ABINIT 8.10.3

Give name for formatted input file:

par21-slabPdecutopt041720.in

Give name for formatted output file:

par21-slabPdecutopt041720.out

Give root name for generic input files:

par21-slabPdecutopt041720i

Give root name for generic output files:

par21-slabPdecutopt041720o

Give root name for generic temporary files:

bulkNiecutopt\_6

--- !COMMENT

src\_file: m\_dtfil.F90

src\_line: 1159

message: |

Output file par21-slabPdecutopt041720.out

already exists.

...

--- !COMMENT

src\_file: m\_dtfil.F90

src\_line: 1183

message: |

Renaming old par21-slabPdecutopt041720.out to par21-slabPdecutopt041720.out0002

...

.Version 8.10.3 of ABINIT

.(MPI version, prepared for a x86\_64\_linux\_gnu5.4 computer)

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ABINIT comes with ABSOLUTELY NO WARRANTY.

It is free software, and you are welcome to redistribute it

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ABINIT is a project of the Universite Catholique de Louvain,

Corning Inc. and other collaborators, see ~abinit/doc/developers/contributors.txt .

Please read https://docs.abinit.org/theory/acknowledgments for suggested

acknowledgments of the ABINIT effort.

For more information, see https://www.abinit.org .

.Starting date : Sat 18 Apr 2020.

- ( at 20h04 )

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=== Build Information ===

Version : 8.10.3

Build target : x86\_64\_linux\_gnu5.4

Build date : 20191008

=== Compiler Suite ===

C compiler : gnu5.4

C++ compiler : gnu5.4

Fortran compiler : gnu5.4

CFLAGS : -g -O2 -mtune=native -march=native

CXXFLAGS : -g -O2 -mtune=native -march=native

FCFLAGS : -g -ffree-line-length-none

FC\_LDFLAGS :

=== Optimizations ===

Debug level : basic

Optimization level : standard

Architecture : intel\_xeon

=== Multicore ===

Parallel build : yes

Parallel I/O : auto

openMP support : no

GPU support : no

=== Connectors / Fallbacks ===

Connectors on : yes

Fallbacks on : yes

DFT flavor : none

FFT flavor : none

LINALG flavor : netlib-fallback

MATH flavor : none

TIMER flavor : abinit

TRIO flavor : none

=== Experimental features ===

Bindings : @enable\_bindings@

Exports : no

GW double-precision : no

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Default optimizations:

-O2 -mtune=native -march=native

Optimizations for 43\_ptgroups:

-O0

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CPP options activated during the build:

CC\_GNU CXX\_GNU FC\_GNU

HAVE\_FC\_ALLOCATABLE\_DT... HAVE\_FC\_ASYNC HAVE\_FC\_BACKTRACE

HAVE\_FC\_COMMAND\_ARGUMENT HAVE\_FC\_COMMAND\_LINE HAVE\_FC\_CONTIGUOUS

HAVE\_FC\_CPUTIME HAVE\_FC\_EXIT HAVE\_FC\_FLUSH

HAVE\_FC\_GAMMA HAVE\_FC\_GETENV HAVE\_FC\_IEEE\_EXCEPTIONS

HAVE\_FC\_INT\_QUAD HAVE\_FC\_IOMSG HAVE\_FC\_ISO\_C\_BINDING

HAVE\_FC\_ISO\_FORTRAN\_2008 HAVE\_FC\_LONG\_LINES HAVE\_FC\_MOVE\_ALLOC

HAVE\_FC\_PRIVATE HAVE\_FC\_PROTECTED HAVE\_FC\_STREAM\_IO

HAVE\_FC\_SYSTEM HAVE\_FORTRAN2003 HAVE\_LIBPAW\_ABINIT

HAVE\_LIBTETRA\_ABINIT HAVE\_MPI HAVE\_MPI2

HAVE\_MPI\_IALLREDUCE HAVE\_MPI\_IALLTOALL HAVE\_MPI\_IALLTOALLV

HAVE\_MPI\_INTEGER16 HAVE\_MPI\_IO HAVE\_MPI\_TYPE\_CREATE\_S...

