EMTO best practices workshop

⚙ Prerequisites

In case people would like to do some practices during the workshop with the installed emto excutables you need to have access to one of these resource:

- Leonardo booster (CINECA, Italy).
- Tetralith (NSC, NAISS, Sweden).

All documented commands for the practices are tested on these clusters.

Who is the course for?

This course is for students, researchers, engineers who would like to get started with EMTO code using a HPC resource. Basic knowledge of electronic structure theory and/or DFT calculations and using Linux will be required.

Schedule

Time	Content
10:00-10:30	Introduction to ENCCS
10:30-12:00	EMTO lectures
12:00-13:00	Lunch break
13:00-15:00	Hands-on session (guided)
15:00-17:00	Hands-on session

About the course

quick setup for this workshop

Tetralith | Leonardo_Booster

```
module use /proj/vasp-ws2024/emto_ws/emto/modules
ml emtoworkshop
```

```
usereservation emtoworkshop-2024-04-16
```

copy exercise to your own place (e.g home)

```
cp -r /proj/vasp-ws2024/emto_ws/exercise ~/
```

optional settings:

```
export SQUEUE_FORMAT="%.15i %.8u %.15a %.15j %.3t %.10M %.10L %.5D %.4C %.10Q %16R %P"
alias sinfo='sinfo -o "%10D %20F %P"'
alias all-myjobs='squeue --me'
```

EMTO leture

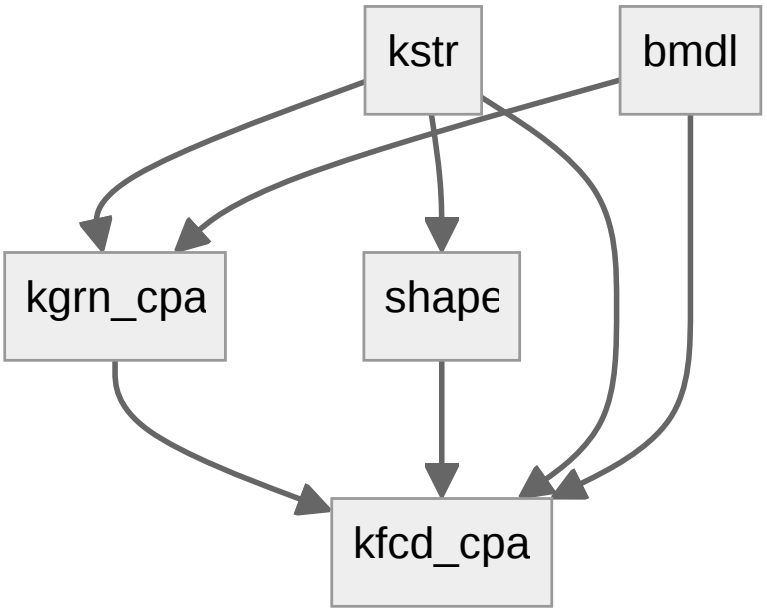
The EMTO Method Fundamentals, Implementation and Demonstration

by Prof. Levente Vitos

Basic About How to Run EMTO Code

exe	function
bmdl	Calculates the Madelung potentials
kstr	Computes the energy dependent slope matrix in real space.
shape	Computes the so called shape function, which transforms any integral over the unit cell into an integral over a sphere surrounding the unit cell.
kgrn_cpa	Solves the actual self-consistent Kohn-Sham equations And calculate the Full charge density
kfcd_cpa	Evaluate the total energy functional from the full charge density generated by kgrn

Running dependence of EMTO subprograms



Commands to run the code looks like:

```
exe < input
```

exercise/00

```
tree 00
00
├── bmdl
│   └── fcc.dat
├── kfcd
│   └── cu.dat
├── kgrn
│   └── cu.dat
├── kstr
│   └── fcc.dat
└── shape
    └── fcc.dat

6 directories, 5 files
```

- please try to run these “dat” file as input for each “exe” inside its folder. for example:

  ```
  cd 00/bmdl
  bmdl < fcc.dat
  ```

  there will be errors, so what should we do ?

  Hint

  ```
  mkdir mdl
  bmdl < fcc.dat
  ```

Caution

EMTO input files have very strict format, an extra space may cause some problems.

KSTR

The input file (kstr/fcc.dat)

```
KSTR      HP......=N                                22 Jan 08
JOBNAM...=fcc        MSGL.=  0 MODE...=B STORE..=Y HIGH...=Y
DIR001=smx/
DIR006=./
Slope matrices, fcc (spdf), (kappa*w)^2= 0.0
NL.....= 4 NLH...=11 NLW...= 9 NDER..= 6 ITRANS= 3 NPRN..= 0
(K*W)^2..=  0.000000 DMAX....=    1.7000 RWATS...=      0.10
NQ3...=  1 LAT...= 2 IPRIM.= 0 NGHBP.=13 NQR2..= 0
A........= 1.0000000 B.......= 1.0000000 C.......= 1.0000000
BSX......= 0.5000000 BSY.....= 0.5000000 BSZ.....= 0.0000000
BSX......= 0.0000000 BSY.....= 0.5000000 BSZ.....= 0.5000000
BSX......= 0.5000000 BSY.....= 0.0000000 BSZ.....= 0.5000000
QX(IQ)...= 0.0000000 QY......= 0.0000000 QZ......= 0.0000000
a/w(IQ)..= 0.70 0.70 0.70 0.70
LAMDA....=    2.5000 AMAX....=    4.5000 BMAX....=    4.5000
```

A part of the input file of `kstr` describes the lattice informations:

- Total number of sites is set by NQ3.
- The symmetry is set by `LAT`, more in the online manual.
- The lattice parameters are renormalized to the length of first lattice vector A (`A=1`).
- **Cartesian Coordinates** are used for sites/"atom" with `QX,QY,QZ`.

Commands for run the `kstr`:

```
kstr < fcc.dat
```

Or add `time` in front to have a feeling about the how much time each code consumes:

```
time kstr < fcc.dat
```

- `DIR006=./` and `JOBNAM...=fcc`: a file `fcc.prn` will be generated in the current directory.
- `DIR001=smx`: "slop matrix" will save to `smx/fcc.tfh`.
- `MSGL.=  0` could silence the screen printing.

BMDL

The input file (bmdl/fcc.dat)

```
BMDL      HP......=N                                22 Jan 08
JOBNAM...=fcc        MSGL.=  1 NPRN.=  0
DIR001=mdl/
DIR006=
Madelung potential for fcc bulk
NL.....= 7
LAMDA....=      2.50 AMAX....=      4.50 BMAX....=      4.50
NQ....=  1 LAT...= 2 IPRIM.= 0 NQR2..= 0
A........= 1.0000000 B.......= 1.0000000 C.......= 1.0000000
BSX......= 0.5000000 BSY.....= 0.5000000 BSZ.....= 0.0000000
BSX......= 0.0000000 BSY.....= 0.5000000 BSZ.....= 0.5000000
BSX......= 0.5000000 BSY.....= 0.0000000 BSZ.....= 0.5000000
QX(IQ)...= 0.0000000 QY......= 0.0000000 QZ......= 0.0000000
```

The Lattice information must be consistent with `kstr`, and the output files will be `./fcc.prn` and `mdl/fcc.mdl`

SHAPE

The input file (shape/fcc.dat) for `bmdl` contains similar lattice information as `kstr`:

The input file (shape/fcc.dat)

```
SHAPE     HP......=N                              22 Jan 08
JOBNAM...=fcc        MSGL.=  0
FOR001=../kstr/smx/fcc.tfh
DIR002=shp/
DIR006=./
Lmax..= 30 NSR..=129 NFI..= 11
NPRN..=  0 IVEF.=  3
```

`FOR001=../kstr/smx/fcc.tfh` shows `shape` will need the “slop matrix” from the result of `kstr`. The output will be `shp/fcc.shp`.

Hint

`kstr,bmdl` and `shape` only contains lattice information with a reduced unit, They could be reused for any system which present with same lattice setup.

