HiLAPW – Practice & Tips

Some Practical Points @ CMD Cluster Systems

- **HiLAPW**
  - **Specifications**
  - **Executables**
- **GETTING STARTED 1, 2, & 3**
- **JOB SUBMISSION**
- **OUTPUT GRAPH**
- **LAcopy**

HiLAPW – Specifications

- 100% Original Code
  - LAPW basis functions
  - LSDA, GGA, Hubbard-*U*
  - Scalar relativity, Spin-orbit coupling
  - All-electron SCF full-potential scheme
  - BZ integration with tetrahedron method
  - Group theory
  - Crystal structure & element data base
  - Total E, forces, DOS, ...
  - XAS, Berry phase, ...

optional functionalities

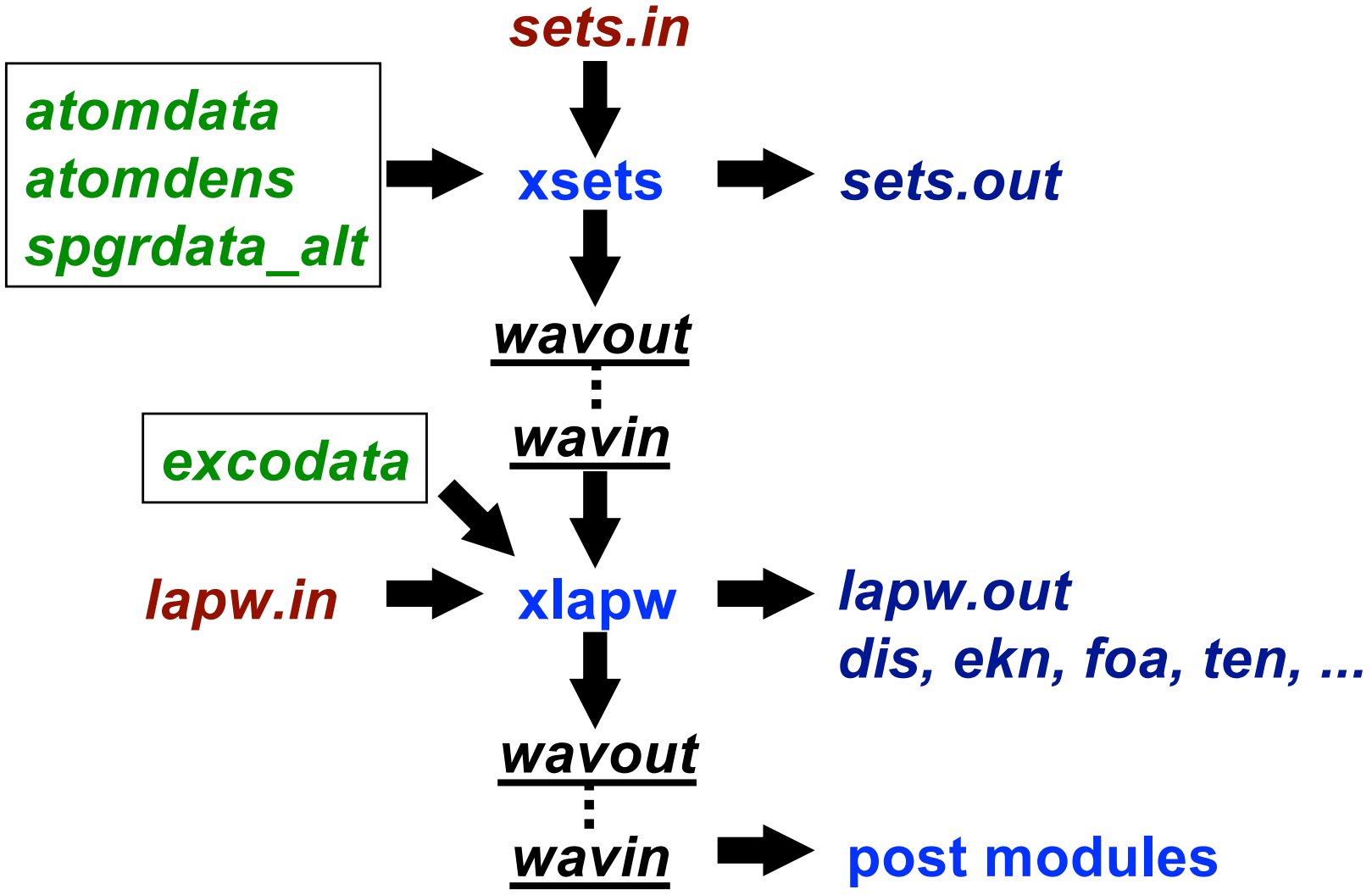
HiLAPW – Specifications

- 100% