Karlsruhe Institute of Technology

The ABC of DFT: hands-on training AIMS 1

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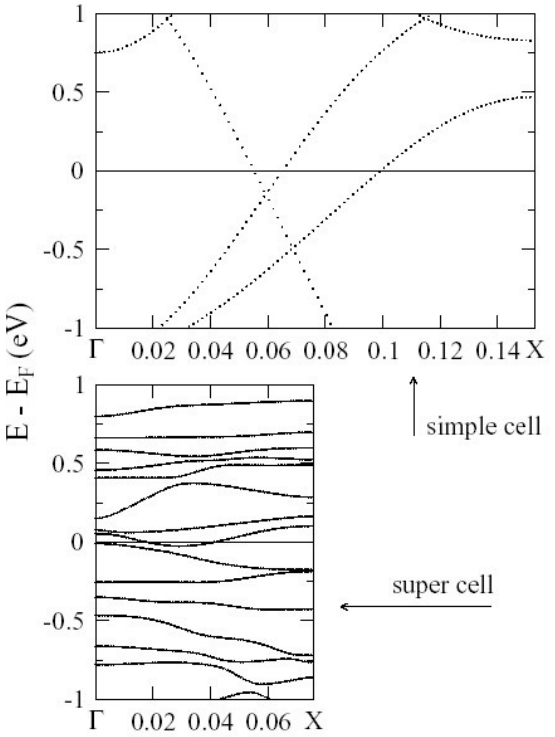
INSTITUTE OF NANOTECHNOLOGY

December 14th Solids: basic calculations

- New type of basis
- **k**-space
- Setting up an AIMS calculation
  - Input files
  - Which parameters you should check always
  - What you should keep in mind
- Demonstration of a simple calculation
  - Reading the output
- Set of exercises to get acquainted
  - Structure optimization
  - Plot a DOS and band-structure
  - Example on diamond



FHI-aims

- Fritz Haber Institute *ab initio* simulations package

  - **Finite systems** and **solids** with periodic boundary conditions
  - Preconstructed numerical strictly local orbitals
  - Various options for Exchange Correlation
  - Runs parallel on 10000+ cores
  - Up to ~100000 atoms massive parallel

  - All the basics quantities,
  - Many advanced options, hybrid functionals, GW, linear response, STM simulation ….

  - Use it if your questions involve solids of surfaces…..

Structure of AIMS

- Two (main) input files: control.in and geometry.in
- One executable
- Main output to standard out

- For the most basic calculations
  aims is called only once,
  some more complicated tasks
  require multiple executions

- Full manual you'll find on the accounts

The task at hand

- Solve

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}} + V_{\text{H}} + V_{\text{xc}}\right\}\phi_{i,\mathbf{k}}(\mathbf{r}) = \varepsilon_{i,\mathbf{k}}\phi_{i,\mathbf{k}}(\mathbf{r})$$

  - For all relevant values of i
  - For a sufficient dense sampling of k
  - Using a sufficiently large basis
  - Using an appropriate approximation for V_{xc}

- Relevant, sufficient and appropriate are dependent on
  - The type of material: which atoms, metal or semi-conductor
  - What quantity we need: total energy, forces, electronic structure..

For all relevant values of i

- The electrons of a single unit cell need to be accommodated
- In AIMS always all electrons are treated, no effective core potentials like in TM
- The numerical basis is comparable in size to the ones Gaussians or atomic orbitals
- empty_states keyword
  Default: $(l+1)^2+2$ for each atom, l is the maximum valence angular momentum

For a sufficient dense sampling of k

- The most important thing to carefully check

- Molecule : only one (no sampling)
- Insulator : few ~ 10 - 100
- Metal : many ~ 1000+

- Different quantities converge differently

- Different smearings/integration methods converge differently

- Keywords: `k_grid k_offset`

Broadening

- Keyword `occupation_type` *`type width`*
  - Gaussian, methfessel-paxton, fermi

- For metallic / small gap systems:
  broadening of ~ 0.1 eV is nessesary to obtain a stable convergence
  a broadening to 0 extrapolation is calculated