KGRN

```
KGRN                                                  13 Oct 12
JOBNAM=cu
STRT..=  A MSGL.=  0 EXPAN.= S FCD..=  Y FUNC..= SCA
FOR001=../kstr/smx/fcc.tfh
FOR001=../kstr/smx/fcc30.tfh
DIR002=pot/
DIR003=pot/
FOR004=../bmdl/mdl/fcc.mdl
DIR006=
DIR009=pot/
DIR010=chd/
DIR011=/tmp/
Self-consistent KKR calculation for fcc Cu
Band: 10 lines
NITER.= 50 NLIN.= 31 NPRN.=  0 NCPA.=  7 NT...=  1 MNTA.=  1
MODE..= 3D FRC..=  N DOS..=  N OPS..=  N AFM..=  P CRT..=  M
Lmaxh.=  8 Lmaxt=  4 NFI..= 31 FIXG.=  2 SHF..=  0 SOFC.=  N
KMSH...= G IBZ..=  2 NKX..=  0 NKY..= 13 NKZ..=  0 FBZ..=  N
KMSH2..= G IBZ2.=  1 NKX2.=  4 NKY2.=  0 NKZ2.= 51
ZMSH...= C NZ1..= 16 NZ2..=  8 NZ3..=  8 NRES.=  4 NZD.=1500
DEPTH..=  1.000 IMAGZ.=  0.020 EPS...=  0.200 ELIM..= -1.000
AMIX...=  0.100 EFMIX.=  1.000 VMTZ..=  0.000 MMOM..=  0.000
TOLE...= 1.d-07 TOLEF.= 1.d-07 TOLCPA= 1.d-06 TFERMI=  500.0 (K)
SWS......=2.686842   NSWS.=  1 DSWS..=   0.05 ALPCPA= 0.6020
Setup: 2 + NQ*NS lines
EFGS...=  0.000 HX....=  0.100 NX...=  5 NZ0..=  6 STMP..= N
Symb   IQ IT ITA NZ  CONC   Sm(s)  S(ws) WS(wst) QTR SPLT Fix
Cu      1  1  1  29  1.000  1.000  1.000  1.000  0.0  0.0  N
Atom:  4 lines + NT*NTA*6 lines
IEX...=  4 NP..= 251 NES..= 15 NITER=100 IWAT.=  0 NPRNA=  0
VMIX.....=  0.300000 RWAT....=  3.500000 RMAX....= 20.000000
DX.......=  0.030000 DR1.....=  0.002000 TEST....=  1.00E-12
TESTE....=  1.00E-12 TESTY...=  1.00E-12 TESTV...=  1.00E-12
Cu
Iz=  29 Norb= 10 Ion=  0 Config= 3d10_4s1
n      1  2  2  2  3  3  3  3  3  4
Kappa -1 -1  1 -2 -1  1 -2  2 -3 -1
Occup  2  2  2  4  2  2  4  4  6  1
Valen  0  0  0  0  0  0  0  1  1  1
```

- need `chd\` and `pot\` to be exist.
- `JOBNAM=cu` will decide the output files start with `cu`: cu.prn, chd/cu.chd, pot/cu.pot ...
- `FOR001=../kstr/smx/fcc.tfh` and `FOR004=../bmdl/mdl/fcc.mdl`.
- `IBZ..=  2` should consistent with `LAT=2` in `kstr` and `bmdl` for `fcc`.
- `NITER.= 50`, `TOLE...= 1.d-07 TOLEF.= 1.d-07`, check with `egrep "erre|Converged|NOS|finished" cu.prn`.
- `AMIX...=  0.100` mixing factor for new charge.
- `SWS......=2.686842`: The average Wigner-Seitz radius (bohr) to scale the lattice.

Note

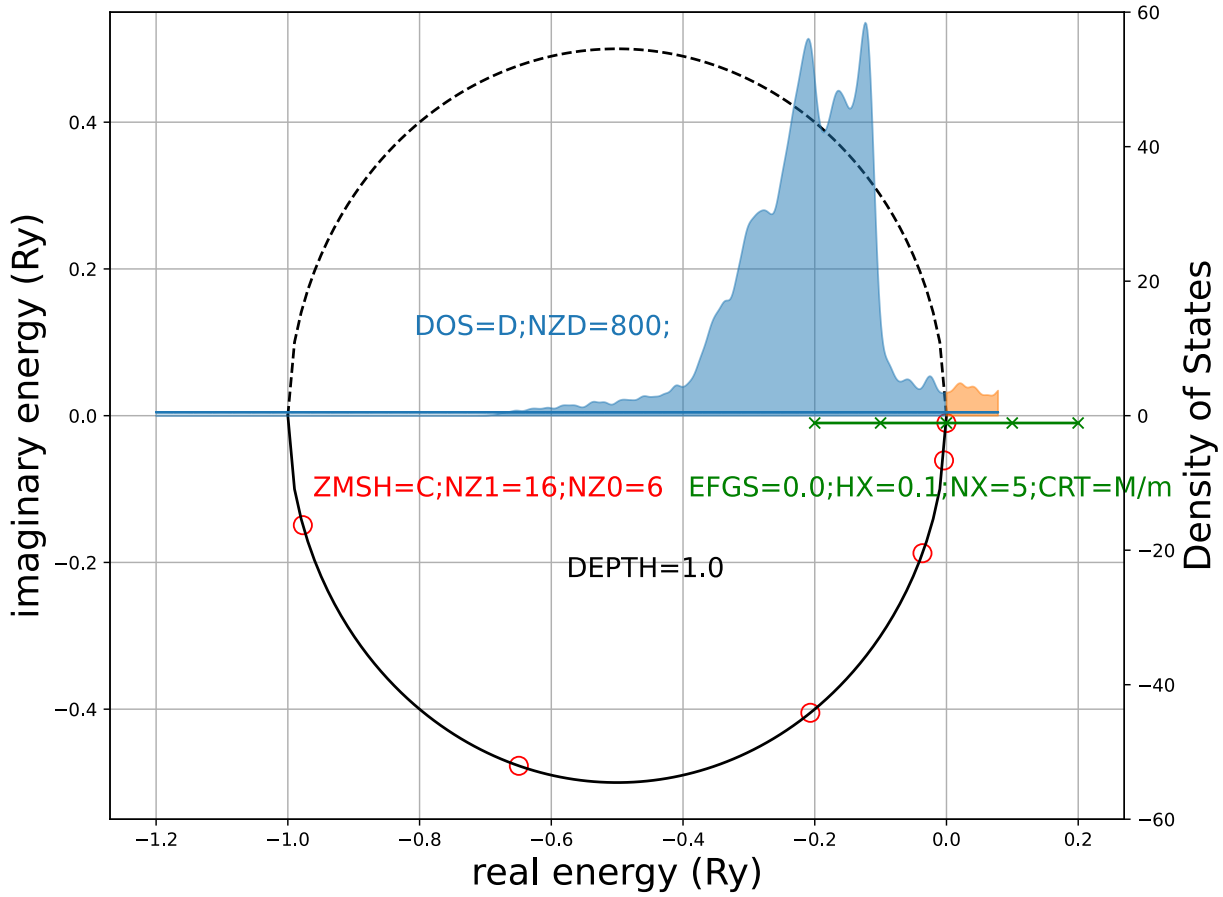
e.g bcc lattice parameters (a) to SWS (\(\omega\)):

$$2\times \frac{4\pi}{3} \omega^3 = a^3$$

units:

- length: Bohr, 1 Bhor = 0.529177249 Angstrom
- energy: Rydberg, 1 Ry = 13.605703976 eV

$$N(\epsilon_F)=\frac{1}{2\pi i}\oint_{\epsilon_F} G(z)~dz$$



exercise/01: 4 sites conventional fcc cell for Cu

In this exercise we will use a different setups for fcc lattice.

1. Copy all input files from exercise/00:

Hint

make sure we are in the path `exercise/`

```
cp -r 00/* 01/
rm -f 01/*/*.{prn,log,kstr,bmdl,shape,bmdl,kgrn,kfcd,out} 01/*/*/*
```

2. Modify kstr and bmdl for conventional fcc unit cell:

Hint

- `NQ` and `LAT` for kstr and bmdl
- `a/w` in kstr

```
--- /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/00/kstr/fcc.dat
+++ /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/01/kstr/fcc.dat
@@ -5,11 +5,17 @@
 Slope matrices, fcc (spdf), (kappa*w)^2= 0.0
 NL.....= 4 NLH...=11 NLW...= 9 NDER..= 6 ITRANS= 3 NPRN..= 0
 (K*W)^2..=  0.000000 DMAX....=    1.7000 RWATS...=      0.10
-NQ3...=  1 LAT...= 2 IPRIM.= 0 NGHBP.=13 NQR2..= 0
+NQ3...=  4 LAT...= 1 IPRIM.= 0 NGHBP.=13 NQR2..= 0
 A........= 1.0000000 B.......= 1.0000000 C.......= 1.0000000
-BSX......= 0.5000000 BSY.....= 0.5000000 BSZ.....= 0.0000000
-BSX......= 0.0000000 BSY.....= 0.5000000 BSZ.....= 0.5000000
-BSX......= 0.5000000 BSY.....= 0.0000000 BSZ.....= 0.5000000
+BSX......= 1.0000000 BSY.....= 0.0000000 BSZ.....= 0.0000000
+BSX......= 0.0000000 BSY.....= 1.0000000 BSZ.....= 0.0000000
+BSX......= 0.0000000 BSY.....= 0.0000000 BSZ.....= 1.0000000
 QX(IQ)...= 0.0000000 QY......= 0.0000000 QZ......= 0.0000000
+QX(IQ)...= 0.5000000 QY......= 0.5000000 QZ......= 0.0000000
+QX(IQ)...= 0.5000000 QY......= 0.0000000 QZ......= 0.5000000
+QX(IQ)...= 0.0000000 QY......= 0.5000000 QZ......= 0.5000000
+a/w(IQ)..= 0.70 0.70 0.70 0.70
+a/w(IQ)..= 0.70 0.70 0.70 0.70
+a/w(IQ)..= 0.70 0.70 0.70 0.70
 a/w(IQ)..= 0.70 0.70 0.70 0.70
 LAMDA....=    2.5000 AMAX....=    4.5000 BMAX....=    4.5000
```

