The Augmented Spherical Wave Package

Hands on Session I

Volker Eyert

Institut für Physik, Universität Augsburg

Electronic Structure in a Nutshell

Outline

Outline

Installation I

Unpack

unpack the file *aswbin_2.3*.tar.gz
$\Rightarrow$ *sub*directory *aswbin_2.3* is created

Adapt environment

include the directory *aswbin_2.3* into your PATH variable typing, from within *aswbin_2.3*, “export PATH=$PATH:$PWD” (bash)

A very first test

type “mnmpr.run” (from within *aswbin_2.3*)
$\Rightarrow$ one-page output of machine parameters

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$\Rightarrow$ one-page output of machine parameters

Installation II

The First ASW Output

```
ASW-2.3, program MNMPR started on asterix at Wed, 17 Jan 2007, 16:32:46.

    Copyright (C) 1992-2007 Volker Eyert
    Please see file COPYRIGHT for details

Machine-specific parameters affecting floating-point arithmethic:

ibase:          2                 (base of the machine)
it:            53                 (number of (base) digits in the mantissa)
xeps:      2.22044604925031D-16   (= min, such that 1.0 + xeps > 1.0)
xepsn:     1.11022302462516D-16   (= min, such that 1.0 - xepsn < 1.0)
minexp:     -1021                 (min exponent before (gradual) underflow)
xzer:      2.22507385850720-308   (underflow threshold = base**(minexp-1))
xmin:      2.22507385850720-308   (safe min, 1/xmin does not overflow)
maxexp:      1024                 (largest exponent before overflow)
xinf:      1.79769313486232+308   (overflow threshold = base**maxexp*(1-xepsn))
irnd:           1                 (= 0/1 for chopping/rounding in addition)

task  1, total       :  cpu time:     0.00400 sec

ASW-2.3, program MNMPR ended on asterix at Wed, 17 Jan 2007, 16:32:46.
```

Installation III

Update shell scripts

from within *aswbin_2.3* run the shell script “upshl”
$\Rightarrow$ all files *.x have a line like “BINDIR=/home/user/aswbin_2.3”
$\Rightarrow$ all files *.run and *.x can be used from everywhere

Summary: installation directory

- executables (files mn*.run, pl*.run)
- shell scripts (files mn*.x, pl*.x)
- info files (README, COPYRIGHT, NEW2.3, HELP, . . .)

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Outline

Preparing for the Application

Create a directory tree

- create e.g. /home/user/appl/ (applications)
- create e.g. /home/user/appl/cu (copper)
- create e.g. /home/user/appl/cu/nm (spin-deg. calcs.)

Generate the main input file: CTRL

within /home/user/appl/cu/nm:

- copy the CTRL file from the database or
- write the CTRL file from scratch

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Generate the main input file: CTRL

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- copy the CTRL file from the database or
- write the CTRL file from scratch

The CTRL File I

CTRL $\Longrightarrow$ main and only input file for all main programs

contains information about, inter alia

- crystal structure
- constituing atoms (type and positions)
- symmetry lines
- options and control parameters
  - non-relativistic $\leftrightarrow$ scalar-relativistic
  - spin-degenerate $\leftrightarrow$ spin-polarized
  - Brillouin-zone sampling scheme and number of **k**-points
  - LDA/GGA-parametrization

all other files are automatically created and deleted

The CTRL File II

A Minimum CTRL File

```
HEADER  Cu fcc
        data by Landolt-Boernstein
VERSION ASW-2.3
STRUC   ALAT=6.83079 CNTR=F
CLASS   ATOM=CU Z=29
SITE    ATOM=CU POS= 0.0  0.0  0.0
```

CTRL: Rules

- “free format” (no tabs)
- sections (categories, cols. 1-8) each containing
- a set of catchwords (tokens, cols. 9-80)

Creating a More Detailed CTRL File

Use new tokens (and run mnsym.x/mnsym.run)

- set HELP=T in category IO

  ```
  IO          HELP=T
  ```

  $\Longrightarrow$: new file HELP describes all tokens
- set VERBOS=40 in category IO

  ```
  IO          VERBOS=40
  ```

  $\Longrightarrow$: new file CALL: a maximum CTRL file

A Standard CTRL File I

```
HEADER  Cu fcc
        data by Landolt-Boernstein
VERSION ASW-2.3
IO      HELP=F SHOW=T VERBOS=30 CLEAN=T
OPTIONS REL=T OVLCHK=T
STRUC   ALAT=6.83079 CNTR=F
CLASS   ATOM=CU Z=29 R=2.6694476 LMXL=2 CONF=4 4 3 4 COORB=0 1 2
                QVAL= 1.0  0.0  10.0  0.0
SITE    ATOM=CU POS= 0.0  0.0  0.0
SYMGRP
ENVEL   EKAP=-0.015
BZSMP   NKBAB=6 BZINT=LTM EMIN=-1.0 EMAX=1.5 NDOS=3000
        NORD=5 WIDTH=0.02 SAVDOS=F SAVCOOP=F SAVFERM=F
CONTROL START= QUIT= FREE=F NITBND=99 CNVG=1.0D-08 CNVGET=1.0D-08
        NITATM=50 CNVGQA=1.0D-10
MIXING  NMIXB=5 BETAB=0.5 INCBB=T NMIXA=5 BETAA=0.5
...
```

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A Standard CTRL File II

```
SYMLIN   NPAN=5 NPTS=400 ORBWGT=F CARTE=F
         LABEL=W ENDPT= 0.500  0.250  0.750
         LABEL=L ENDPT= 0.500  0.500  0.500
         LABEL=g ENDPT= 0.000  0.000  0.000
         LABEL=X ENDPT= 0.500  0.000  0.500
         LABEL=W ENDPT= 0.500  0.250  0.750
         LABEL=K ENDPT= 0.375  0.375  0.750
PLOT     CARTV=T
         ORIGIN= 0.0  0.0  0.0
         RPLOT1= 1.0  0.0  0.0
         RPLOT2= 0.0  1.0  0.0
         RPLOT3= 0.0  0.0  1.0
         NPDIV1=50 NPDIV2=50
```

Running the Main Programs I

Self-Consistent Field Cycle: mnscf.x/mnscf.run

Summary Generated by Shell Script monic

```
ASW-2.3, program MNSCF started on asterix at Wed, 17 Jan 2007, 20:49:20.
Calculation converged after  12 iteration(s).
                     Start of Iteration   12
    47 irreducible k-points generated from    1000 ( 10, 10, 10).
           Fermi energy - MTZ =     0.690175 Ryd
The system is a metal:
           DOS at Fermi energy:     3.878797 1/Ryd
           Gamma * (f.u./cell):     0.671990 mJ/(mole*K**2)
Mean-square residual:                   0.417823D-23
Total free atom energies     :  -3304.550572 Ryd
Total variational energy     :  -3304.871499 Ryd
Cohesive energy              :      0.320927 Ryd
 qdiff =       0.00000000  <        0.00000001
 ediff =       0.00000001  <        0.00000001
ASW-2.3, program MNSCF ended on asterix at Wed, 17 Jan 2007, 20:49:31.
```