- Large gap / semiconductors:
  default value of 0.01 eV is usually good
  too large > fractional occupation
  too smalll > no formal Fermi-level

- in any case:
  - careful checks for k-point convergence are necessary

Using a sufficiently large basis

- Size of the basis is controlled in the final part of the control.in file by inserting basis function definitions
- All predefined functions are given in the species_defaults folder
- Four preset accuracies, light_194, light, tight, really_tight
- Prerelaxation, test calculations : light
- Final relaxation : tight
- Final convergence test : really_tight

Using an appropriate approximation for V_{xc}

- Keyword `xc` *`xc-type`*

- LDA's

  `pw-lda, pz-lda, vwn`

- GGA's

  `am05, blyp, pbe, pbeint, pbesol, revpbe`

- Hybrid functionals (including non-local exchange)

  `b3lyp, hse03, hse06, pbe0, pbesol0`

  - Mostly GGA correlation + 0.75 GGA exchange + 0.25 Fock exchange

- Approaches strickly beyond DFT

  `hf, mp2, screx, cohex`

Running aims

- Create a working directory
- Prepare the input files
  control.in
  geometry.in
- Run aims
- Post process the output
  - Various scripts are available for the most general tasks

Files used by AIMS: Input

- Geometry.in

Atomic structure, unit cell, and atom specific details

```
#
#  fcc Al
#  Equilibrium lattice parameter: 3.98 A (LDA)
#
  atom 0. 0. 0. Al
#
# unit cell
#
lattice_vector  1.99 1.99 0.0
lattice_vector  0.0  1.99 1.99
lattice_vector  1.99 0.0  1.99
```

- Output structures can be retrieved using some scripts:

create_geometry_zip.pl
create_xyz_movie.pl
create_xyz.pl

Files used by AIMS: Input

- Control.in
  - What to do and how to do it
  - Which physical model
    xc-functional, spin, relativistic effects, …
  - What kind of calculation
    structure optimization, calculating electronic properties, …
    specifying output
  - What basis to use
    add species defaults from the database.

Getting started

- The input files for and descriptions of the exercises are contained in a tar file
  `handsonsession.6.tar`
  under `/net/intact/home/dft20>`
- Please copy them to your account and unpack

```
> cp ~/../dft20/handsonsession.6.tar ~/ABC_of_DFT/hands-on-sessions/
> cd ~/ABC_of_DFT/hands-on-sessions
> tar -xvf handsonsession.6.tar
> cp ~/../dft20/setupaims .
> ./setupaims
```

