Elastic constants calculation for α-Pt_2Si step by step

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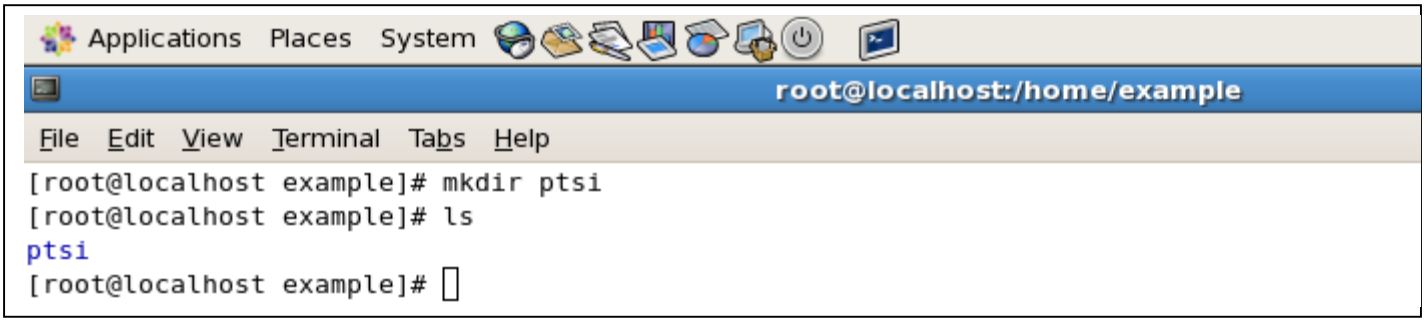
(09.02.2013)

α-Pt_2Si compound is a test case for elastic constants calculation. It has tetragonal symmetry with space group I4/mmm with number 139. The α-Pt_2Si structure (**PtSi.struct**) is described in detail in the following:

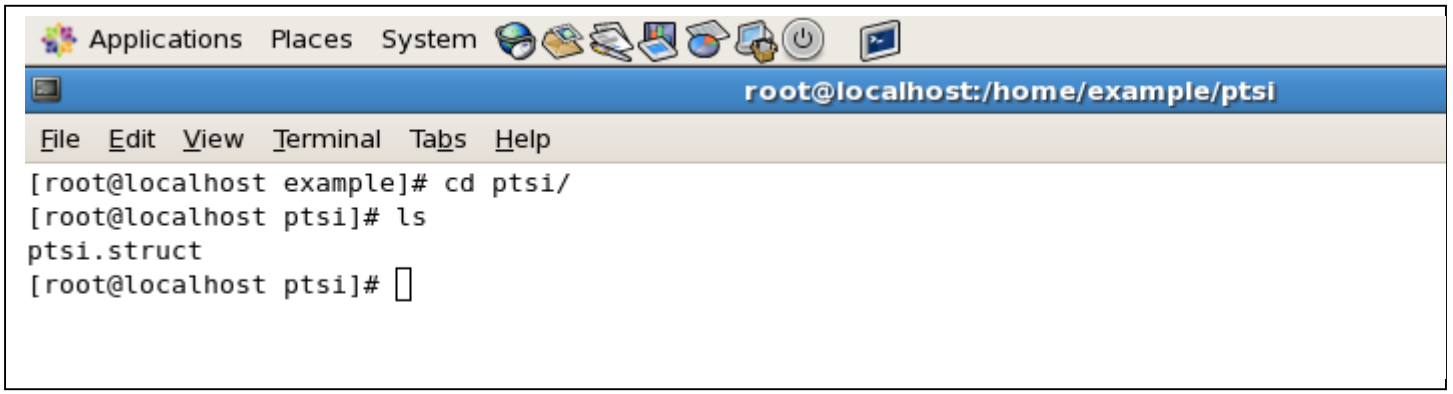
```
alpha Pt2Si
B   LATTICE,NONEQUIV.ATOMS:  2139_I4/mmm
MODE OF CALC=RELA unit=bohr
  7.461000  7.461000 11.268000 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT=-2
      -1: X=0.00000000 Y=0.50000000 Z=0.75000000
Pt         NPT=  781  R0=0.00000500 RMT=    2.4100   Z: 78.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Si         NPT=  781  R0=0.00010000 RMT=    2.1300   Z: 14.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  16      NUMBER OF SYMMETRY OPERATIONS
```

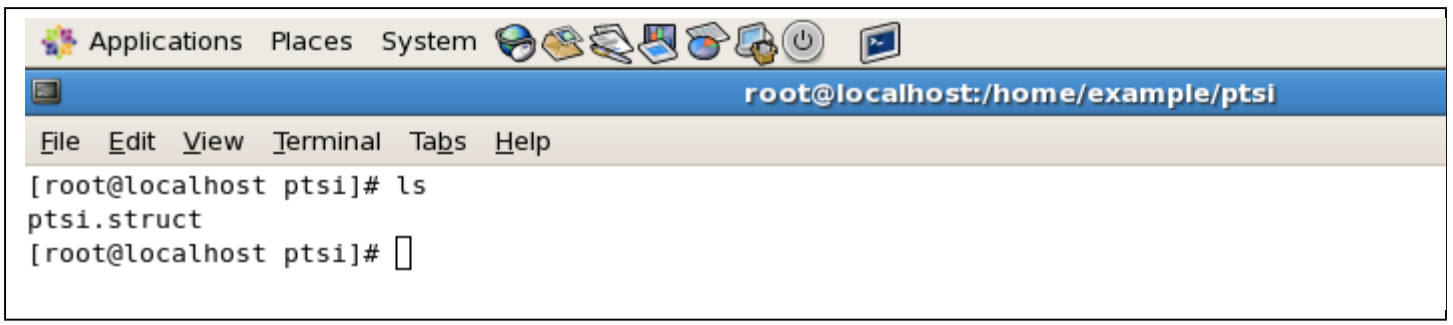
You can find it from example directory.

- Make a directory with name **ptsi .**

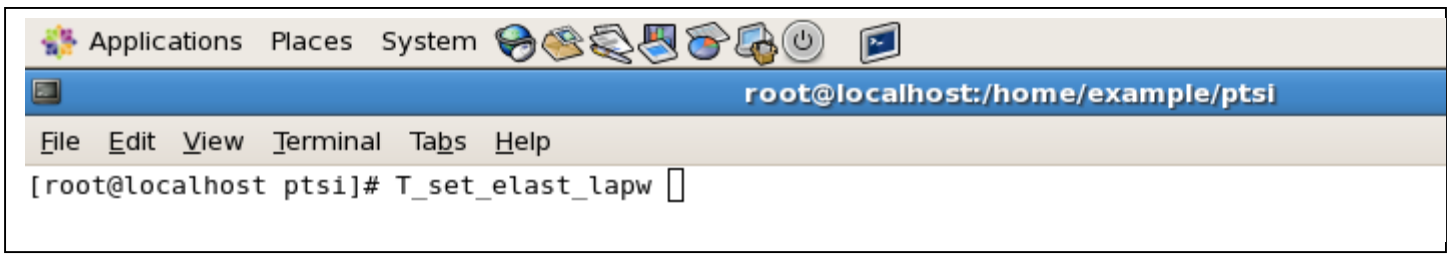


- Change to **ptsi** directory and copy **ptsi.struct** within it from example directory.