Running the Main Programs II

Calculate Properties

Band structure

mnbnd.x/mnbnd.run

DOS, COOP, and Fermi surface

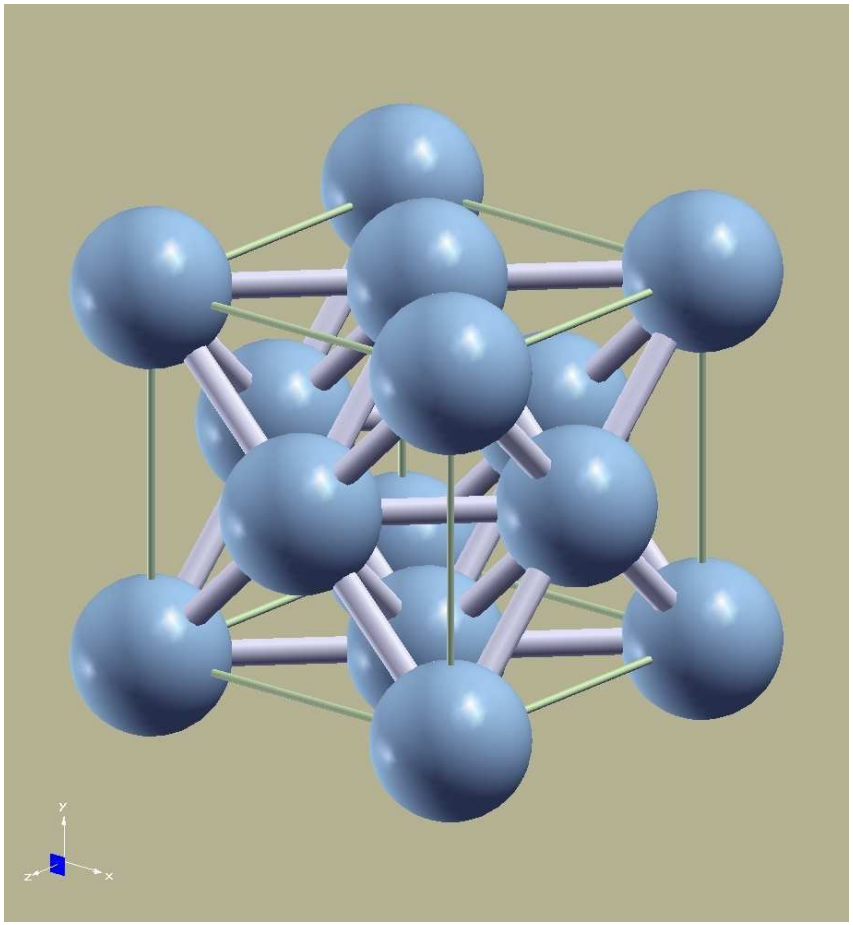
mndos.x/mnscf.run

Optical spectra

mnopt.x/mnscf.run

Running the Plot Programs I

Crystal Structure: plxcr.x



Running the Plot Programs II

Band Structure: plbnd.x/plbnd.run

Interaction with the Program (First Run)

```
 ASW-2.3, program PLBND started on asterix at Fri, 02 Feb 2007, 18:28:37.

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     Please see file COPYRIGHT for details

 All input will be echoed to file PLIB.

 Enter terminal type:
 1 = X-Windows (default)
 2 = PC-Screen (vt220-emulation)
 3 = suppress terminal output
/
 Enter output device (default: 1):
 1 = Color postscript
 2 = Postscript
 3 = PDF (not yet supported)
 4 = JPEG (not yet supported)
 5 = LaTeX
 6 = LaTeX (special)
 7 = HP LaserJet III (PCL5)
 8 = PNG
 9 = GIF
10 = leave decision for later
11 = suppress output to file
/
```

Running the Plot Programs II (cont.)

Band Structure: plbnd.x/plbnd.run

Interaction with the Program (First Run)

```
...
 Portrait (P), landscape (L) or encapsulated postscript plot (E, default)?
/
 Enter title:
/

 Please wait a moment: I'm reading rest of file BNDE.
 Timing for   39 points out of  398:     0.00000 sec.

 Energies in Rydberg (F) or eV (T, default)?
/
 Energies relative to MTZ (0) or EFermi (F, default)?
/
 Energies connected by lines (T) (default F)?
/

 Ebot =    -9.755217 eV , Etop =    28.178791 eV  relative to EF
 Emin =   -10.000000 eV , Emax =     6.000000 eV  relative to EF
 Enter new Emin, Emax to change these defaults:
/
 task  1, total       :  cpu time:     0.04400 sec

 ASW-2.3, program PLBND ended on asterix at Fri, 02 Feb 2007, 18:28:37.
```

Running the Plot Programs II (cont.)

Band Structure: plbnd.x/plbnd.run

The PLIB file

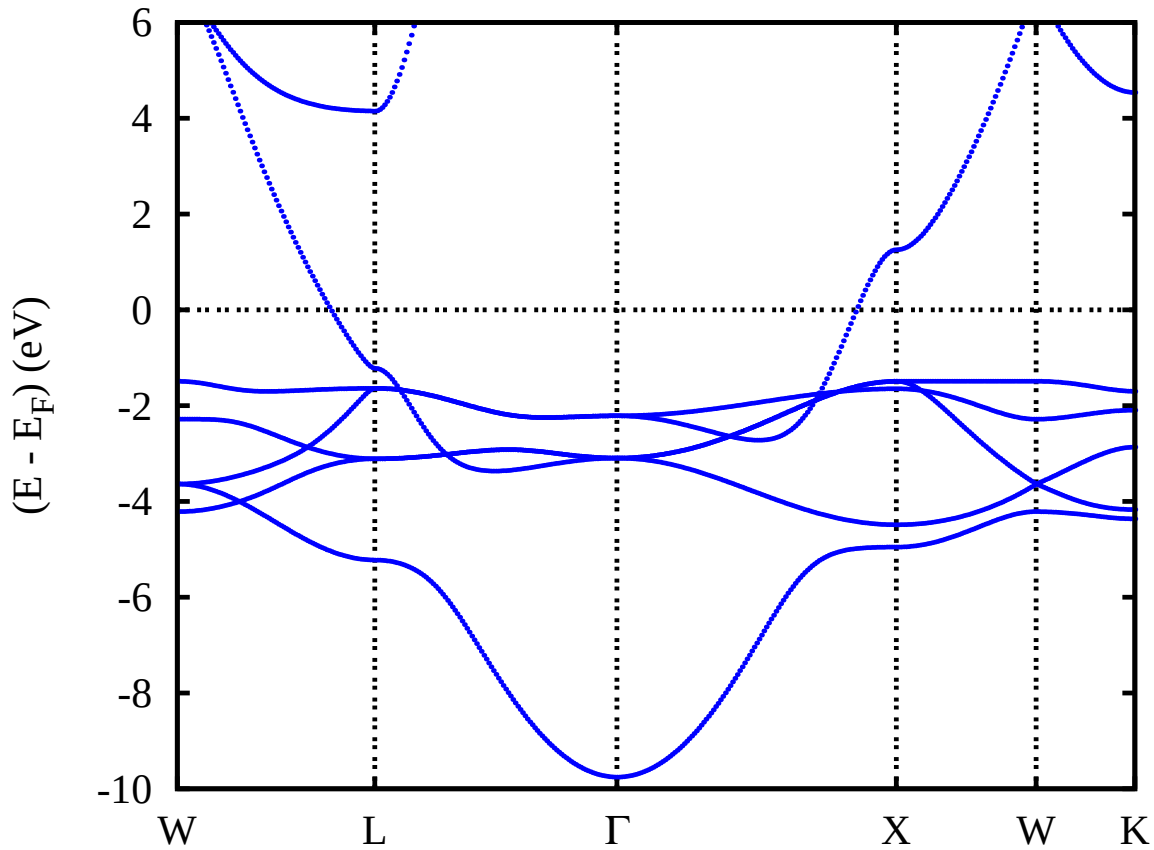
```
 1                          / Terminal type
 1                          / Output device
E                           / Portrait (P), landscape (L) or EPS (E, default)?
Cu fcc
T                           / Rydberg (F) or eV (T, default)?
F                           / E-MTZ (0) or E-EF (F, default)?
F                           / Lines (T) (default F)?
      -10.000000
        6.000000            / Emin, Emax
```

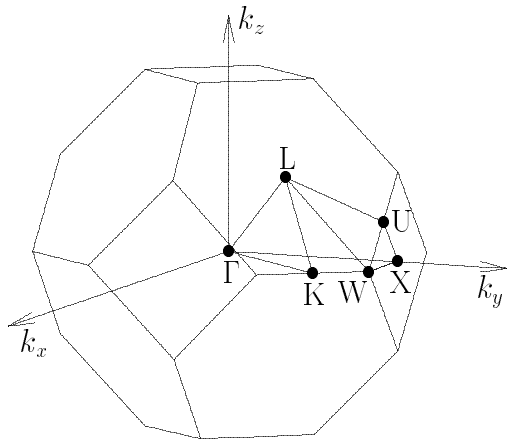
Interaction with the Program (Second Run)