- AIMS can now be executed by typing

```
> aims
```

Or better

```
> aims | tee outputfilename
```

Exercises

- Cubic diamond :
  - convergency tests
  - Volume optimization

- Fcc Al : volume optimization, dos and band-structure plotting

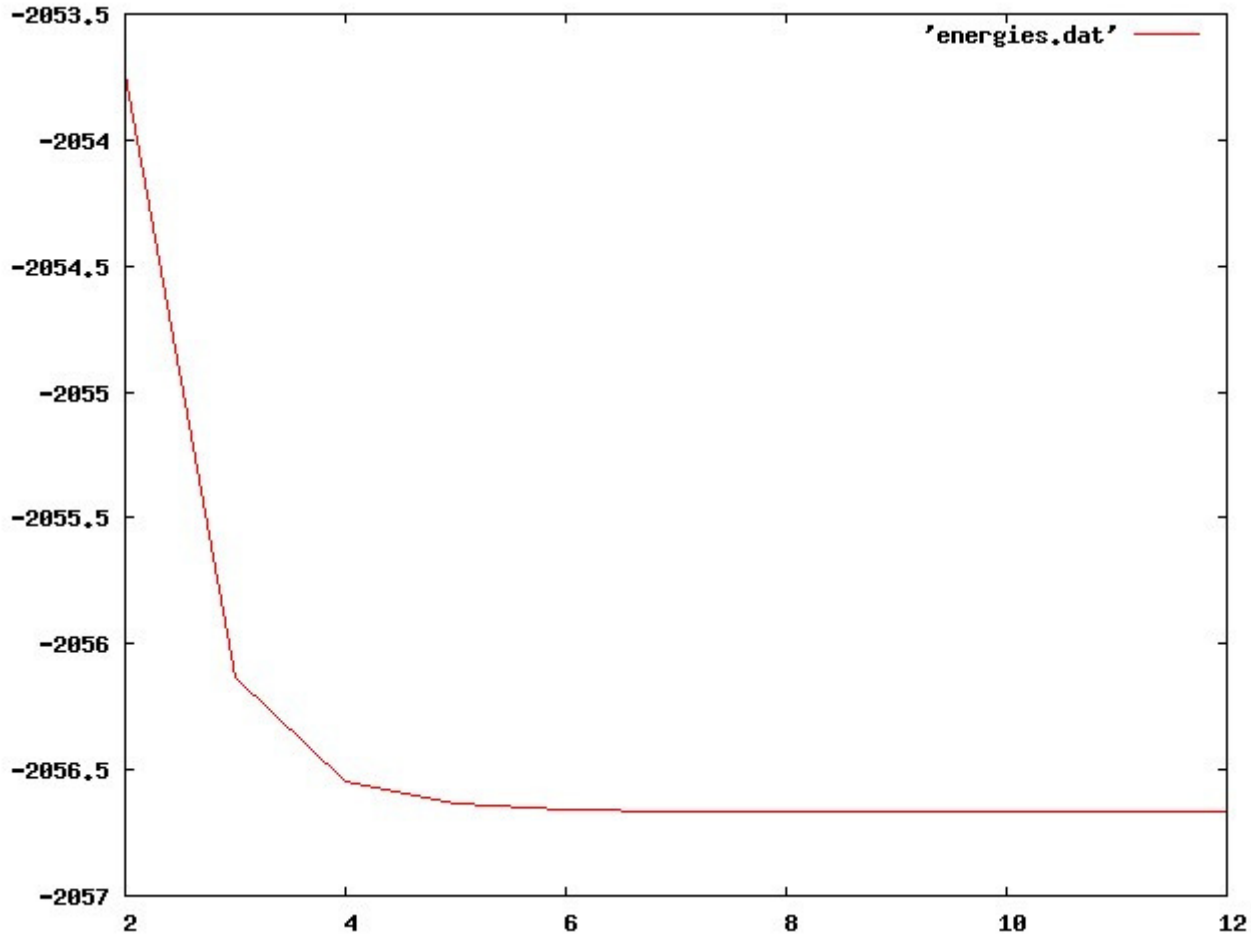
Exercise 1 cubic diamond

- Energy convergence with k-points

- Optimization: in this case symmetry leave only one free parameter, lattice parameter or unit cell volume

