```
      subroutine walk_scan
      Implicit real*8(a-h,o-z)
      double precision:: alpha,beta,beta0,alpha0,r0,pas
      integer:: cont, m, mi
      common/dades1/Z,beta,alpha,r0
      common/dades2/m, mi,sec,encerts
      common/results/ene1,ene2
      double precision E,E2,Ea,Eb,Fa,Fb,EEa,EEb,EFa,EFb,EaEb,Ea2,Eb2
      double precision E0,E20,Ea0,Eb0,Fa0,Fb0,EEa0,EEb0,EFa0,EFb0,EaEb0,Ea20,Eb20
      dimension grad(2),hess(2,2),hessm1(2,2)


      x1=r0*(2*ran2(idum)-1)
      y1=r0*(2*ran2(idum)-1)
      z1=r0*(2*ran2(idum)-1)
      x2=r0*(2*ran2(idum)-1)
      y2=r0*(2*ran2(idum)-1)
      z2=r0*(2*ran2(idum)-1)

      r1=sqrt(x1**2+y1**2+z1**2)
      r2=sqrt(x2**2+y2**2+z2**2)
      dist=sqrt((x1-x2)**2+(y1-y2)**2+(z1-z2)**2)
      grad(1)=alpha
      grad(2)=beta

      p0= prob(r1,r2,dist)

!     write(*,*) "p0 ",p0


      ! termalitzation

    cont=0
    do i=1,mi

      x1b=r0*(2*ran2(idum)-1)
      y1b=r0*(2*ran2(idum)-1)
      z1b=r0*(2*ran2(idum)-1)
      x2b=r0*(2*ran2(idum)-1)
      y2b=r0*(2*ran2(idum)-1)
      z2b=r0*(2*ran2(idum)-1)

      r1b=sqrt(x1b**2+y1b**2+z1b**2)
      r2b=sqrt(x2b**2+y2b**2+z2b**2)
      distb=sqrt((x1b-x2b)**2+(y1b-y2b)**2+(z1b-z2b)**2)

      p1=prob(r1b,r2b,distb)

!     write(*,*) "p1 ",p1

      w=ran2(idum);

      IF(p1/p0>sec*w) THEN
          x1=x1b
          y1=y1b
          z1=z1b
          x2=x2b
          y2=y2b
          z2=z2b
          p0=p1
          cont=cont+1
      ENDIF

    enddo

!   write(*,*) "cont ",cont
!   write(*,*) "initial  step",r0
      pas=r0*cont/(encerts*mi);
!   write(*,*) " fitted step ",pas


    E0=0.d0
```

```
E20=0.d0
Ea0=0.d0
Eb0=0.d0
Fa0=0.d0
Fb0=0.d0
EEa0=0.d0
EEb0=0.d0
EFa0=0.d0
EFb0=0.d0
EaEb0=0.d0
Ea20=0.d0
Eb20=0.d0

E=0.d0
E2=0.d0
Ea=0.d0
Eb=0.d0
Fa=0.d0
Fb=0.d0
EEa=0.d0
EEb=0.d0
EFa=0.d0
EFb=0.d0
EaEb=0.d0
Ea2=0.d0
Eb2=0.d0

cont=0
do i=1,m

    x1b=pas*(2*ran2(idum)-1)
    y1b=pas*(2*ran2(idum)-1)
    z1b=pas*(2*ran2(idum)-1)
    x2b=pas*(2*ran2(idum)-1)
    y2b=pas*(2*ran2(idum)-1)
    z2b=pas*(2*ran2(idum)-1)

    r1b=sqrt(x1b**2+y1b**2+z1b**2)
    r2b=sqrt(x2b**2+y2b**2+z2b**2)
    distb=sqrt((x1b-x2b)**2+(y1b-y2b)**2+(z1b-z2b)**2)

    p1=prob(r1b,r2b,distb)

    w=ran2(idum);

    IF(p1/p0>sec*w) THEN
        cont=cont+1
        E0=Ene(distb,r1b,r2b,x1b,x2b,y1b,y2b,z1b,z2b)
        E20=E0**2
        Ea0=Enea(distb,r1b,r2b,x1b,x2b,y1b,y2b,z1b,z2b)
