cin1.f   
Dec 03, 03 13:34, Printed: August 28, 2004 (Saturday).   
pages 7, 8, 9, 10/42 (4, 5/21):   
c..............   
FUNCTION PLJ(IA,IB)   
INCLUDE "cin.h"   
implicit real \*8 (a-h,o-z)   
common/nnn/ee(NVM),nnn(NVM), kk(NVM),ll(NVM),jj(NVM),nlist   
COMMON /JZ/JZ(NJZMAX) /NH/NH(NJZMAX)   
T=0.d0   
NA=NH(IA)   
NB=NH(IB)   
IF (NA.NE.NB) GOTO 1000   
MA=JZ(IA)   
MB=JZ(IB)   
IF (MA.NE.MB+2) GOTO 1000   
JA=JJ(NA)   
T=JA\*(JA+2)-MA\*MB   
T=dSQRT(T)   
1000 PLJ=T   
RETUN   
END   
c   
SUBROUTINE DETS(IC,N1,N2)   
INCLUDE "cin.h"   
COMMON /NDC/NDC(NCMAX)   
IF(IC.EQ.1)THEN   
N1=1   
N2=NDC(1)   
ELSE   
II=0   
DO I=1,IC-1   
II=II+NDC(I)   
END DO   
N1=II+1   
N2=II+NDC(IC)   
END IF   
RETURN   
END   
c   
SUBROUTINE FORMH   
INCLUDE "cin.h"   
implicit real\*8 (a-h,o-z)   
COMMON /NC/NC /NE/NE /NV/NV   
COMMON /NCJ/NCJ(NCMAX) /COEF/COEF(NCOEF)   
c COMMON/AAA/MAA,III(NSTJ),JJJ(NSTJ)/AAAA/AA(NSTJ)   
common /aline/al(NXX) /nline/nind(NXX) /diag/diag(NXX)   
REAL COEF   
logical iwl   
real \*8, allocatable :: a(:)   
integer, allocatable :: iii(:),jjj(:)   
INTEGER \*2 nind   
IF(NV.GT.NXX)THEN   
PRINT 1,NV,NXX   
--   
1 FORMAT('' Too big matrix: NV='', i5,'' NXX='',i5)   
STOP   
END IF   
NDCMAX=0   
DO IC=1,NC   
NDCMAX=MAX0(NDCMAX,NDC(IC))   
END DO   
c IF(NDCMAX.GT.NSTJ)THEN   
c PRINT 23,NCMAX,NSTJ   
c 23 FORMAT('' NDCMAX='',I5,'' greater then (than?) NSTJ='',I5)   
c STOP   
c END IF   
ndcm2=NDCMAX\*\*2   
allocate (aa(ndcm2),iii(ndcm2),jjj(ndcm2))   
if(allocated(aa).and.allocated(iii).and.allocated(jjj))then   
print \*,''OK''   
else   
stop ''allocation failed in FORMH''   
end if   
print \*, '' Calculation of H:''   
c open (11,file=''/erased\_at\_5am\_monday/dzuba/cin.buf'',   
c , status=''unknown'',form=''UNFORMATTED'')   
  
IND=0   
IVV=0   
c print \*,'' nv='',nv   
DO 10 IV=1,NV   
ICI=NCJ(IV)   
CALL DETS(ICI,NI1,NI2)   
call coretest(ni1,idc1)   
NDI=NI2-NI2+1   
JVV=0   
ICJ0=0   
ii=0   
DO 20 JV=1,IV   
c iwl=iv.eq.1.and.jv.eq.1   
ICJ=NCJ(JV)   
CALL DETS(ICJ,NJ1,NJ2)   
call coretest(nj1,idc2)   
c if(idc1.eq.1.and.idc2.eq.1.and.iv.ne.jv) go to 21   
c if(iv.gt.1.and.jv.gt.1.and.iv.ne.jv) go to 21   
IF(ICJ0.NE.ICJ)THEN   
CALL MATRCO(ICI,ICJ,NI1,NI2,NJ1,NJ2,   
, MAA,III(1),JJJ(1)AA(1))   
ICJ0=ICJ   
END IF   
NDJ=NJ2-NJ1+1   
T=0.   
