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