HAVE\_OS\_LINUX HAVE\_TIMER\_ABINIT USE\_MACROAVE

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- input file -> par21-slabPdecutopt041720.in

- output file -> par21-slabPdecutopt041720.out

- root for input files -> par21-slabPdecutopt041720i

- root for output files -> par21-slabPdecutopt041720o

-instrng: 98 lines of input have been read from file par21-slabPdecutopt041720.in

Please give name of formatted atomic psp file

iofn2 : for atom type 1, psp file is ../../ni/pseudopotential/Pd.psp8

read the values zionpsp= 18.0 , pspcod= 8 , lmax= 2

inpspheads: deduce mpsang = 3, n1xccc = 2501.

invars1 : treat image number: 1

ingeo: use angdeg to generate rprim.

symlatt : the Bravais lattice is hP (primitive hexagonal)

xred is defined in input file

ingeo: takes atomic coordinates from input array xred

symlatt : the Bravais lattice is hP (primitive hexagonal)

symlatt : the Bravais lattice is hP (primitive hexagonal)

symspgr : spgroup= 164 P-3 m 1 (=D3d^3)

symspgr : optical characteristics = uniaxial

Optical axis (in reduced coordinates, real space ) : 0 0 1

ingeo: angdeg(1:3)= 90.00000000 90.00000000 120.00000000

chkneu : initialized the occupation numbers for occopt= 4, spin-unpolarized or antiferromagnetic case :

2.00 2.00 2.00 2.00 2.00 2.00 2.00 2.00 2.00 2.00 2.00 2.00

2.00 2.00 2.00 2.00 2.00 2.00 2.00 2.00 2.00 2.00 2.00 2.00

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0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

mpi\_setup: mkmem undefined in the input file.Use default mkmem = nkpt

mpi\_setup: With nkpt\_me=4 and mkmem = 4, ground state wf handled in core.

mpi\_setup: mkqmem undefined in the input file.Use default mkqmem = nkpt

mpi\_setup: With nkpt\_me=4 and mkqmem = 4, ground state wf handled in core.

mpi\_setup: mk1mem undefined in the input file.Use default mk1mem = nkpt

mpi\_setup: With nkpt\_me=4 and mk1mem = 4, ground state wf handled in core.

For input ecut= 4.200000E+01 best grid ngfft= 30 30 270

max ecut= 4.201850E+01

==== FFT mesh ====

FFT mesh divisions ........................ 30 30 270

Augmented FFT divisions ................... 31 31 270

FFT algorithm ............................. 112

FFT cache size ............................ 16

getmpw: optimal value of mpw= 13445

Symmetries : space group P-3 m 1 (#164); Bravais hP (primitive hexag.)

getdim\_nloc : deduce lmnmax = 18, lnmax = 6,

lmnmaxso= 18, lnmaxso= 6.

For input ecut= 1.304062E+01 best grid ngfft= 18 18 150

max ecut= 1.375729E+01

==== FFT mesh ====

FFT mesh divisions ........................ 18 18 150

Augmented FFT divisions ................... 19 19 150

FFT algorithm ............................. 101

FFT cache size ............................ 16

getmpw: optimal value of mpw= 167

memory : analysis of memory needs

================================================================================

Values of the parameters that define the memory need of the present run

intxc = 0 ionmov = 0 iscf = 7 lmnmax = 6

lnmax = 6 mgfft = 270 mpssoang = 3 mqgrid = 3001

natom = 3 nloc\_mem = 1 nspden = 1 nspinor = 1

nsppol = 1 nsym = 12 n1xccc = 2501 ntypat = 1

occopt = 4 xclevel = 2

- mband = 48 mffmem = 1 mkmem = 4

mpw = 13445 nfft = 243000 nkpt = 4

For the susceptibility and dielectric matrices, or tddft :

mgfft = 150 nbnd\_in\_blk= 6 nfft = 48600 npw = 167

================================================================================

P This job should need less than 214.316 Mbytes of memory.