- plbnd.run < PLIB or
- plbnd.x PLIB

Running the Plot Programs III

Band Structure: plbnd.x/plbnd.run





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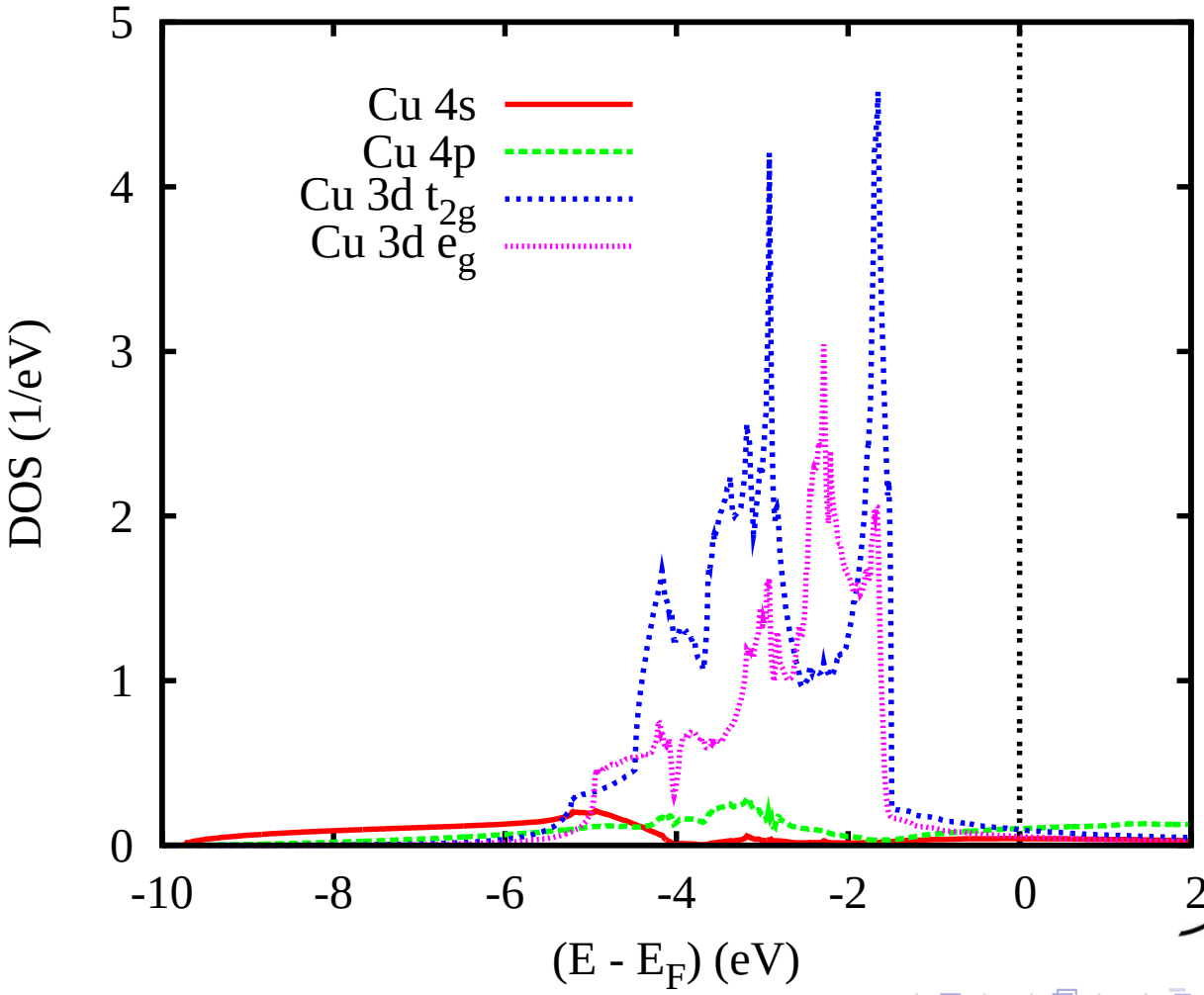
Running the Plot Programs IV

Densities of States: pldos.x/pldos.run



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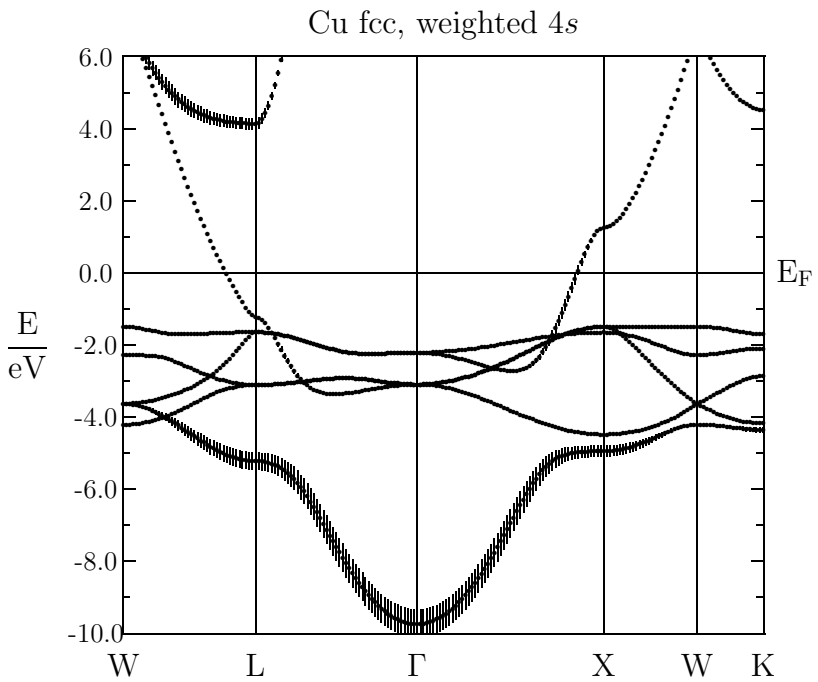
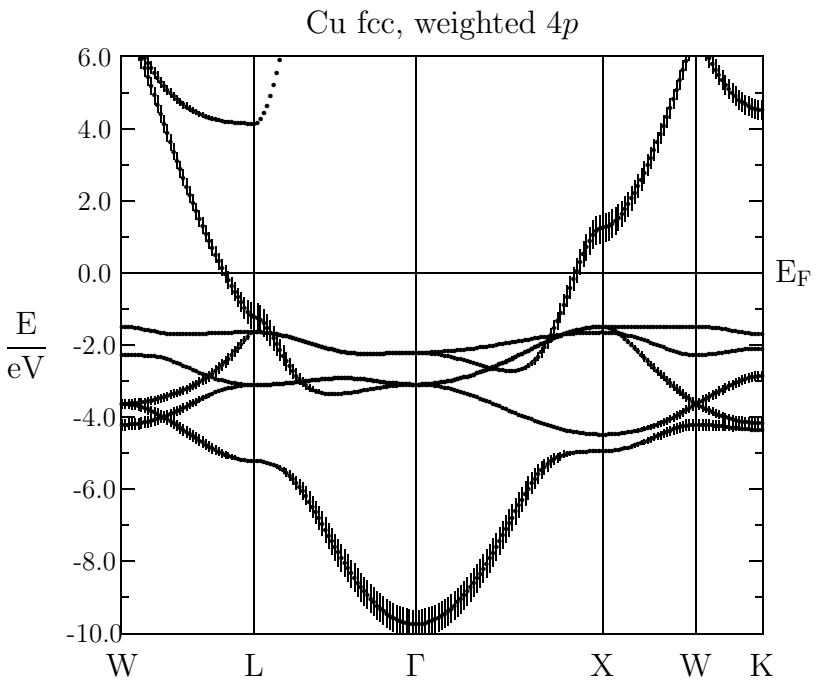
Running the Plot Programs V

Weighted Band Structure: plbnd.x/plbnd.run





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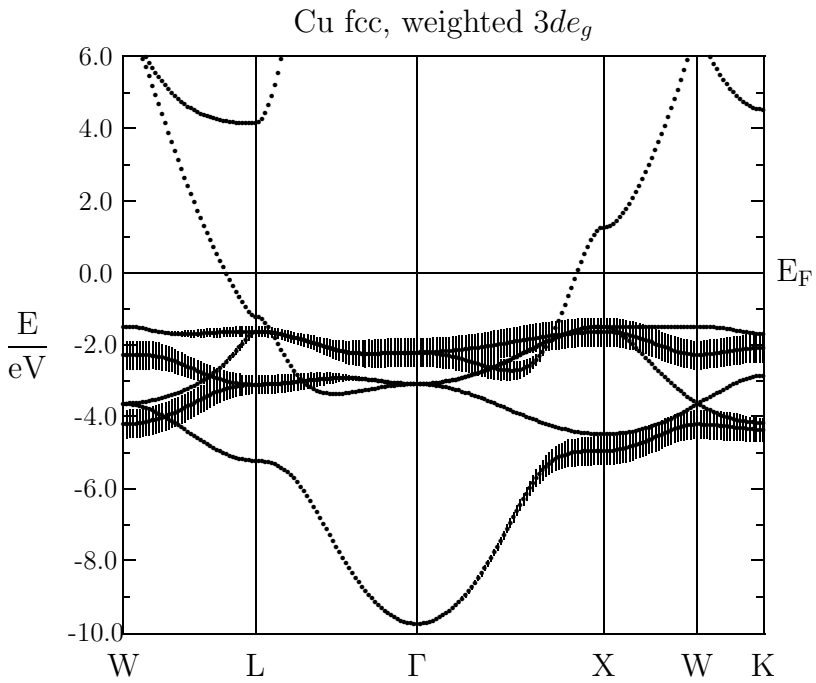
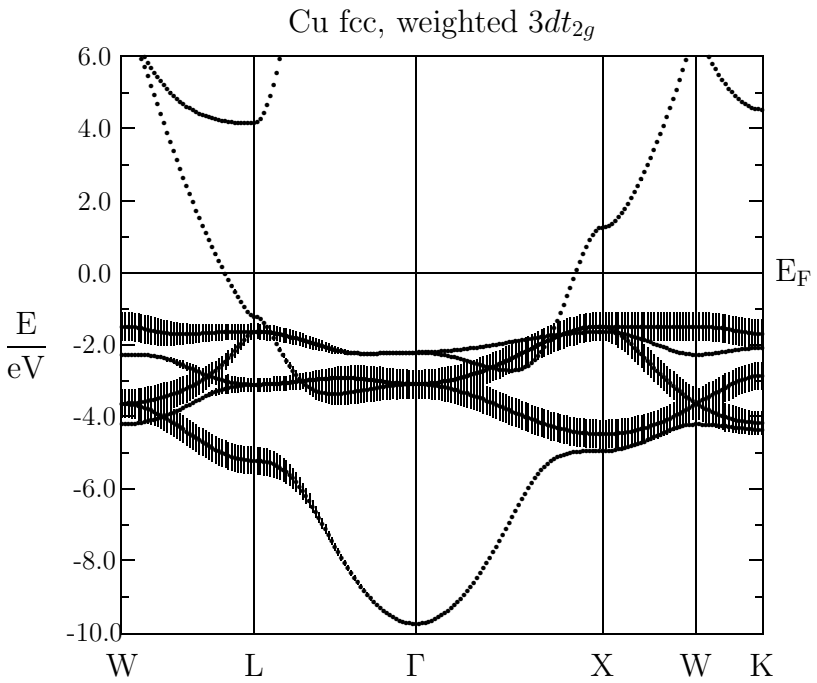
Running the Plot Programs VI