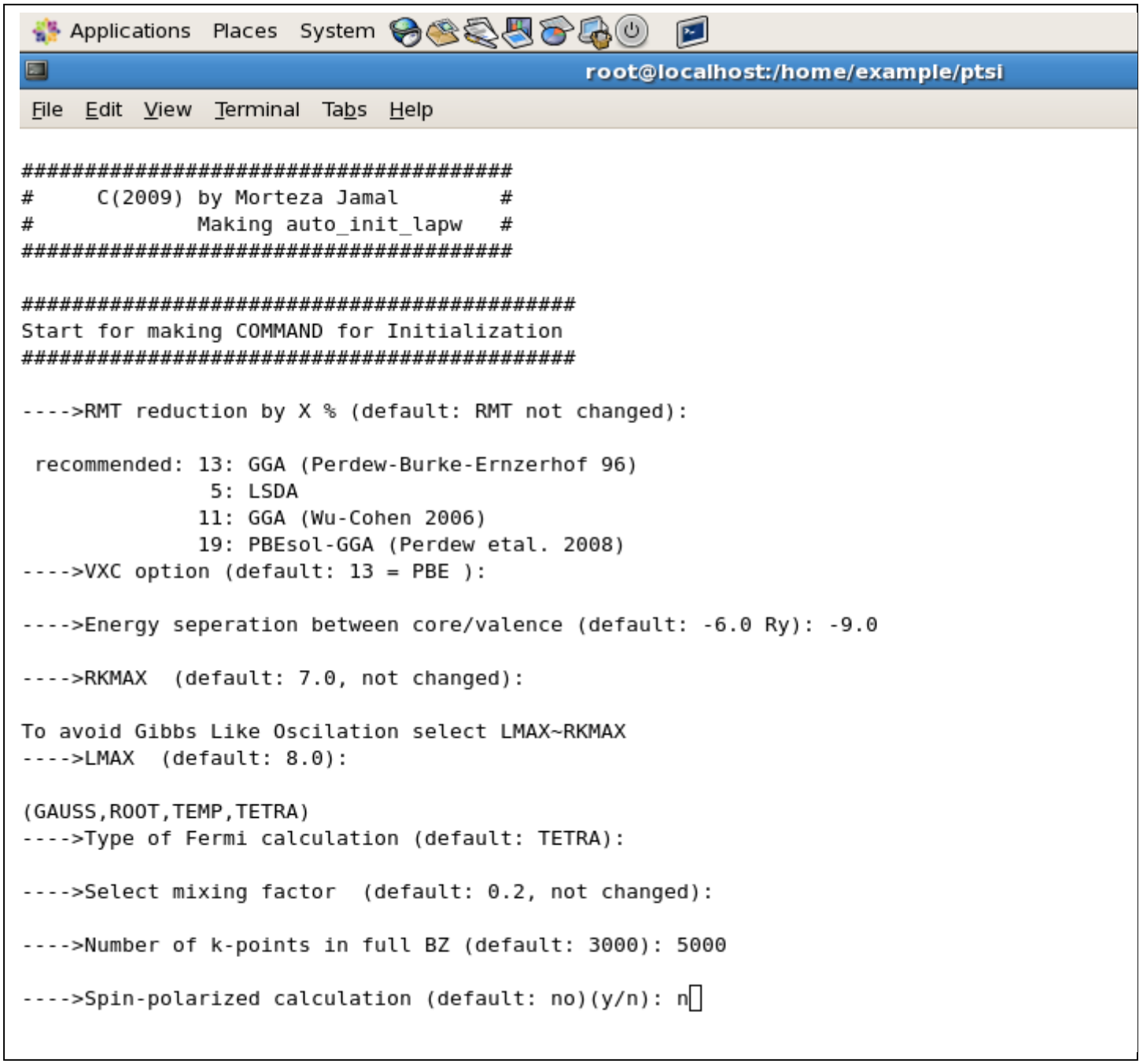


- Run **T_set_elast_lapw**

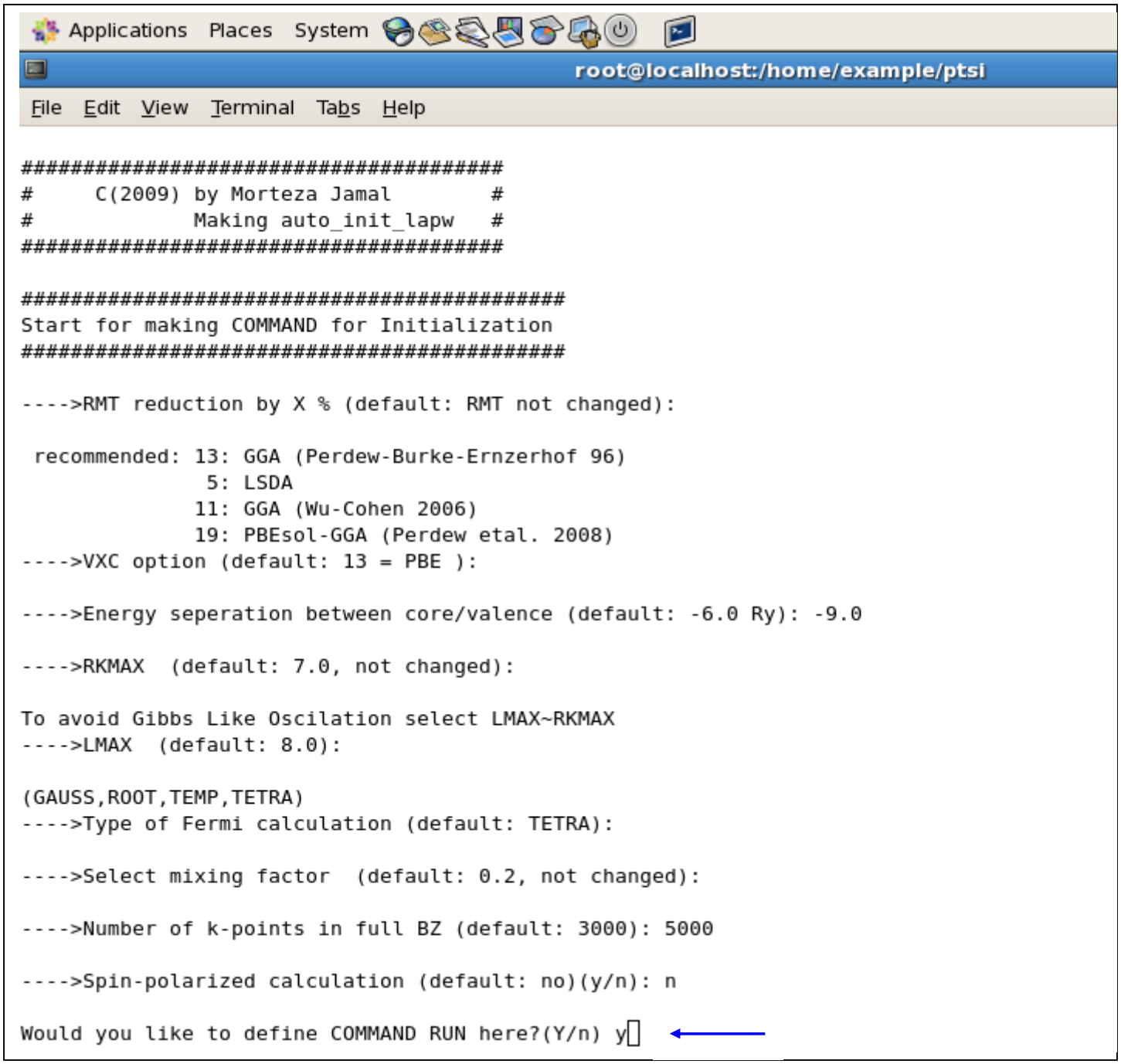


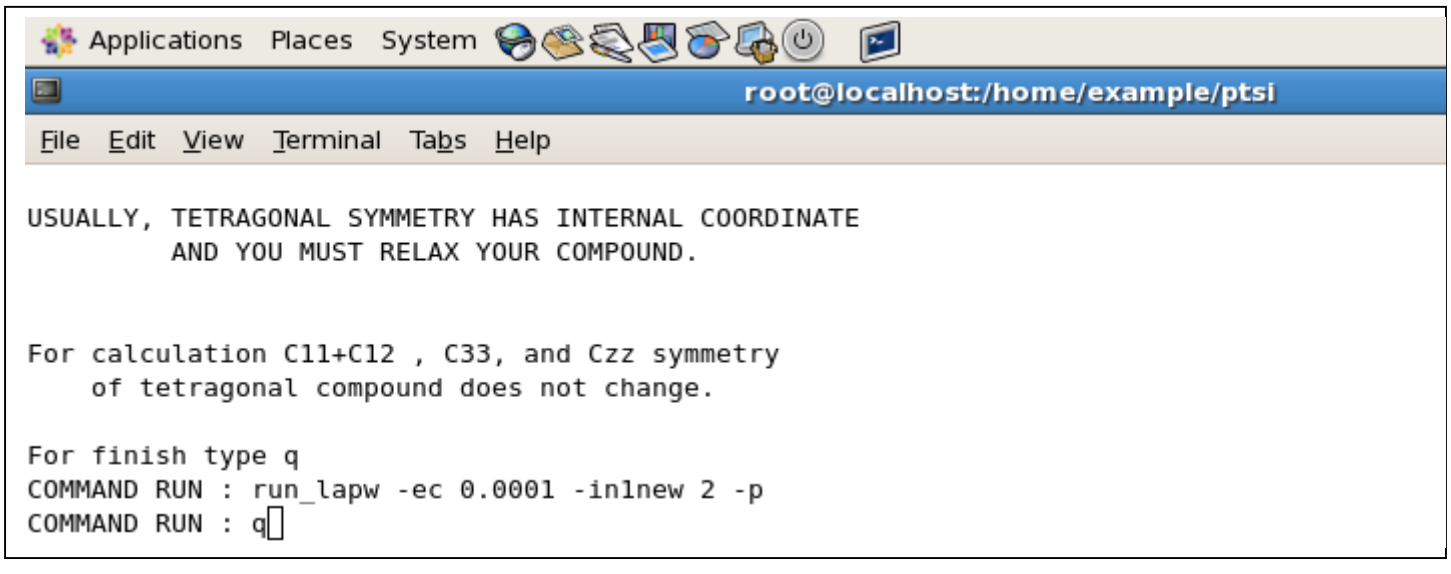
- I selected the following parameters for calculation :

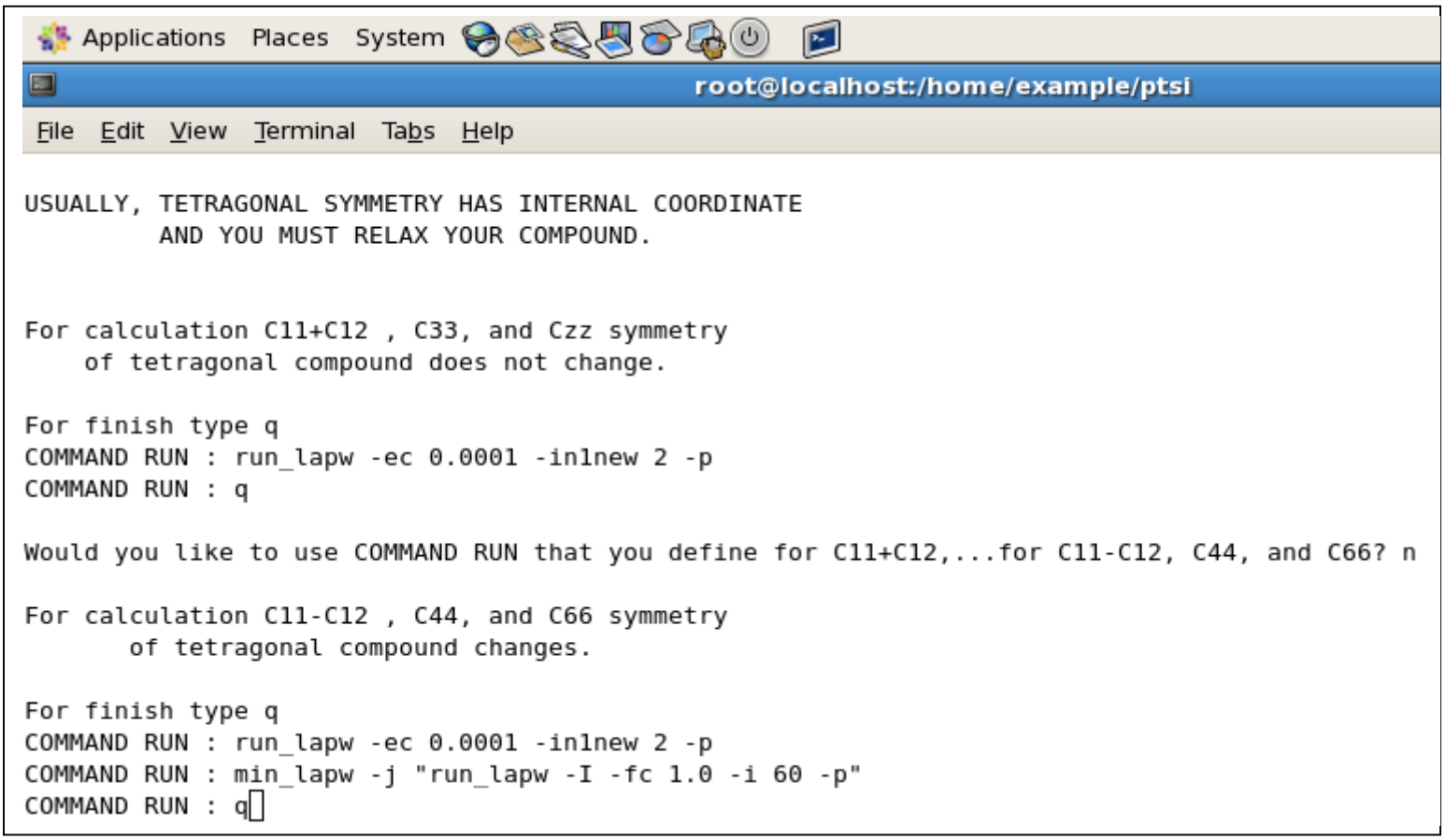
RMT reduction = default (RMT not changed), Xc = default (PBE), Energy seperaction = -9.0, R_Kmax = 7, L_max = 8, Type of Fermi calculation = default (TETRA), mixing factor = default (0.2), nkpoint = 5000, and Spin-polarized calculation = default (no).



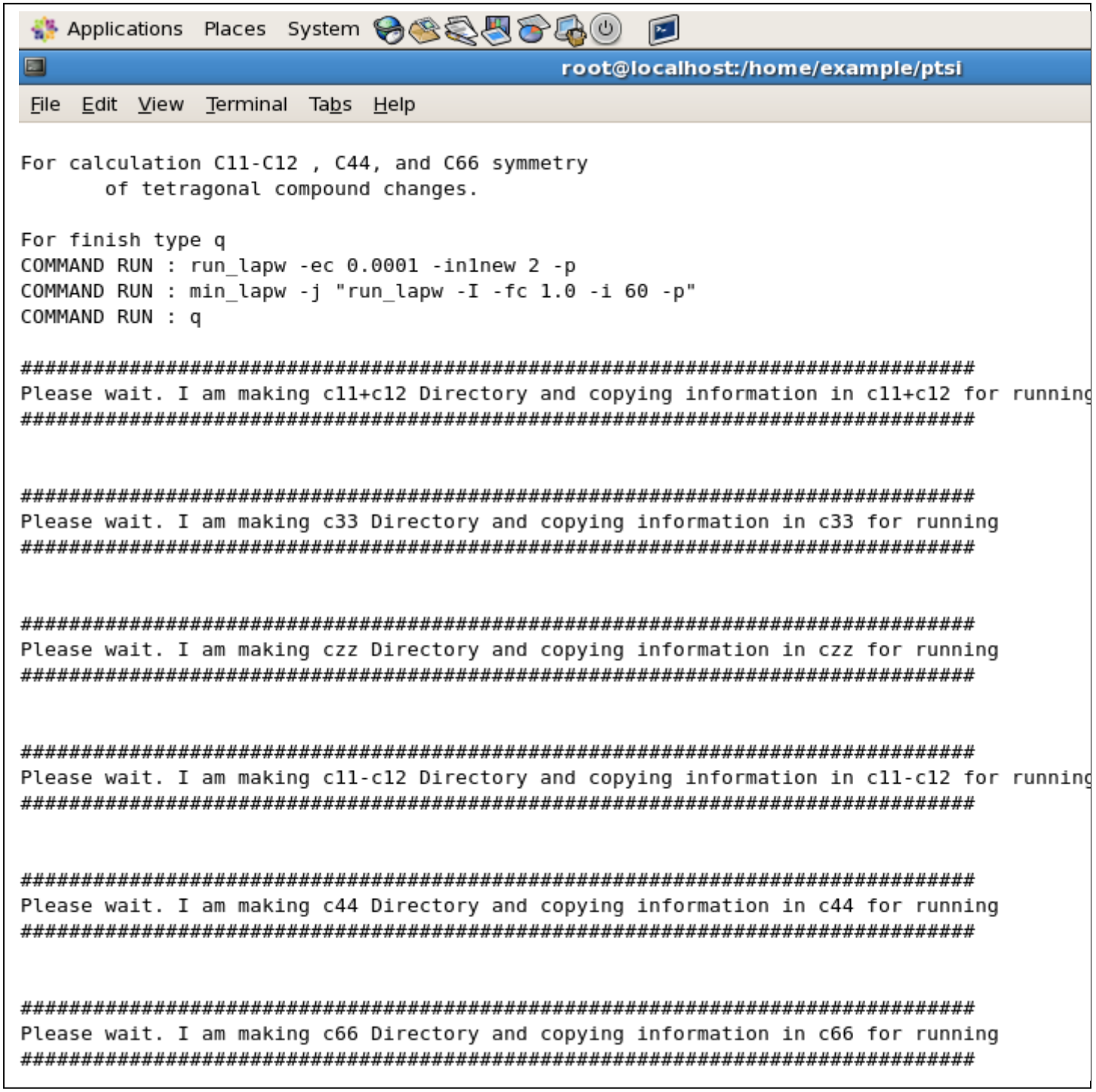
- Define **command run**


Applications Places System
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help
##
C(2009) by Morteza Jamal
Making auto_init_lapw
##
##
Start for making COMMAND for Initialization
##
---->RMT reduction by X % (default: RMT not changed):
recommended: 13: GGA (Perdew-Burke-Ernzerhof 96)
5: LSDA
11: GGA (Wu-Cohen 2006)
19: PBEsol-GGA (Perdew etal. 2008)
---->VXC option (default: 13 = PBE):
---->Energy seperation between core/valence (default: -6.0 Ry): -9.0
---->RKMAX (default: 7.0, not changed):
To avoid Gibbs Like Oscilation select LMAX~RKMAX
---->LMAX (default: 8.0):
(GAUSS,ROOT,TEMP,TETRA)
---->Type of Fermi calculation (default: TETRA):
---->Select mixing factor (default: 0.2, not changed):
---->Number of k-points in full BZ (default: 3000): 5000
---->Spin-polarized calculation (default: no)(y/n): n
Would you like to define COMMAND RUN here?(Y/n) y

