```
C**********************************************************************
C     MOVIE CREATION PROGRAM USING ANM EIGENVALUE/EIGENVECTOR OUTPUT
C**********************************************************************
C     VERSION 4 9/27/05
C     WRITTEN/ARRANGED BY TANER Z SEN
C
C     PLEASE REFER TO THE FOLLOWING PAPERS FOR MORE INFO:
C
C     ANM:
C     Atilgan AR, Durell SR, Jernigan RL, Demirel MC, Keskin O,
C     Bahar I, Biophys. J., 80:505-15, 2001.
C
C     GNM:
C     Bahar I, Atilgan AR, Erman B, Fold. & Des., 2:173-81, 1997
C
C**********************************************************************
C     VARIABLES
C**********************************************************************
      PARAMETER(SITE=104)
      INTEGER I,LN,NEIG,IC,NSITE
      REAL X(SITE),Y(SITE),Z(SITE),W(SITE*3),V(SITE*3,SITE*3),WI,VIJ,SUM
      REAL FAC,BETA(SITE),SCA,DX(SITE),DY(SITE),DZ(SITE)
      CHARACTER*3 NNAM,CNAM(SITE),DUMMY3
      CHARACTER*6 DUMMY6
      CHARACTER*4 ATNAME,ANAME(SITE)
      CHARACTER*1 A1,CHA(SITE)
      CHARACTER*12 AA
      CHARACTER*30 FILEOUT
      REAL OCCUP(SITE*3),VMAX,VMAXIN,OCCUPMAX,OCCUPMAXIN,TOP,R1
      INTEGER NMODE,D1INT,D2INT,ANUM(SITE),RNUM(SITE)

      OPEN(50,FILE='1hrc.pdb')
      OPEN(71,FILE='eigenvectors.txt')

C**********************************************************************
C     READ ALPHA CARBONS COORDINATES, AND B-FACTORS
C**********************************************************************

310   READ(50,'(A6)') DUMMY6
      IF(DUMMY6.NE.'ATOM  ') GOTO 310
      BACKSPACE(50)

      ICA=1
320   READ(50,'(A6)') DUMMY6
      IF(DUMMY6.NE.'ATOM  ') THEN
       IF(DUMMY6.EQ.'END   ') THEN
        GOTO 330
       ELSE
        GOTO 320
       ENDIF
      ENDIF
      BACKSPACE(50)
      READ(50,55) DUMMY6,D1INT,ATNAME,DUMMY3,A1,D2INT,XXX,YYY,ZZZ,R1,BBB

      IF(ATNAME.EQ.' CA ') THEN
       ANUM(ICA)=D1INT
       ANAME(ICA)=ATNAME
       CNAM(ICA)=DUMMY3
       CHA(ICA)=A1
       RNUM(ICA)=D2INT
```

```
        X(ICA)=XXX
        Y(ICA)=YYY
        Z(ICA)=ZZZ
        BETA(ICA)=BBB
        ICA=ICA+1
       ENDIF
       GOTO 320

55     FORMAT(A6,I5,1X,A4,1X,A3,1X,A1,I4,4X,3F8.3,2F6.2)

330    IF(SITE.NE.(ICA-1)) THEN
        WRITE(*,*) 'THERE IS A PROBLEM WITH THE NUMBER OF RESIDUES!'
        WRITE(*,*) 'GIVEN RESNUM=',SITE,'CALCULATED RESNUM=',ICA-1
        GOTO 666
       ENDIF

C*************************************************************************
C      READING THE EIGENVALUES & EIGENVECTORS as created by ANM program
C*************************************************************************
       READ(71,*) LN, NEIG
       DO I=1,NEIG
       READ (71,*) W(I)
       ENDDO

       NSITE=LN/3

       IF(NSITE.NE.SITE) THEN
        WRITE(*,*) 'NSITE is not equal to SITE'
        GOTO 666
       ENDIF

C      THE FIRST SET OF DATA IS: J=1 AND THEN I=1,LN (V(1,1) V(2,1) etc.
       READ(71,*) ((V(I,j), I=1,LN),J=1,NEIG)

C*************************************************************************
C      CREATING THE MOVIE TO BE SHOWN IN VMD (freeware software)
C      http://www.ks.uiuc.edu/Research/vmd/
C*************************************************************************

C      USER INPUT

10     WRITE(*,*) 'Which mode do you want to visualize?'
       WRITE(*,*) '(the first 6 modes correspond to zero eigenvalues, so'
       WRITE(*,*) ' 7 -> 1st slowest mode,'
       WRITE(*,*) ' 8 -> 2nd slowest mode, etc)'
       READ(*,*) NMODE
       WRITE(*,*) 'How many frames do you want? (e.g. 20)'
       WRITE(*,*) '(output is in -1 to +1 displacement using cosine)'
       READ(*,*) IFRAME
       WRITE(*,*) 'Enter amplification factor: (e.g. 5)'
       READ(*,*) AMP_FACTOR
       WRITE(*,*) 'Enter a filename for the output pdbfile: (e.g. "1agb.")'