Weighted Band Structure: plbnd.x/plbnd.run





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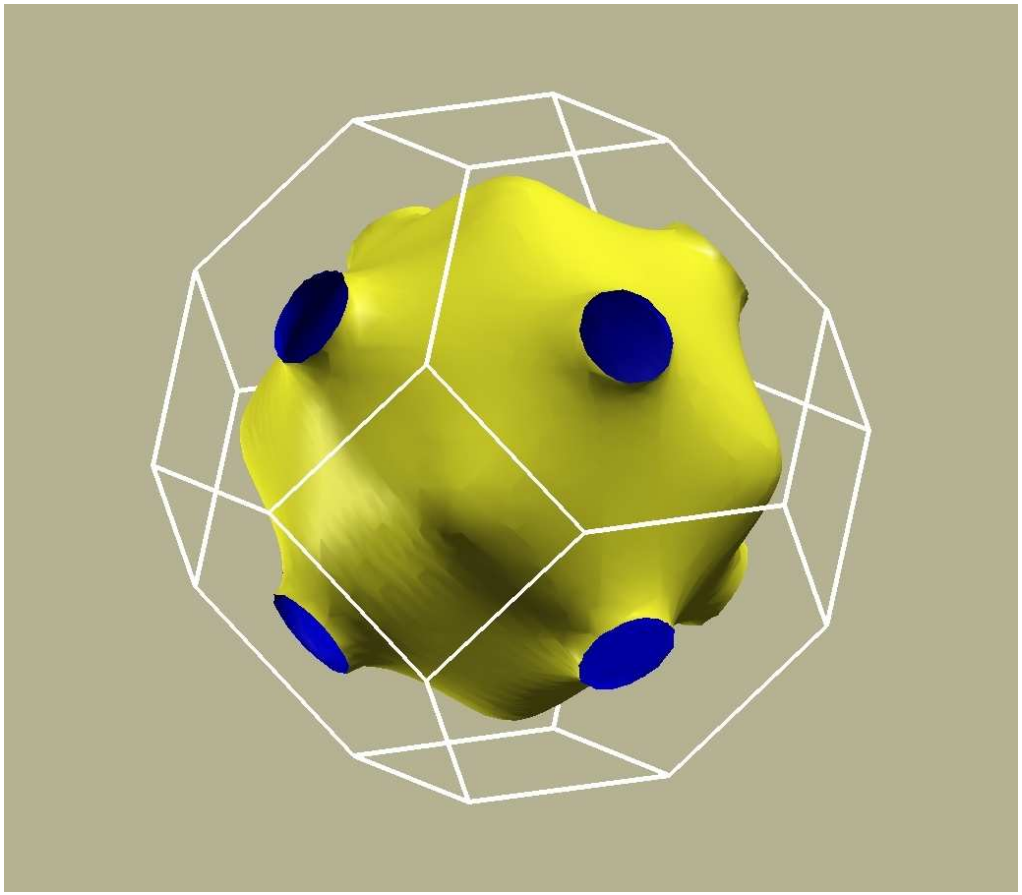
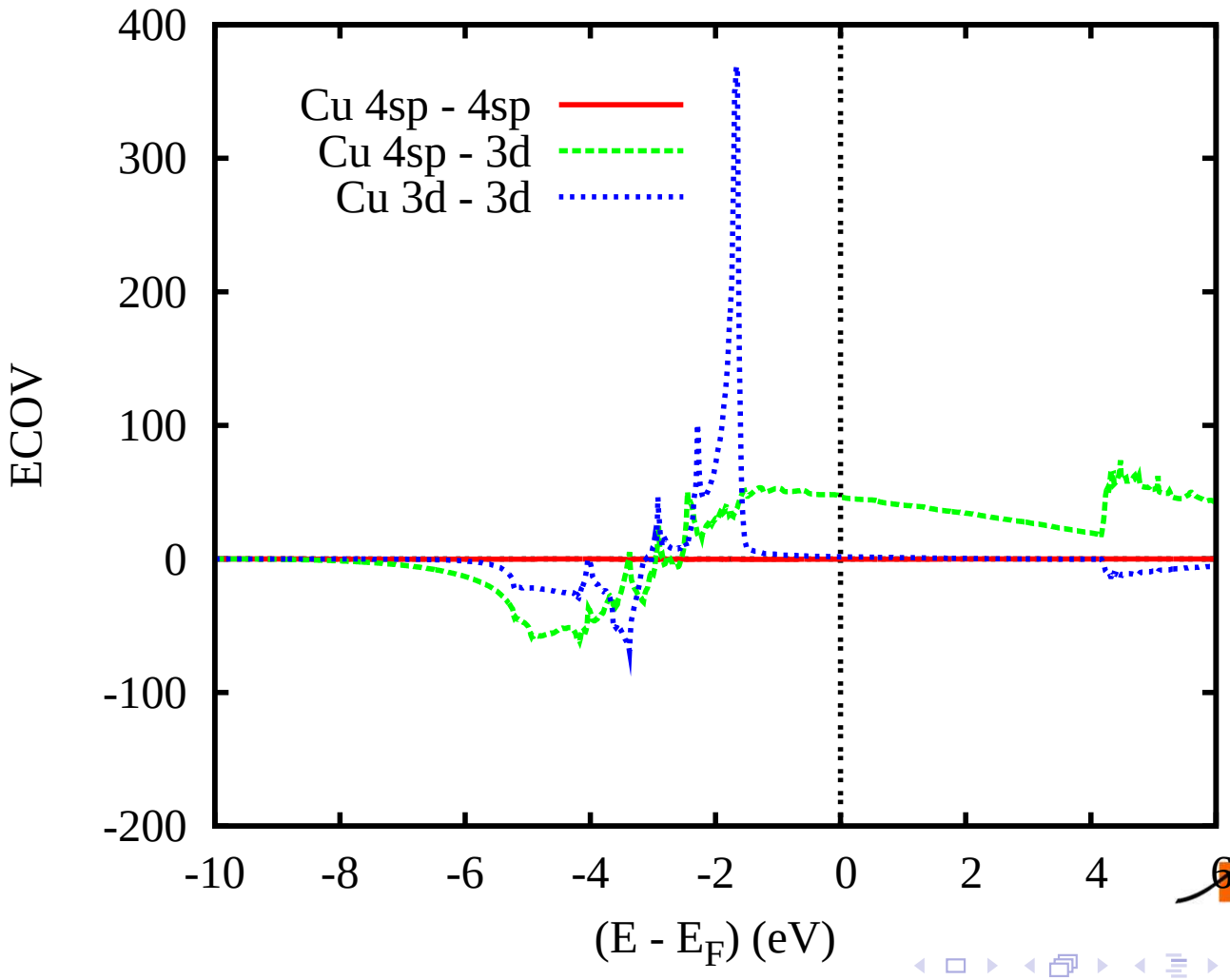
Running the Plot Programs VII

