
      DO 410 I=1,K
      IPOS=2*I
      IAREA=IPOS+1
      TI=(X-XT(IPOS))/SIGRT2
      PI=TI-1.0/SIGRT2
      SERTI=SERIN(TI)
      SERPI=SERIN(PI)
  410 SPECTR=SPECTR+XT(IAREA)*C(IAREA)*(SERTI-SERPI)
      SPECTR=SPECTR/ROOTPI
C
C          C. EXIT LOGIC
      IF(IC.EQ.2)GO TO 210
      V(1)=SPECTR
      RETURN
C
C CALCULATE PURE BACKGROUND
C
C          A. PREPARATORY STAGE
  500 IINBGR=2*K+2
      XSHIFT=Q(1)+FLOAT(M-1)/2.0
C
C          B. BRANCH ON L
      IF(L)505,510,515
  505 BGR=0.0
      GO TO 590
  510 BGR=XT(N)*C(N)
      GO TO 590
C
C          C. HORNER'S SCHEME AT L>0
  515 IEND=N-1
      BGR=XT(N)*C(N)
      DO 520 I=IINBGR,IEND
      KK=N-I+IINBGR-1
  520 BGR=BGR*(X-XSHIFT)+XT(KK)*C(KK)
C
C          D. EXIT LOGIC
  590 IF(IC.EQ.2)GO TO 220
      V(1)=BGR
      RETURN
      END
```

```
C
C
C HANDLES I/O OPERATIONS OF "KATOK" (SEE DESCRIPTION OF COMMONS THERE)
C
C DESCRIPTION OF ARGUMENTS:
C   IC    - REGIME SWITCH; HAS THE FOLLOWING VALUES:
C           1  DIALOGUE SET OF OUTPUT OPTIONS
C           2  INPUT SPECTRUM IDENTIFIER & STREAM SIZE MM; PRINT HEADER
C           3  INPUT A DATA SECTION
C           4  PREPARE DATA FOR COMPUTATION: A. REQUEST N
C                                            B. CALCULATE X0
C                                            C. RENORMALIZE (SCALE)
C                                            D. CHECK CONSISTENCY
C           5  POINT-DATA OUTPUT
C           6  PARAMETER OUTPUT (WITH OR WITHOUT GRAPHS)
C           7  PRINT PROGRAM STATUS VECTOR & DATA DURING EXECUTION
C           8  PRINT ERROR MESSAGES
C           9  CHECK AND - IF NEEDED - REDUCE PEAK NUMBER "K"
C   YDER - FUNCTION-CUM-DERIVATIVES SUBROUTINE
C
C
C PERIPHERAL-UNIT ALLOCATION OF PRESENT VERSION:
C     3 - LINE PRINTER
C     4 - SYSTEM CONSOLE
C     5 - PAPER-TAPE READER
C
C
C SUBROUTINE CHOPPED ARTIFICIALLY DUE TO OVERCORE IN FORTD-COMPILER
      SUBROUTINE INOUT(IC,YDER)
C
C
C
      LOGICAL PSV,OOV
      COMMON PSV(5)
      COMMON OOV(3)
      COMMON MM,M,K,L,N
      COMMON         Q(100),YQ(100),X0(40),IDENTF(36),NFC,NLC
      COMMON         W(100),FXT(100),FIXT(100,40),YQT(100),XT(40),
     1               ETOT(40),C(40),BGPC(6),WEIGHT(5),STACK(5),DUM(280),
     2               V(40,40),DELTXT(40),
     3                     MSWICH,NSECT,ITER,THETAT,THETIG,THETLT,REG,
     4               THECPS,THECPL,INTERR,DET
      COMMON         LENGTH
      COMMON         THETLM,TLIM,LMIN,LMAX,NMIN,NMAX,KMIN,KMAX,MMAX,
     1               MMDMAX,DEGER,ITRMAX,DEVMIN,SRCOEF
C
C
C
C
C
C
C REGIME SWITCH
      GO TO(100,200,300,400,500,600,700,800,900),IC
C
C
  100 CALL INOU1
      RETURN
C
C
```