Rough estimation (10% accuracy) of disk space for files :

\_ WF disk file : 39.392 Mbytes ; DEN or POT disk file : 1.856 Mbytes.

================================================================================

Biggest array : f\_fftgr(disk), with 114.9465 MBytes.

memana : allocated an array of 114.946 Mbytes, for testing purposes.

memana: allocated 214.316Mbytes, for testing purposes.

The job will continue.

--------------------------------------------------------------------------------

------------- Echo of variables that govern the present computation ------------

--------------------------------------------------------------------------------

-

- outvars: echo of selected default values

- iomode0 = 0 , fftalg0 =112 , wfoptalg0 = 0

-

- outvars: echo of global parameters not present in the input file

- max\_nthreads = 0

-

-outvars: echo values of preprocessed input variables --------

- iomode 1

acell 5.1443120781E+00 5.1443120781E+00 4.4918955770E+01 Bohr

amu 1.06420000E+02

chksymbreak 0

densfor\_pred 6

diemac 1.00000000E+08

ecut 4.20000000E+01 Hartree

- fftalg 112

iprcel 45

istwfk 2 0 1 0

ixc 11

kpt 0.00000000E+00 0.00000000E+00 0.00000000E+00

2.50000000E-01 0.00000000E+00 0.00000000E+00

5.00000000E-01 0.00000000E+00 0.00000000E+00

2.50000000E-01 2.50000000E-01 0.00000000E+00

kptrlatt 4 0 0 0 4 0 0 0 1

kptrlen 2.05772483E+01

max\_ncpus 48

P mkmem 4

natom 3

nband 48

nbdbuf 6

ngfft 30 30 270

nkpt 4

nline 6

nnsclo 3

npulayit 30

nstep 10

nsym 12

ntypat 1

occ 2.000000 2.000000 2.000000 2.000000 2.000000 2.000000

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0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