Fermi Surface: plfrm.x



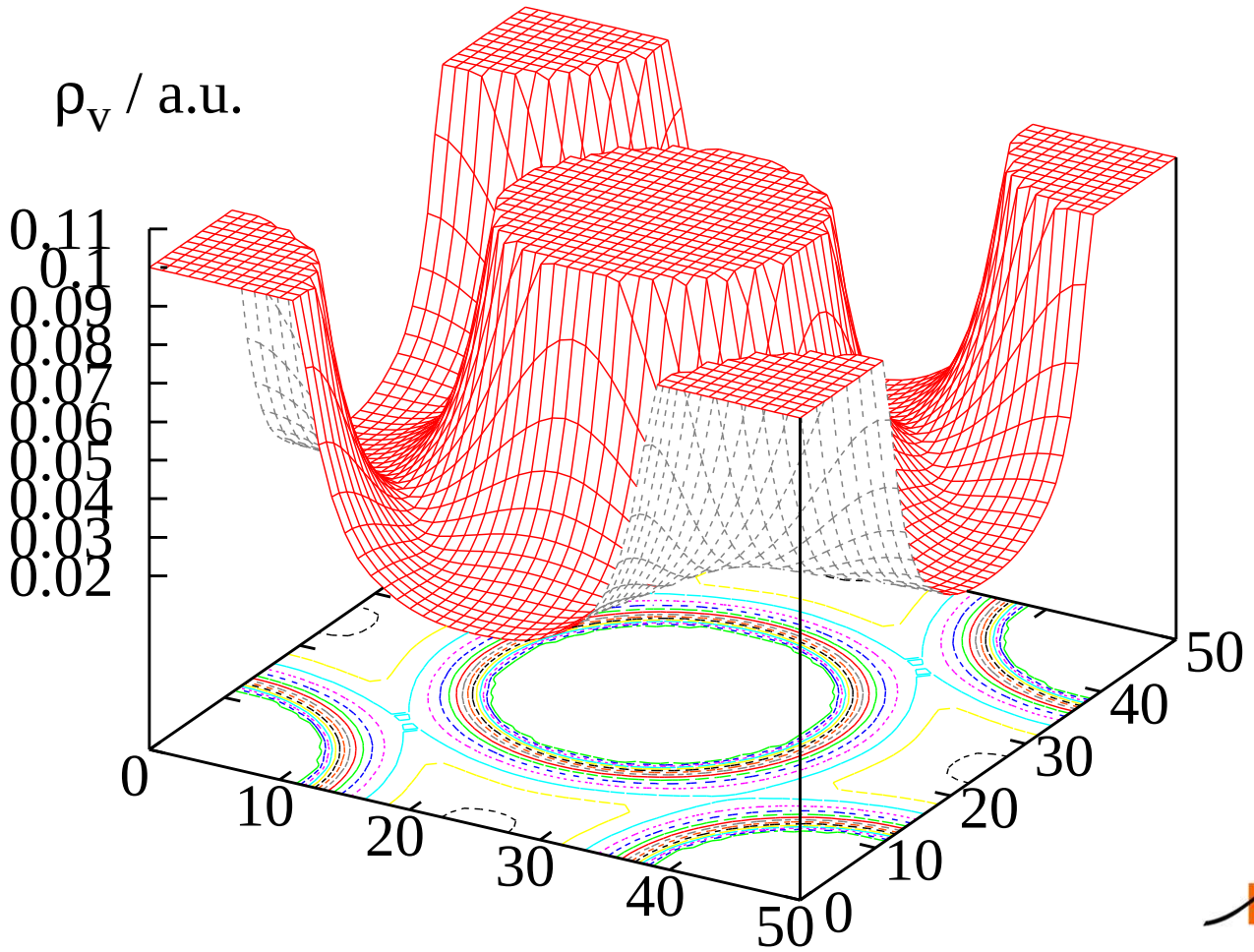
Running the Plot Programs VIII

Covalence Energy (COOP, COHP): plcop.x/plcop.run



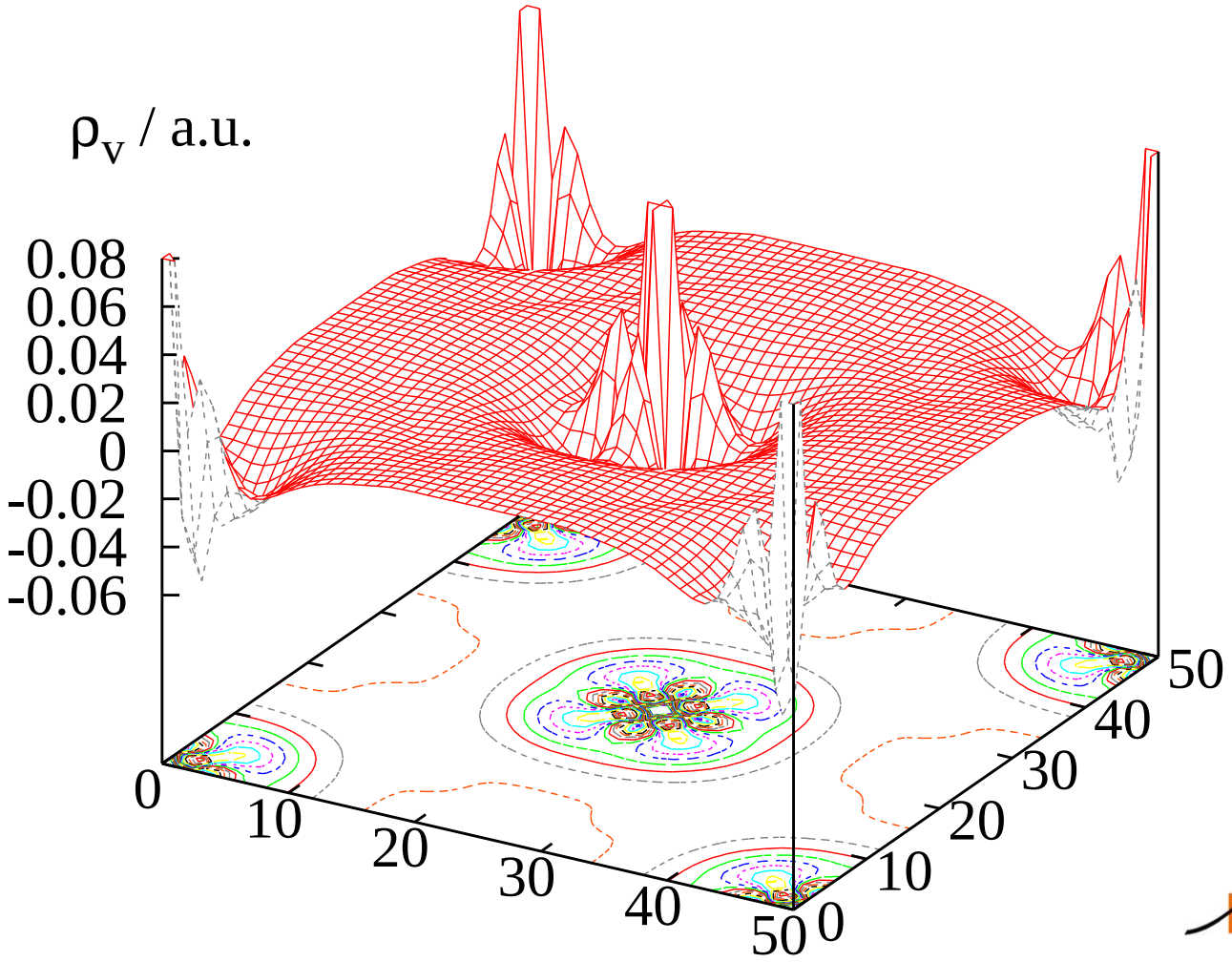
Running the Plot Programs IX

Valence Electron Density: plrho.x/plrho.run



Running the Plot Programs X

Valence Electron Density: plrho.x/plrho.run



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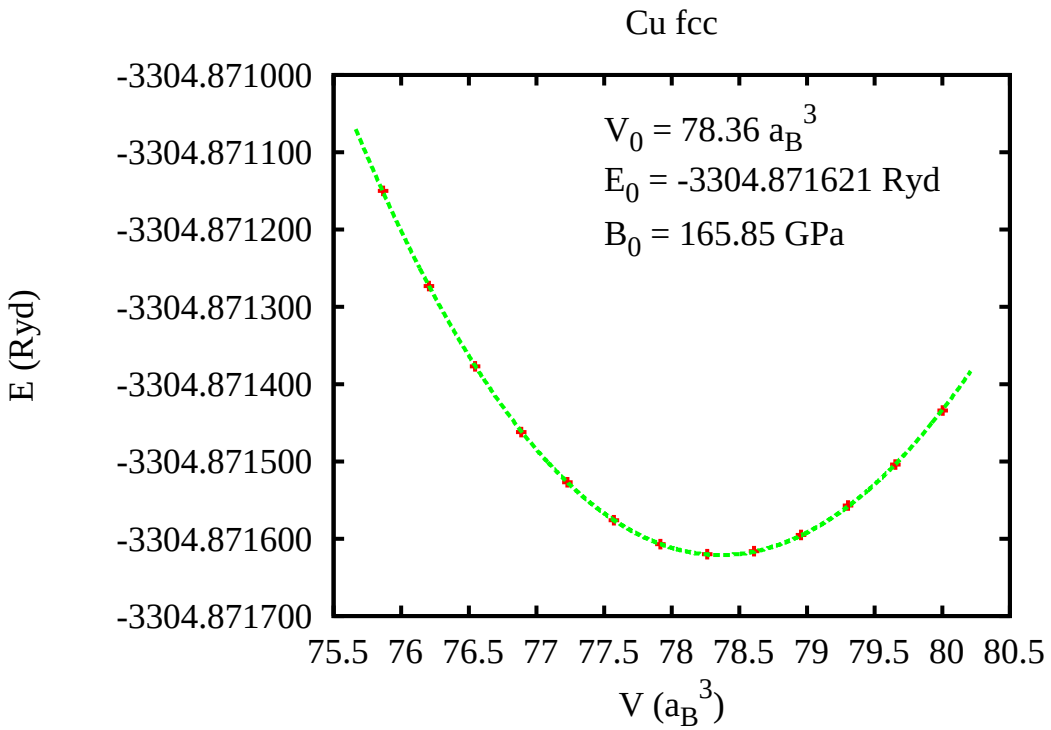
Running the Plot Programs XI

Total Energy and Bulk Modulus: plblk.x



Theory/Exp.