3. put 4 Cu on these 4 sites in kgrn

Hint

- `NT=1` and all `IT` should be same: 4 Cu atoms should be equivalent.
- `IBZ=1` for simple cubic symmetry.

```
--- /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/00/kgrn/cu.dat
+++ /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/01/kgrn/cu.dat
@@ -15,7 +15,7 @@
 NITER.= 50 NLIN.= 31 NPRN.=  0 NCPA.=  7 NT...=  1 MNTA.=  1
 MODE..= 3D FRC..=  N DOS..=  N OPS..=  N AFM..=  P CRT..=  M
 Lmaxh.=  8 Lmaxt=  4 NFI..= 31 FIXG.=  2 SHF..=  0 SOFC.=  N
-KMSH...= G IBZ..=  2 NKX..=  0 NKY..= 13 NKZ..=  0 FBZ..=  N
+KMSH...= G IBZ..=  1 NKX..=  0 NKY..= 13 NKZ..=  0 FBZ..=  N
 KMSH2..= G IBZ2.=  1 NKX2.=  4 NKY2.=  0 NKZ2.= 51
 ZMSH...= C NZ1..= 16 NZ2..=  8 NZ3..=  8 NRES.=  4 NZD.=1500
 DEPTH..=  1.000 IMAGZ.=  0.020 EPS...=  0.200 ELIM..= -1.000
@@ -26,6 +26,9 @@
 Cu      1  1  1  29  1.000  1.000  1.000  1.000  0.0  0.0  N
+Cu      2  1  1  29  1.000  1.000  1.000  1.000  0.0  0.0  N
+Cu      3  1  1  29  1.000  1.000  1.000  1.000  0.0  0.0  N
+Cu      4  1  1  29  1.000  1.000  1.000  1.000  0.0  0.0  N
 Atom:  4 lines + NT*NTA*6 lines
 IEX...=  4 NP..= 251 NES..= 15 NITER=100 IWAT.=  0 NPRNA=  0
 VMIX.....=  0.300000 RWAT....=  3.500000 RMAX....= 20.000000
```

4. run all of the calculations and compare the total energy in kfcd for these 2 different fcc setups.

The energy of two setups should be same/close, but if not ?

Hint

we could play with the k-points for convergence test.

e.g:

- NKY=37 for 00/kgrn/cu.dat
- NKY=19 for 01/kgrn/cu.dat

exercise/02: equilibrium volume for fcc Cu

In this exercise we will practice how to get lattice parameters for fcc copper with EMTO code. The main idea is to calculate total energy vs. different volumes, $E(\omega)$ curve, and fit to an “Equation of State” function. Here we choose “Morse function”:

$$E(\omega)=a+be^{-\lambda\omega}+ce^{-2\lambda\omega}$$

System-specific instructions

Select instructions for the system you are using:

Tetralith | Leonardo_Booster

Instructions for use on the NAISS cluster Tetralith (NSC)

Attention

make sure we are in the path at `exercise/02`

1. we could reuse the kstr, bmdl and shape from exercise/00

Hint

```
ln -vs ../00/kstr
ln -vs ../00/bmdl
ln -vs ../00/shape
```

2. base on 00/kgrn/cu.dat, change to different SWS and also the jobname and file name

Hint

```
for sws in `seq 2.60 0.02 2.76`
do
  sed -e "s/JOBNAM=.*/JOBNAM=cu_${sws}/" \
      -e "s/SWS......=......../SWS......=${sws}0000/" \
    ../00/kgrn/cu.dat > kgrn/cu_${sws}.dat
done

# maybe we need reduce the AMIX
      # -e 's/AMIX...=  0.100/AMIX...=  0.020/' \
# soft core apprixmation is important for equilibrium volume calculation
      # -e 's/SOFC.=  N/SOFC.=  Y/' \
```

3. base on 00/kfcd/cu.dat change to different jobnam and file name

Hint

```
mkdir -vp kfcd
for sws in `seq 2.60 0.02 2.76`
do
  sed -e "s/JOBNAM...=.*/JOBNAM...=cu_${sws}/" \
      ../00/kfcd/cu.dat > kfcd/cu_${sws}.dat
done
# maybe we want to silence the output
      # -e 's/MSGL..=  1/MSGL..=  0/' \
```

4. run all calculations and get \(E(\omega)\)

- submit all kgrn jobs to the queue, use following sbatch script.

Tetralith | Leonardo_Booster

```
cd kgrn
sbatch -A naiss2024-22-241 -c 2 -a 1-9 -t 10:00 ../../emto.sbatch
```

- check if the kgrn jobs are finished correctly.

Hint

```
cd kgrn
grep -L "finished" *.prn
```

- submit all kfcd jobs to the queue, use following sbatch script.

Tetralith | Leonardo_Booster

```
cd kfcd
sbatch -A naiss2024-22-241 -c 1 -a 1-9 -t 10:00 ../../emto.sbatch
```

5. get total energy vs. `SWS` from kfcd output

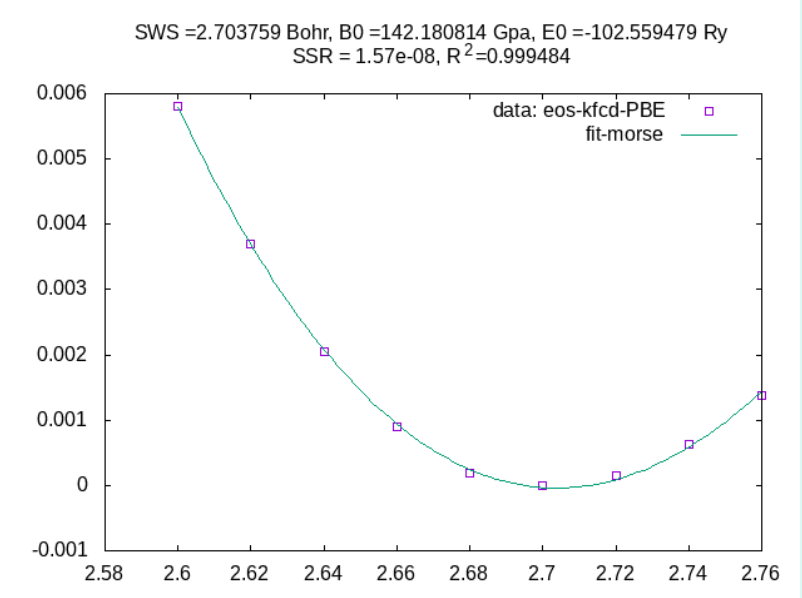
Hint

```
cd kfcd
grep TOT-PBE *.prn
```

here we choose PBE EXC

```
#              EXC                                    5th
8th
cu_2.60.prn:    TOT-PBE         -102.553631 (Ry)    -102.553631 (Ry/site)   S=
2.600000 Bohr
cu_2.62.prn:    TOT-PBE         -102.555746 (Ry)    -102.555746 (Ry/site)   S=
2.620000 Bohr
cu_2.64.prn:    TOT-PBE         -102.557381 (Ry)    -102.557381 (Ry/site)   S=
2.640000 Bohr
cu_2.66.prn:    TOT-PBE         -102.558531 (Ry)    -102.558531 (Ry/site)   S=
2.660000 Bohr
cu_2.68.prn:    TOT-PBE         -102.559243 (Ry)    -102.559243 (Ry/site)   S=
2.680000 Bohr
cu_2.70.prn:    TOT-PBE         -102.559439 (Ry)    -102.559439 (Ry/site)   S=
2.700000 Bohr
cu_2.72.prn:    TOT-PBE         -102.559283 (Ry)    -102.559283 (Ry/site)   S=
2.720000 Bohr
cu_2.74.prn:    TOT-PBE         -102.558814 (Ry)    -102.558814 (Ry/site)   S=
2.740000 Bohr
cu_2.76.prn:    TOT-PBE         -102.558060 (Ry)    -102.558060 (Ry/site)   S=
2.760000 Bohr
```

fit the 5th and 8th for morse function



exercise/03: elastic constance calculation for fcc Cu

In this exercise we will practice how to get elastic constance for fcc copper with EMTO code.

Orthorhombic distortion

$$\begin{split}D_o(\delta_o) + I = \left[\begin{matrix} 1+\delta_o&0&0\\ 0&1-\delta_o&0\\ 0&0&\frac{1}{(1-\delta_o^2)}\\ \end{matrix}\right]\end{split}$$

leads to energy change

$$\Delta E(\delta_o) = 2Vc'\delta_o^2+O(\delta_o^4)$$

Monoclinic distortion

$$D_m(\delta_m) + I = \left[\begin{matrix} 1&\delta_m&0\\ \delta_m&1&0\\ 0&0&\frac{1}{(1-\delta_m^2)}\\ \end{matrix}\right]$$

leads to energy change

$$\Delta E(\delta_m) = 2Vc_{44}\delta_m^2+O(\delta_m^4)$$
$$B=\frac{1}{3}(c_{11}+2c_{12})$$
$$c'=\frac{1}{2}(c_{11}-c_{12})$$

- Isochoric stain
  - volume not changed: SWS not changed.
  - only even order of δ.
- Orthorhombic distortion apply to fcc: face center orthorhombic (fco).
- Monoclinic distortion apply to fcc: body center orthorhombic (bco).