occopt 4

optforces 0

ortalg -2

paral\_kgb 1

prtden 0

prtebands 0

prteig 0

prtwf 0

rprim 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

-5.0000000000E-01 8.6602540378E-01 0.0000000000E+00

6.1232339957E-17 1.0605752387E-16 1.0000000000E+00

spgroup 164

symrel 1 0 0 0 1 0 0 0 1 -1 0 0 0 -1 0 0 0 -1

-1 0 0 1 1 0 0 0 1 1 0 0 -1 -1 0 0 0 -1

0 1 0 -1 -1 0 0 0 1 0 -1 0 1 1 0 0 0 -1

0 -1 0 -1 0 0 0 0 1 0 1 0 1 0 0 0 0 -1

-1 -1 0 1 0 0 0 0 1 1 1 0 -1 0 0 0 0 -1

1 1 0 0 -1 0 0 0 1 -1 -1 0 0 1 0 0 0 -1

timopt -3

tnons 0.0000000 0.0000000 0.0000000 -0.3333333 0.3333333 0.2000000

0.0000000 0.0000000 0.0000000 -0.3333333 0.3333333 0.2000000

0.0000000 0.0000000 0.0000000 -0.3333333 0.3333333 0.2000000

0.0000000 0.0000000 0.0000000 -0.3333333 0.3333333 0.2000000

0.0000000 0.0000000 0.0000000 -0.3333333 0.3333333 0.2000000

0.0000000 0.0000000 0.0000000 -0.3333333 0.3333333 0.2000000

tolvrs 1.00000000E-12

tsmear 5.00000000E-04 Hartree

typat 1 1 1

wfoptalg 114

wtk 0.06250 0.37500 0.18750 0.37500

xangst 0.0000000000E+00 0.0000000000E+00 0.0000000000E+00

6.0990131703E-16 1.5716933324E+00 2.3770087627E+00

1.3611263528E+00 7.8584666619E-01 4.7540175254E+00

xcart 0.0000000000E+00 0.0000000000E+00 0.0000000000E+00

1.1525464573E-15 2.9700699631E+00 4.4918955770E+00

2.5721560390E+00 1.4850349815E+00 8.9837911540E+00

xred 0.0000000000E+00 0.0000000000E+00 0.0000000000E+00

3.3333333333E-01 6.6666666667E-01 1.0000000000E-01

6.6666666667E-01 3.3333333333E-01 2.0000000000E-01

znucl 46.00000

================================================================================

chkinp: Checking input parameters for consistency.

DATA TYPE INFORMATION:

REAL: Data type name: REAL(DP)

Kind value: 8

Precision: 15

Smallest nonnegligible quantity relative to 1: 0.22204460E-15

Smallest positive number: 0.22250739-307

Largest representable number: 0.17976931+309

INTEGER: Data type name: INTEGER(default)

Kind value: 4

Bit size: 32

Largest representable number: 2147483647

LOGICAL: Data type name: LOGICAL

Kind value: 4

CHARACTER: Data type name: CHARACTER Kind value: 1

==== OpenMP parallelism is OFF ====

==== Using MPI-2 specifications ====

MPI-IO support is ON

xmpi\_tag\_ub ................ 2147483647

xmpi\_bsize\_ch .............. 1

xmpi\_bsize\_int ............. 4

xmpi\_bsize\_sp .............. 4

xmpi\_bsize\_dp .............. 8

xmpi\_bsize\_spc ............. 8

xmpi\_bsize\_dpc ............. 16

xmpio\_bsize\_frm ............ 4

xmpi\_address\_kind .......... 8

xmpi\_offset\_kind ........... 8

MPI\_WTICK .................. 9.9999999999999995E-007

================================================================================

== DATASET 1 ==================================================================

- nproc = 1

--- !COMMENT

src\_file: m\_xgScalapack.F90

src\_line: 251

message: |

xgScalapack in auto mode

...

getdim\_nloc : deduce lmnmax = 18, lnmax = 6,

lmnmaxso= 18, lnmaxso= 6.

Exchange-correlation functional for the present dataset will be:

GGA: Perdew-Burke-Ernzerhof functional - ixc=11

Citation for XC functional:

J.P.Perdew, K.Burke, M.Ernzerhof, PRL 77, 3865 (1996)

Unit cell volume ucvol= 1.0294728E+03 bohr^3

Angles (23,13,12)= 9.00000000E+01 9.00000000E+01 1.20000000E+02 degrees

getcut: wavevector= 0.0000 0.0000 0.0000 ngfft= 30 30 270

ecut(hartree)= 42.000 => boxcut(ratio)= 2.00044

- pspini: atom type 1 psp file is ../../ni/pseudopotential/Pd.psp8

- pspatm: opening atomic psp file ../../ni/pseudopotential/Pd.psp8

- Pd ONCVPSP r\_core= 1.41 1.46 1.55

- 46.00000 18.00000 150807 znucl, zion, pspdat

8 11 2 4 600 0.00000 pspcod,pspxc,lmax,lloc,mmax,r2well

5.99000000000000 7.00000000000000 0.00000000000000 rchrg,fchrg,qchrg

nproj 2 2 2

extension\_switch 1

valence charge integrates to: 17.981741043196138

pspatm : epsatm= 26.08747418

--- l ekb(1:nproj) -->

0 7.863783 -2.278114

1 3.250522 -0.649532

2 -4.140429 -0.914990

pspatm: atomic psp has been read and splines computed

4.22617082E+03 ecore\*ucvol(ha\*bohr\*\*3)

==== Info on pseudopotentials ====

Norm-conserving pseudopotentials

Number of pseudopotentials .. 1

Number of types of atoms .. 1

Scalar calculation (no spin-orbit term)

Nonlocal part applied using Legendre polynomials

Max number of non-local projectors over l and type 2

Highest angular momentum +1 ....... 3

Max number of (l,n) components .. 6

Max number of (l,m,n) components .. 6

Pseudo-Core Charge Info:

Number of radial points for pseudo-core charge .. 2501

XC core-correction treatment (optnlxccc) ........ 1

Radius for pseudo-core charge for each type .....

