

```
!$omp parallel do reduction(+: pdot)
do i=1,Nconf
    pdot=pdot+q(i)*bqp(i)
enddo
a(iter)=pdot
c bqp=bqp-a(iter)*q
c call daxpy(Nconf,-a(iter),q,1,bqp,1)
cc now bqp=(H-a(iter))#H-b(iter-1)*q(iter-1)
c b(iter)=dnrm2(Nconf,bqp,1)
pnorm=0d0
!$omp parallel do reduction(+: pnorm)
do i=1,Nconf
    bqp(i)=bqp(i)-a(iter)*q(i)
    pnorm=pnorm+bqp(i)*bqp(i)
enddo
b(iter)=sqrt(pnorm)

if (abs(ipass).eq.1) then
c --- diagonalize real symmetric tridiagonal matrix
call trieigen(iter,a,b, ee,ev)
write(*,'(A2,I5,E20.10,2E12.4)')
c istr, iter, ee(1), a(iter), b(iter-1)
if (abs(b(iter)).lt.1d-10) goto 100
if(ipass.eq.1) then
c add minimum number of iterations for restarting!
if (abs(ee(1)-eold).lt.1d-14*abs(ee(1))) goto 100
eold=ee(1)
endif
endif
if (ipass.eq.2) then
```



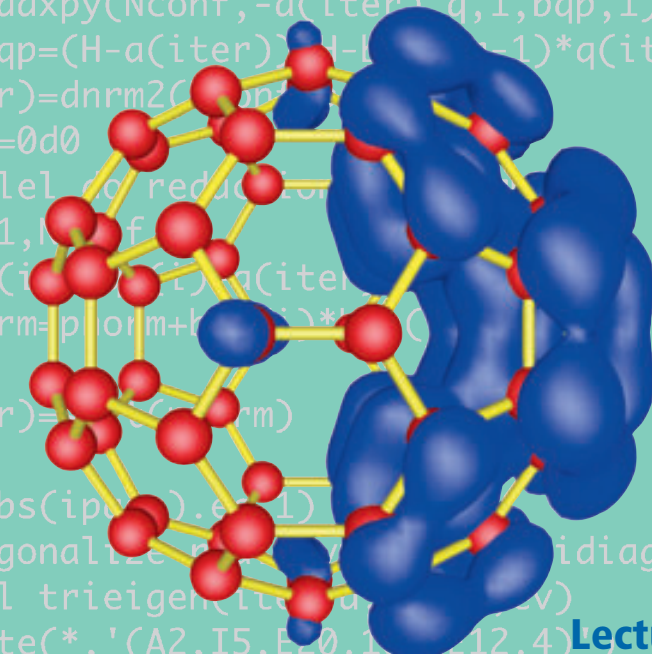
```
do iter=2,niter
c now q=q(iter-1), bqp=b(iter-1)*q(iter)
!$omp parallel do private(t)
do i=1,Nconf
    t=q(i)
    q(i)=bqp(i)/b(iter-1)
    bqp(i)=-b(iter-1)*t
enddo
```



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c bqp=bqp-a(iter)*q
c call daxpy(Nconf,-a(iter),q,1,bqp,1)
cc now bqp=(H-a(iter))#H-b(iter-1)*q(iter-1)
c b(iter)=dnrm2(Nconf,bqp,1)
pnorm=0d0
!$omp parallel do reduction(+: pnorm)
do i=1,Nconf
    bqp(i)=bqp(i)-a(iter)*q(i)
    pnorm=pnorm+bqp(i)*bqp(i)
enddo
b(iter)=sqrt(pnorm)

if (abs(ipass).eq.1) then
c --- diagonalize real symmetric tridiagonal matrix
call trieigen(iter,a,b, ee,ev)
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endif
endif
if (ipass.eq.2) then
```



```
c add minimum number of iterations for restarting!
if (abs(ee(1)-eold).lt.1d-14*abs(ee(1))) goto 100
eold=ee(1)
endif
endif
if (ipass.eq.2) then
c --- accumulate lowest eigenvector: Psi0=Psi0+ev(iter,1)*
call daxpy(Nconf, ev(iter,1),q,1,Psi0,1)
endif
enddo
```