Note

All files for this exercise are in the path exercise/03

fco lattice in emto

$\delta=0.00$

The input file (kstr/fco0.dat)

```
KSTR      HP......=N                                22 Jan 08
JOBNAM...=fco0       MSGL.=  0 MODE...=B STORE..=Y HIGH...=Y
DIR001=smx/
DIR006=./
Slope matrices, fco (spdf) DeltaE/V = (C11-C12)*e^2+O[e^4] (e=0.00)
NL.....= 4 NLH...=11 NLW...= 9 NDER..= 6 ITRANS= 3 NPRN..= 0
(K*W)^2..=  0.000000 DMAX....=    1.6000 RWATS...=      0.10
NQ3...=  1 LAT...=11 IPRIM.= 1 NGHBP.=13 NQR2..= 0
A........= 1.0000000 B.......= 1.0000000 C.......= 1.0000000
ALPHA....=     90.d0 BETA....=     90.d0 GAMMA...=     90.d0
QX(.1)...= 0.0000000 QY......= 0.0000000 QZ......= 0.0000000
a/w(.2)..= 0.70 0.70 0.70 0.70
LAMDA....=    2.5000 AMAX....=    4.5000 BMAX....=    4.5000
```

In the output file (kstr/fco0.prn)

```
PRIMV:    Default choice of primitive vectors.

          A     =  1.000000 B     =  1.000000 C     =  1.000000
          ALPHA = 90.000000 BETA  = 90.000000 GAMMA = 90.000000

          Primitive vectors for  Fco lattice in
          units of the lattice spacing a:

          (   0.50000,   0.00000,   0.50000 )
          (   0.50000,   0.50000,   0.00000 )
          (   0.00000,   0.50000,   0.50000 )

          Basis vectors:            NQ3 =   1

          (   0.00000,   0.00000,   0.00000 )
```

\(\delta=0.05\)

The input file (kstr/fco5.dat)

```
1   KSTR      HP......=N                              22 Jan 08
2   JOBNAM...=fco5       MSGL.=  0 MODE...=B STORE..=Y HIGH...=Y
3   DIR001=smx/
4   DIR006=./
5   Slope matrices, fco (spdf) DeltaE/V = (C11-C12)*e^2+O[e^4] (e=0.05)
6   NL.....= 4 NLH...=11 NLW...= 9 NDER..= 6 ITRANS= 3 NPRN..= 0
7   (K*W)^2..=  0.000000 DMAX....=    1.6000 RWATS...=      0.10
8   NQ3...=  1 LAT...=11 IPRIM.= 1 NGHBP.=13 NQR2..= 0
9   A........= 1.0000000 B.......=0.90476190 C.......=0.95476786
10  ALPHA....=     90.d0 BETA....=     90.d0 GAMMA...=     90.d0
11  QX(.1)...= 0.0000000 QY......= 0.0000000 QZ......= 0.0000000
12  a/w(.2)..= 0.70 0.70 0.70 0.70
13  LAMDA....=    2.5000 AMAX....=    4.5000 BMAX....=    4.5000
```

In the output file (kstr/fco5.prn)

```
PRIMV:    Default choice of primitive vectors.

          A     =  1.000000 B     =  0.904762 C     =  0.954768
          ALPHA = 90.000000 BETA  = 90.000000 GAMMA = 90.000000

          Primitive vectors for  Fco lattice in
          units of the lattice spacing a:

          (   0.50000,   0.00000,   0.47738 )
          (   0.50000,   0.45238,   0.00000 )
          (   0.00000,   0.45238,   0.47738 )

          Basis vectors:            NQ3 =   1

          (   0.00000,   0.00000,   0.00000 )
```

bco lattice in emto

\(\delta=0.00\)

The input file (kstr/bco0.dat)

```
KSTR      HP......=N                                22 Jan 08
JOBNAM...=bco0       MSGL.=  0 MODE...=B STORE..=Y HIGH...=Y
DIR001=smx/
DIR006=./
Slope matrices, bco (spdf) DeltaE/V = 2C44e^2+O[e^4] (e=0.00)
NL.....= 4 NLH...=11 NLW...= 9 NDER..= 6 ITRANS= 3 NPRN..= 0
(K*W)^2..=  0.000000 DMAX....=    2.4000 RWATS...=      0.10
NQ3...=  1 LAT...=10 IPRIM.= 1 NGHBP.=13 NQR2..= 0
A........= 1.0000000 B.......= 1.0000000 C.......=1.41421356
ALPHA....=     90.d0 BETA....=     90.d0 GAMMA...=     90.d0
QX(IQ)...= 0.0000000 QY......= 0.0000000 QZ......= 0.0000000
a/w(IQ)..= 0.70 0.70 0.70 0.70
LAMDA....=    2.5000 AMAX....=    4.5000 BMAX....=    4.5000
```

In the output file (kstr/bco0.prn)

```
PRIMV:    Default choice of primitive vectors.

          A     =  1.000000 B     =  1.000000 C     =  1.414214
          ALPHA = 90.000000 BETA  = 90.000000 GAMMA = 90.000000

          Primitive vectors for  Bco lattice in
          units of the lattice spacing a:

          (   0.50000,  -0.50000,   0.70711 )
          (   0.50000,   0.50000,  -0.70711 )
          (  -0.50000,   0.50000,   0.70711 )

          Basis vectors:            NQ3 =   1

          (   0.00000,   0.00000,   0.00000 )
```

\(\delta=0.05\)

The input file (kstr/bco5.dat)

```
KSTR      HP......=N                                22 Jan 08
JOBNAM...=bco5       MSGL.=  0 MODE...=B STORE..=Y HIGH...=Y
DIR001=smx/
DIR006=./
Slope matrices, bco (spdf) DeltaE/V = 2C44e^2+O[e^4] (e=0.05)
NL.....= 4 NLH...=11 NLW...= 9 NDER..= 6 ITRANS= 3 NPRN..= 0
(K*W)^2..=  0.000000 DMAX....=    2.2000 RWATS...=      0.10
NQ3...=  1 LAT...=10 IPRIM.= 1 NGHBP.=13 NQR2..= 0
A........= 1.0000000 B.......=0.90476190 C.......=1.35024566
ALPHA....=     90.d0 BETA....=     90.d0 GAMMA...=     90.d0
QX(IQ)...= 0.0000000 QY......= 0.0000000 QZ......= 0.0000000
a/w(IQ)..= 0.70 0.70 0.70 0.70
LAMDA....=    2.5000 AMAX....=    4.5000 BMAX....=    4.5000
```

In the output file (kstr/bco5.prn)

```
 PRIMV:    Default choice of primitive vectors.

           A     =  1.000000 B     =  0.904762 C     =  1.350246
           ALPHA = 90.000000 BETA  = 90.000000 GAMMA = 90.000000

           Primitive vectors for  Bco lattice in
           units of the lattice spacing a:

           (   0.50000,  -0.45238,   0.67512 )
           (   0.50000,   0.45238,  -0.67512 )
           (  -0.50000,   0.45238,   0.67512 )

           Basis vectors:            NQ3 =   1

           (   0.00000,   0.00000,   0.00000 )
```