- Atom type 1 has pseudo-core radius .. 5.9900

Info on the Q-grid used for form factors in spline form:

Number of q-points for radial functions ffspl .. 13105

Number of q-points for vlspl ................... 13105

vloc is computed in Reciprocal Space

model core charge treated in real-space

XC functional for type 1 is 11

Pseudo valence available: yes

wfconv: 48 bands initialized randomly with npw= 6717, for ikpt= 1

wfconv: 48 bands initialized randomly with npw= 13445, for ikpt= 2

wfconv: 48 bands initialized randomly with npw= 13288, for ikpt= 3

wfconv: 48 bands initialized randomly with npw= 13312, for ikpt= 4

\_setup2: Arith. and geom. avg. npw (full set) are 13364.938 13364.756

initro: for itypat= 1, take pseudo charge density from pp file

================================================================================

For input ecut= 1.304062E+01 best grid ngfft= 18 18 150

max ecut= 1.375729E+01

==== FFT mesh ====

FFT mesh divisions ........................ 18 18 150

Augmented FFT divisions ................... 19 19 150

FFT algorithm ............................. 100

FFT cache size ............................ 16

getmpw: optimal value of mpw= 167

getcut: wavevector= 0.0000 0.0000 0.0000 ngfft= 30 30 270

ecut(hartree)= 42.000 => boxcut(ratio)= 2.00044

--- !WARNING

src\_file: m\_drivexc.F90

src\_line: 1092

message: |

Density went too small (lower than xc\_denpos) at 41271 points

and was set to xc\_denpos = 1.00E-14. Lowest was -0.16E-05.

Likely due to too low boxcut or too low ecut for pseudopotential core charge.

...

ITER STEP NUMBER 1

vtorho : nnsclo\_now=3, note that nnsclo,dbl\_nnsclo,istep=3 0 1

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13312

You should try to get npband\*bandpp= 48

For information matrix size is 13312

You should try to get npband\*bandpp= 48

For information matrix size is 13312

newocc: new Fermi energy is 0.078879 , with nelect= 54.000000

Number of bissection calls = 52

newocc : computed new occ. numbers for occopt= 4 , spin-unpolarized case.

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

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mkrho: echo density (plane-wave part only)

Total charge density [el/Bohr^3]

Maximum= 1.7959E+00 at reduced coord. 0.4333 0.7333 0.1111

Minimum= 0.0000E+00 at reduced coord. 0.1333 0.4667 0.5519

Integrated= 5.4000E+01

Total charge density [el/Bohr^3]

Maximum= 1.7959E+00 at reduced coord. 0.4333 0.7333 0.1111

Minimum= 0.0000E+00 at reduced coord. 0.1333 0.4667 0.5519

Integrated= 5.4000E+01

rhotov : is\_hybrid\_ncpp= F

rhotov : n3xccc= 243000

ETOT 1 -406.16038814135 -4.062E+02 1.283E-06 1.264E+04

scprqt: <Vxc>= -1.9022967E-01 hartree

dielmt : 15 largest eigenvalues of the hermitian RPA dielectric matrix

1-5 : 3.00815E+01 1.03637E+01 3.74536E+00 3.30438E+00 2.79132E+00

6-10 : 2.42897E+00 2.42897E+00 2.42362E+00 2.42362E+00 2.37212E+00

11-15: 2.37212E+00 2.34492E+00 2.15828E+00 1.93860E+00 1.64757E+00

dielmt : 5 smallest eigenvalues of the hermitian RPA dielectric matrix

1-5 :-1.38182E+03 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00

Simple mixing update:

residual square of the potential : 1658.2573826503378

scfcv\_core: previous iteration took 50 [s]