        Eb0=Eneb(distb,r1b,r2b,x1b,x2b,y1b,y2b,z1b,z2b)
        Fa0=Funa(distb)
        Fb0=Funb(distb)
        EEa0=E0*Ea0
        EEb0=E0*Eb0
        EFa0=E0*Fa0
        EFb0=E0*Fb0
        EaEb0=Ea0*Eb0
        Ea20=Ea0**2
        Eb20=Eb0**2

        E=E+E0
        E2=E2+E20
        Ea=Ea+Ea0
        Eb=Eb+Eb0
        Fa=Fa+Fa0
        Fb=Fb+Fb0
        EEa=EEa+EEa0
        EEb=EEb+EEb0
        EFa=EFa+EFa0
        EFb=EFb+EFb0
        EaEb=EaEb+EaEb0
```

```
            Ea2=Ea2+Ea20
            Eb2=Eb2+Eb20

            p0=p1

        ENDIF

    enddo

    alpha0=alpha
    beta0=beta

    E=E/cont
    E2=E2/cont
    Ea=Ea/cont
    Eb=Eb/cont
    Fa=Fa/cont
    Fb=Fb/cont
    EEa=EEa/cont
    EEb=EEb/cont
    EFa=EFa/cont
    EFb=EFb/cont
    EaEb=EaEb/cont
    Ea2=Ea2/cont
    Eb2=Eb2/cont


    ene1=E
    ene2=E2
    grad(1)=2.d0*(EEa-E*Ea)
    grad(2)=2.d0*(EEb-E*Eb)
    hess(1,1)=2.d0*(Ea2-EFa*Ea+E*Fa*Ea-Ea*EFa+EFa**2-E*Fa*EFa+Ea*E*Fa-EFa*E*Fa+E**2*Fa**2)
    hess(2,2)=2.d0*(Eb2-EFb*Eb+E*Fb*Eb-Eb*EFb+EFb**2-E*Fb*EFb+Eb*E*Fb-EFb*E*Fb+E**2*Fb**2)
    hess(1,2)=2.d0*(Ea*Eb-EFb*Ea+E*Fb*Ea-Eb*EFa+EFb*EFa-E*Fb*EFa+Eb*E*Fa-EFb*E*Fa+E**2*Fb*Fa)
    hess(2,1)=hess(1,2)
    det=hess(1,1)*hess(2,2)-hess(1,2)*hess(2,1)
    hessm1(1,1)=hess(2,2)/det
    hessm1(2,2)=hess(1,1)/det
    hessm1(1,2)=-hess(1,2)/det
    hessm1(2,1)=hessm1(1,2)

!   write(*,*) "det = ",det
!   write(*,*) "Hessià = ",hess(1,1),hess(1,2),hess(2,1),hess(2,2)
!   write(40,*) "energia ", E,"  variancia  ", E2-E**2
!   write(40,*) "gradient ", grad(1:2)
!   write(40,*) "det = ",det
!   write(40,*) "Hessià = ",hess(1,1),hess(1,2),hess(2,1),hess(2,2)
!   write(40,*) "E,E2,Ea,Eb,Fa,Fb,EEa,EEb,EFa,EFb,EaEb,Ea2,Eb2"
!   write(40,*) E," ",E2," ",Ea," ",Eb," ",Fa," ",Fb," ",EEa," ",EEb," ",EFa," ",EFb,"
",EaEb," ",Ea2," ",Eb2
!   write(*,*) " gradient ", grad(1:2)
!   write(*,*) "hessia  ", hess(1:2,1:2)
!   write(*,*) "alpha0 = ",alpha0,"  beta0 = ",beta0

    alpha=alpha0-(hessm1(1,1)*grad(1)+hessm1(1,2)*grad(2))
    beta=beta0-(hessm1(2,1)*grad(1)+hessm1(2,2)*grad(2))

    write(40,*) "alpha0 = ",alpha0,"  beta0 = ",beta0
    write(40,*) "alpha = ",alpha,"  beta = ",beta
!   write(*,*) "E = ",ene1,"  var = ",ene2-ene1**2
!   write(*,*) "alpha = ",alpha,"  beta = ",beta
!   write(*,*) "punts encertats ",cont,"   punts fallits ",m-cont;


return
end
```