kgrn inputs

```
--- /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/00/kgrn/cu.dat
+++ /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/03/kgrn/cuf5.dat
@@ -1,25 +1,25 @@
 KGRN                                              13 Oct 12
-JOBNAM=cu
+JOBNAM=cuf5
 STRT..=  A MSGL.=  0 EXPAN.= S FCD..=  Y FUNC..= SCA
-FOR001=../kstr/smx/fcc.tfh
-FOR001=../kstr/smx/fcc30.tfh
+FOR001=../kstr/smx/fco5.tfh
+FOR001=../kstr/smx/fco510.tfh
 DIR002=pot/
 DIR003=pot/
-FOR004=../bmdl/mdl/fcc.mdl
+FOR004=../bmdl/mdl/fco5.mdl
 DIR006=
 DIR009=pot/
 DIR010=chd/
 DIR011=/tmp/
-Self-consistent KKR calculation for fcc Cu
+Self-consistent KKR calculation for fcc Cu, (C11-C12)/2
 Band: 10 lines
 NITER.= 50 NLIN.= 31 NPRN.=  0 NCPA.=  7 NT...=  1 MNTA.=  1
 MODE..= 3D FRC..=  N DOS..=  N OPS..=  N AFM..=  P CRT..=  M
 Lmaxh.=  8 Lmaxt=  4 NFI..= 31 FIXG.=  2 SHF..=  0 SOFC.=  N
-KMSH...= G IBZ..=  2 NKX..=  0 NKY..= 13 NKZ..=  0 FBZ..=  N
+KMSH...= G IBZ..= 11 NKX..= 27 NKY..= 27 NKZ..= 27 FBZ..=  N
 KMSH2..= G IBZ2.=  1 NKX2.=  4 NKY2.=  0 NKZ2.= 51
 ZMSH...= C NZ1..= 16 NZ2..=  8 NZ3..=  8 NRES.=  4 NZD.=1500
 DEPTH..=  1.000 IMAGZ.=  0.020 EPS...=  0.200 ELIM..= -1.000
-AMIX...=  0.100 EFMIX.=  1.000 VMTZ..=  0.000 MMOM..=  0.000
+AMIX...=  0.050 EFMIX.=  1.000 VMTZ..=  0.000 MMOM..=  0.000
 TOLE...= 1.d-07 TOLEF.= 1.d-07 TOLCPA= 1.d-06 TFERMI=  500.0 (K)
 SWS.....=2.686842   NSWS.=  1 DSWS..=   0.05 ALPCPA= 0.6020
 Setup: 2 + NQ*NS lines
```

```
--- /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/00/kgrn/cu.dat
+++ /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/03/kgrn/cuo5.dat
@@ -1,25 +1,25 @@
 KGRN                                                13 Oct 12
-JOBNAM=cu
+JOBNAM=cuo5
 STRT..=  A MSGL.=  0 EXPAN.= S FCD..=  Y FUNC..= SCA
-FOR001=../kstr/smx/fcc.tfh
-FOR001=../kstr/smx/fcc30.tfh
+FOR001=../kstr/smx/bco5.tfh
+FOR001=../kstr/smx/bco510.tfh
 DIR002=pot/
 DIR003=pot/
-FOR004=../bmdl/mdl/fcc.mdl
+FOR004=../bmdl/mdl/bco5.mdl
 DIR006=
 DIR009=pot/
 DIR010=chd/
 DIR011=/tmp/
-Self-consistent KKR calculation for fcc Cu
+Self-consistent KKR calculation for fcc Cu, C44
 Band: 10 lines
 NITER.= 50 NLIN.= 31 NPRN.=  0 NCPA.=  7 NT...=  1 MNTA.=  1
 MODE..= 3D FRC..=  N DOS..=  N OPS..=  N AFM..=  P CRT..=  M
 Lmaxh.=  8 Lmaxt=  4 NFI..= 31 FIXG.=  2 SHF..=  0 SOFC.=  N
-KMSH...= G IBZ..=  2 NKX..=  0 NKY..= 13 NKZ..=  0 FBZ..=  N
+KMSH...= G IBZ..= 10 NKX..= 27 NKY..= 27 NKZ..= 37 FBZ..=  N
 KMSH2..= G IBZ2.=  1 NKX2.=  4 NKY2.=  0 NKZ2.= 51
 ZMSH...= C NZ1..= 16 NZ2..=  8 NZ3..=  8 NRES.=  4 NZD.=1500
 DEPTH..=  1.000 IMAGZ.=  0.020 EPS...=  0.200 ELIM..= -1.000
-AMIX...=  0.100 EFMIX.=  1.000 VMTZ..=  0.000 MMOM..=  0.000
+AMIX...=  0.050 EFMIX.=  1.000 VMTZ..=  0.000 MMOM..=  0.000
 TOLE...= 1.d-07 TOLEF.= 1.d-07 TOLCPA= 1.d-06 TFERMI=  500.0 (K)
 SWS.....=2.686842   NSWS.=  1 DSWS..=   0.05 ALPCPA= 0.6020
 Setup: 2 + NQ*NS lines
```

kfcd inputs

```
--- /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/00/kfcd/cu.dat
+++ /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/03/kfcd/cuf5.dat
@@ -1,6 +1,6 @@
-KFCD      MSGL..=  1                                22 Jan 08
-JOBNAM...=cu
-STRNAM...=fcc
+KFCD      MSGL..=  0                                22 Jan 08
+JOBNAM...=cuf5
+STRNAM...=fco5
 DIR001=../kstr/smx/
 DIR002=../kgrn/chd/
 DIR003=../shape/shp/
```

```
--- /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/00/kfcd/cu.dat
+++ /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/03/kfcd/cuo5.dat
@@ -1,6 +1,6 @@
-KFCD      MSGL..=  1                                  22 Jan 08
-JOBNAM...=cu
-STRNAM...=fcc
+KFCD      MSGL..=  0                                  22 Jan 08
+JOBNAM...=cuo5
+STRNAM...=bco5
 DIR001=../kstr/smx/
 DIR002=../kgrn/chd/
 DIR003=../shape/shp/
```

run the exercise03

- submit all kstr, bmdl and shape jobs to the queue, use following sbatch script.

Tetralith | Leonardo_Booster

```
cd kstr
sbatch -A naiss2024-22-241 -c 1 -a 1-12 -t 10:00 ../../emto.sbatch
```

- submit all kgrn jobs to the queue, use following sbatch script.

Tetralith | Leonardo_Booster

```
cd kgrn
sbatch -A naiss2024-22-241 -c 8 -a 1-12 -t 10:00 ../../emto.sbatch
```

- check if the kgrn jobs are finished correctly.

Hint

```
cd kgrn
grep -L "finished" *.prn
```

- submit all kfcd jobs to the queue, use following sbatch script.

Tetralith | Leonardo_Booster

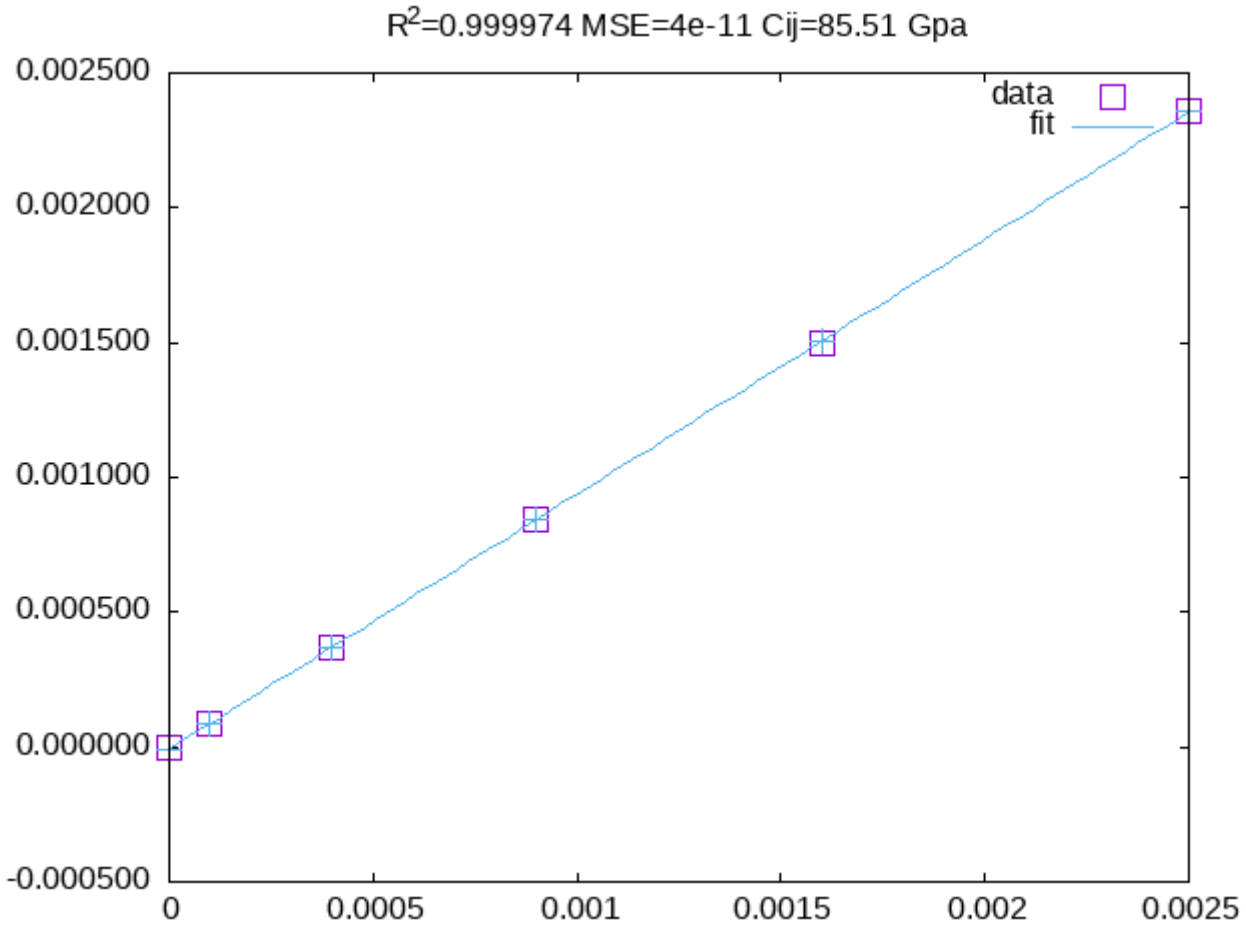
```
cd kfcd
sbatch -A naiss2024-22-241 -c 1 -a 1-12 -t 10:00 ../../emto.sbatch
```