ITER STEP NUMBER 2

vtorho : nnsclo\_now=3, note that nnsclo,dbl\_nnsclo,istep=3 0 2

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13312

You should try to get npband\*bandpp= 48

For information matrix size is 13312

You should try to get npband\*bandpp= 48

For information matrix size is 13312

newocc: new Fermi energy is 0.052911 , with nelect= 54.000000

Number of bissection calls = 52

newocc : computed new occ. numbers for occopt= 4 , spin-unpolarized case.

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0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 1.333 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

mkrho: echo density (plane-wave part only)

Total charge density [el/Bohr^3]

Maximum= 1.9122E+00 at reduced coord. 0.4667 0.7667 0.1074

Minimum= 0.0000E+00 at reduced coord. 0.4000 0.1333 0.4815

Integrated= 5.4000E+01

Total charge density [el/Bohr^3]

Maximum= 1.9122E+00 at reduced coord. 0.4667 0.7667 0.1074

Minimum= 0.0000E+00 at reduced coord. 0.4000 0.1333 0.4815

Integrated= 5.4000E+01

rhotov : is\_hybrid\_ncpp= F

rhotov : n3xccc= 243000

ETOT 2 -406.32122713801 -1.608E-01 5.824E-10 4.516E+03

scprqt: <Vxc>= -1.6880193E-01 hartree

Pulay update with 1 previous iterations:

mixing of old trial potential : alpha(m:m-4)= 0.559 0.441

scfcv\_core: previous iteration took 41 [s]

ITER STEP NUMBER 3

vtorho : nnsclo\_now=3, note that nnsclo,dbl\_nnsclo,istep=3 0 3

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13312

You should try to get npband\*bandpp= 48

For information matrix size is 13312

You should try to get npband\*bandpp= 48

For information matrix size is 13312

newocc: new Fermi energy is 0.074725 , with nelect= 54.000000

Number of bissection calls = 50

newocc : computed new occ. numbers for occopt= 4 , spin-unpolarized case.

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 1.796 1.796 0.000 0.000 0.000 0.000 0.000 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.068 0.000 0.000 0.000 0.000 0.000 0.000 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

mkrho: echo density (plane-wave part only)

Total charge density [el/Bohr^3]

Maximum= 1.8618E+00 at reduced coord. 0.4333 0.7667 0.1111

Minimum= 4.4820E-08 at reduced coord. 0.0000 0.0000 0.5963

Integrated= 5.4000E+01

Total charge density [el/Bohr^3]

Maximum= 1.8618E+00 at reduced coord. 0.4333 0.7667 0.1111

Minimum= 4.4820E-08 at reduced coord. 0.0000 0.0000 0.5963

Integrated= 5.4000E+01

rhotov : is\_hybrid\_ncpp= F

rhotov : n3xccc= 243000

ETOT 3 -406.42526467537 -1.040E-01 4.619E-10 6.100E+03

scprqt: <Vxc>= -1.8271744E-01 hartree

Pulay update with 2 previous iterations:

mixing of old trial potential : alpha(m:m-4)= 0.436 0.348 0.216

scfcv\_core: previous iteration took 41 [s]

ITER STEP NUMBER 4

vtorho : nnsclo\_now=3, note that nnsclo,dbl\_nnsclo,istep=3 0 4

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13312

You should try to get npband\*bandpp= 48

For information matrix size is 13312

You should try to get npband\*bandpp= 48

For information matrix size is 13312

newocc: new Fermi energy is 0.065593 , with nelect= 54.000000

Number of bissection calls = 10

newocc : computed new occ. numbers for occopt= 4 , spin-unpolarized case.