```
  200 CALL INOU2
      RETURN
C
C
  300 CALL INOU3
      RETURN
C
C
C PREPARATORY BLOCK - CHECKS, INITIAL GUESSES, SCALING, WEIGHTS
C
C
C CARRY OUT FIRST 4 CHECKS ON DATA CORRECTNESS (DIMENSION CHECKS)
  400 IF((L.LT.LMIN).OR.(L.GT.LMAX))MSWICH=1
      IF(MSWICH.EQ.1)GO TO 810
C
      IF((N.LT.NMIN).OR.(N.GT.NMAX))MSWICH=2
      IF(MSWICH.EQ.2)GO TO 820
C
      IF((K.LT.KMIN).OR.(K.GT.KMAX))MSWICH=3
      IF(MSWICH.EQ.3)GO TO 830
C
      IF((M.LT.(N+1)).OR.(M.GT.MMAX))MSWICH=4
      IF(MSWICH.EQ.4)GO TO 840
C
C CALCULATE INITIAL GUESSES OF PEAK PARAMETERS; THREE MORE DATA CHECKS
      X0(1)=0.0
      DO 410 I=1,K
      I1=4*(I-1)+1
      I2=I1+1
      I3=I2+1
      I4=I3+1
      QDEL=ABS(W(I1)-W(I3))
      YDEL=W(I2)-W(I4)
      IW1=INT(W(I1))
      IW3=INT(W(I3))
C
      IF(((IW1.LT.NFC).OR.(IW1.GT.NLC)).OR.
     *   ((IW3.LT.NFC).OR.(IW3.GT.NLC)))MSWICH=6
      IF(MSWICH.EQ.6)GO TO 860
C
      IF(IW1.EQ.IW3)MSWICH=8
      IF(MSWICH.EQ.8)GO TO 880
C
      IYQ2=IW1-NFC+1
      IYQ4=IW3-NFC+1
C
      IF((W(I2).NE.YQ(IYQ2)).OR.(W(I4).NE.YQ(IYQ4)))MSWICH=7
      IF(MSWICH.EQ.7)GO TO 870
C
C SET INITIAL GUESS OF POSITION
      IF(YDEL)405,405,406
  405 X0(2*I)=W(I3)
      GO TO 407
  406 X0(2*I)=W(I1)
  407 C(2*I)=1.0
C
C SET INITIAL GUESS OF AREA; RENORMALIZE
      AUXIL=QDEL*ABS(YDEL)
      IYQ2=INT(ALOG(AUXIL)/.693147+.5)
      C(2*I+1)=2.0**(IYQ2-3)
      X0
```

```
      X0(2*I+1)=AUXIL/C(2*I+1)
C
C PILE UP SUM OF FULL WIDTH AT HALF MAXIMUM (FWHM)
      X0(1)=X0(1)+QDEL
C
  410 CONTINUE
      X0(1)=X0(1)/(2.35482*FLOAT(K))
      C(1)=1.0
C
C          NOTE: IN COMPUTATION THE FIRST PARAMETER HAS THE
C                USUAL MEANING OF THE VARIANCE IN THE GAUSS
C                DISTRIBUTION. HOWEVER, THE PHYSICAL VALUE
C                OF FULL-WIDTH-AT-HALF-MAXIMUM IS
C                PRINTED OUT INSTEAD.
C
C FINAL CHECK & BACKGROUND INITIAL GUESSES; STATISTICAL WEIGHTS
      YQMIN=1.0E+20
      DO 420 I=1,M
      IF(YQ(I))412,414,416
  412 MSWICH=9
      GO TO 890
  414 W(I)=1.0
      GO TO 418
  416 W(I)=1.0/YQ(I)
  418 IF(YQ(I).LT.YQMIN)YQMIN=YQ(I)
  420 CONTINUE
C
      IF(L)490,440,440
  440 L1=L+1
      DO 450 I=1,L1
      I1=2*K+I+1
      C(I1)=BGPC(I)
      X0(I1)=0.0
      IF(I.EQ.1)X0(I1)=YQMIN/BGPC(1)
  450 CONTINUE
  490 DEVMIN=SQRT(YQMIN)
      RETURN
C
C
  500 CALL INOU5
      RETURN
C
C
  600 CALL INOU6
      RETURN
C
C
  700 CALL INOU7
      RETURN
C
C
C PRINT ERROR MESSAGES (MESSAGE NUMBER IS "MSWICH")
  800 IF(MSWICH.EQ.0)GO TO 899
      GO TO(810,820,830,840,850,860,870,880,890,892,894,896),MSWICH
  810 WRITE(1,2100)L
      RETURN
  820 WRITE(1,2101)
      RETURN
  830 WRITE(1,2102)
      RETURN
```