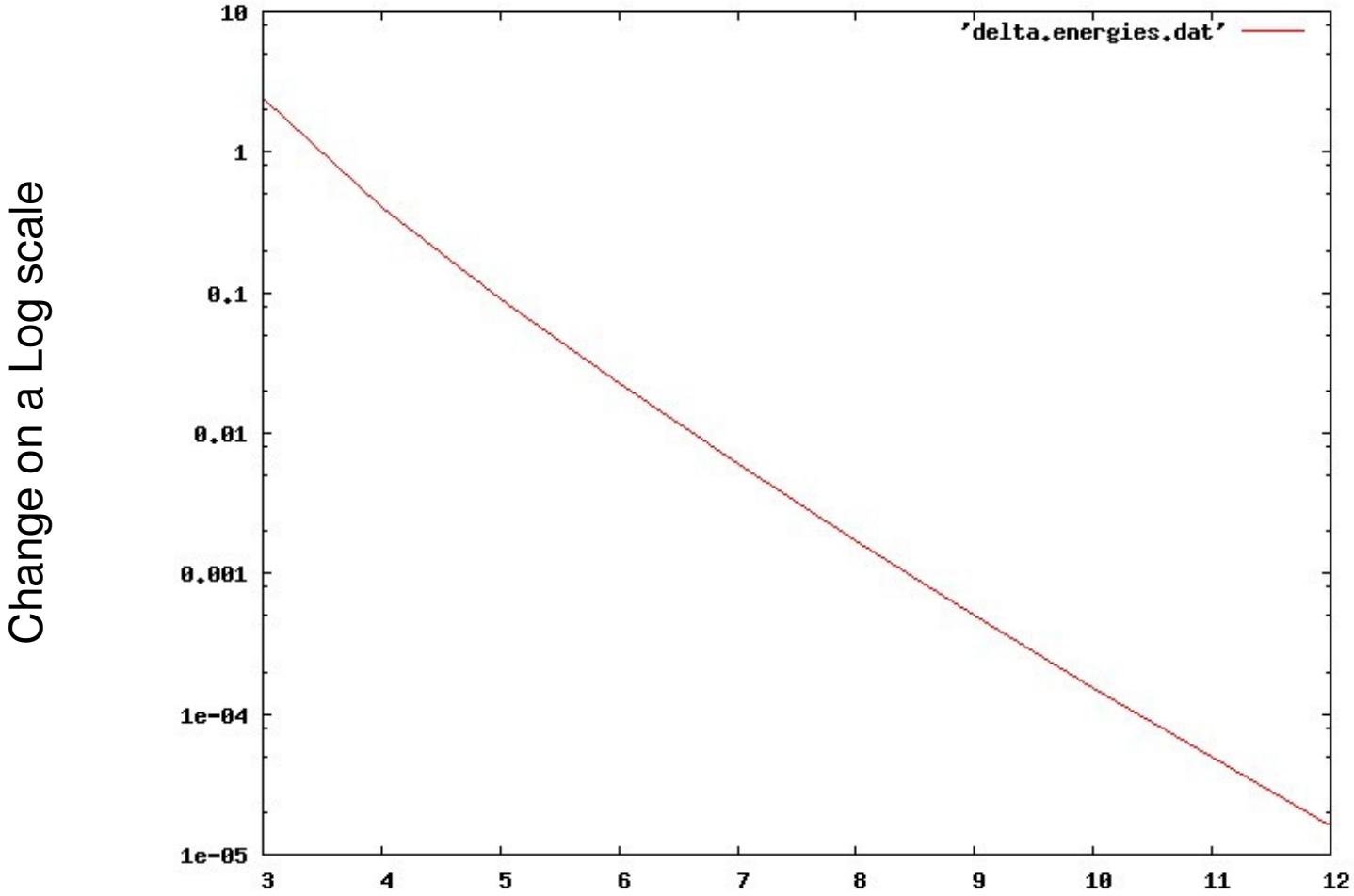
Exercise 1 cubic diamond

- Energy convergence with k-points



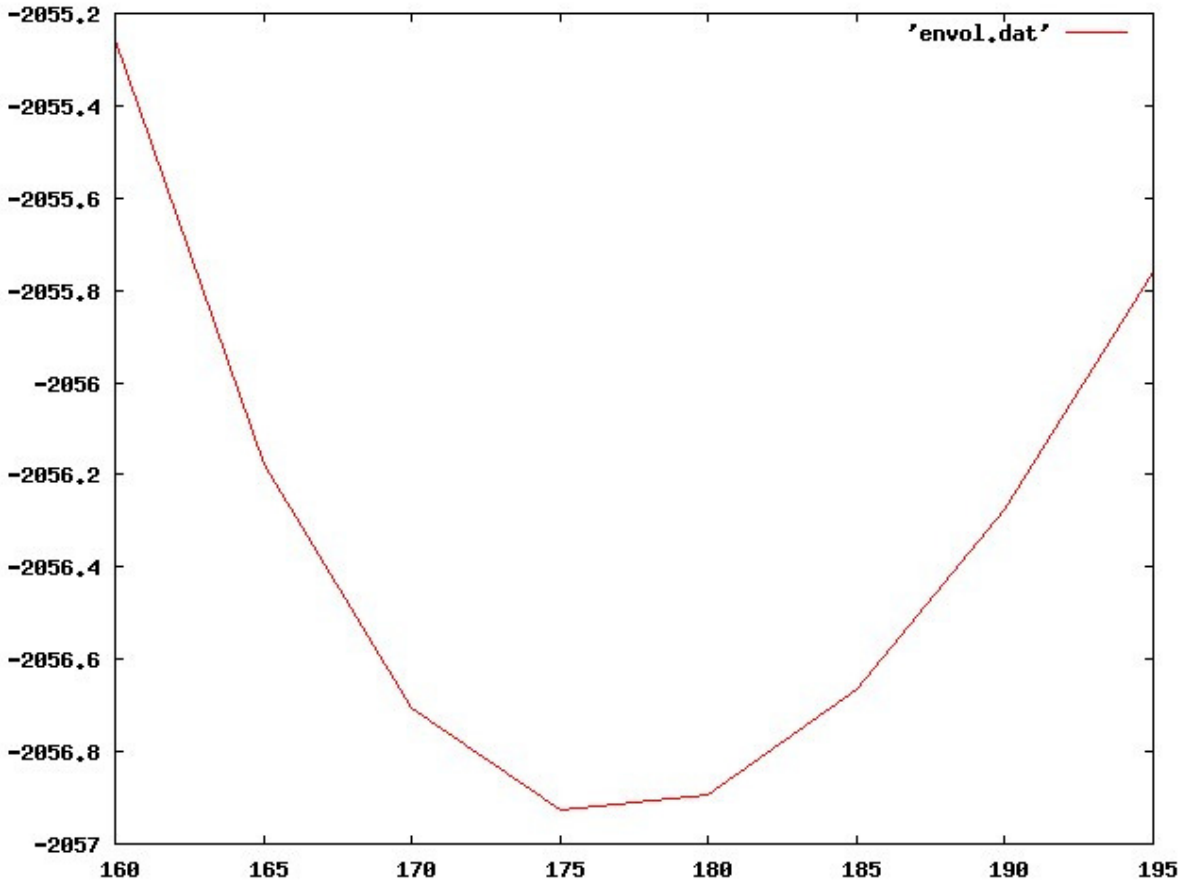
Exercise 1 cubic diamond

- Energy convergence with k-points



Exercise 1 cubic diamond

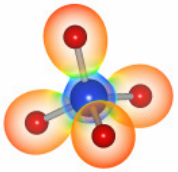
- Optimization: in this case symmetry leave only one free parameter, lattice parameter or unit cell volume