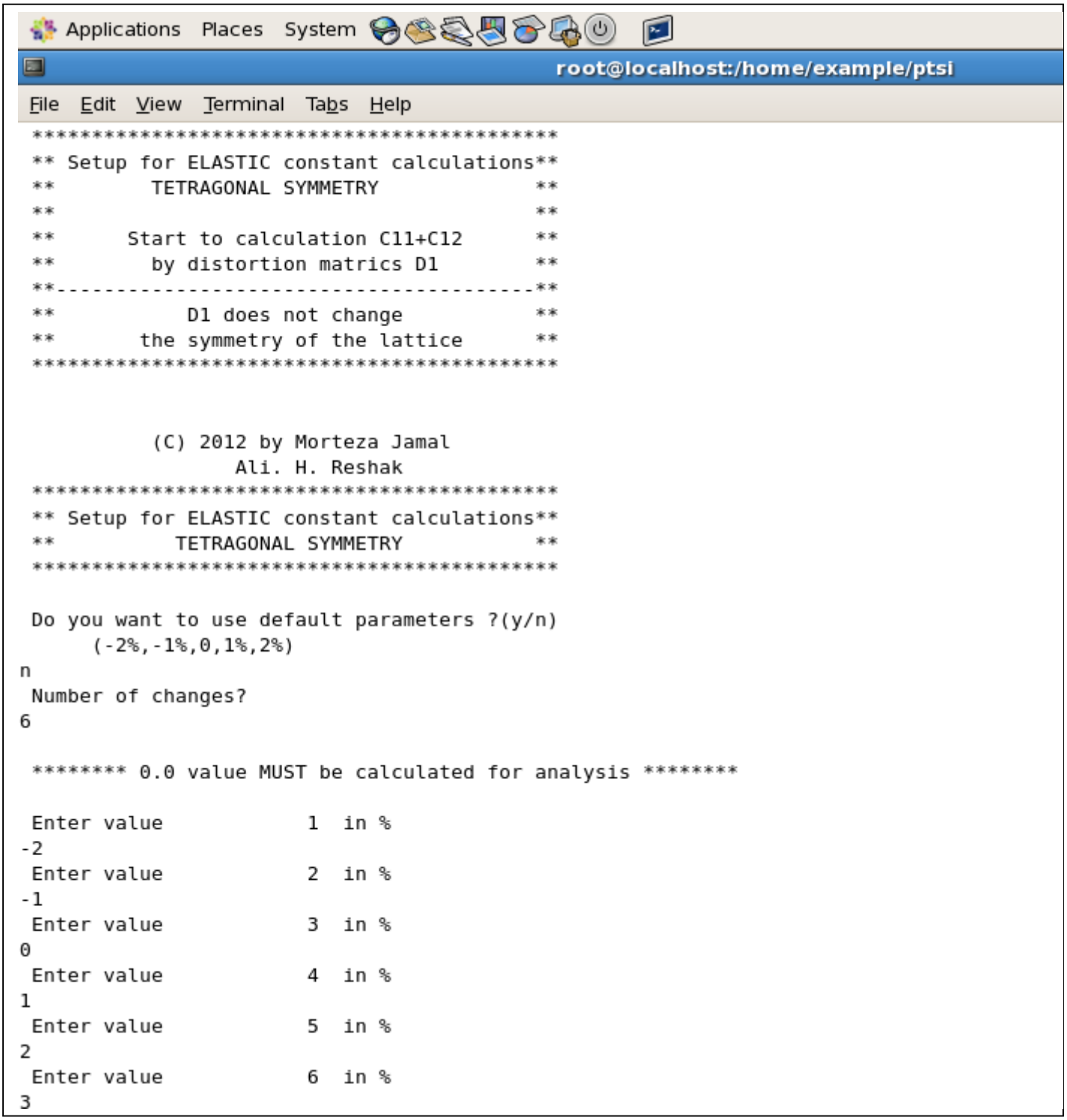

Applications Places System
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help
USUALLY, TETRAGONAL SYMMETRY HAS INTERNAL COORDINATE
AND YOU MUST RELAX YOUR COMPOUND.
For calculation C11+C12 , C33, and Czz symmetry
of tetragonal compound does not change.
For finish type q
COMMAND RUN : run_lapw -ec 0.0001 -in1new 2 -p
COMMAND RUN : q


Applications Places System
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help
USUALLY, TETRAGONAL SYMMETRY HAS INTERNAL COORDINATE
AND YOU MUST RELAX YOUR COMPOUND.
For calculation C11+C12 , C33, and Czz symmetry
of tetragonal compound does not change.
For finish type q
COMMAND RUN : run_lapw -ec 0.0001 -in1new 2 -p
COMMAND RUN : q
Would you like to use COMMAND RUN that you define for C11+C12,...for C11-C12, C44, and C66? n
For calculation C11-C12 , C44, and C66 symmetry
of tetragonal compound changes.
For finish type q
COMMAND RUN : run_lapw -ec 0.0001 -in1new 2 -p
COMMAND RUN : min_lapw -j "run_lapw -I -fc 1.0 -i 60 -p"
COMMAND RUN : q

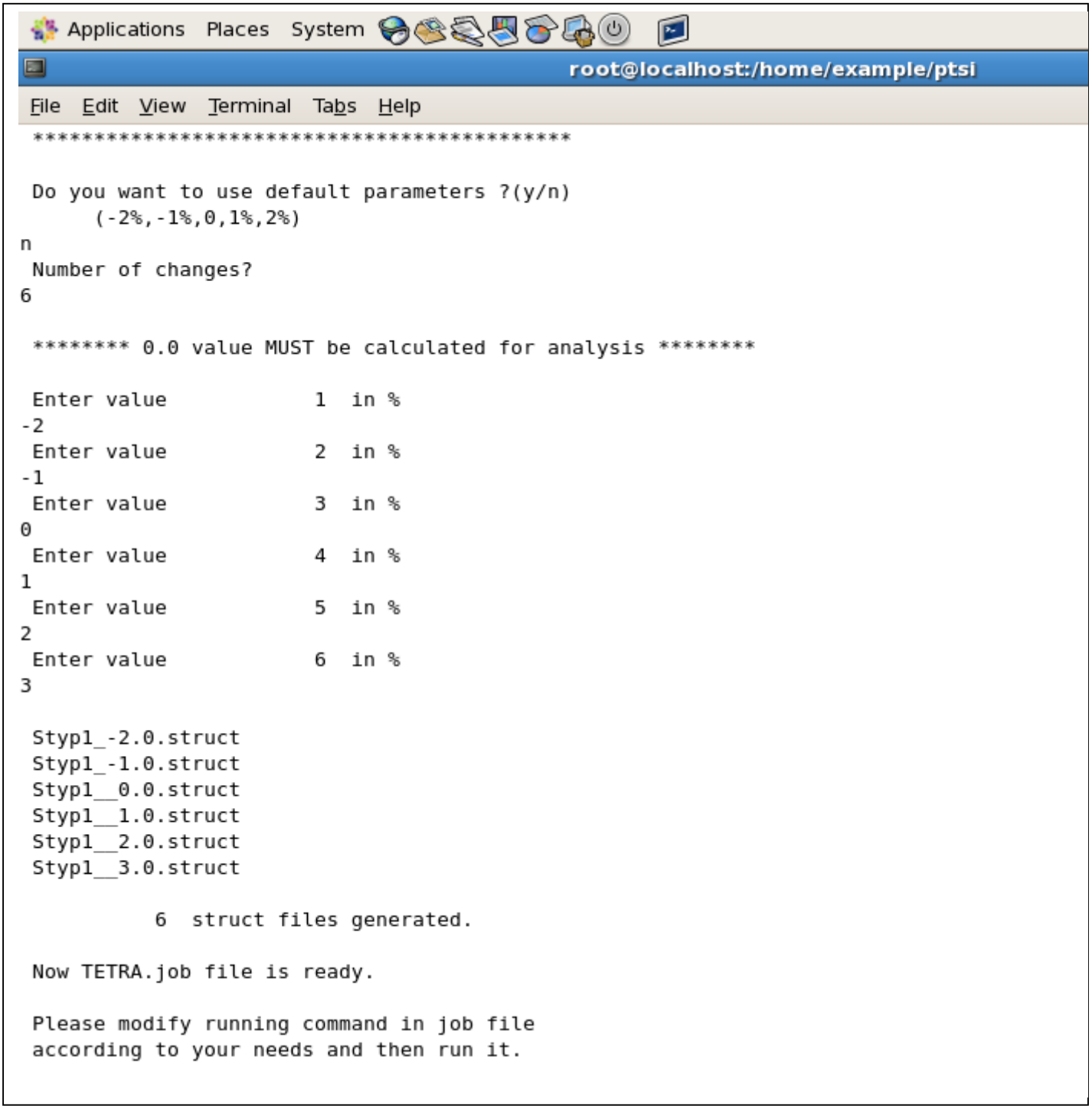
Now, we see



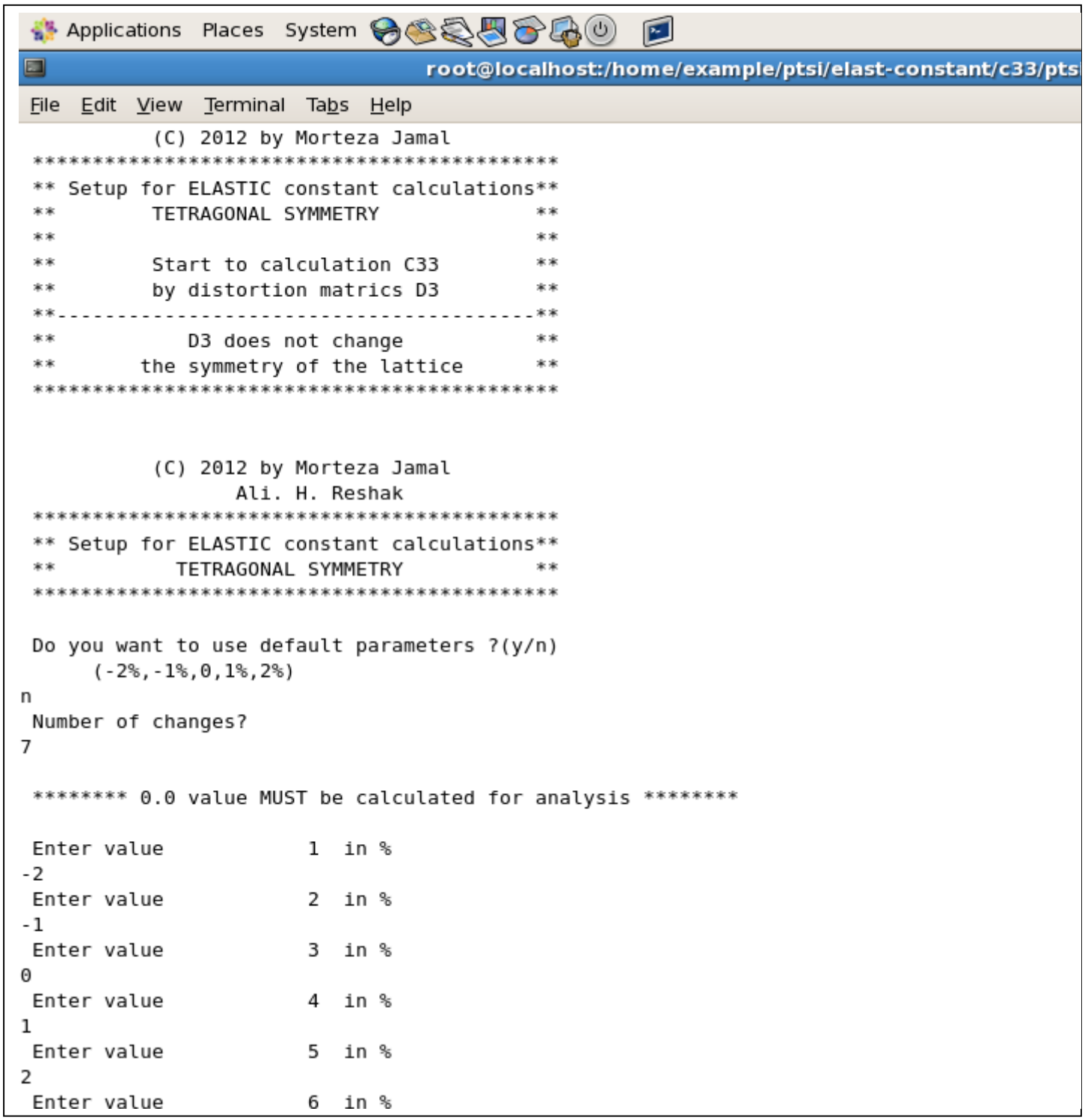
- I didn't use default parameters for (C11+C12) calculations. I selected number of changes 6 and value of changes -2, -1, 0, 1, 2, 3.