extract the results

In kfcd folder

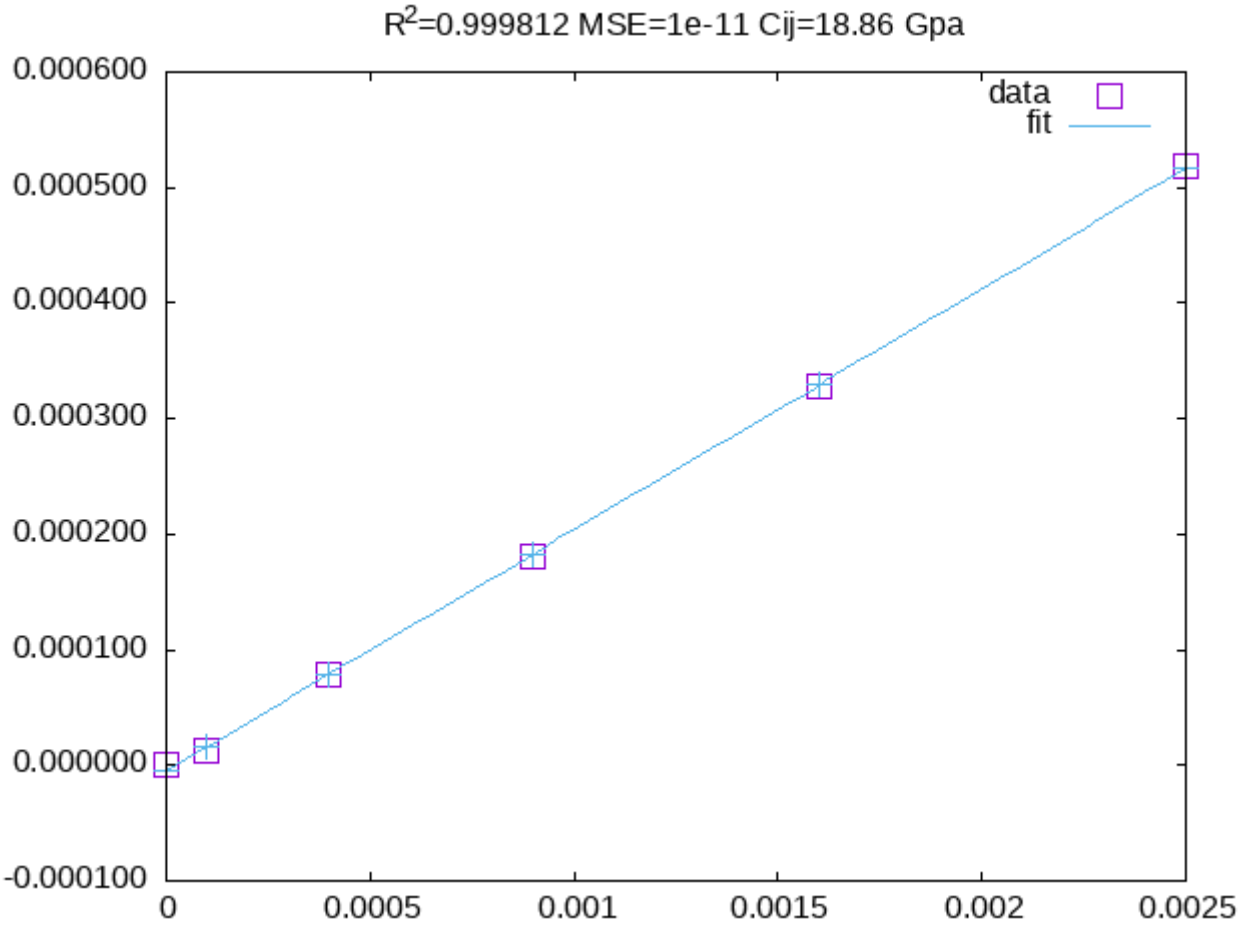
```
grep TOT-PBE cuo?.prn | awk '{if(NR==1)e0=$5;printf "%s %.6f %.6f\n"
$1,NR*NR*0.0001,$5-e0}'
```

fit \(\delta_o^2\) vs. \(\Delta E\) with the 2nd and 3th column to get \(c'\).




```
grep TOT-PBE cuf?.prn | awk '{if(NR==1)e0=$5;printf "%s %.6f %.6f\n"
$1,NR*NR*0.0001,$5-e0}'
```

fit \(\delta_m^2\) vs. \(\Delta E\) with the 2nd and 3th column to get \(c_{44}\).



exercise/04: Mixing enthalpy for bcc FeCrx alloy: FM

In this exercise we will practice how to get Mixing enthalpy of bcc \(Fe_{ (1-x) }Cr_x\) alloy with EMTO.

$$H = E_{Fe_{(1-x)}Cr_x} - (1-x)E_{Fe_{bcc}} - x E_{Cr_{bcc}}$$

The reference states are chosen as FM Fe and NM Cr, both in bcc structure. [1]
For each \(Fe_{ (1-x) }Cr_x\), we need its equilibrium volume and correspond energy.

alloy setup with CPA in kgrn

create an input files for \(Fe_{50}Cr_{50}\)

- we could copy the kgrn input from exercise00 and make some changes.
  - `JOBNAM=fecr_FM`
  - `FOR001=../kstr/smx/bcc.tfh`, `FOR004=../bmdl/mdl/bcc.mdl` and `IBZ..=  3`
  - `MNTA.=  2`
  - `AFM..=  F`
  - `SOFC.=  Y`
  - `AMIX...=  0.010`
  - ```
    Symb   IQ IT ITA NZ  CONC   Sm(s)  S(ws) WS(wst) QTR SPLT Fix
    Fe      1  1  1  26  50.00  1.000  1.000  1.000  0.0  2.0  N
    Cr      1  1  2  24  50.00  1.000  1.000  1.000  0.0 -1.0  N
    ```
    ```

```
Fe
Iz=  26 Norb= 10 Ion=  0 Config= 3d7_4s1
n      1  2  2  2  3  3  3  3  3  4
Kappa -1 -1  1 -2 -1  1 -2  2 -3 -1
Occup  2  2  2  4  2  2  4  4  3  1
Valen  0  0  0  0  0  0  0  1  1  1
Cr
Iz=  24 Norb=  9 Ion=  0 Config= 3d4_4s2
n      1  2  2  2  3  3  3  3  4
Kappa -1 -1  1 -2 -1  1 -2  2 -1
Occup  2  2  2  4  2  2  4  4  2
Valen  0  0  0  0  0  0  0  1  1
```

Hint

```
--- /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/00/kgrn/cu.dat
+++ /home/runner/work/emto-best-practices/emto-best-
practices/content/exercise/solutions/04/kgrn/fecr_FM.dat
@@ -1,21 +1,21 @@
 KGRN                                                13 Oct 12
-JOBNAM=cu
+JOBNAM=fecr_FM
 STRT..=  A MSGL.=  0 EXPAN.= S FCD..=  Y FUNC..= SCA
-FOR001=../kstr/smx/fcc.tfh
-FOR001=../kstr/smx/fcc30.tfh
+FOR001=../kstr/smx/bcc.tfh
+FOR001=../kstr/smx/bcc30.tfh
 DIR002=pot/
 DIR003=pot/
-FOR004=../bmdl/mdl/fcc.mdl
+FOR004=../bmdl/mdl/bcc.mdl
 DIR006=
 DIR009=pot/
 DIR010=chd/
 DIR011=/tmp/
-Self-consistent KKR calculation for fcc Cu
+Self-consistent KKR calculation for bcc FeCrX
 Band: 10 lines
-NITER.= 50 NLIN.= 31 NPRN.=  0 NCPA.=  7 NT...=  1 MNTA.=  1
-MODE..= 3D FRC..=  N DOS..=  N OPS..=  N AFM..=  P CRT..=  M
-Lmaxh.=  8 Lmaxt=  4 NFI..= 31 FIXG.=  2 SHF..=  0 SOFC.=  N
-KMSH...= G IBZ..=  2 NKX..=  0 NKY..= 13 NKZ..=  0 FBZ..=  N
+NITER.= 50 NLIN.= 31 NPRN.=  0 NCPA.=  7 NT...=  1 MNTA.=  2
+MODE..= 3D FRC..=  N DOS..=  N OPS..=  N AFM..=  F CRT..=  M
+Lmaxh.=  8 Lmaxt=  4 NFI..= 31 FIXG.=  2 SHF..=  0 SOFC.=  Y
+KMSH...= G IBZ..=  3 NKX..=  0 NKY..= 13 NKZ..=  0 FBZ..=  N
 KMSH2..= G IBZ2.=  1 NKX2.=  4 NKY2.=  0 NKZ2.= 51
 ZMSH...= C NZ1..= 16 NZ2..=  8 NZ3..=  8 NRES.=  4 NZD.=1500
 DEPTH..=  1.000 IMAGZ.=  0.020 EPS...=  0.200 ELIM..= -1.000
@@ -25,15 +25,22 @@
 EFGS...=  0.000 HX....=  0.100 NX...=  5 NZ0..=  6 STMP..= N
 Symb   IQ IT ITA NZ  CONC   Sm(s)  S(ws) WS(wst) QTR SPLT Fix
-Cu      1  1  1  29  1.000  1.000  1.000  1.000  0.0  0.0  N
+Fe      1  1  1  26  50.00  0.000  1.000  1.000  0.0  2.0  N
+Cr      1  1  2  24  50.00  0.000  1.000  1.000  0.0 -1.0  N
 Atom:  4 lines + NT*NTA*6 lines
 IEX...=  4 NP..= 251 NES..= 15 NITER=100 IWAT.=  0 NPRNA=  0
 VMIX.....=  0.300000 RWAT....=  3.500000 RMAX....= 20.000000
 DX.......=  0.030000 DR1.....=  0.002000 TEST....=  1.00E-12
 TESTE....=  1.00E-12 TESTY...=  1.00E-12 TESTV...=  1.00E-12
-Cu
-Iz=  29 Norb= 10 Ion=  0 Config= 3d10_4s1
+Fe
+Iz=  26 Norb= 10 Ion=  0 Config= 3d7_4s1
 n      1  2  2  2  3  3  3  3  3  4
 Kappa -1 -1  1 -2 -1  1 -2  2 -3 -1
-Occup  2  2  2  4  2  2  4  4  6  1
+Occup  2  2  2  4  2  2  4  4  3  1
 Valen  0  0  0  0  0  0  0  1  1  1
+Cr
+Iz=  24 Norb=  9 Ion=  0 Config= 3d4_4s2
+n      1  2  2  2  3  3  3  3  4
+Kappa -1 -1  1 -2 -1  1 -2  2 -1
+Occup  2  2  2  4  2  2  4  4  2
+Valen  0  0  0  0  0  0  0  1  1
```

- kstr, bmdl, shape and kfcd input files

Hint

The input file (kstr/bcc.dat)