IF(MAA.GT.0)THEN   
DO M=1,MAA   
T=T+COEF(IVV+III(M))\*COEF(JVV+JJJ(M))\*AA(M)   
END DO   
IND=IND+1   
ii=ii+1   
if(JV.EQ.IV)then   
AL(1)=T   
nind(1)=ii   
else   
AL(ii+1)=T   
nind(ii+1)=JV   
----   
end if   
c if(t.ne.0.d0)print 6,iv,jv,ici,icj,t   
c 6 format(''H:'',2i5,'' :'',2i5,f12.6)   
end if   
21 JVV=JVV+NDJ   
20 CONTINUE   
diag(iv)=T   
IF((IV/50)\*50+1.EQ.IV)PRINT 5,IV,NT,T   
5 FORMAT(''H:'',2I6,F12.6)   
call dumpline(IV,ii)   
11 IVV=IVV+NDI   
10 CONTINUE   
call flush(ind)   
IF(NV.LT.6)PRINT 22, (AL(I),I=1,NV\*(NV+1)/2)   
22 FORMAT(5E12.4)   
deallocate(aa,iii,jjj)   
RETURN   
END   
c   
subroutine coretest(id,ind)   
INCLUDE "cin.h"   
implicit real\*8 (a-h,o-z)   
dimension idet(128)   
common/nh/nh(njzmax) /ne/ne   
common/nnn/ee(NVM), nnn(NVM), kk(NVM), ll(NVM),jj(NVM),nlist   
call gdet(id,idet)   
ind=0   
do i=1,ne   
na=nh(idet(i))   
if(nnn(na).eq.3.and.ll(na).eq.1)ind=ind+1   
end do   
if(ind.ne.6)then   
ind=1   
else   
ind=0   
end if   
return   
end   
c   
subroutine flush(ind)   
INCLUDE "cin.h"   
implicit real\*8 (a-h,o-z)   
common/matrix/a(NBLOCK) /matind/indx(NBLOCK)   
common/block/last,nb /NV/NV /MJ/MJ /NE/NE /diag/diag(NXX)   
INTEGER \*2 indx   
if(last.gt.0)then   
write(11)(a(l),l=1,last)   
write(11)(indx(l),l=1,last)   
if(last.le.6)then   
print \*,''Matrix:''   
print 1, (indx(l),l=1,last)   
1 format(6i13)   
print 2, (a(l),l=1,last)   
2 format(6e13.5)   
end if   
nb=nb+1   
else   
last=NBLOCK   
end if   
close(11)   
open(12,file=''mat.par'',status=''UNKNOWN'' ,   
! form=''UNFORMATTED'')   
--   
pro=200.\*ind/(nv\*(nv+1))   
c print \*,'' nv='' ,nv   
c print \*,'' ind='' , ind   
c print \*,'' pro='' ,pro   
c print \*,'' nb='' ,nb   
c print \*,'' nblock='' , nblock   
c print \*,'' last='' , last   
print 11,nv,nv\*(nv+1)/2,ind,pro,nb,NBLOCK,last   
11 format(''Number of states '',i10/   
/ '' Total matrix size '', i10/   
/ '' Number of non-zeros '',i10/   
/ '' Non-zero fraction '',f10.2,''%''/   
/ '' Number of blocks '', i10/   
/ '' Block size: NBLOCK= '',i10, ''last='',i10)   
write(12)mj,ne,NBLOCK,nv,ind,nb,last   
write(12)(diag(l),l=1,NV)   
close(12)   
return   
end   
с   
subroutine dumpline(iv,ii)   
INCLUDE "cin.h"   
implicit real\*8 (a-h,o-z)   
common/aline/a1(NXX) /nline/nind(NXX) /block/last,nb   
common/matrix/a(NBLOCK) /matind/indx(NBLOCK)   
INTEGER \*2 nind,indx   
if(iv.eq.1)then   
last=0   
nb=0   
end if   
nind(1)=ii   
do i=1,ii   
last=last+1   
if(last.gt.NBLOCK)then   
nb=nb+1   
print 1,nb   
1 format(''Writing block #'',i3,''...'')   
write(11)(a(l),l=1,NBLOCK)   
write(11)(indx(l),l=1,NBLOCK)   
last=1   
end if   
a(last)=al(i)   
indx(last)=nind(i)   
end do   
return   
end