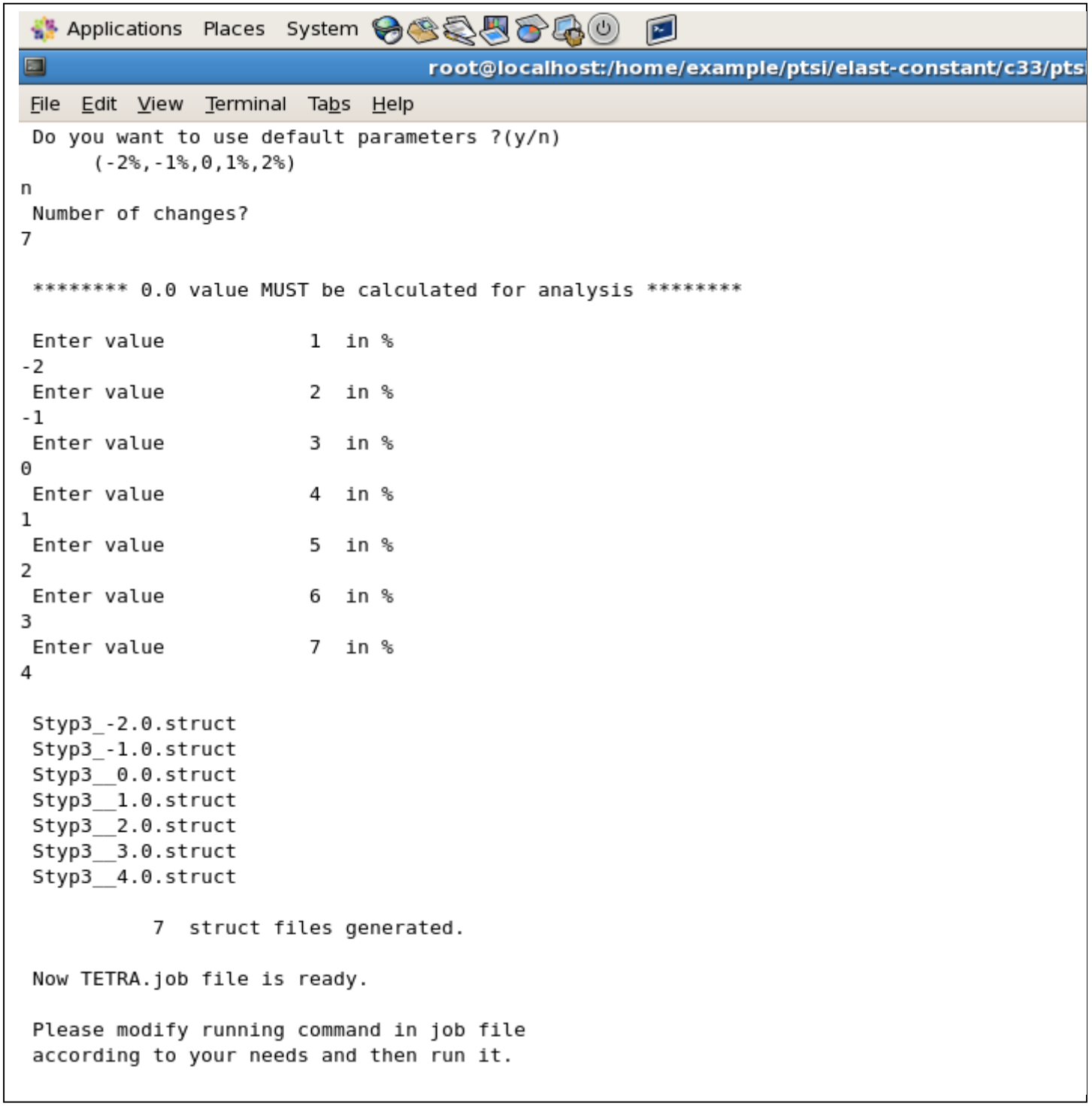

Applications Places System
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help
****
** Setup for ELASTIC constant calculations**
** TETRAGONAL SYMMETRY **
** **
** Start to calculation C11+C12 **
** by distortion matrics D1 **

** D1 does not change **
** the symmetry of the lattice **
****
(C) 2012 by Morteza Jamal
Ali. H. Reshak
****
** Setup for ELASTIC constant calculations**
** TETRAGONAL SYMMETRY **
****
Do you want to use default parameters ?(y/n)
(-2%,-1%,0,1%,2%)
n
Number of changes?
6
******** 0.0 value MUST be calculated for analysis ********
Enter value 1 in %
-2
Enter value 2 in %
-1
Enter value 3 in %
0
Enter value 4 in %
1
Enter value 5 in %
2
Enter value 6 in %
3

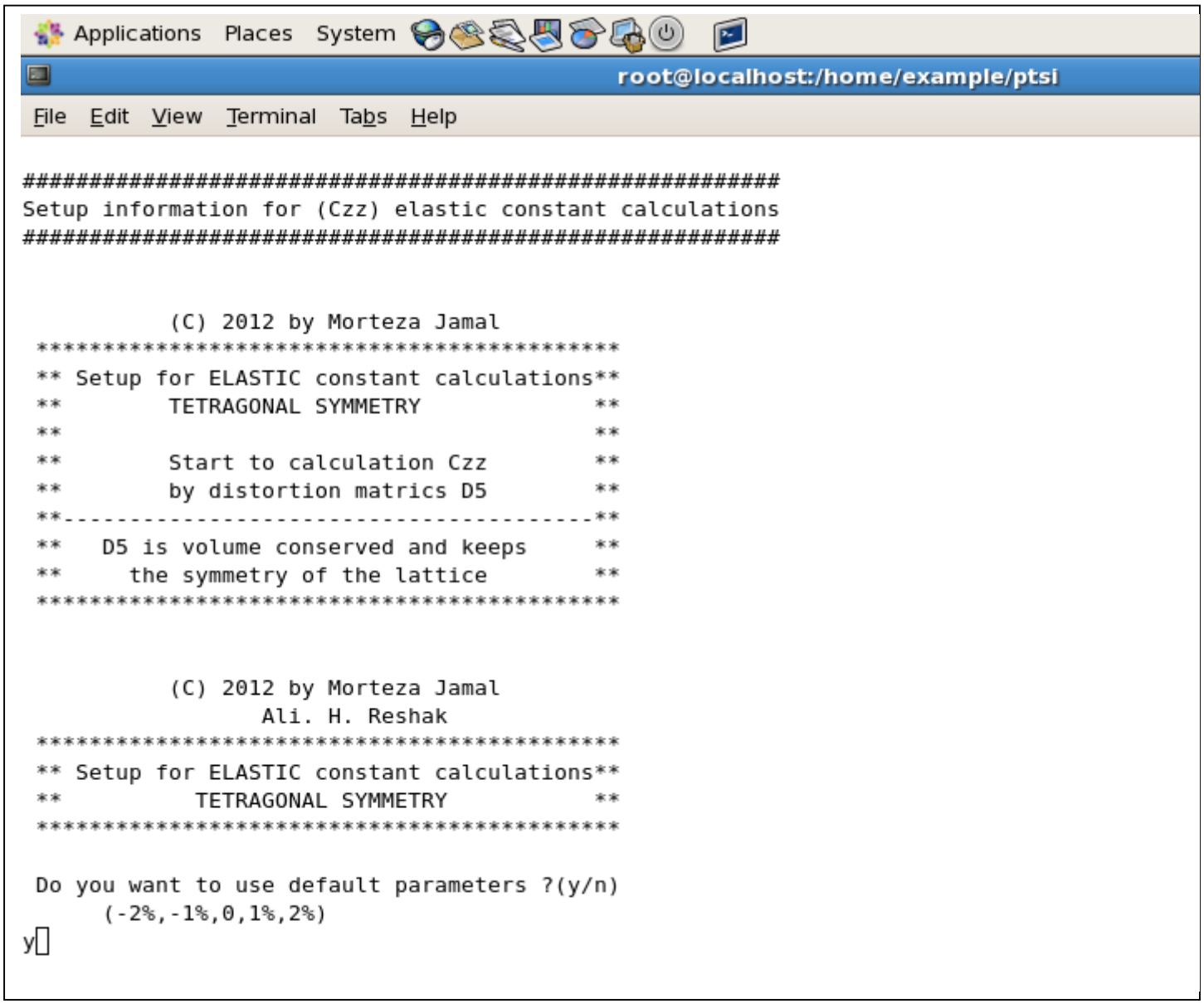


- I didn't use default parameters for (C33) calculations. I selected number of changes 7 and value of changes -2, -1, 0, 1, 2, 3, 4.

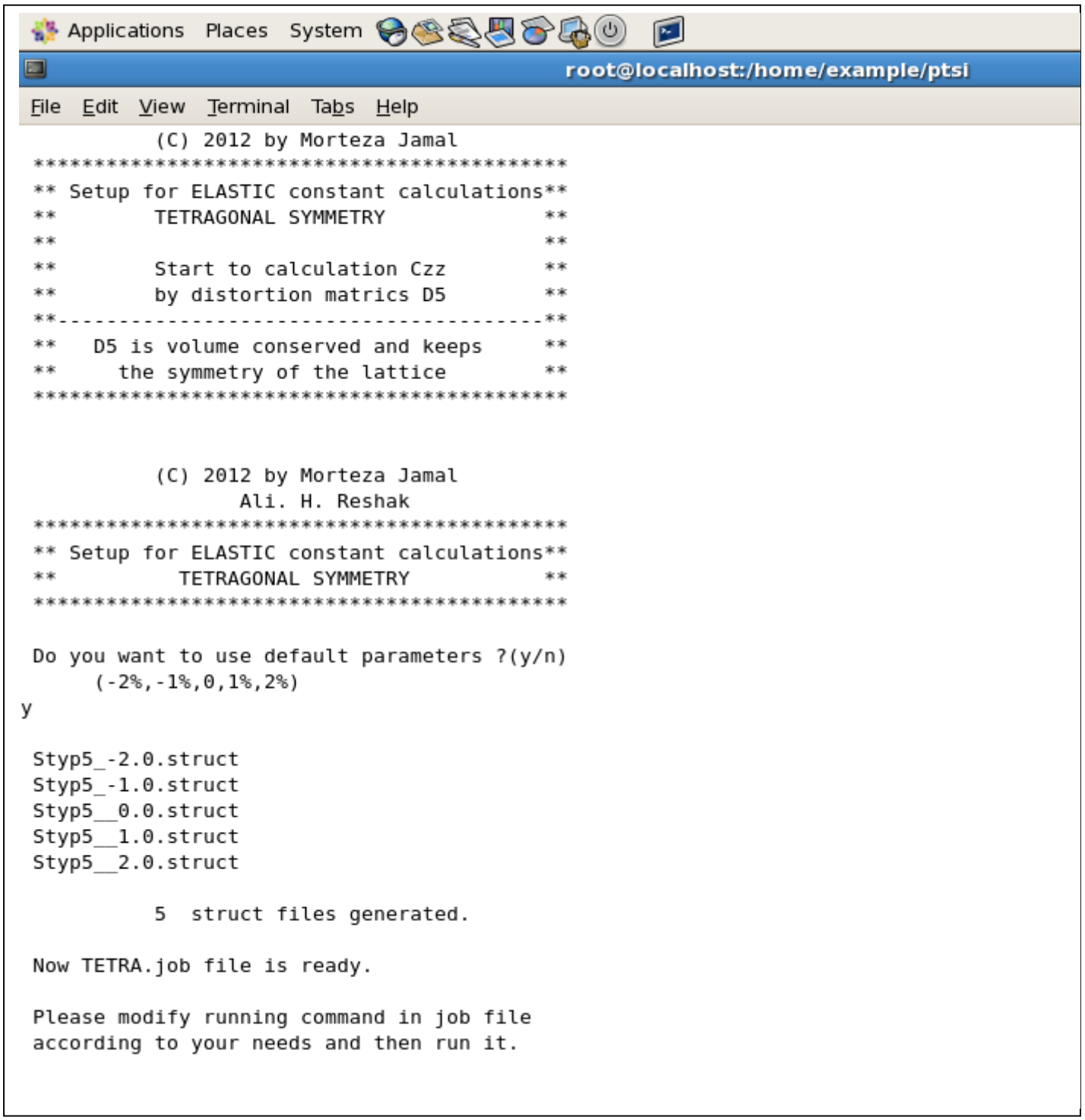

Applications Places System
root@localhost:/home/example/ptsi/elast-constant/c33/pts
File Edit View Terminal Tabs Help
(C) 2012 by Morteza Jamal
** Setup for ELASTIC constant calculations**
** TETRAGONAL SYMMETRY **
** Start to calculation C33 **
** by distortion matrics D3 **
** D3 does not change **
** the symmetry of the lattice **
(C) 2012 by Morteza Jamal
Ali. H. Reshak
** Setup for ELASTIC constant calculations**
** TETRAGONAL SYMMETRY **
Do you want to use default parameters ?(y/n)
(-2%,-1%,0,1%,2%)
n
Number of changes?
7
******** 0.0 value MUST be calculated for analysis ********
Enter value 1 in %
-2
Enter value 2 in %
-1
Enter value 3 in %
0
Enter value 4 in %
1
Enter value 5 in %
2
Enter value 6 in %



- I used default parameters for (Czz) calculations.