```
KSTR      HP......=N                                22 Jan 08
JOBNAM...=bcc        MSGL.=  1 MODE...=B STORE..=Y HIGH...=Y
DIR001=smx/
DIR006=
Slope matrices, bcc (spdf), (kappa*w)^2= 0.0
NL.....= 4 NLH...=11 NLW...= 9 NDER..= 6 ITRANS= 3 NPRN..= 0
(K*W)^2..=  0.000000 DMAX....=    2.2000 RWATS...=      0.10
NQ3...=  1 LAT...= 3 IPRIM.= 0 NGHBP.=13 NQR2..= 0
A........= 1.0000000 B.......= 1.0000000 C.......= 1.0000000
BSX......= 0.5000000 BSY.....= 0.5000000 BSZ.....=-0.5000000
BSX......= 0.5000000 BSY.....=-0.5000000 BSZ.....= 0.5000000
BSX......=-0.5000000 BSY.....= 0.5000000 BSZ.....= 0.5000000
QX.......= 0.0000000 QY......= 0.0000000 QZ......= 0.0000000
a/w......= 0.70 0.70 0.70 0.70
LAMDA....=    2.5000 AMAX....=    4.5000 BMAX....=    4.5000
```

The input file (bmdl/bcc.dat)

```
BMDL      HP......=N                                22 Jan 08
JOBNAM...=bcc        MSGL.=  1 NPRN.=  0
DIR001=mdl/
DIR006=
Madelung potential for bcc bulk
NL.....= 7
LAMDA....=      2.50 AMAX....=      4.50 BMAX....=      4.50
NQ....=  1 LAT...= 3 IPRIM.= 1 NQR2..= 0
A........=     1.000 B.......=     1.000 C.......=     1.000
ALFA.....=      90.0 BETA....=      90.0 GAMMA...=      90.0
QX(1)....=       0.0 QY(1)...=       0.0 QZ(1)...=       0.0
```

- run all calculations

```
tree
  .
├── bmdl
│   ├── bcc.dat
│   └── mdl
├── kfcd
│   └── fecr_FM.dat
├── kgrn
│   ├── chd
│   ├── fecr_FM.dat
│   └── pot
├── kstr
│   ├── bcc.dat
│   └── smx
└── shape
    ├── bcc.dat
    └── shp

11 directories, 5 files
```

- check `NOS` from kgrn/fecr_FM.prn

```
grep -H NOS *.prn
fecr_FM.prn: KKRFCD: NOS(Ef) =      7.000025 ELT =      7.000000
fecr_FM.prn: KKRFCD: NOS(Ef) =      7.000025 ELT =      7.000000
```

Hint

increase `NCPA` to make sure cpa loop converged

```
sed -i 's/NCPA.=  7/NCPA.= 17/' fecr_FM.dat
```

create input files with different volumes for each \(Fe_{(1-x)}Cr_x\)

```
#! /bin/bash
# generate kgrn and kfcd input files based on kgrn/fecr_FM.dat
for i in `seq 0 2 10`  `seq 30 20 90` 100
do
  cr=$(printf "%03d" $i)
  fe=$(printf "%03d" $((100-i)))
  folder=FM/FeCr$cr
  mkdir -p $folder/{kgrn,kfcd}

  ln -s $(pwd)/kstr  $folder/kstr
  ln -s $(pwd)/bmdl  $folder/bmdl
  ln -s $(pwd)/shape $folder/shape

  for sws in `seq 2.59 0.02 2.69`
  do
        # -e "s/NCPA.=.../NCPA.= 17/"  \
        # -e "s/NKY..=.../NKY..= 21/" \
    sed -e "s/JOBNAM=.*/JOBNAM=fecr-$sws/" \
        -e "28 s/ 50.00/$fe.00/"  \
        -e "29 s/ 50.00/$cr.00/"  \
        -e "s/SWS......=......../SWS......=${sws}0000/" \
        kgrn/fecr_FM.dat > $folder/kgrn/fecr-$sws.dat

    sed -e "s/JOBNAM...=.*/JOBNAM...=fecr-$sws/" \
        kfcd/fecr_FM.dat > $folder/kfcd/fecr-$sws.dat
  done
done
```

- get equilibrium state for each concentration.

```
Eos.sh FeCr* > eos
cat eos
```

---

[1] Electronic origin of the anomalous stability of Fe-rich bcc Fe-Cr alloys

exercise/05: Mixing enthalpy for bcc FeCrx alloy: PM

In this exercise we will practice how to treat magnetic disorder with CPA. It is the same story as exercise/04[1], but here we treat the system within paramagnetic (PM) state.

$$H = E_{Fe^\uparrow_{(1-x/2)}Fe^\downarrow_{(1-x/2)}Cr^\uparrow_{x/2}Cr^\downarrow_{x/2}} - (1-x)E_{Fe^\uparrow_{50}Fe^\downarrow_{50}} - x E_{Cr^\uparrow_{50}Cr^\downarrow_{50}}$$

- copy kgrn and kfcd input form exercise/04 and reuse its kstr, bmdl and shape.

```
cp -r ../04/{kgrn,kfcd} 05/
cd 05
ln -s ../04/kstr
ln -s ../04/bmdl
ln -s ../04/shape
cp kgrn/{fecr_FM,fecr_PM}.dat
cp kfcd/{fecr_FM,fecr_PM}.dat
```

- spin \(\uparrow\) and \(\downarrow\) as “alloy components”.

split the components to half in kgrn input

```
27  Symb   IQ IT ITA NZ  CONC   Sm(s)  S(ws) WS(wst) QTR SPLT Fix
28  Fe      1  1  1  26  25.00  0.000  1.000  1.000  0.0  2.0  N
29  Fe      1  1  2  26  25.00  0.000  1.000  1.000  0.0 -2.0  N
30  Cr      1  1  3  24  25.00  0.000  1.000  1.000  0.0 -1.0  N
31  Cr      1  1  4  24  25.00  0.000  1.000  1.000  0.0  1.0  N
```

  - remember change `MNTA.=  4`.

- add “atomic config” for the extra components.

```
37  Fe
38  Iz=  26 Norb= 10 Ion=  0 Config= 3d7_4s1
39  n      1  2  2  2  3  3  3  3  3  4
40  Kappa -1 -1  1 -2 -1  1 -2  2 -3 -1
41  Occup  2  2  2  4  2  2  4  4  3  1
42  Valen  0  0  0  0  0  0  0  1  1  1
43  Fe
44  Iz=  26 Norb= 10 Ion=  0 Config= 3d7_4s1
45  n      1  2  2  2  3  3  3  3  3  4
46  Kappa -1 -1  1 -2 -1  1 -2  2 -3 -1
47  Occup  2  2  2  4  2  2  4  4  3  1
48  Valen  0  0  0  0  0  0  0  1  1  1
49  Cr
50  Iz=  24 Norb=  9 Ion=  0 Config= 3d4_4s2
51  n      1  2  2  2  3  3  3  3  4
52  Kappa -1 -1  1 -2 -1  1 -2  2 -1
53  Occup  2  2  2  4  2  2  4  4  2
54  Valen  0  0  0  0  0  0  0  1  1
55  Cr
56  Iz=  24 Norb=  9 Ion=  0 Config= 3d4_4s2
57  n      1  2  2  2  3  3  3  3  4
58  Kappa -1 -1  1 -2 -1  1 -2  2 -1
59  Occup  2  2  2  4  2  2  4  4  2
60  Valen  0  0  0  0  0  0  0  1  1
```

- calculations and results processing are same as exercise/04

---

[1] Electronic origin of the anomalous stability of Fe-rich bcc Fe-Cr alloys

exercise/06 diamond

Carbon in A4 structure.

2 Fcc lattice shift along the diagonal from (0,0,0) to (1/4,1/4,1/4)

```
KSTR      HP......=N                                22 Jan 08
JOBNAM...=A4         MSGL.=  1 MODE...=B STORE..=Y HIGH...=Y
DIR001=smx/
DIR006=./
Slope matrices, l21 (spdf), (kappa*w)^2= 0.0
NL.....= 3 NLH...=11 NLW...= 9 NDER..= 6 ITRANS= 3 NPRN..= 0
(K*W)^2..=  0.000000 DMAX....=    1.0980 RWATS...=      0.10
NQ3...=  2 LAT...= 2 IPRIM.= 0 NGHBP.=13 NQR2..= 0
A........= 1.0000000 B.......= 1.0000000 C.......= 1.0000000
BSX......= 0.5000000 BSY.....= 0.5000000 BSZ.....= 0.0000000
BSX......= 0.0000000 BSY.....= 0.5000000 BSZ.....= 0.5000000
BSX......= 0.5000000 BSY.....= 0.0000000 BSZ.....= 0.5000000
QX(IQ)...= 0.0000000 QY......= 0.0000000 QZ......= 0.0000000
QX(IQ)...= 0.2500000 QY......= 0.2500000 QZ......= 0.2500000
a/w(IQ)..= 0.70 0.70 0.70 0.70
a/w(IQ)..= 0.70 0.70 0.70 0.70
LAMDA....=    2.5000 AMAX....=    4.5000 BMAX....=    4.5000
```

Run kstr for this A4 structure, check the output file if there are some warnings. Will be problem ?

How about we also fill up the (1/2,1/2,1/2) and (3/4,3/4,3/4), what lattice it should be?