```
  840 WRITE(1,2103)
      RETURN
  850 WRITE(1,2104)
      RETURN
  860 WRITE(1,2106)
      RETURN
  870 WRITE(1,2107)
      RETURN
  880 WRITE(1,2108)
      RETURN
  890 WRITE(1,2105)
      RETURN
  892 WRITE(1,2109)
      RETURN
  894 WRITE(1,2110)K
      RETURN
  896 WRITE(1,2111)
  899 RETURN
C
C
C CHECK & COMPRESS (REDUCE PROBLEM)
  900 IR=0
  901 IF(K-1)999,999,902
  902 KEND1=K-1
      CRIT=2.50663*XT(1)*YQMIN/SRCOEF
      DO 990 K1=1,KEND1
      KPOS1=2*K1
      KAREA1=KPOS1+1
      AREA1=XT(KAREA1)*C(KAREA1)

      IF(AREA1.LE.CRIT)GO TO 930
      KIN2=K1+1
      DO 980 K2=KIN2,K
      KPOS2=2*K2
      KAREA2=KPOS2+1
      AREA2=XT(KAREA2)*C(KAREA2)
      IF(AREA2.LE.CRIT)GO TO 940
      IF(ABS(XT(KPOS1)-XT(KPOS2)).LE.2.35482*XT(1)/SRCOEF)GO TO 950
      GO TO 980
C
C FIRST PEAK NEGLIGIBLE
  930 DO 931 I=KPOS1,N
      XT(I)=XT(I+2)
  931 C(I)=C(I+2)
      GO TO 960
C
C SECOND PEAK NEGLIGIBLE
  940 DO 941 I=KPOS2,N
      XT(I)=XT(I+2)
  941 C(I)=C(I+2)
      GO TO 960
C
C TWO PEAKS TOO NEAR
  950 XT(KPOS1)=(XT(KPOS1)+XT(KPOS2))/2.0
      XT(KAREA1)=XT(KAREA1)*C(KAREA1)+XT(KAREA2)*C(KAREA2)
      C(KAREA1)=AMAX1(C(KAREA1),C(KAREA2))
      XT(KAREA1)=XT(KAREA1)/C(KAREA1)
      DO 951 I=KPOS2,N
      XT(I)=XT(I+2)
  951 C(I)=C(I+2)
  960 K=K-1
```