       READ(*,'(a)') FILEOUT

       I=INDEX(FILEOUT,'.')-1
       OPEN(12,FILE=FILEOUT(1:I)//".pdb")
       OPEN(13,FILE=FILEOUT(1:I)//"_FLUCTUATIONS.pdb")
       OPEN(14,FILE=FILEOUT(1:I)//"_COLOR.pdb")
       OPEN(15,FILE=FILEOUT(1:I)//"_FLUC.TXT")
```

```
C     ADJUSTING THE FLUCTUATION AMPLITUDES

      OCCUPMAX=0.0
      VMAX=0.0
      DO J=1,NSITE
      OCCUP(J)=v(3*J-2,NMODE)*v(3*J-2,NMODE)+v(3*J-1,NMODE)*v(3*J-1,NMODE)
     $ +v(3*J,NMODE)*v(3*J,NMODE)
      OCCUP(J)=OCCUP(J)/W(NMODE)
      IF(OCCUPMAX.LE.OCCUP(J)) OCCUPMAX=OCCUP(J)
      IF(VMAX.LE.ABS(v(3*J-2,NMODE))) VMAX=ABS(v(3*J-2,NMODE))
      IF(VMAX.LE.ABS(v(3*J-1,NMODE))) VMAX=ABS(v(3*J-1,NMODE))
      IF(VMAX.LE.ABS(v(3*J,NMODE))) VMAX=ABS(v(3*J,NMODE))
      ENDDO

      WRITE(*,*) 'The largest fluctuation OCCUPMAX is',OCCUPMAX
      WRITE(*,*) 'If you want to change OCCUPMAX, put in a smaller value'
      READ(*,*) OCCUPMAXIN

      IF(OCCUPMAX.GT.OCCUPMAXIN) OCCUPMAX=OCCUPMAXIN
      WRITE(*,*) 'Largest VMAX  absolute is',VMAX
      WRITE(*,*) 'If you want to adjust it, enter a smaller value'
      READ(*,*) VMAXIN
      IF(VMAX.GT.VMAXIN) VMAX=VMAXIN


      DO J=1,NSITE
         IF(OCCUP(J).GT.OCCUPMAX) THEN
            OCCUP(J)=1.0
         ELSE
            OCCUP(J)=OCCUP(J)/OCCUPMAX
         ENDIF
         IF(ABS(V(3*J-2,NMODE)).GT.VMAX) THEN
            TOP=SIGN(VMAX,v(3*J-2,NMODE))
            V(3*J-2,NMODE)=TOP
         ENDIF
         IF(ABS(V(3*J-1,NMODE)).GT.VMAX) THEN
            TOP=SIGN(VMAX,V(3*J-1,NMODE))
            V(3*J-1,NMODE)=TOP
         ENDIF
         IF(ABS(V(3*j,NMODE)).GT.VMAX) THEN
            TOP=SIGN(VMAX,v(3*J,NMODE))
            V(3*J,NMODE)=TOP
         ENDIF
      ENDDO

C     FOR EACH FRAME
      DO IFR=1,IFRAME+1

C     CALCULATION OF COORDINATE CHANGES DURING MOTION
         XTEMP=(IFR-1)*3.14156/(IFRAME)
         IF(W(NMODE).GT.1.0E-05) THEN
            XTEMP=AMP_FACTOR*COS(XTEMP)/SQRT(W(NMODE))
         ELSE
            WRITE(*,*) 'Please enter a non-zero eigenvalue!'
            GOTO 666
         ENDIF

         DO J=1,NSITE
            DX(J)=V(3*J-2,NMODE)*XTEMP
            DY(J)=V(3*J-1,NMODE)*XTEMP
```

```
            DZ(J)=V(3*J,NMODE)*XTEMP
          ENDDO

C     WRITING COORDINATES TO A FILE IN PDB FORMAT
          DO I=1,NSITE
           WRITE(12,55) 'ATOM  ',ANUM(I),ANAME(I),CNAM(I),CHA(I),RNUM(I),
     *       X(I)+DX(I),Y(I)+DY(I),Z(I)+DZ(I),R1,BETA(I)
          ENDDO

          WRITE(12,'(a)')'END'

C     WRITING COORDINATES TO A FILE IN COLORFUL PDB FORMAT
          DO I=1,NSITE
           WRITE(14,55) 'ATOM  ',ANUM(I),ANAME(I),CNAM(I),CHA(I),RNUM(I),
     *       X(I)+DX(I),Y(I)+DY(I),Z(I)+DZ(I),R1,
     *       (DX(I)**2+DY(I)**2+DZ(I)**2)
          ENDDO

          WRITE(14,'(a)')'END'
        ENDDO
        CLOSE(12)

C     THE FLUCTUATIONS ARE GIVEN IN THE B-FACTOR COLUMN
        DO I=1,NSITE
              IFR=1
              XTEMP=(IFR-1)*3.14156/(IFRAME)
              XTEMP=AMP_FACTOR*COS(XTEMP)/SQRT(W(NMODE))
              DX(I)=V(3*I-2,NMODE)*XTEMP
              DY(I)=V(3*I-1,NMODE)*XTEMP
              DZ(I)=V(3*I,NMODE)*XTEMP


         WRITE(13,55) 'ATOM  ',ANUM(I),ANAME(I),CNAM(I),CHA(I),RNUM(I),
     *       X(I)+DX(I),Y(I)+DY(I),Z(I)+DZ(I),R1,
     *       (DX(I)**2+DY(I)**2+DZ(I)**2)

         WRITE(15,*) RNUM(I),(DX(I)**2+DY(I)**2+DZ(I)**2)

         ENDDO

           WRITE(13,'(a)')'END'


C     VISUALIZATION OF OTHERS MODES
        WRITE(*,*) 'Do you want to visualize another mode?'
        WRITE(*,*) 'Enter 1 for yes, any other DIGIT for no'
        READ(*,*) IANSWER
        IF(IANSWER.eq.1) GOTO 10


        WRITE(*,*) 'Program finished successfully!'
666     STOP
        END
```