$a = 6.79/6.81 a_B$

$E_{coh} = 321/256 mRyd$

$B_0 = 166/137 GPa$

Summary Cu
New files

Output of main programs

outscf, outbnd, outdos

Copy of CTRL

CBAK

Atomic file

CU

Echo files of plot programs

PLI*

Output files of main programs $\Longrightarrow$ input to the plot routines

BNDE, BNDV, DOS, COOP, FERM, FREE, OPT, RHO, STRU, STRX

Output files of plot programs

blk.ps, bnd.ps, dos.ps, coop.ps, ferm.ps, opt.ps, rho.ps

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Outline

Preparing for the Application

Create a directory tree

- create e.g. /home/user/appl/be (beryllium)
- create e.g. /home/user/appl/be/nm (spin-deg. calcs.)

A minimum CTRL file

```
HEADER  Be hcp
VERSION ASW-2.3
STRUC   ALAT=4.321048 CLAT=6.771078 GAMMA=120.0
CLASS   ATOM=BE Z= 4
SITE    CARTP=F
        ATOM=BE POS= 0.333333 -0.333333  0.250000
        ATOM=BE POS=-0.333333  0.333333 -0.250000
```

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CLASS    ATOM=BE Z= 4
SITE     CARTP=F
         ATOM=BE POS= 0.333333 -0.333333  0.250000
         ATOM=BE POS=-0.333333  0.333333 -0.250000
```

A Standard CTRL File I

```
HEADER  Be hcp
VERSION ASW-2.3
IO      HELP=F SHOW=T VERBOS=30 CLEAN=T
OPTIONS REL=T OVLCHK=T
STRUC   ALAT=4.321048 CLAT=6.771078 GAMMA=120.0 CNTR=P
CLASS   ATOM=BE Z= 4 R=2.35549765 LMXL=1 CONF=2 2 3
                QVAL= 2.0  0.0  0.0
SITE    CARTP=F
        ATOM=BE POS= 0.333333 -0.333333  0.250000
        ATOM=BE POS=-0.333333  0.333333 -0.250000
SYMGRP
ENVEL   EKAP=-0.015
BZSMP   NKBAB=6 BZINT=LTM EMIN=-0.5 EMAX=1.5 NDOS=1000
        NORD=5 WIDTH=0.02 SAVDOS=F SAVFERM=F SAVOPT=F
CHARGE  NETA=2 EETA=-1.0 -3.0 SAVRHO=F
CONTROL START= QUIT= FREE=F NITBND=99 CNVG=1.0D-08 CNVGET=1.0D-08
        NITATM=50 CNVGQA=1.0D-10
MIXING  NMIXB=5 BETAB=0.5 INCBB=T NMIXA=5 BETAA=0.5
...
```

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A Standard CTRL File II

```
SYMLIN   NPAN=7 NPTS=400 CARTE=F
         LABEL=g ENDPT= 0.000000  0.000000  0.000000
         LABEL=M ENDPT= 0.000000  0.500000  0.000000
         LABEL=K ENDPT=-0.333333  0.666667  0.000000
         LABEL=g ENDPT= 0.000000  0.000000  0.000000
         LABEL=A ENDPT= 0.000000  0.000000  0.500000
         LABEL=L ENDPT= 0.000000  0.500000  0.500000
         LABEL=H ENDPT=-0.333333  0.666667  0.500000
         LABEL=A ENDPT= 0.000000  0.000000  0.500000
PLOT     CARTV=F
         ORIGIN= 0.65 0.35 0.0
         RPLOT1=-1.0  1.0  0.0
         RPLOT2= 0.0  0.0  1.0
         RPLOT3= 1.0  1.0  0.0
         NPDIV1=100 NPDIV2=100
```

Running the Main Programs

Complete set of calculations: mnall.x

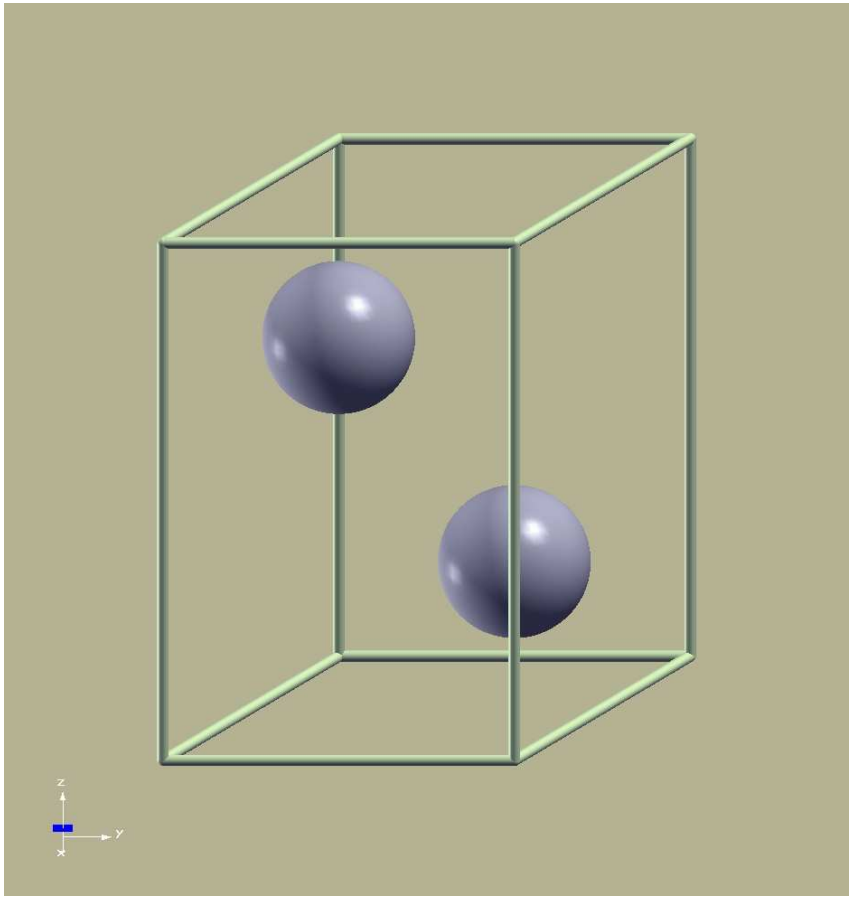
scf-cycle + band structure + DOS, COOP, Fermi surface

Summary Generated by Shell Script monic