```
      N=N-2
      IR=1
      DO 962 I=1,N
  962 XØ(I)=XT(I)
      GO TO 9Ø1
C
  98Ø CONTINUE
  99Ø CONTINUE
  999 IF(IR.EQ.1)MSWICH=11
      IR=Ø
      RETURN
C
C
C FORMAT STATEMENTS - TO BE REVISED FOR 8Ø-COLUMN PRINT
C FORMAT STATEMENTS
 21ØØ FORMAT(     "***L=",I3," : OUTSIDE PERMITTED LIMITS [-1,5]")
 21Ø1 FORMAT(     "***UNKNOWN PARAMETERS OUTSIDE LIMITS [3,4Ø]")
 21Ø2 FORMAT(     "***NUMBER OF PEAKS OUTSIDE LIMITS [1,19]")
 21Ø3 FORMAT(     "***SECTION EITHER TOO SHORT OR TOO LONG")
 21Ø4 FORMAT(     "***RECONSIDER OPTIONS - TOO MUCH PRINTING REQUESTED")
 21Ø5 FORMAT(     "***ERROR: NEGATIVE VALUE OF COUNTS IN SECTION")
 21Ø6 FORMAT(     "***ERROR: CHARACTERISTIC POINTS OUTSIDE SECTION",
     *" BOUNDARIES")
 21Ø7 FORMAT(     "***ERROR: BAD ORDINATES OF CHARACTERISTIC POINTS")
 21Ø8 FORMAT(     "***ERROR: CHARACTERISTIC POINTS OF A PEAK ",
     *"COINCIDE")
 21Ø9 FORMAT(     ">>>WARNING: PROBLEM DEGENERATES AT SOLUTION POINT")
 211Ø FORMAT(     ">>>WARNING: PROBLEM REDUCED TO ",I2," PEAKS")
 2111 FORMAT(    /"######## END OF PROCESSING ########")
C
C
      END
C
C
C A CHOPPED PIECE OF INOUT-SUBROUTINE
      SUBROUTINE INOU1
C
C
C
C
C
      LOGICAL PSV,OOV
      COMMON PSV(5)
      COMMON OOV(3)
      COMMON MM,M,K,L,N
      COMMON         Q(1ØØ),YQ(1ØØ),XØ(4Ø),IDENTF(36),NFC,NLC
      COMMON         W(1ØØ),FXT(1ØØ),FIXT(1ØØ,4Ø),YQT(1ØØ),XT(4Ø),
     1               ETOT(4Ø),C(4Ø),BGPC(6),WEIGHT(5),STACK(5),DUM(28Ø),
     2               V(4Ø,4Ø),DELTXT(4Ø),
     3                     MSWICH,NSECT,ITER,THETAT,THETIG,THETLT,REG,
     4               THECPS,THECPL,INTERR,DET
      COMMON         LENGTH
      COMMON         THETLM,TLIM,LMIN,LMAX,NMIN,NMAX,KMIN,KMAX,MMAX,
     1               MMDMAX,DEGER,ITRMAX,DEVMIN,SRCOEF
C
C
      DATA IYES/2HY /
C
C DIALOGUE INPUT OF OPERATOR"S OUTPUT OPTIONS
      WRITE(1,19ØØ)
```



```
      READ(1,19Ø3)IAUX
      IF(IAUX.EQ.IYES)GO TO 2
      OOV(1)=.FALSE.
      GO TO 3
    2 OOV(1)=.TRUE.
    3 WRITE(1,19Ø1)
      READ(1,19Ø3)IAUX
      IF(IAUX.EQ.IYES)GO TO 5
      OOV(2)=.FALSE.
      GO TO 6
    5 OOV(2)=.TRUE.
    6 WRITE(1,19Ø2)
      READ(1,19Ø3)IAUX
      IF(IAUX.EQ.IYES)GO TO 8
      OOV(3)=.FALSE.
      GO TO 9
    8 OOV(3)=.TRUE.
    9 RETURN
C
 19ØØ FORMAT(     "SHOULD RESULTS BE PRINTED BY ITERATIONS ?")
 19Ø1 FORMAT(     "IS REGIME INFORMATION REQUIRED ?")
 19Ø2 FORMAT(     "SHOULD A PICTURE OF FINAL RESULTS BE DRAWN ?")
 19Ø3 FORMAT(A1)
      END
C
C
C A CHOPPED PIECE OF INOUT-SUBROUTINE
      SUBROUTINE INOU2
C
C
C
C
C
C
      LOGICAL PSV,OOV
      COMMON PSV(5)
      COMMON OOV(3)
      COMMON MM,M,K,L,N
      COMMON         Q(1ØØ),YQ(1ØØ),XØ(4Ø),IDENTF(36),NFC,NLC
      COMMON         W(1ØØ),FXT(1ØØ),FIXT(1ØØ,4Ø),YQT(1ØØ),XT(4Ø),
     1               ETOT(4Ø),C(4Ø),BGPC(6),WEIGHT(5),STACK(5),DUM(28Ø),
     2               V(4Ø,4Ø),DELTXT(4Ø),
     3                     MSWICH,NSECT,ITER,THETAT,THETIG,THETLT,REG,
     4               THECPS,THECPL,INTERR,DET
      COMMON         LENGTH
      COMMON         THETLM,TLIM,LMIN,LMAX,NMIN,NMAX,KMIN,KMAX,MMAX,
     1               MMDMAX,DEGER,ITRMAX,DEVMIN,SRCOEF
C
C
C
C INPUT SPECTRUM IDENTIFIER & STREAM SIZE; PRINT HEADER
      READ(5,1998)(IDENTF(I),I=1,36)
      READ(5,1999)MM
      WRITE(1,2ØØØ)
      WRITE(1,2ØØ1)
      WRITE(1,2ØØ2)(IDENTF(I),I=1,36),MM
 1998 FORMAT(36A2)
 1999 FORMAT(I3)
 2ØØØ FORMAT( ///1ØX,"DISCRETE SPECTRA PROCESSING ",
     *"BY 'KATOK' AUTOMATIC SUBROUTINE")
 2
```