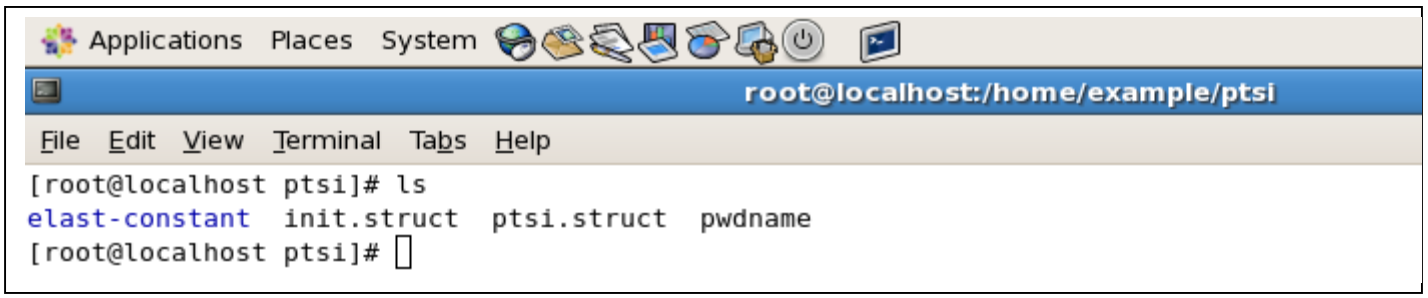

Applications Places System
root@localhost:/home/example/ptsi
File Edit View Terminal Tabs Help
##
Setup information for (Czz) elastic constant calculations
##
(C) 2012 by Morteza Jamal
****
** Setup for ELASTIC constant calculations**
** TETRAGONAL SYMMETRY **
** **
** Start to calculation Czz **
** by distortion matrics D5 **

** D5 is volume conserved and keeps **
** the symmetry of the lattice **
****
(C) 2012 by Morteza Jamal
Ali. H. Reshak
****
** Setup for ELASTIC constant calculations**
** TETRAGONAL SYMMETRY **
****
Do you want to use default parameters ?(y/n)
(-2%,-1%,0,1%,2%)
y

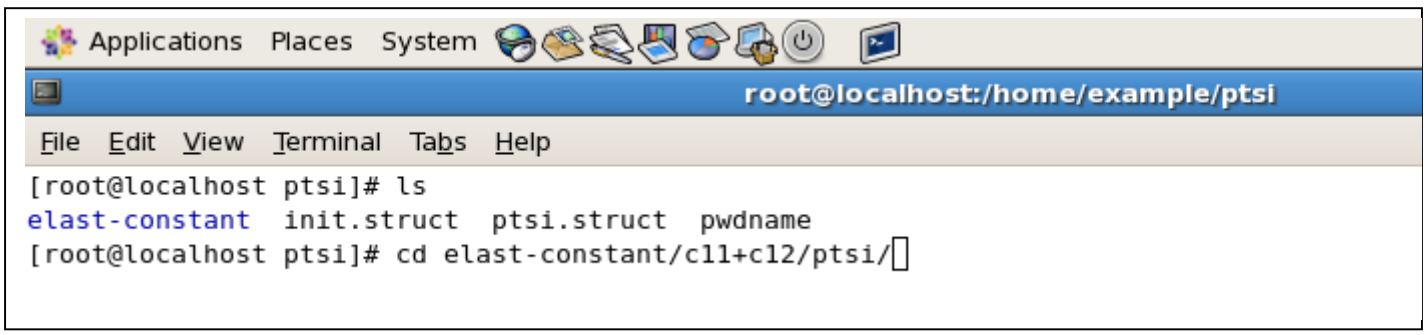


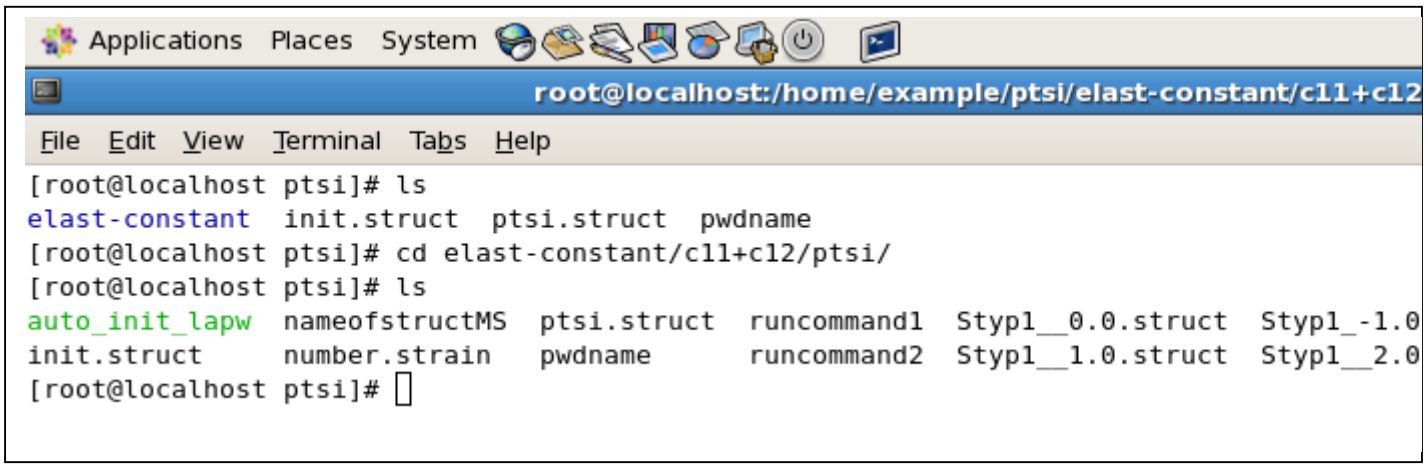
- I used default parameters for (C44), (C11-C12), and (C66) calculations.
  I did the same producer such as above pictures .

Now, if we get a list we will see a directory with name **elast-constant**

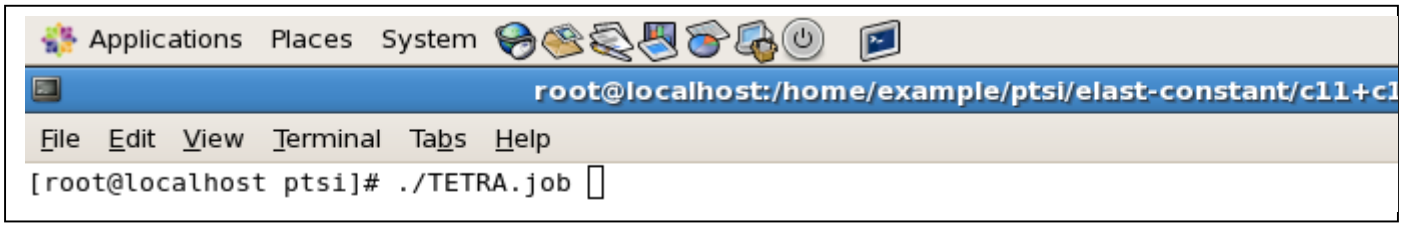


- Now, we have to run created **TETRA.job** file. You can use **T_calljob_lapw** but, I prefer to run them by hand because I want to check steps of running by WIEN2k. For this goal, I change to **elast-constant** directory and then to **c11+c12** and **ptsi**.

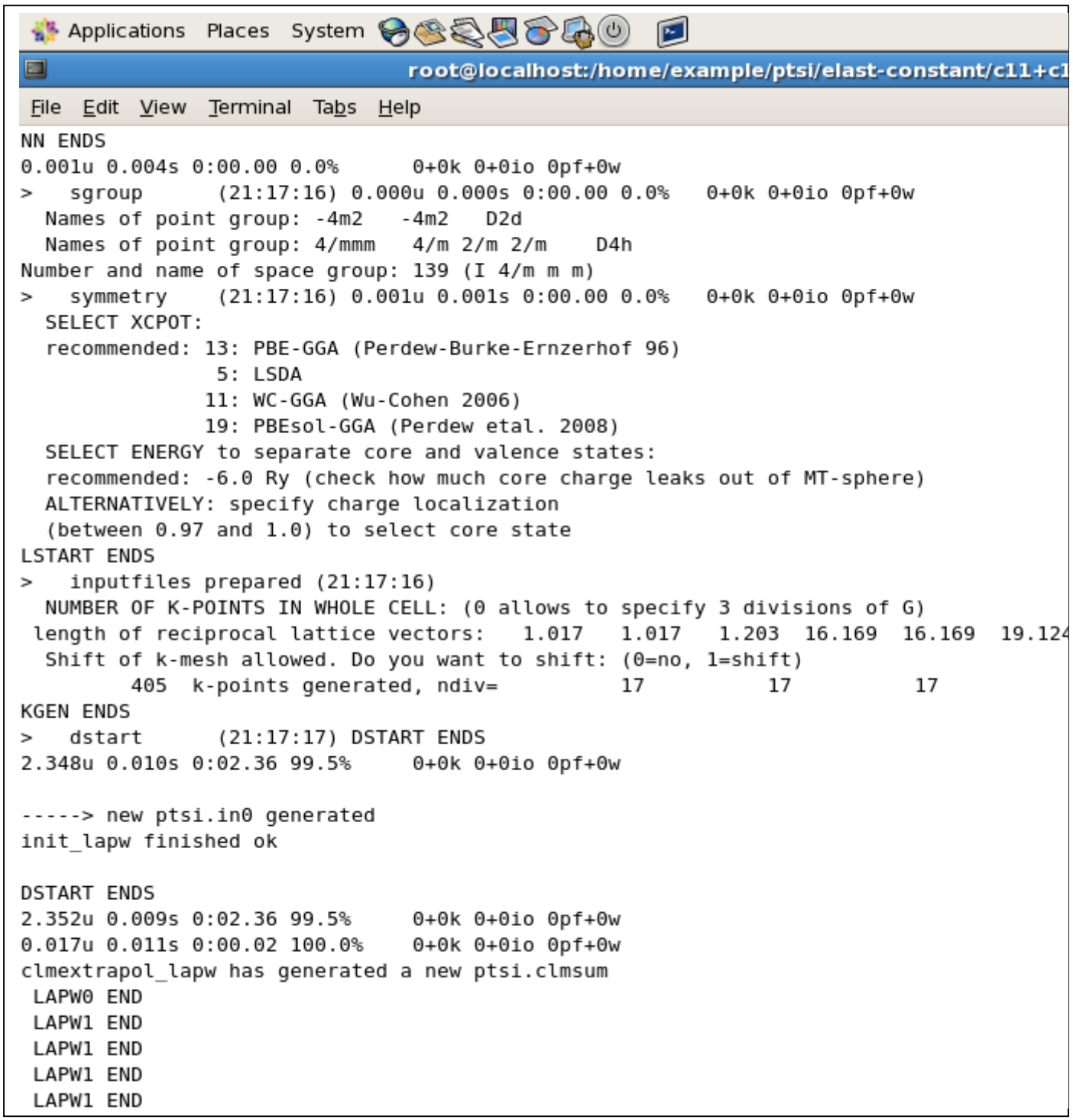




- Now, I call **TETRA.job** and calculations start. It will take time.


Applications Places System
root@localhost:/home/example/ptsi/elast-constant/c11+c1
File Edit View Terminal Tabs Help
[root@localhost ptsi]# ./TETRA.job