```
ASW-2.3, program MNSCF started on asterix at Thu, 18 Jan 2007, 11:42:57.
Calculation converged after   6 iteration(s).
                      Start of Iteration    6
   819 irreducible k-points generated from   15300 ( 30, 30, 17).
           Fermi energy - MTZ =     0.863599 Ryd
The system is a metal:
           DOS at Fermi energy:     1.377990 1/Ryd
           Gamma * (f.u./cell):     0.238733 mJ/(mole*K**2)
Mean-square residual:                   0.717071D-23
Total free atom energies     :    -57.800152 Ryd
Total variational energy     :    -58.371920 Ryd
Cohesive energy              :      0.571767 Ryd
 qdiff =       0.00000000  <        0.00000001
 ediff =       0.00000001  <        0.00000001
ASW-2.3, program MNSCF ended on asterix at Thu, 18 Jan 2007, 11:44:12.
```

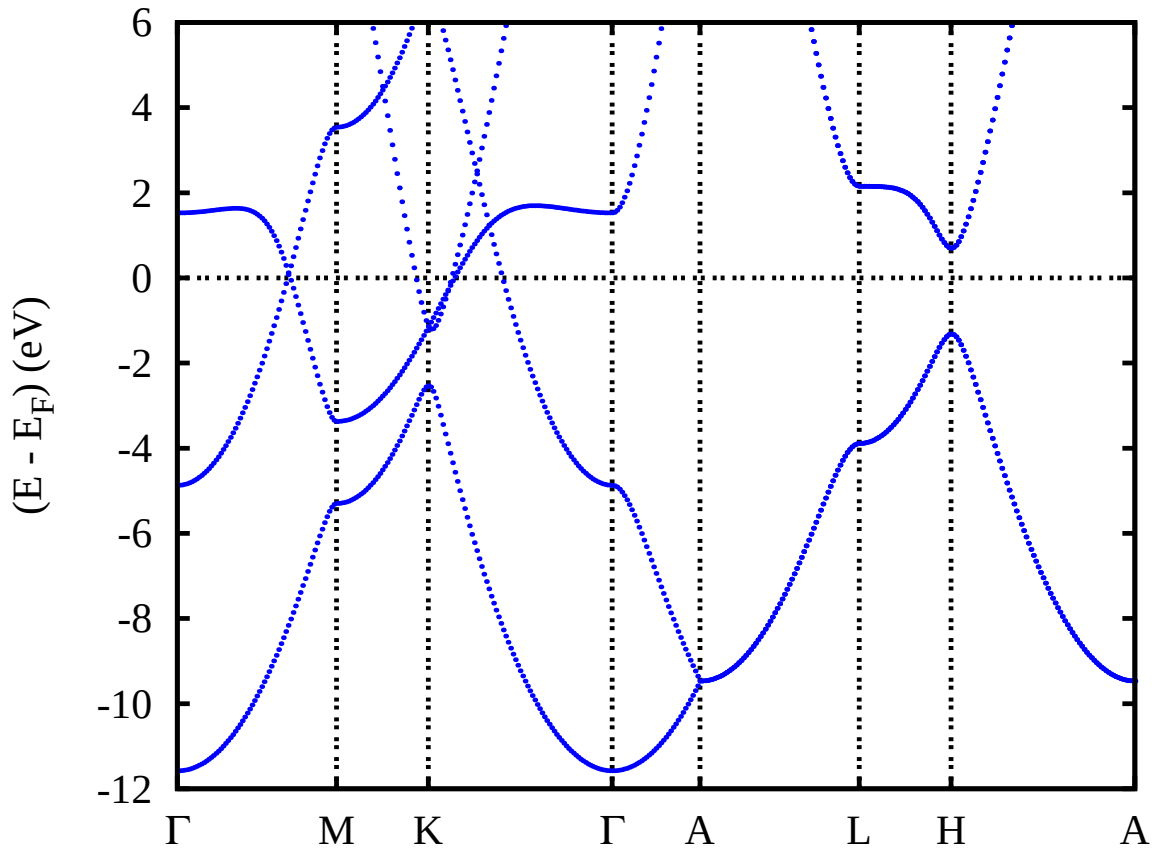
Running the Plot Programs I

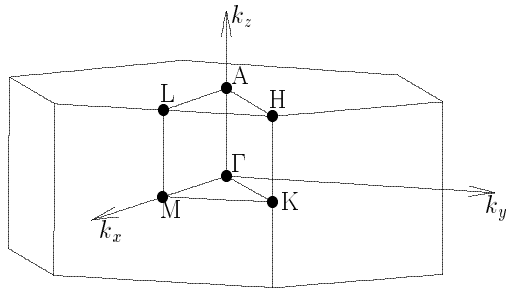
Crystal Structure: plxcr.x



Running the Plot Programs II

Band Structure: plbnd.x/plbnd.run