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 0.000 0.000 0.000 0.000 0.000 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

mkrho: echo density (plane-wave part only)

Total charge density [el/Bohr^3]

Maximum= 1.8631E+00 at reduced coord. 0.4333 0.7667 0.1111

Minimum= 7.1133E-08 at reduced coord. 0.0000 0.0000 0.5963

Integrated= 5.4000E+01

Total charge density [el/Bohr^3]

Maximum= 1.8631E+00 at reduced coord. 0.4333 0.7667 0.1111

Minimum= 7.1133E-08 at reduced coord. 0.0000 0.0000 0.5963

Integrated= 5.4000E+01

rhotov : is\_hybrid\_ncpp= F

rhotov : n3xccc= 243000

ETOT 4 -406.43587597968 -1.061E-02 2.525E-10 5.058E+03

scprqt: <Vxc>= -1.8283509E-01 hartree

Pulay update with 3 previous iterations:

mixing of old trial potential : alpha(m:m-4)= 0.290 0.290 0.273 0.147

scfcv\_core: previous iteration took 41 [s]

ITER STEP NUMBER 5

vtorho : nnsclo\_now=3, note that nnsclo,dbl\_nnsclo,istep=3 0 5

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13434

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13445

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13288

You should try to get npband\*bandpp= 48

For information matrix size is 13312

You should try to get npband\*bandpp= 48

For information matrix size is 13312

You should try to get npband\*bandpp= 48

For information matrix size is 13312

newocc: new Fermi energy is 0.065187 , with nelect= 54.000000

Number of bissection calls = 10

newocc : computed new occ. numbers for occopt= 4 , spin-unpolarized case.

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 0.000 0.000 0.000 0.000 0.000 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

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0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000

2.000 2.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

mkrho: echo density (plane-wave part only)

Total charge density [el/Bohr^3]

Maximum= 1.8641E+00 at reduced coord. 0.4333 0.7667 0.1111

Minimum= 8.7759E-08 at reduced coord. 0.5333 0.1000 0.6000

Integrated= 5.4000E+01

Total charge density [el/Bohr^3]

Maximum= 1.8641E+00 at reduced coord. 0.4333 0.7667 0.1111

Minimum= 8.7759E-08 at reduced coord. 0.5333 0.1000 0.6000

Integrated= 5.4000E+01

rhotov : is\_hybrid\_ncpp= F

rhotov : n3xccc= 243000

ETOT 5 -406.43991043678 -4.034E-03 6.870E-12 4.651E+03

scprqt: <Vxc>= -1.8288438E-01 hartree

dielmt : 15 largest eigenvalues of the hermitian RPA dielectric matrix

1-5 : NaN NaN NaN NaN NaN

6-10 : NaN NaN NaN NaN NaN

11-15: NaN NaN NaN NaN NaN

dielmt : 5 smallest eigenvalues of the hermitian RPA dielectric matrix

1-5 : NaN NaN NaN NaN NaN

Pulay update with 4 previous iterations:

mixing of old trial potential : alpha(m:m-4)= NaN NaN NaN NaN NaN

scfcv\_core: previous iteration took 46 [s]

ITER STEP NUMBER 6

vtorho : nnsclo\_now=3, note that nnsclo,dbl\_nnsclo,istep=3 0 6

You should try to get npband\*bandpp= 48

For information matrix size is 13434

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

This is embarrasing. Let's pray

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

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--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

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--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

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--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

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...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

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--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

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--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

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--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

This is embarrasing. Let's pray

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

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--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

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src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

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src\_file: m\_lobpcg2.F90

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mpi\_rank: 0

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src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

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--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

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...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

This is embarrasing. Let's pray

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

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...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

This is embarrasing. Let's pray

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

This is embarrasing. Let's pray

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

This is embarrasing. Let's pray

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

This is embarrasing. Let's pray

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

This is embarrasing. Let's pray

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 502

message: |

This is embarrasing. Let's pray

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 720

message: |

An old style abi\_xorthonormalize happened but now I'll try to continue ;-)

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

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message: |

But before that, I want to recalculate H|Psi> and S|Psi>

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You should try to get npband\*bandpp= 48

For information matrix size is 13434

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src\_file: m\_lobpcg2.F90

src\_line: 559

message: |

But before that, I want to recalculate H|Psi> and S|Psi>

...