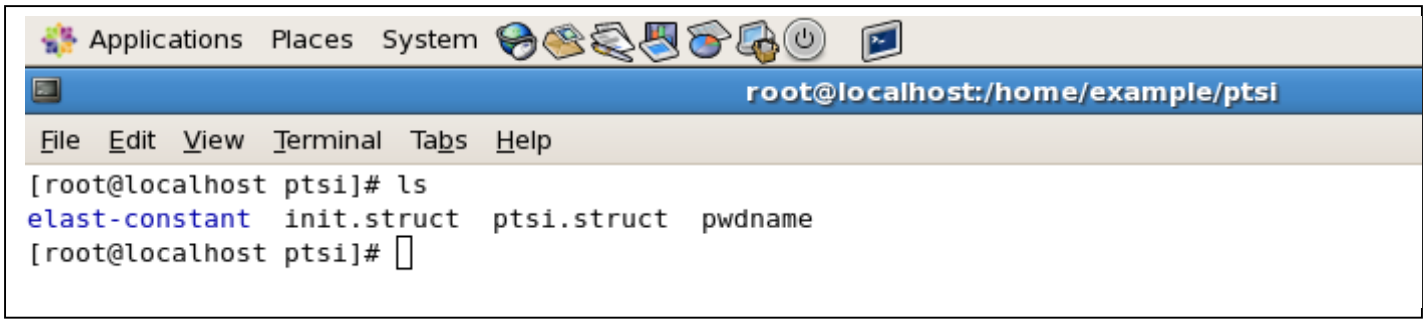
Now, we see

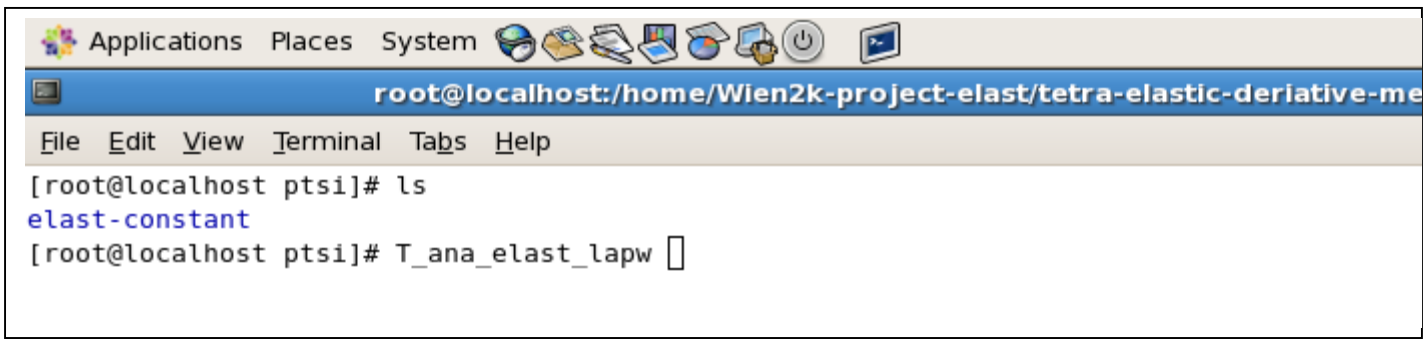

Applications Places System
root@localhost:/home/example/ptsi/elast-constant/c11+c1
File Edit View Terminal Tabs Help
NN ENDS
0.001u 0.004s 0:00.00 0.0% 0+0k 0+0io 0pf+0w
> sgroup (21:17:16) 0.000u 0.000s 0:00.00 0.0% 0+0k 0+0io 0pf+0w
Names of point group: -4m2 -4m2 D2d
Names of point group: 4/mmm 4/m 2/m 2/m D4h
Number and name of space group: 139 (I 4/m m m)
> symmetry (21:17:16) 0.001u 0.001s 0:00.00 0.0% 0+0k 0+0io 0pf+0w
SELECT XCPOT:
recommended: 13: PBE-GGA (Perdew-Burke-Ernzerhof 96)
5: LSDA
11: WC-GGA (Wu-Cohen 2006)
19: PBEsol-GGA (Perdew etal. 2008)
SELECT ENERGY to separate core and valence states:
recommended: -6.0 Ry (check how much core charge leaks out of MT-sphere)
ALTERNATIVELY: specify charge localization
(between 0.97 and 1.0) to select core state
LSTART ENDS
> inputfiles prepared (21:17:16)
NUMBER OF K-POINTS IN WHOLE CELL: (0 allows to specify 3 divisions of G)
length of reciprocal lattice vectors: 1.017 1.017 1.203 16.169 16.169 19.124
Shift of k-mesh allowed. Do you want to shift: (0=no, 1=shift)
405 k-points generated, ndiv= 17 17 17
KGEN ENDS
> dstart (21:17:17) DSTART ENDS
2.348u 0.010s 0:02.36 99.5% 0+0k 0+0io 0pf+0w
-----> new ptsi.in0 generated
init_lapw finished ok
DSTART ENDS
2.352u 0.009s 0:02.36 99.5% 0+0k 0+0io 0pf+0w
0.017u 0.011s 0:00.02 100.0% 0+0k 0+0io 0pf+0w
clmextrapol_lapw has generated a new ptsi.clmsum
LAPW0 END
LAPW1 END
LAPW1 END
LAPW1 END
LAPW1 END

- We repeat the same steps for running **TETRA.job** within c11-c12 , c33, czz, c44, and c66 directories.

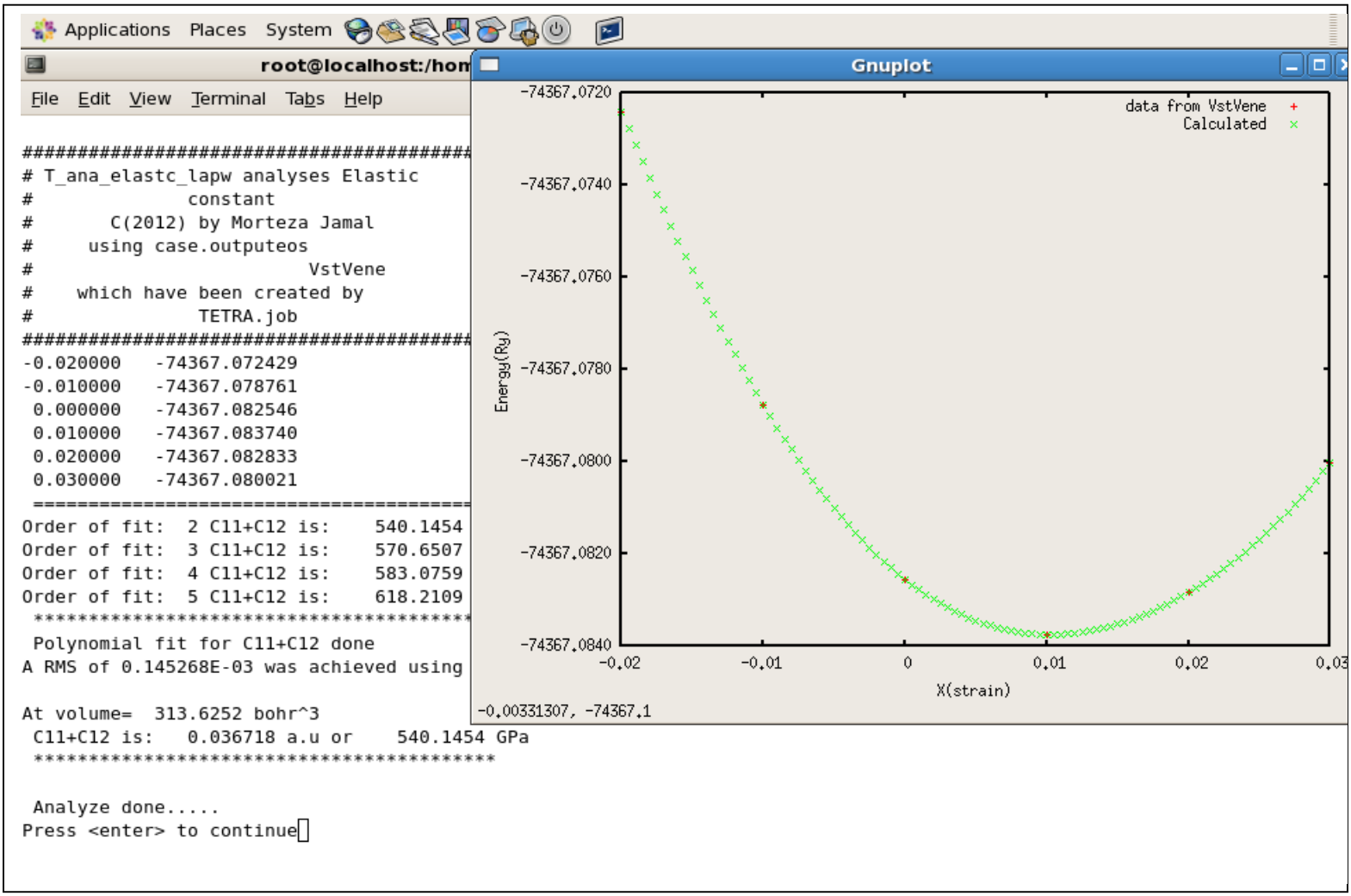
After calculations, we analyze our calculation for finding C11 , C12 , C44 and ….
For this goal, we change to main directory i.e. **ptsi** directory and run