```
2001 FORMAT(     14X,"VERSION F4/HP-21MX     DUBNA/AUGUST'78     ",
     *"V.GADJOKOV")
2002 FORMAT(     "STREAM PROCESSED -"/     36A2,/
     *48X,"- CONSISTS OF ",I3," SECTIONS")
      RETURN
      END
C
C
C A CHOPPED PIECE OF INOUT-SUBROUTINE
      SUBROUTINE INOU3
C
C
C
C
      LOGICAL PSV,OOV
      COMMON PSV(5)
      COMMON OOV(3)
      COMMON MM,M,K,L,N
      COMMON          Q(100),YQ(100),X0(40),IDENTF(36),NFC,NLC
      COMMON          W(100),FXT(100),F1XT(100,40),YQT(100),XT(40),
     1                ETOT(40),C(40),BGPC(6),WEIGHT(5),STACK(5),DUM(280),
     2                V(40,40),DELTXT(40),
     3                      MSWICH,NSECT,ITER,THETAT,THETIG,THETLT,REG,
     4                THECPS,THECPL,INTERR,DET
      COMMON          LENGTH
      COMMON          THETLM,TLIM,LMIN,LMAX,NMIN,NMAX,KMIN,KMAX,MMAX,
     1                MMDMAX,DEGER,ITRMAX,DEVMIN,SRCOEF
C
C
C
C
C
C INPUT A DATA SECTION; PRINT SECTION HEADER-CUM-NUMBER
      READ(5,1903)M,K,L
      READ(5,1904)NFC
      NLC=NFC+M-1
      DO 310 I=1,M
      Q(I)=FLOAT(NFC+I-1)
  310 CONTINUE
      READ(5,1905)(YQ(I),I=1,M)
      DO 320 I=1,K
      I1=4*(I-1)+1
      I2=I1+1
      I3=I2+1
      I4=I3+1
      READ(5,1906)W(I1),W(I2),W(I3),W(I4)
C W-ARRAY SERVES HERE AS TEMPORARY STORAGE FOR CHARACTERISTIC POINTS
  320 CONTINUE
      WRITE(1,2003)(IDENTF(I),I=1,12),NSECT
C CONTROL PRINT OF INPUT DATA (MAY BE ELIMINATED)
      WRITE(1,1903)M,K,L
      WRITE(1,1904)NFC,NLC
      WRITE(1,1905)(YQ(I),I=1,M)
      KKKKK=4*K
      WRITE(1,1906)(W(I),I=1,KKKKK)
C END OF CONTROL PRINT
      RETURN
C
 1903 FORMAT(3I3)
 1904 FORMAT(I7)
```