8 8 8 k-point mesh

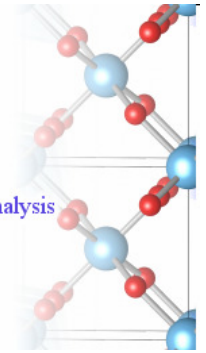
Exercise 1 cubic diamond

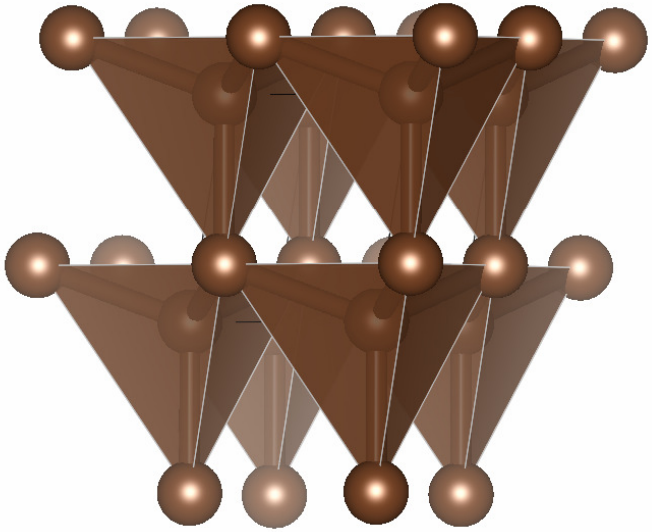
- Visualizing structure using VESTA



VESTA

Visualization for Electronic and STructural Analysis





Exercise 2 fcc Aluminum

- Plotting the DOS

```
> gnuplot
gnuplot> plot 'KS_DOS_total.dat'  w l
```

