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c-- program to compute the partial autocorrelation function pACF
c-- of the time-derivative of the X-H bond length in order to
c-- further calculate the partial vibrational density of states
c-- corresponding to the local X-H stretching mode, i.e.
c-- the contribution of this motion to the overall vibrational
c-- density of states - vDOS - by Lj. Pejov



      dimension xdr(20000)
      dimension xr(20000)
      dimension xt(20000)
      dimension xc(20000)
      dimension xcnor(20000)
      dimension xrp(20000)


c--  definition of the number of steps

      nstep=10000


c--  read the input data
c--  xt(i) - time; xr(i) - X-H distance;
c--  xdr(i) - time derivative of the X-H distance


       do i=1,nstep

      read (1,*) xt(i), xr(i), xdr(i)

       enddo


c--  computation of the pACF


      xsum=0

       do i=1,nstep

        xsum = xsum + xdr(i)

       enddo


      xav=xsum/nstep


       do i=1,nstep
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        xrp(i) = xdr(i) - xav

       enddo


c--  definition of the maximum number of lags
c--  that are physically/numerically acceptable


      nlags=int(10*log10(10.0*nstep))


      xc(1)=0

       do i=1,nstep

       xc(1)=xc(1) + xrp(i)*xrp(i)

      enddo
        xc(1) = xc(1)/nstep




       do j=2,nlags

        xc(j)=0

         do i=1,nstep-(j-1)

           xc(j) = xc(j) + xrp(i)*xrp(i+(j-1))

         enddo

           xc(j)= xc(j)/(nstep-(j-1))

       enddo


       do i=1,nlags

       xcnor(i)=xc(i)/xc(1)

       enddo


c-- write an output
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```
c--  xt(i) - time; xc(i) - autocorrelation function;
c--  xcnor(i) - normalized autocorrelation function


       do i=1,nlags

      write (2,*) xt(i), xc(i), xcnor(i)

       enddo




 10    format(i5,4f10.6)

       stop
       end
```