```
 1905 FORMAT(10F7.0)
 1906 FORMAT(4F7.0)
 2003 FORMAT(////     15X,"SPECTRUM: ",12A2,"..., SECTION NO.",I3/
     1                15X,"*******************************",
     2                    "**********************")
C
      END
C
C
C A CHOPPED PIECE OF INOUT-SUBROUTINE
      SUBROUTINE INOU5
C
C
C
C
      LOGICAL PSV,OOV
      COMMON PSV(5)
      COMMON OOV(3)
      COMMON MM,M,K,L,N
      COMMON          Q(100),YQ(100),X0(40),IDENTF(36),NFC,NLC
      COMMON          W(100),FXT(100),F1XT(100,40),YQT(100),XT(40),
     1                ETOT(40),C(40),BGPC(6),WEIGHT(5),STACK(5),DUM(280),
     2                V(40,40),DELTXT(40),
     3                      MSWICH,NSECT,ITER,THETAT,THETIG,THETLT,REG,
     4                THECPS,THECPL,INTERR,DET
      COMMON          LENGTH
      COMMON          THETLM,TLIM,LMIN,LMAX,NMIN,NMAX,KMIN,KMAX,MMAX,
     1                MMDMAX,DEGER,ITRMAX,DEVMIN,SRCOEF
C
C
C
C
C POINT-DATA OUTPUT (OPTIONAL - WHEN OOV(1)=.T.)
      WRITE(1,1910)ITER
      WRITE(1,1911)
C
C SELECT MAXIMUM ABSOLUTE DEVIATION
      DMAX=-1.0
      DO 510 I=1,M
      AUXIL=ABS(FXT(I))
      IF(DMAX.LT.AUXIL)DMAX=AUXIL
  510 CONTINUE
C
C STORE TEMPORARILY NORMALIZED RELATIVE DEVIATION IN AUXIL; PRINT DATA

      DO 520 I=1,M
      AUXIL=FXT(I)/DMAX
      I1=INT(Q(I))
      I2=INT(YQ(I))
      WRITE(1,1912)I1,I2,W(I),YQT(I),FXT(I),AUXIL
  520 CONTINUE
      RETURN
C
 1910 FORMAT(     /"ITERATION ",I2)
 1911 FORMAT(     "============",44X,"DELTA"/       "CHANNEL",
     1        5X,"COUNTS",4X,"STAT.WEIGHT",4X,"APPROXIMATION",
     5        3X,"(APPR-COUNT)",4X,"DLT/DMX")
 1912 FORMAT(     I6,4X,I7,4X,1PE11.3,4X,0PF12.3,4X,F12.3,4X,F7.2)
      END
C
C
```

```
 C A CHOPPED PIECE OF INOUT-SUBROUTINE

      SUBROUTINE INOU6
C
C
C
C
      LOGICAL PSV,OOV
      COMMON PSV(5)
      COMMON OOV(3)
      COMMON MM,M,K,L,N
      COMMON        Q(100),YQ(100),X0(40),IDENTF(36),NFC,NLC
      COMMON        W(100),FXT(100),F1XT(100,40),YQT(100),XT(40),
     1              ETOT(40),C(40),BGPC(6),WEIGHT(5),STACK(5),DUM(280),
     2              V(40,40),DELTXT(40),
     3                    MSWICH,NSECT,ITER,THETAT,THETIG,THETLT,REG,
     4              THECPS,THECPL,INTERR,DET
      COMMON        LENGTH
      COMMON        THETLM,TLIM,LMIN,LMAX,NMIN,NMAX,KMIN,KMAX,MMAX,

     1              MMDMAX,DEGER,ITRMAX,DEVMIN,SRCOEF
C
C
C
C
C
C PARAMETER OUTPUT: OPTIONAL FOR INTERNAL ITERATIONS (WHEN OOV(1)=.T.)
C                   MANDATORY AT SOLUTION POINT WHERE A GRAPH IS
C                           DRAWN OPTIONALLY (WHEN OOV(3)=.T.)
      IF(PSV(4))GO TO 610
      WRITE(1,1930)ITER,INTERR
      WRITE(1,1931)
  610 WRITE(1,1920)THETAT
      WRITE(1,1921)THETLT
      WRITE(1,1923)
      WRITE(1,1925)
      DO 620 I=1,K
      IPOS=2*I
      IAREA=2*I+1
      AREA=XT(IAREA)*C(IAREA)
      ERRAR=ETOT(IAREA)*C(IAREA)

