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C
  PROGRAM SMERG
C
C Fortran-77 sort-merge solution for Siena exercise
C
  PARAMETER (NX=200000)
  INTEGER IH (NX) , IK (NX) , IL (NX) , IP (NX) , IQ (NX)
  REAL FF (NX) , SI (NX) , SY (12,24)
C
C Read data from standard input
C
  READ (*, '( /) ')
  READ (*, *) NS
  READ (*, *) ((SY (I, J) , I=1, 12) , J=1, NS)
  NR=0
1  N=NR+1
  IF (N.GT.NX) STOP '** Too many reflections **'
  READ (*, *, END=5) IH (N) , IK (N) , IL (N) , FF (N) , SI (N)
  IP (N)=N
  NR=N
C
C Convert reflection indices to standard setting
C
  U=REAL (IH (N))
  V=REAL (IK (N))
  W=REAL (IL (N))
  DO 4 M=-1, 1, 2
    DO 3 J=1, NS
      I=M*NINT (SY (1, J) *U+SY (4, J) *V+SY (7, J) *W)
      K=M*NINT (SY (2, J) *U+SY (5, J) *V+SY (8, J) *W)
      L=M*NINT (SY (3, J) *U+SY (6, J) *V+SY (9, J) *W)
      IF (L.LT.IL (N)) GOTO 3
      IF (L.GT.IL (N)) GOTO 2
      IF (K.LT.IK (N)) GOTO 3
      IF (K.GT.IK (N)) GOTO 2
      IF (I.LE.IH (N)) GOTO 3
2    IH (N)=I
      IK (N)=K
      IL (N)=L
3    CONTINUE
4    CONTINUE
  GOTO 1
C
C Sort pointer arrays on h, then k, then l
C
5  CALL INSORT (NR, IP, IQ, IH)
  CALL INSORT (NR, IQ, IP, IK)
  CALL INSORT (NR, IP, IQ, IL)
C
C Combine equivalents - now contiguous
C
  R=0.
  S=0.
  NU=NR
  NC=0
  N=1
6  IF (N.GT.NR) GOTO 16
  M=N
  MQ=IQ (M)
  P=0.
  Q=0.
7  NQ=IQ (N)
  IF (IH (NQ) .NE. IH (MQ) .OR. IK (NQ) .NE. IK (MQ) .OR. IL (NQ) .NE. IL (MQ)) GOTO 8
  P=P+FF (NQ)
  Q=Q+1./SI (NQ) **2
  N=N+1
  IF (N.LE.NR) GOTO 7

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8   P=P/REAL(N-M)
   Q=1./SQRT(Q)
C
C Detect systematic absences and centric reflections
C
   U=REAL(IH(MQ))
   V=REAL(IK(MQ))
   W=REAL(IL(MQ))
   NT=0
   DO 13 J=2,NS
     I=NINT(SY(1,J)*U+SY(4,J)*V+SY(7,J)*W)
     K=NINT(SY(2,J)*U+SY(5,J)*V+SY(8,J)*W)
     L=NINT(SY(3,J)*U+SY(6,J)*V+SY(9,J)*W)
     IF(I.NE.IH(MQ).OR.K.NE.IK(MQ).OR.L.NE.IL(MQ))GOTO 12
     IF(MOD(NINT(12.*(SY(10,J)*U+SY(11,J)*V+SY(12,J)*W)),12).EQ.0)
11  + GOTO 13
     FORMAT(' Reflection',3i4,' syst. abs., I/sigma =',F8.2)
     WRITE(*,11) IH(MQ), IK(MQ), IL(MQ), P/Q
     GOTO 6
12  IF(-I.EQ.IH(MQ).AND.-K.EQ.IK(MQ).AND.-L.EQ.IL(MQ))NT=1
13  CONTINUE
   NC=NC+NT
   NU=NU+1
   IF(NU.GT.NX)STOP '** Too many reflections **'
   IH(NU)=IH(MQ)
   IK(NU)=IK(MQ)
   IL(NU)=IL(MQ)
   FF(NU)=P
   SI(NU)=Q
   IF(N.LE.M+1)GOTO 6
   DO 14 I=M,N-1
     R=R+ABS(FF(IQ(I))-P)
     S=S+P
14  CONTINUE
   GOTO 6
C
C Unique reflections now in IH(NR+1..NU) etc. Output statistics.
C
15  FORMAT(/I6,' Unique reflections, of which',I5,' centric ',
+ 'R(int) =',F8.4/)
16  WRITE(*,15)NU-NR,NC,R/S
   END
C
C -----
C
   SUBROUTINE INSORT(N,IP,IQ,ID)
C
C Sort-merge integer data in order of ascending ID(I). IP is the
C current pointer array to ID and IQ becomes the new pointer array.
C
   INTEGER IP(N),IQ(N),ID(N),IT(9999)
   L=ID(1)
   M=L
   DO 1 I=2,N
     L=MIN0(ID(I),L)
     M=MAX0(ID(I),M)
1  CONTINUE
   L=L-1
   M=M-L
   DO 2 I=1,M
     IT(I)=0
2  CONTINUE
   DO 3 I=1,N
     J=ID(I)-L
     IT(J)=IT(J)+1
3  CONTINUE
   J=0

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DO 4 I=1,M
K=J
J=J+IT(I)
IT(I)=K
4 CONTINUE
DO 5 I=1,N
J=ID(IP(I))-L
IT(J)=IT(J)+1
J=IT(J)
IQ(J)=IP(I)
5 CONTINUE
RETURN
END
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