```
KSTR      HP......=N                                22 Jan 08
JOBNAM...=L21        MSGL.=  1 MODE...=B STORE..=Y HIGH...=Y
DIR001=smx/
DIR006=./
Slope matrices, l21 (spdf), (kappa*w)^2= 0.0
NL.....= 3 NLH...=11 NLW...= 9 NDER..= 6 ITRANS= 3 NPRN..= 0
(K*W)^2..=  0.000000 DMAX....=    1.0980 RWATS...=      0.10
NQ3...=  4 LAT...= 2 IPRIM.= 0 NGHBP.=13 NQR2..= 0
A........= 1.0000000 B.......= 1.0000000 C.......= 1.0000000
BSX......= 0.5000000 BSY.....= 0.5000000 BSZ.....= 0.0000000
BSX......= 0.0000000 BSY.....= 0.5000000 BSZ.....= 0.5000000
BSX......= 0.5000000 BSY.....= 0.0000000 BSZ.....= 0.5000000
QX(IQ)...= 0.0000000 QY......= 0.0000000 QZ......= 0.0000000
QX(IQ)...= 0.2500000 QY......= 0.2500000 QZ......= 0.2500000
QX(IQ)...= 0.5000000 QY......= 0.5000000 QZ......= 0.5000000
QX(IQ)...= 0.7500000 QY......= 0.7500000 QZ......= 0.7500000
a/w(IQ)..= 0.70 0.70 0.70 0.70
a/w(IQ)..= 0.70 0.70 0.70 0.70
a/w(IQ)..= 0.70 0.70 0.70 0.70
a/w(IQ)..= 0.70 0.70 0.70 0.70
LAMDA....=    2.5000 AMAX....=    4.5000 BMAX....=    4.5000
```

Check the `CMDL` value from its output, and compare with bcc (exercise/04/kstr/bcc.prn)

```
grep CMDL L21.prn
grep ../04/kstr/bcc.prn
```

Let’s use this more “close packed” structure for diamond

```
KGRN                                                13 Oct 12
JOBNAM=c
STRT..=  A MSGL.=  0 EXPAN.= M FCD..=  Y FUNC..= SCA
FOR001=../kstr/smx/L21.tfh
FOR001=../kstr/smx/L21p.tfh
DIR002=pot/
DIR003=pot/
FOR004=../bmdl/mdl/L21.mdl
DIR006=
DIR009=pot/
DIR010=chd/
DIR011=/tmp/
Self-consistent KKR calculation for A4 C
Band: 10 lines
NITER.= 50 NLIN.= 31 NPRN.=  0 NCPA.=  7 NT...=  4 MNTA.=  1
MODE..= 3D FRC..=  N DOS..=  N OPS..=  N AFM..=  P CRT..=  I
Lmaxh.=  8 Lmaxt=  3 NFI..= 31 FIXG.=  2 SHF..=  0 SOFC.=  Y
KMSH...= G IBZ..=  2 NKX..=  0 NKY..= 13 NKZ..=  0 FBZ..=  N
KMSH2..= G IBZ2.=  1 NKX2.=  4 NKY2.=  0 NKZ2.= 51
ZMSH...= C NZ1..= 32 NZ2..=  8 NZ3..=  8 NRES.=  4 NZD.= 800
DEPTH..=  2.000 IMAGZ.=  0.020 EPS...=  0.200 ELIM..= -1.000
AMIX...=  0.050 EFMIX.=  1.000 VMTZ..=  0.000 MMOM..=  0.000
TOLE...= 1.d-07 TOLEF.= 1.d-07 TOLCPA= 1.d-06 TFERMI=  500.0 (K)
SWS......=1.650000   NSWS.=  1 DSWS..=   0.05 ALPCPA= 0.6020
Setup: 2 + NQ*NS lines
EFGS...=  0.000 HX....=  0.200 NX...=  5 NZ0..= 16 STMP..= A
Symb   IQ IT ITA NZ  CONC   Sm(s)  S(ws) WS(wst) QTR SPLT Fix
C       1  1  1   6  1.000  1.000  1.000  1.000  0.0  0.0  N
C       2  2  1   6  1.000  1.000  1.000  1.000  0.0  0.0  N
Em      3  3  1   0  1.000  1.000  1.000  1.000  0.0  0.0  N
Em      4  4  1   0  1.000  1.000  1.000  1.000  0.0  0.0  N
Atom:  4 lines + NT*NTA*6 lines
IEX...=  4 NP..= 251 NES..= 15 NITER=100 IWAT.=  0 NPRNA=  0
VMIX.....=  0.300000 RWAT....=  3.500000 RMAX....= 20.000000
DX.......=  0.030000 DR1.....=  0.002000 TEST....=  1.00E-12
TESTE....=  1.00E-12 TESTY...=  1.00E-12 TESTV...=  1.00E-12
C
Iz=   6 Norb=  3 Ion=  0 Config= 2s2 2p2
n      1  2  2
Kappa -1 -1  1
Occup  2  2  2
Valen  0  1  1
C
Iz=   6 Norb=  3 Ion=  0 Config= 2s2 2p2
n      1  2  2
Kappa -1 -1  1
Occup  2  2  2
Valen  0  1  1
Em
Iz=   0 Norb=  0 Ion=  0 Config= 1s0
n      1
Kappa -1
Occup  0
Valen  1
Em
Iz=   0 Norb=  0 Ion=  0 Config= 1s0
n      1
Kappa -1
Occup  0
Valen  1
```

- `Em` : empty sites
- `CRT..=  I`
- kstr: `NL.....= 3`

Lattice constants for diamond ?

Convert to SWS ?

Hint

diamond structure in cubic conventional cells contains 8 atoms, we add extra 8 emtpy sites:

$$16\times \frac{4\pi}{3} \omega^3 = a^3$$

Eqation of state for diamond

```
#! /bin/bash

mkdir -vp diamond/kgrn/{chd,pot}
mkdir -vp diamond/kfcd/

cd diamond
ln -s ../kstr
ln -s ../shape
ln -s ../bmdl
cd -

for sws in `seq 1.60 0.02 1.70`
do
  sed -e "s/JOBNAM=.*/JOBNAM=c_${sws}/" \
      -e "s/SWS......=......../SWS......=${sws}0000/" \
      kgrn/c.dat > diamond/kgrn/c_${sws}.dat

  sed -e "s/JOBNAM...=.*/JOBNAM...=c_${sws}/" \
      kfcd/c.dat > diamond/kfcd/c_${sws}.dat
done
```

Maybe Heusler Alloy ?

See also

- EMTO website
- EMTO Manual
- Book by Prof. Levente Vitos: Computational Quantum Mechanics for Materials Engineers

Credits

The lesson file structure and browsing layout is inspired by and derived from work by CodeRefinery licensed under the MIT license. We have copied and adapted most of their license text.

Use of EMTO code should follow the EMTO license (https://emto.gitlab.io/license.html):

- **NO WARRANTY**: We are not responsible for any damage, defect or loss incurred as a result of operating the software.
- Only **non-commercial** use allowed.
- **CANNOT** redistribute source-code or its executable binaries.
- Can modify source-code but **CANNOT** redistribute modifications (derivative works, include its executable binaries).
- Parts of the software are provided under separate licenses, as follows:
  - BLAS routines under the BLAS License (http://www.netlib.org/blas/#_licensing)
  - LAPACK routines under the modified BSD license (http://www.netlib.org/lapack/LICENSE.txt)

Instructional Material

This instructional material is made available under the Creative Commons Attribution license (CC-BY-4.0). The following is a human-readable summary of (and not a substitute for) the full legal text of the CC-BY-4.0 license. You are free to:

- **share** - copy and redistribute the material in any medium or format
- **adapt** - remix, transform, and build upon the material for any purpose, even commercially.

The licensor cannot revoke these freedoms as long as you follow these license terms:

- **Attribution** - You must give appropriate credit (mentioning that your work is derived from work that is Copyright (c) ENCCS and individual contributors and, where practical, linking to https://enccs.github.io/sphinx-lesson-template), provide a link to the license, and indicate if changes were made. You may do so in any reasonable manner, but not in any way that suggests the licensor endorses you or your use.
- **No additional restrictions** - You may not apply legal terms or technological measures that legally restrict others from doing anything the license permits.

With the understanding that:

- You do not have to comply with the license for elements of the material in the public domain or where your use is permitted by an applicable exception or limitation.

- No warranties are given. The license may not give you all of the permissions necessary for your intended use. For example, other rights such as publicity, privacy, or moral rights may limit how you use the material.

Software

Except where otherwise noted, the example programs and other software provided with this repository are made available under the OSI-approved MIT license.