- **T_ana_elast_lapw**

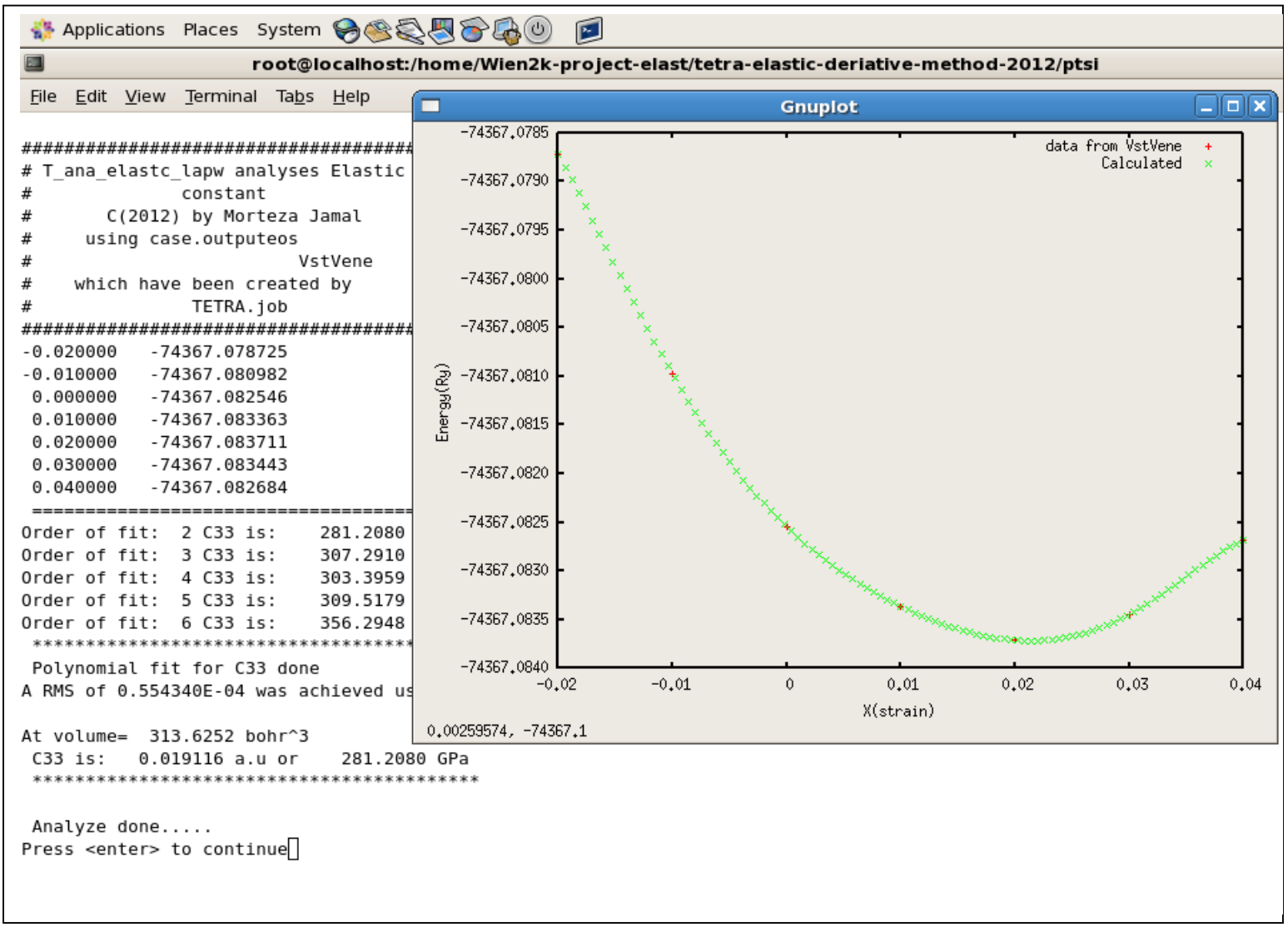




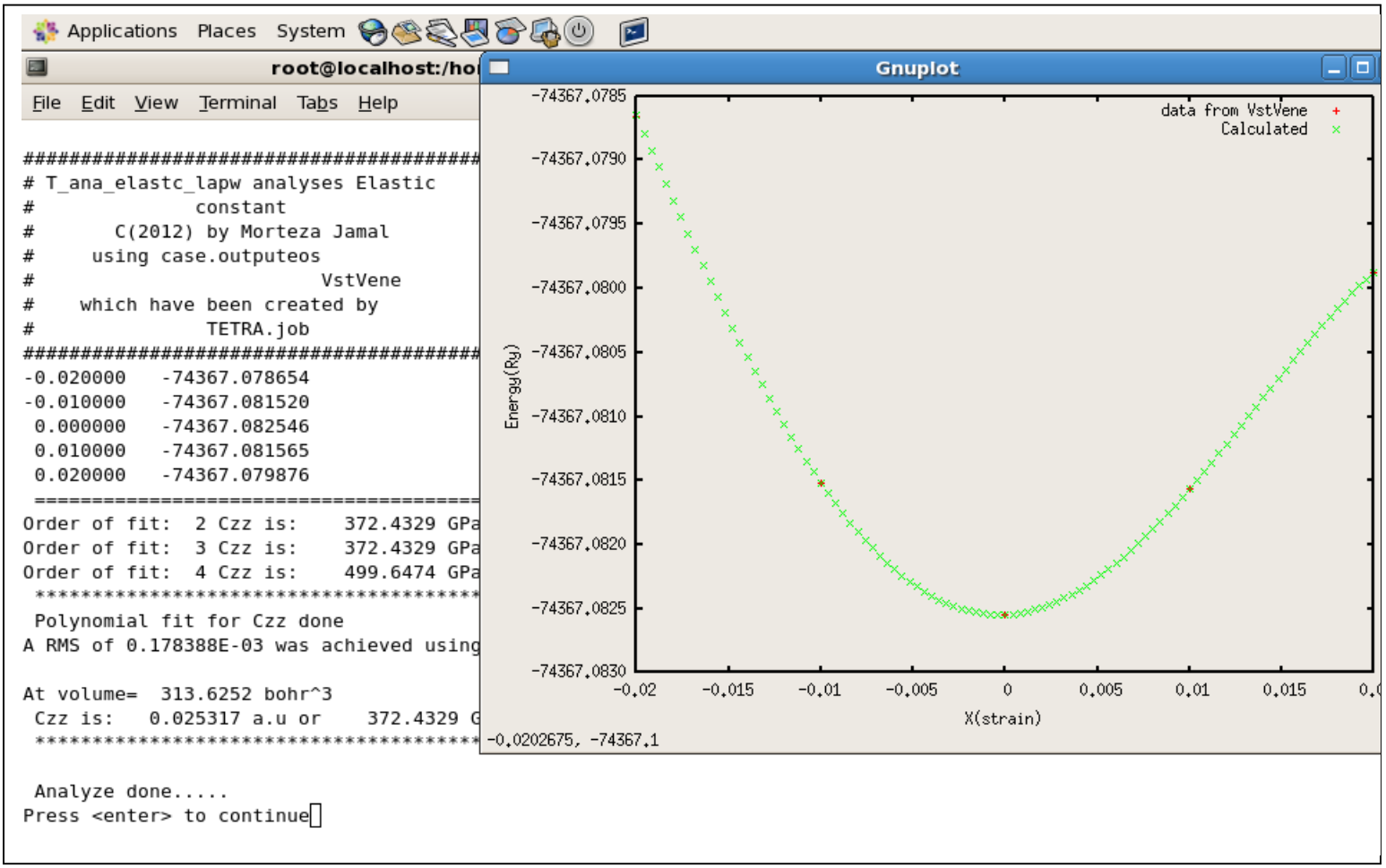
Now, we see


Applications Places System
root@localhost:/hom
File Edit View Terminal Tabs Help
##
T_ana_elastc_lapw analyses Elastic
constant
C(2012) by Morteza Jamal
using case.outputeos
VstVene
which have been created by
TETRA.job
##
-0.020000   -74367.072429
-0.010000   -74367.078761
 0.000000   -74367.082546
 0.010000   -74367.083740
 0.020000   -74367.082833
 0.030000   -74367.080021
 ==
Order of fit: 2 C11+C12 is: 540.1454
Order of fit: 3 C11+C12 is: 570.6507
Order of fit: 4 C11+C12 is: 583.0759
Order of fit: 5 C11+C12 is: 618.2109
 ****
 Polynomial fit for C11+C12 done
A RMS of 0.145268E-03 was achieved using
At volume= 313.6252 bohr^3
 C11+C12 is: 0.036718 a.u or   540.1454 GPa
 ****
 Analyze done.....
Press <enter> to continue
Gnuplot
data from VstVene
Calculated
-74367.0720
-74367.0740
-74367.0760
-74367.0780
-74367.0800
-74367.0820
-74367.0840
Energy(Ry)
-0.02
-0.01
0
0.01
0.02
X(strain)
-0.00331307, -74367.1

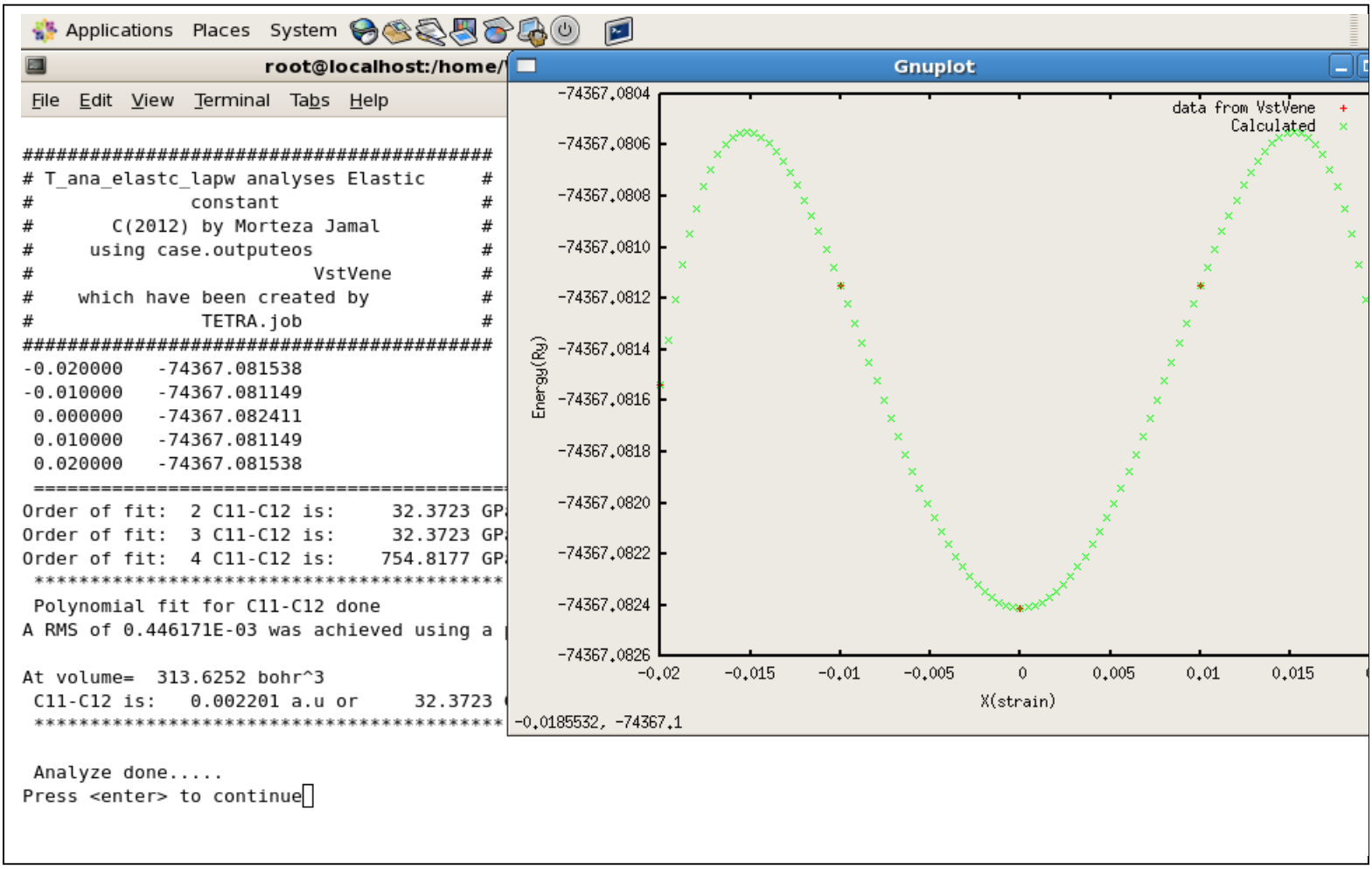
And then



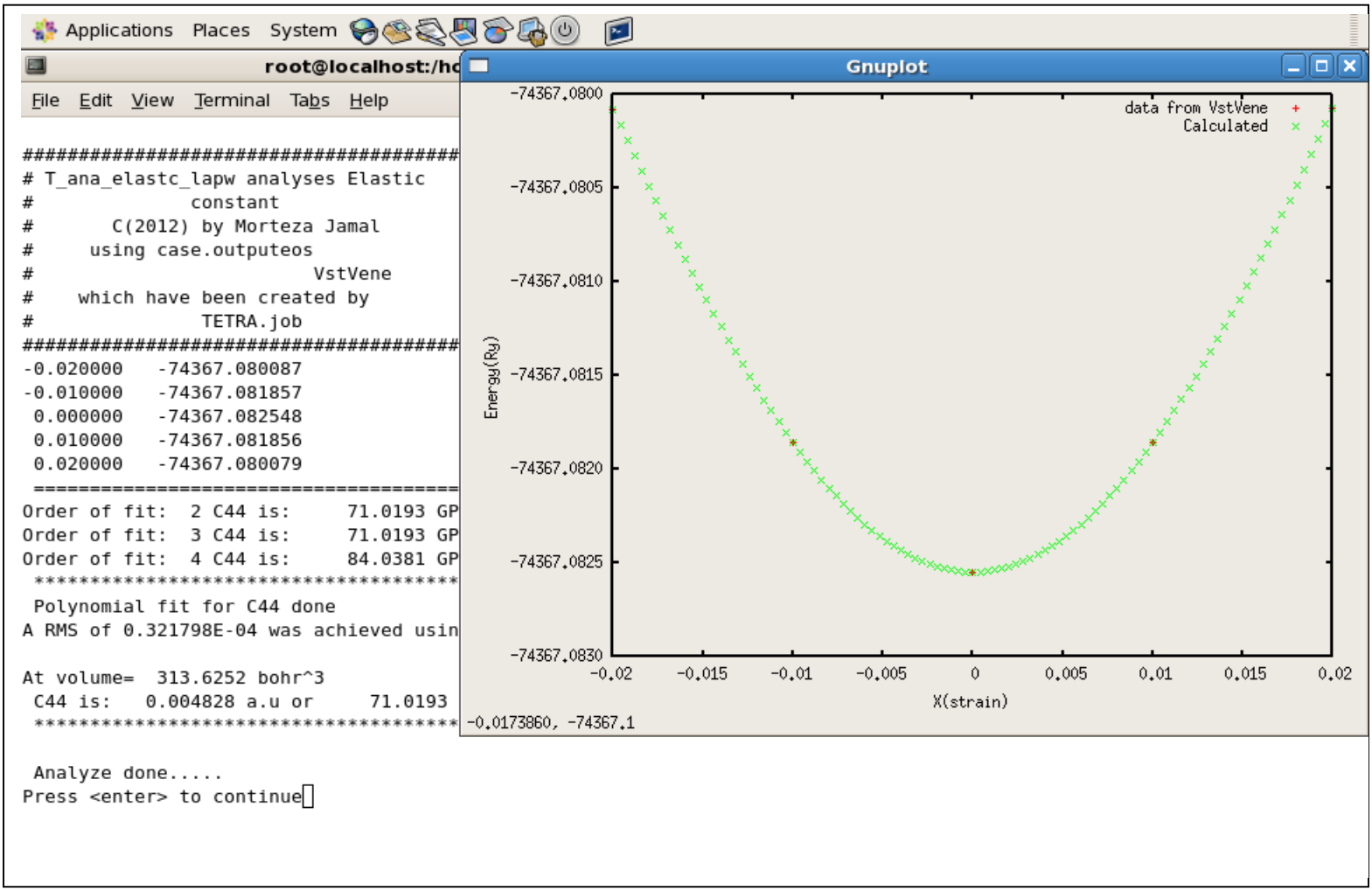
And after that


Applications Places System
root@localhost:/ho
File Edit View Terminal Tabs Help
T_ana_elastc_lapw analyses Elastic
constant
C(2012) by Morteza Jamal
using case.outputeos
VstVene
which have been created by
TETRA.job
-0.020000 -74367.078654
-0.010000 -74367.081520
0.000000 -74367.082546
0.010000 -74367.081565
0.020000 -74367.079876
Order of fit: 2 Czz is: 372.4329 GPa
Order of fit: 3 Czz is: 372.4329 GPa
Order of fit: 4 Czz is: 499.6474 GPa
Polynomial fit for Czz done
A RMS of 0.178388E-03 was achieved using
At volume= 313.6252 bohr^3
Czz is: 0.025317 a.u or 372.4329 G
Analyze done.....
Press <enter> to continue
Gnuplot
data from VstVene
Calculated
Energy(Ry)
X(strain)
-74367.0785
-74367.0790
-74367.0795
-74367.0800
-74367.0805
-74367.0810
-74367.0815
-74367.0820
-74367.0825
-74367.0830
-0.02
-0.015
-0.01
-0.005
0
0.005
0.01
0.015
-0.0202675, -74367.1