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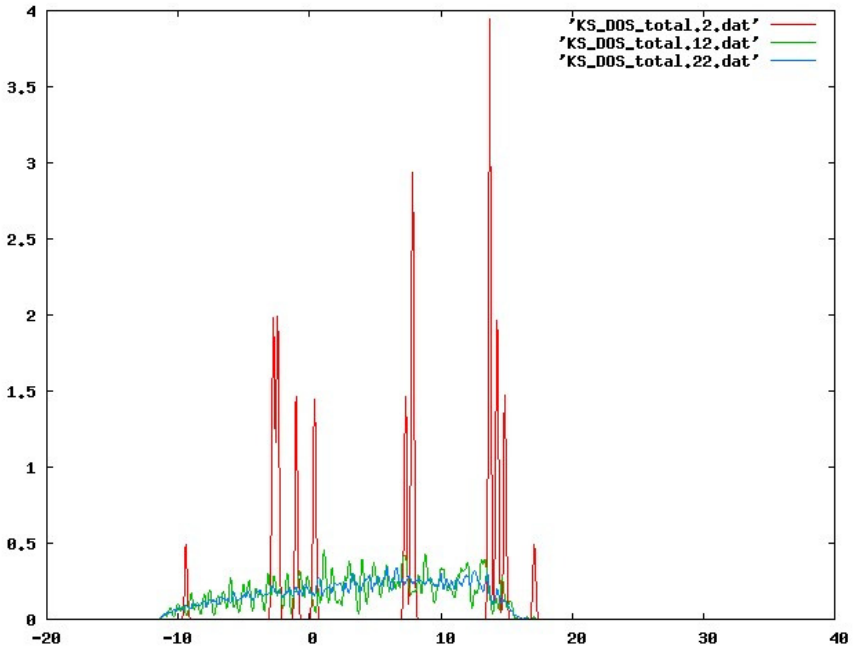
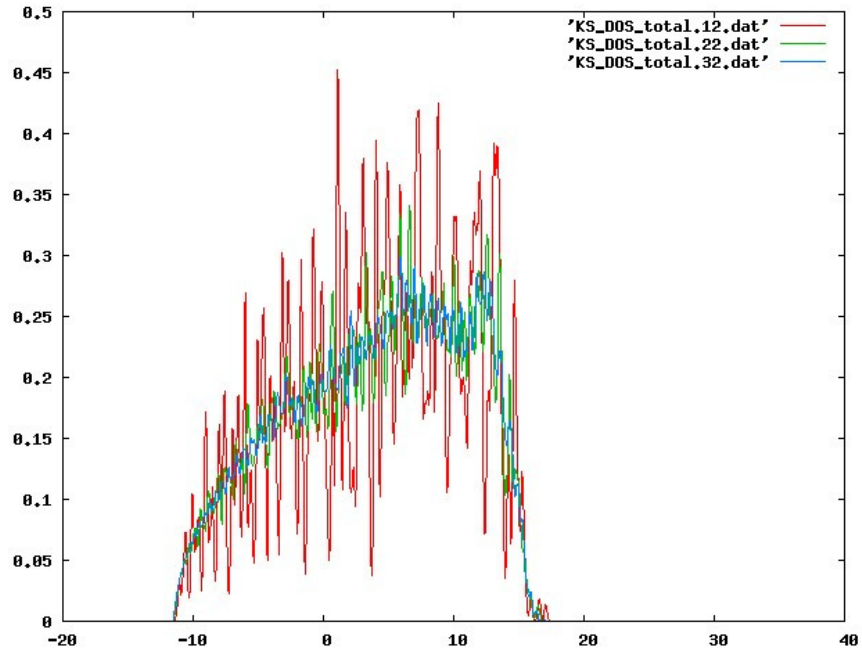
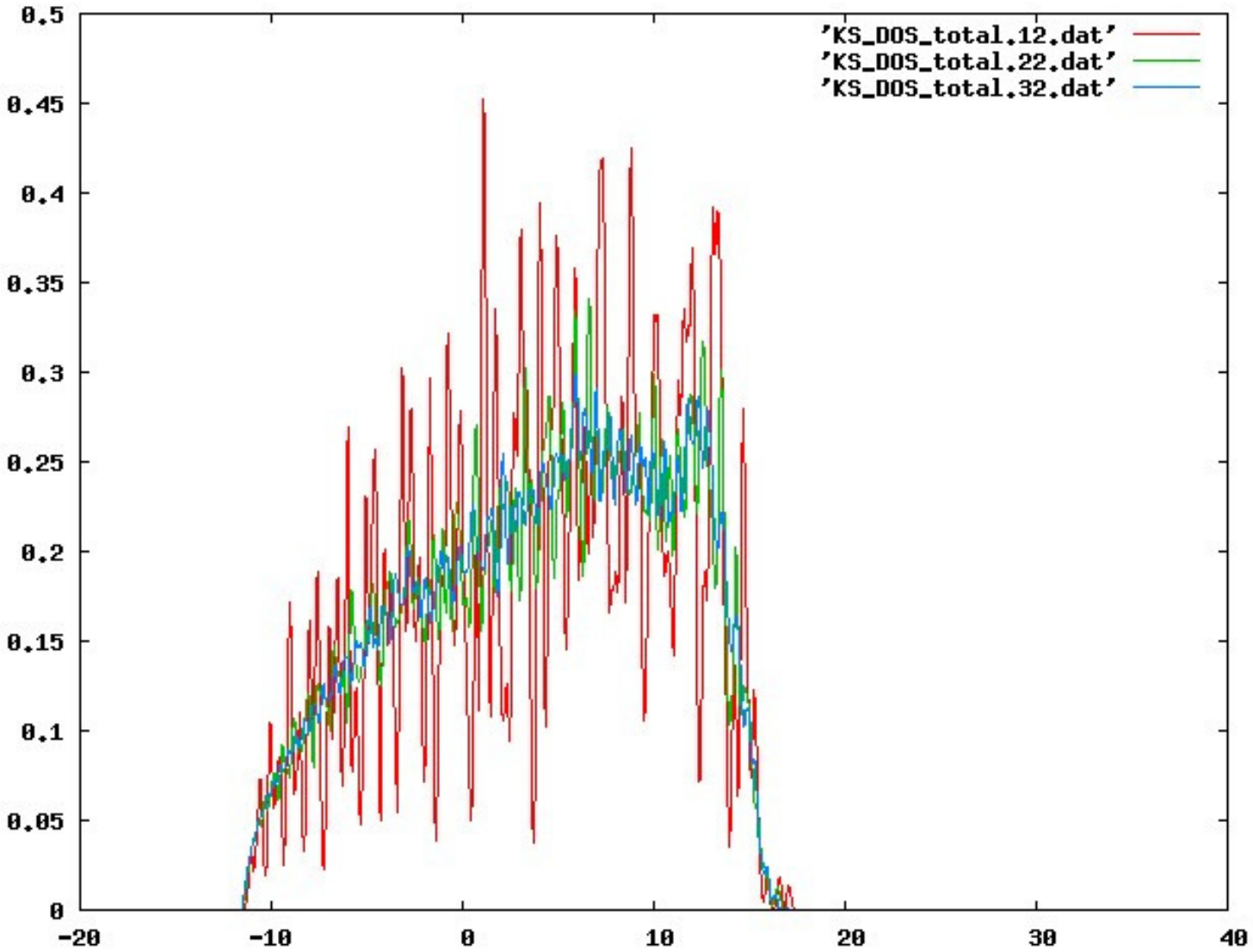
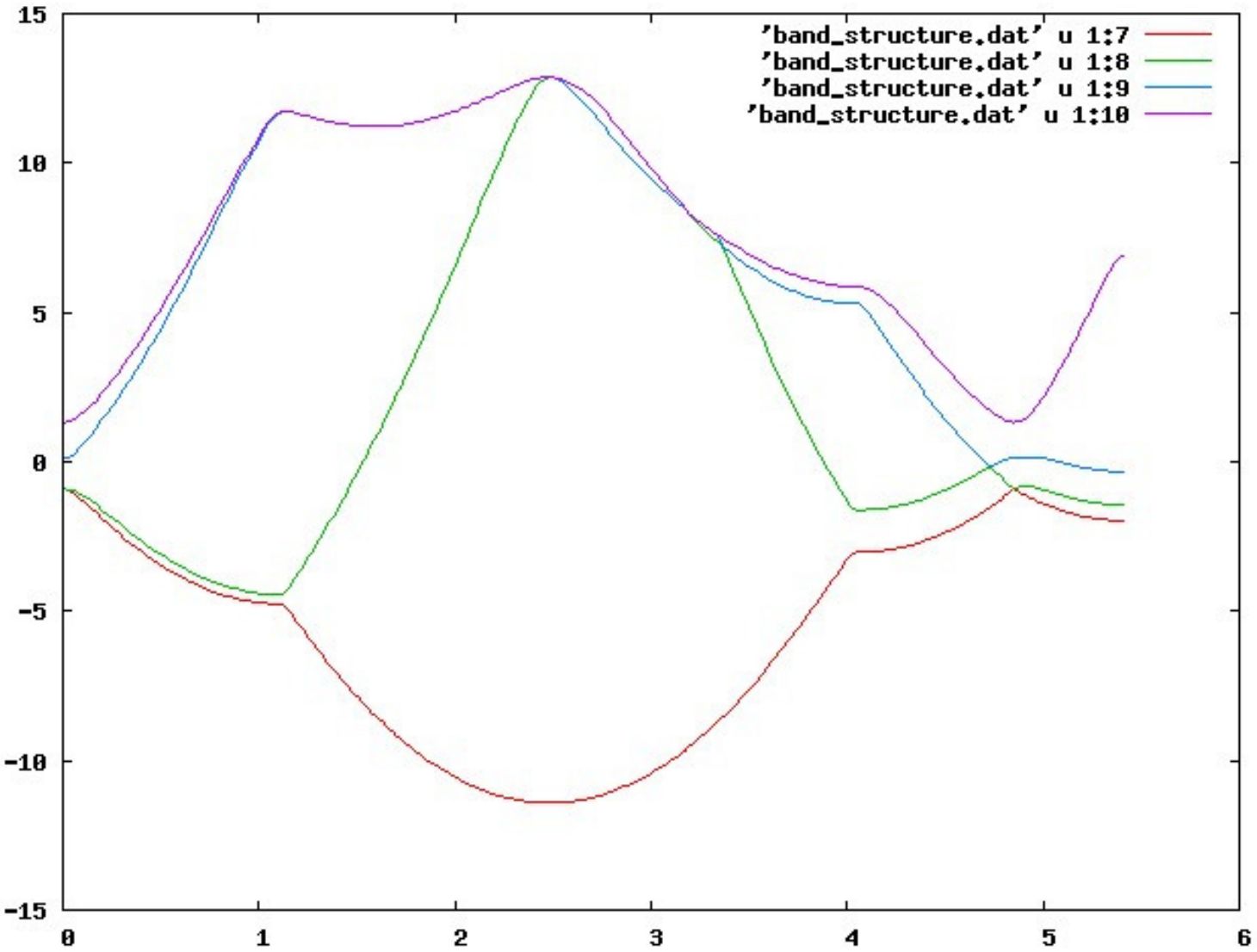





'KS_DOS_total.12.dat'
'KS_DOS_total.22.dat'
'KS_DOS_total.32.dat'
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-20
-10
0
10
20
30
40

Exercise 2 fcc Aluminum

- Plotting the band structure
- Uncomment the output band lines in the control.in file
- Run aims
- Run aims_band_plotting.pl
- Plot using gnuplot


'band_structure.dat' u 1:7
'band_structure.dat' u 1:8
'band_structure.dat' u 1:9
'band_structure.dat' u 1:10
15
10
5
0
-5
-10
-15
0
1
2
3
4
5
6