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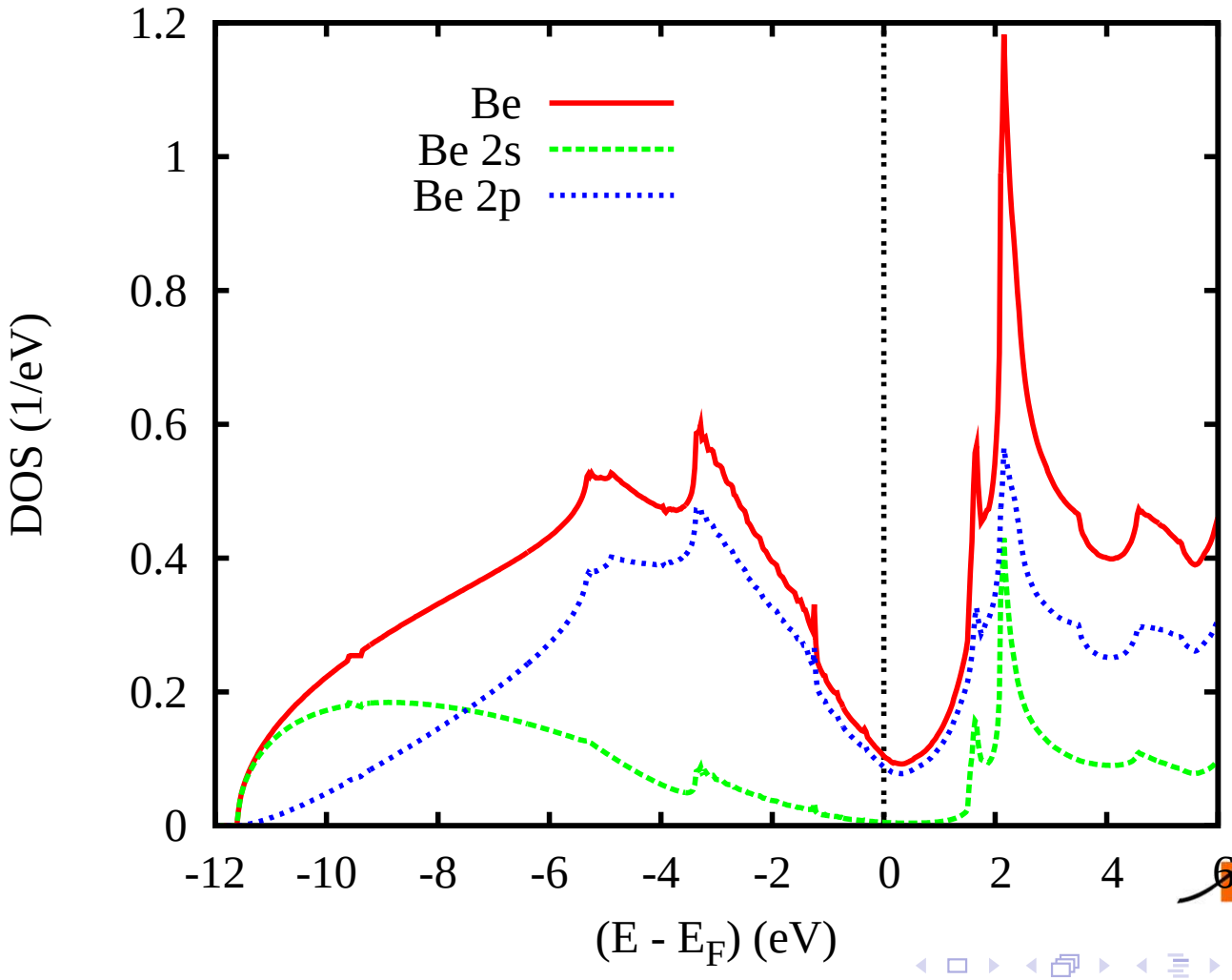
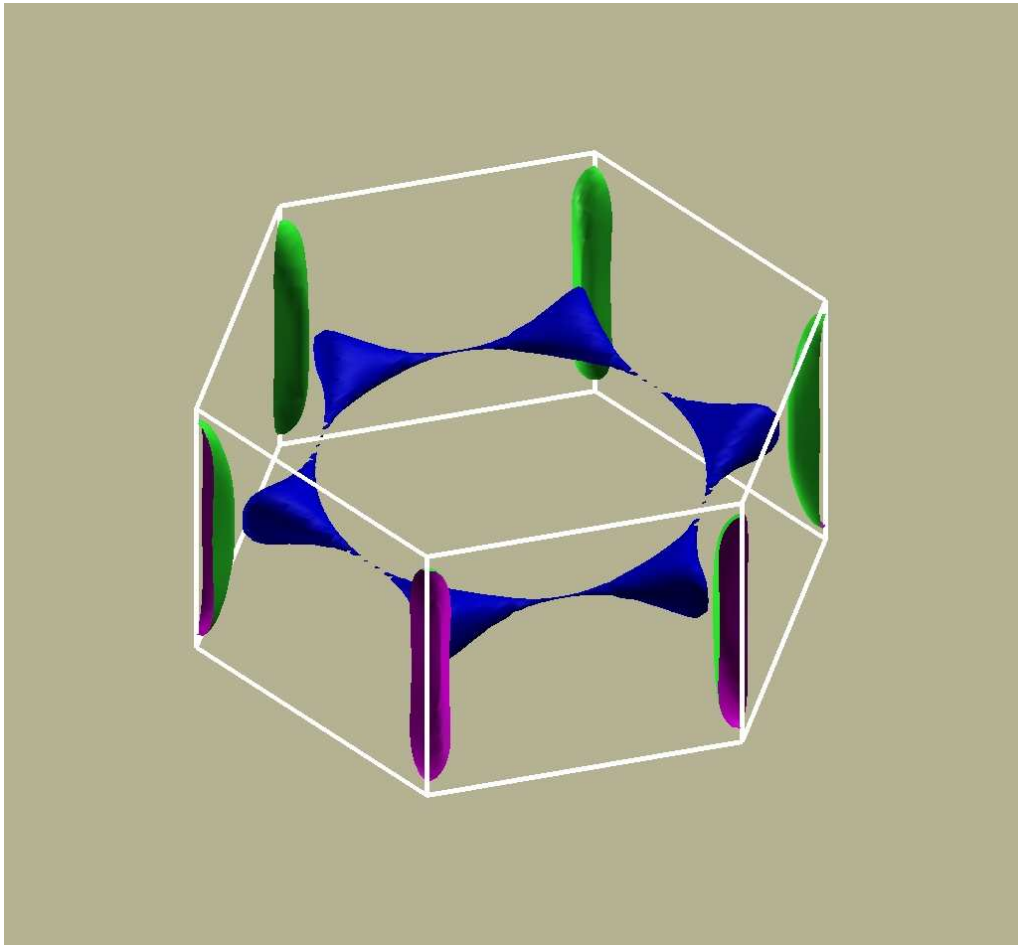
Running the Plot Programs III

Densities of States: pldos.x/pldos.run



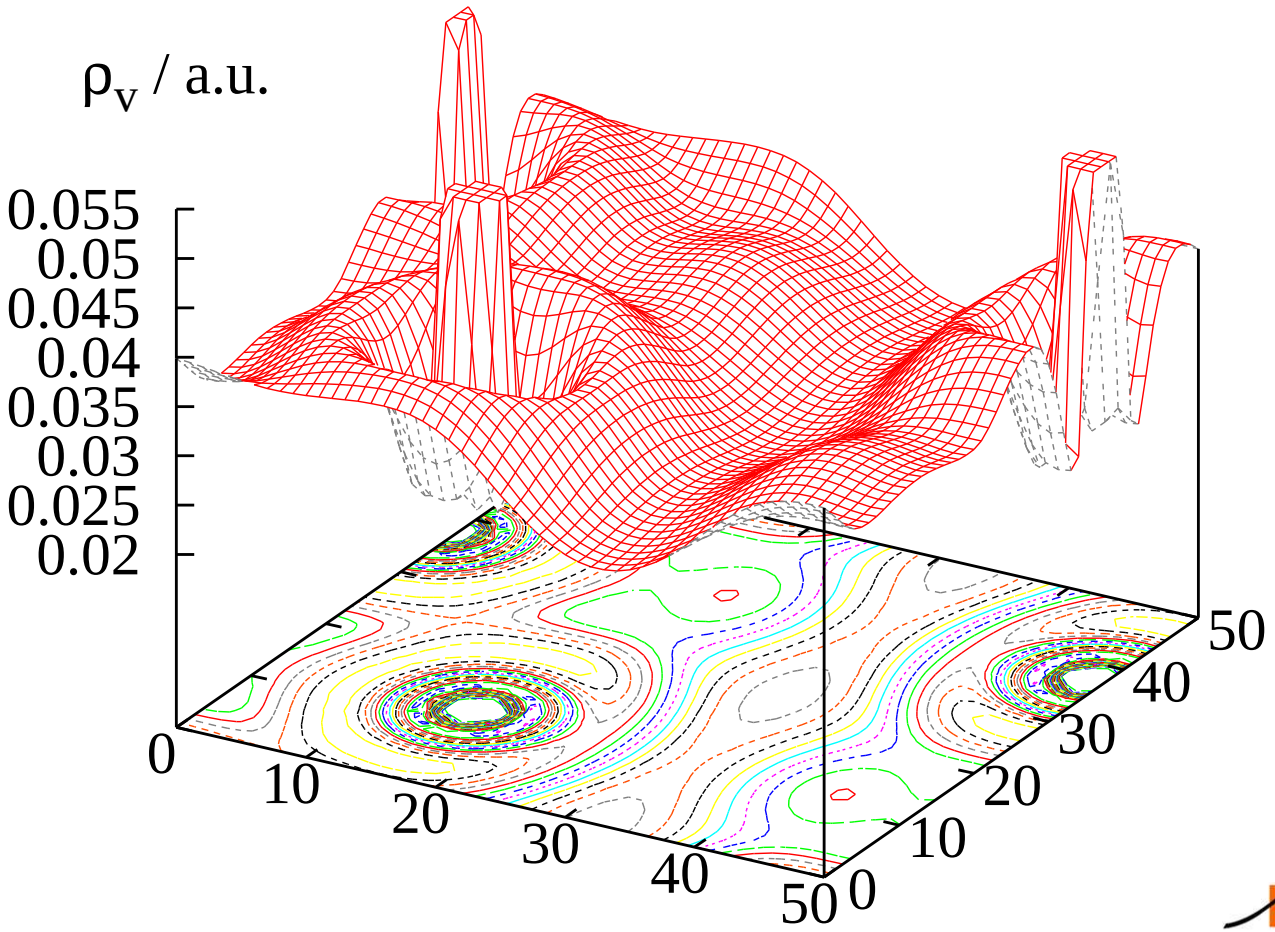
Running the Plot Programs IV

Fermi Surface: plfrm.x



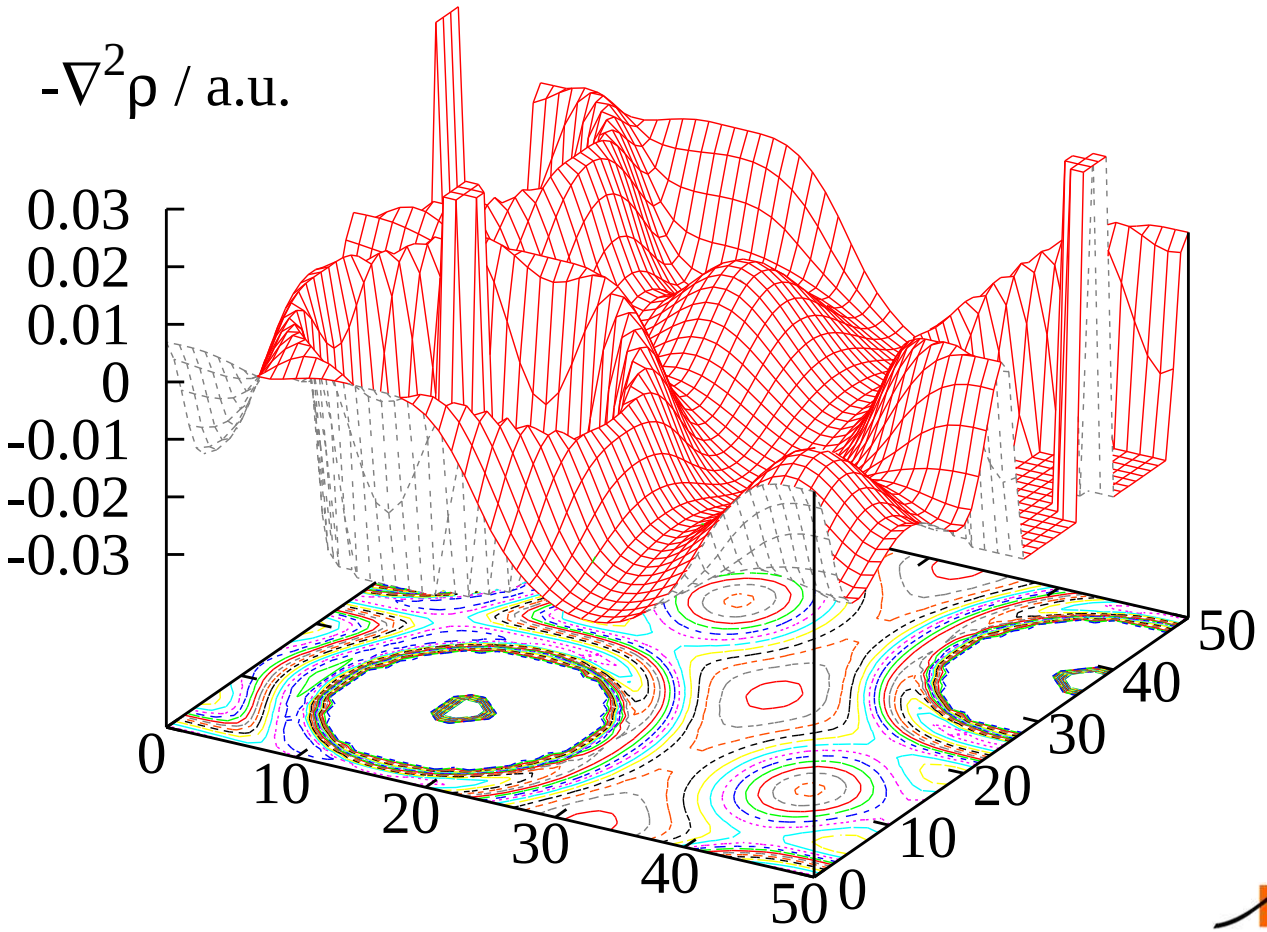
Running the Plot Programs V

Valence Electron Density: plrho.x/plrho.run



Running the Plot Programs VI

Laplacian of Electron Density: plrho.x/plrho.run



INSTITUT für PHYSIK
UNIVERSITÄT AUGSBURG

Summary

Preparation

- generate (copy/edit or write) CTRL file

Complete set of calculations: mnall.x

- self-consistent field calculation (mnscf.run)
- band structure (mnbnd.run)
- DOS, COOP, Fermi surface (mnscf.run)

Analyze results

- check output (use monic or edit)
- plot band structure, DOS, COOP, FS, ρ, $-\nabla^2\rho$, ...
- use PLI* files

Further Reading I

V. Eyert
The Augmented Spherical Wave Method — An Extended User Guide.