      WRITE(1,1924)I,XT(IPOS),ETOT(IPOS),AREA,ERRAR
  620 CONTINUE
      AREA=XT(1)*2.35482
      ERRAR=ETOT(1)*2.35482
      WRITE(1,1922)AREA,ERRAR
      IF(L)630,640,640
  630 WRITE(1,1940)
      RETURN
  640 WRITE(1,1926)
      WRITE(1,1927)
      WRITE(1,1928)
      L1=L+1
      DO 650 I=1,L1
      IAUXIL=I-1
      IAREA=2*K+I+1
      AREA=XT(IAREA)*C(IAREA)
      ERRAR=ETOT(IAREA)*C(IAREA)
      WRITE(1,1929)IAUXIL,AREA,ERRAR
```



```
  650 CONTINUE
      RETURN
C
 1930 FORMAT(   /"SOLUTION FOUND AT ",I2," ITERATION ",

     *           "(INTERRUPT NO.",I1,")")
 1931 FORMAT(    "**********************************************")
 1920 FORMAT(   /"SOLUTION DEFECT (USUAL):",F10.4)
 1921 FORMAT(    "SOLUTION DEFECT (LONG): ",F10.4)
 1922 FORMAT(   /"FWHM:",3X,F9.3," +/-",F9.3)
 1923 FORMAT(   /5X,"PEAK NO.",6X,"POSITION",7X,"ERROR",15X,
     *              "AREA",10X,"ERROR")
 1924 FORMAT(    8X,I2,8X,F9.3,4X,F9.3,8X,F12.3,4X,F11.3)

 1925 FORMAT(    5X,"--------",6X,"--------",7X,"-----",15X,

     *              "----",10X,"-----")
 1940 FORMAT(   /10X,"NO BACKGROUND IN THIS SECTION")
 1926 FORMAT(   /10X,"BACKGROUND COEFFICIENTS")
 1927 FORMAT(    10X,"-----------------------")
 1928 FORMAT(   /7X,"DEGREE",7X,"VALUE",8X,"ERROR")
 1929 FORMAT(    9X,I1,6X,1PE11.3,2X,E11.3)
      END
C
C
C A CHOPPED PIECE OF INOUT-SUBROUTINE

      SUBROUTINE INOU7
C
C
C
C
C
      LOGICAL PSV,OOV
      COMMON PSV(5)
      COMMON OOV(3)
      COMMON MM,M,K,L,N
      COMMON        Q(100),YQ(100),X0(40),IDENTF(36),NFC,NLC
      COMMON        W(100),FXT(100),F1XT(100,40),YQT(100),XT(40),
     1              ETOT(40),C(40),BGPC(6),WEIGHT(5),STACK(5),DUM(280),
     2              V(40,40),DELTXT(40),
     3                    MSWICH,NSECT,ITER,THETAT,THETIG,THETLT,REG,
     4              THECPS,THECPL,INTERR,DET
      COMMON        LENGTH
      COMMON        THETLM,TLIM,LMIN,LMAX,NMIN,NMAX,KMIN,KMAX,MMAX,
     1              MMDMAX,DEGER,ITRMAX,DEVMIN,SRCOEF
C
C
C
C PRINT PROGRAM STATUS VECTOR & REGIME DATA DURING EXECUTION
      WRITE(1,2004)(PSV(I),I=1,5),ITER,THETAT,THETLT,REG,DET
      RETURN
C
 2004 FORMAT(   /"  REGIME: ",5L3,";",2X,"ITERATION=",I2,2X,
     1           "THETA=",F8.4,2X,"THETAL=",F8.4/
     2           36X,"REGULARIZER=",F8.4,2X,"DETR=",1PE10.2)
C
      END
      END$
```

This code has been edited and debugged on various computers before its final installment on HP 21MX. The author is gratefull to Mrs.R.Pabst and to A.Gilyov for their help in introducing him into the respective ES1010 and HP 21MX disk operating systems. Sincere thanks are also due to Dr.Dr.M.Ya.Kuznetsova and M.Enikova for the preparation of sample input and for the useful discussion of the results.

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Received by Publishing Department
on May 17 1979.