You should try to get npband\*bandpp= 48

For information matrix size is 13434

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message: |

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...

You should try to get npband\*bandpp= 48

For information matrix size is 13445

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src\_file: m\_lobpcg2.F90

src\_line: 559

message: |

But before that, I want to recalculate H|Psi> and S|Psi>

...

You should try to get npband\*bandpp= 48

For information matrix size is 13445

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message: |

But before that, I want to recalculate H|Psi> and S|Psi>

...

You should try to get npband\*bandpp= 48

For information matrix size is 13445

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src\_file: m\_lobpcg2.F90

src\_line: 559

message: |

But before that, I want to recalculate H|Psi> and S|Psi>

...

You should try to get npband\*bandpp= 48

For information matrix size is 13288

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But before that, I want to recalculate H|Psi> and S|Psi>

...

You should try to get npband\*bandpp= 48

For information matrix size is 13288

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--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 559

message: |

But before that, I want to recalculate H|Psi> and S|Psi>

...

You should try to get npband\*bandpp= 48

For information matrix size is 13288

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But before that, I want to recalculate H|Psi> and S|Psi>

...

You should try to get npband\*bandpp= 48

For information matrix size is 13312

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src\_line: 502

message: |

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--- !COMMENT

src\_file: m\_lobpcg2.F90

src\_line: 559

message: |

But before that, I want to recalculate H|Psi> and S|Psi>

...

You should try to get npband\*bandpp= 48

For information matrix size is 13312

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--- !COMMENT

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This is embarrasing. Let's pray

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src\_file: m\_lobpcg2.F90

src\_line: 559

message: |

But before that, I want to recalculate H|Psi> and S|Psi>

...

You should try to get npband\*bandpp= 48

For information matrix size is 13312

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I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

...

--- !ERROR

src\_file: m\_lobpcg2.F90

src\_line: 525

mpi\_rank: 0

message: |

I'm so so sorry I could not make it, I did my best but I failed. Sorry. I'm gonna suicide

Program received signal SIGSEGV: Segmentation fault - invalid memory reference.

Backtrace for this error:

#0 0x7FC562177E08

#1 0x7FC562176F90

#2 0x7FC56145D4AF

#3 0x14929FC in \_\_m\_splines\_MOD\_splfit at m\_splines.F90:172

#4 0xD181F7 in \_\_m\_occ\_MOD\_getnel at m\_occ.F90:219

#5 0xD1A572 in \_\_m\_occ\_MOD\_newocc at m\_occ.F90:496

#6 0x56B467 in \_\_m\_vtorho\_MOD\_vtorho at m\_vtorho.F90:1192

#7 0x537144 in \_\_m\_scfcv\_core\_MOD\_scfcv\_core at m\_scfcv\_core.F90:1536

#8 0x52A0DC in \_\_m\_scfcv\_MOD\_scfcv\_scfcv at m\_scfcv.F90:746

#9 0x51A87C in \_\_m\_gstate\_MOD\_gstate at m\_gstate.F90:1331

#10 0x425566 in \_\_m\_gstateimg\_MOD\_gstateimg at m\_gstateimg.F90:566

#11 0x4169BC in \_\_m\_driver\_MOD\_driver at m\_driver.F90:705 (discriminator 22)

#12 0x408F31 in MAIN\_\_ at abinit.F90:444