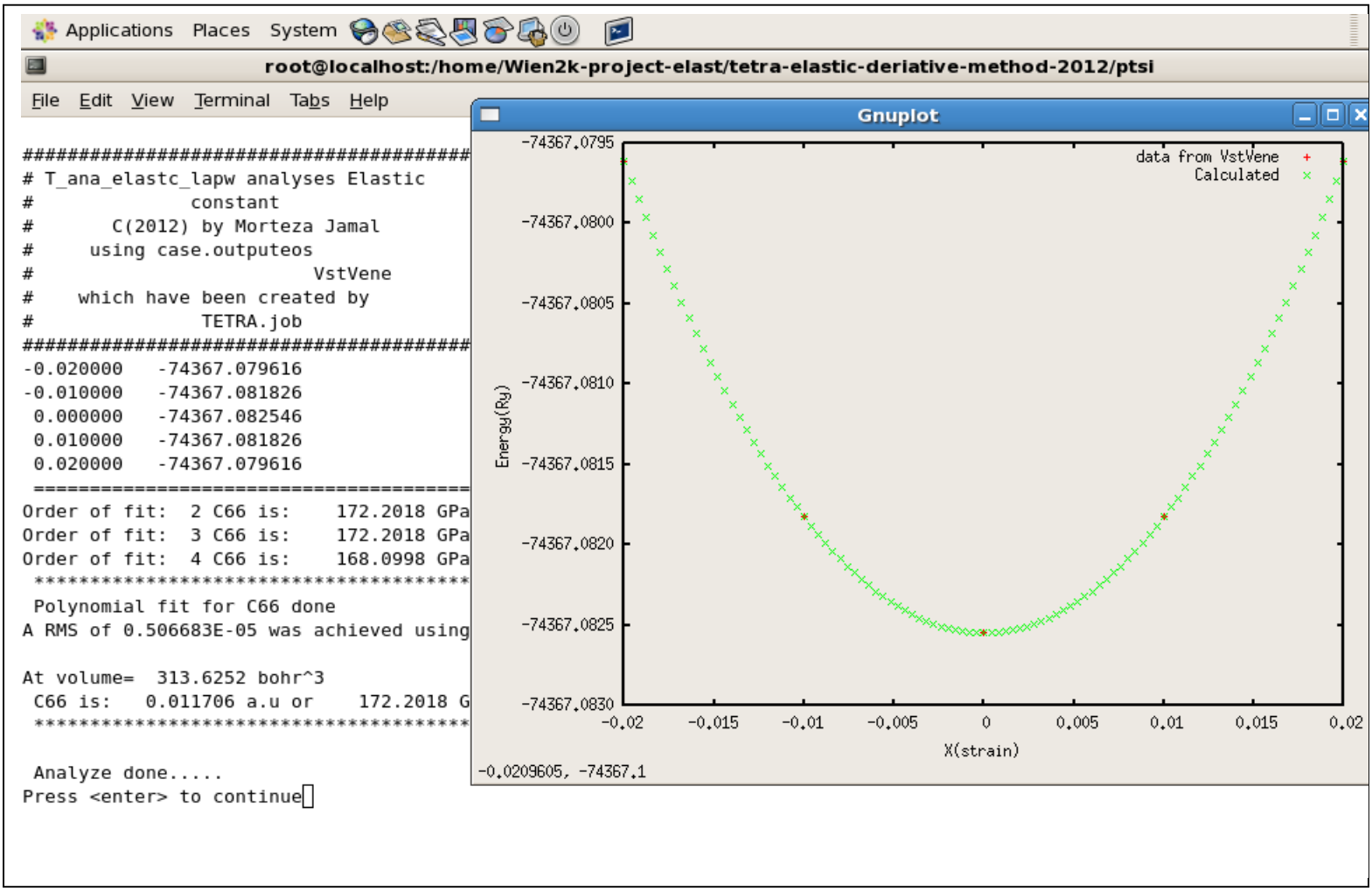
And then



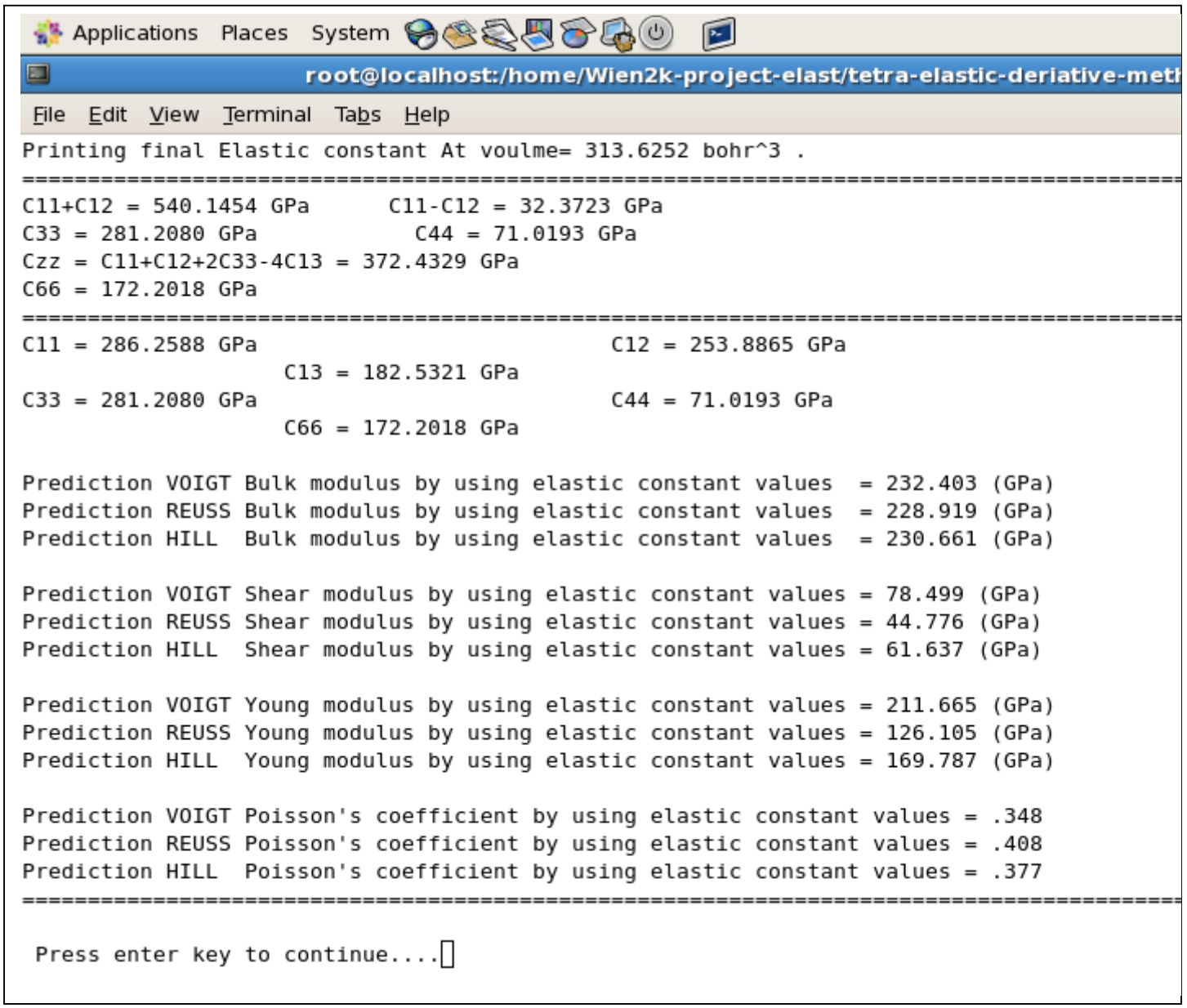
And after that



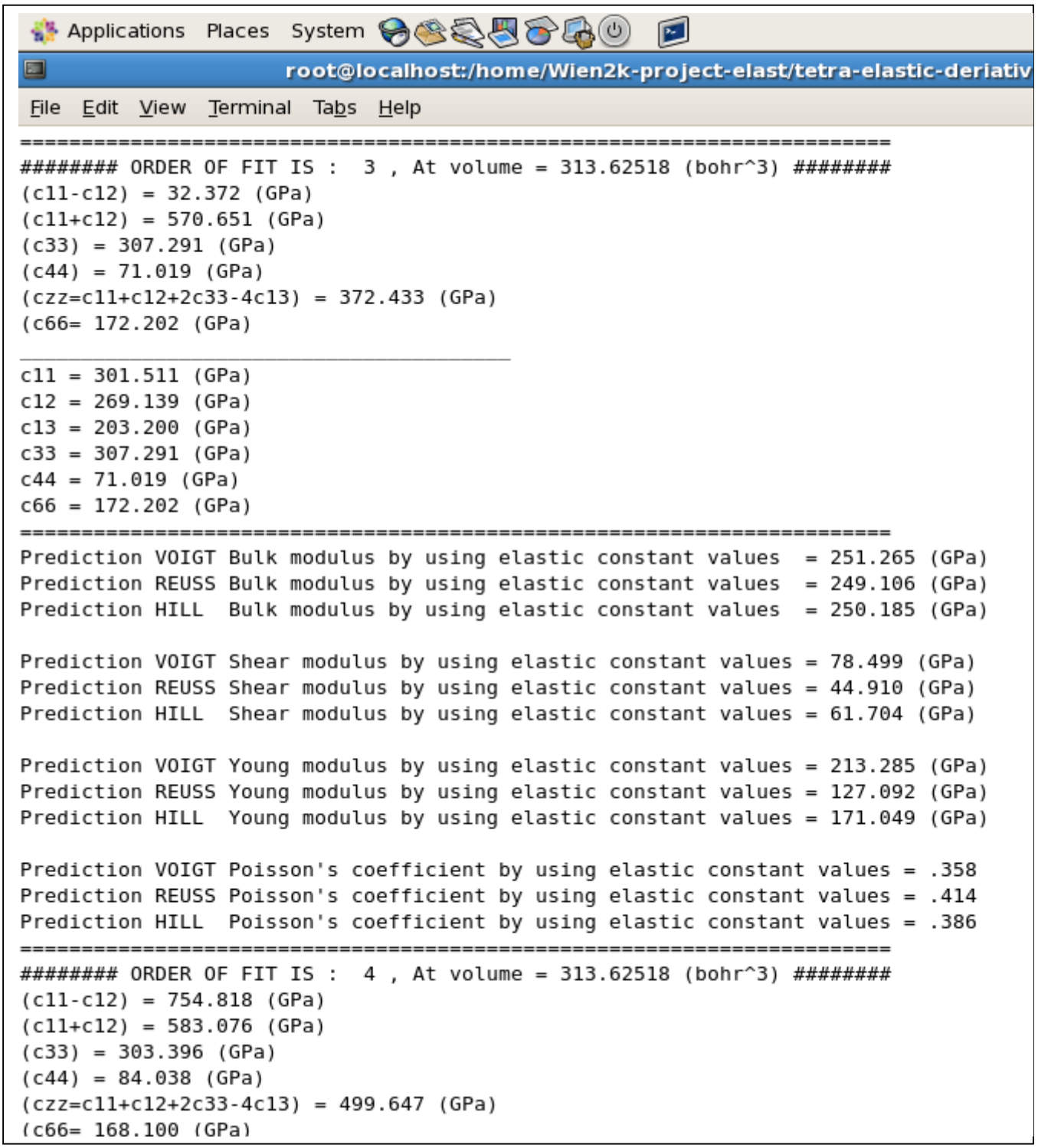
And at the end



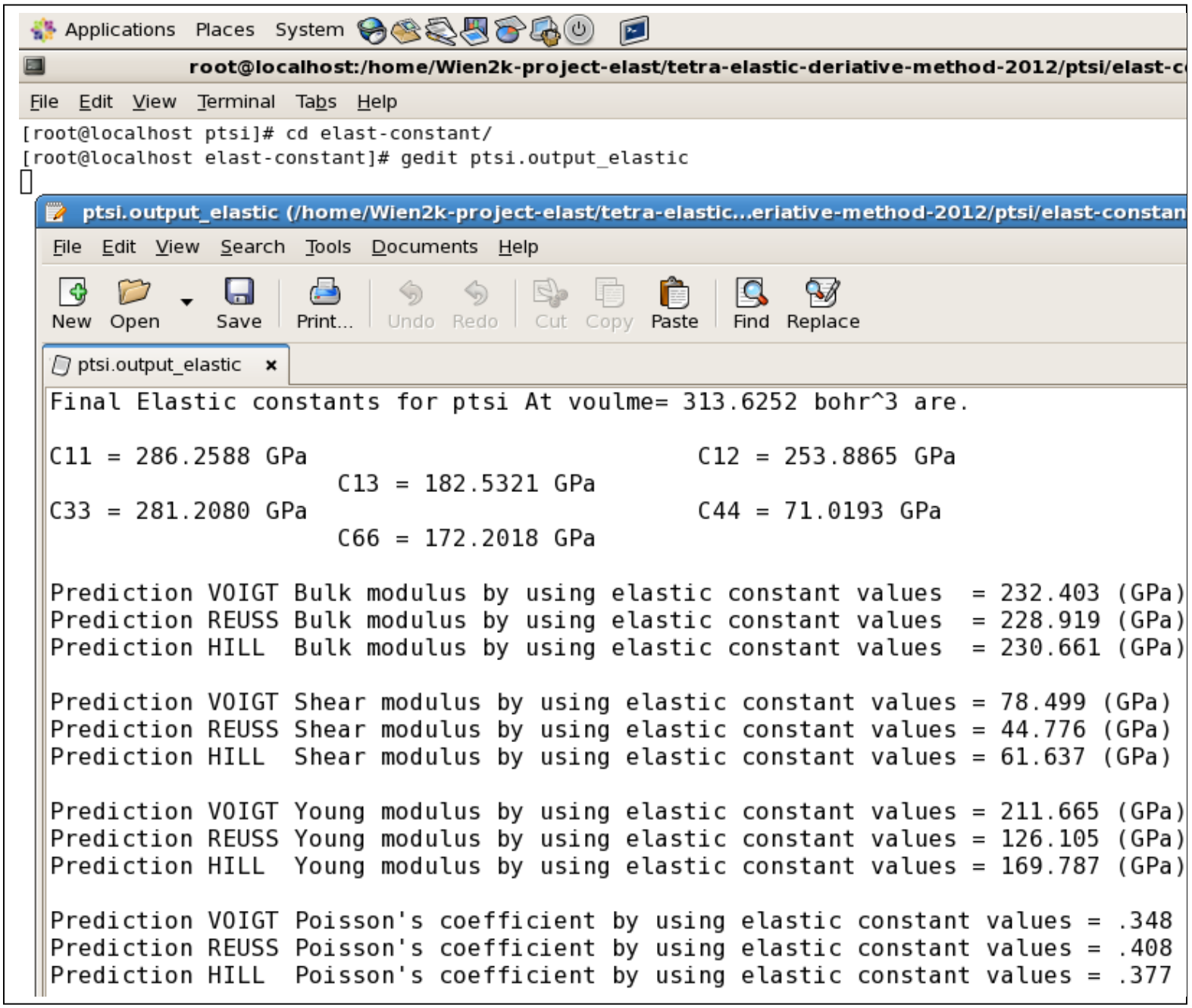
Now, we see results



And then checks the sensitivity of your results to the order of fit.



Now, change to **elast-constant** directory. You can see the results in **ptsi.output_elastic**



Good luck
Morteza Jamal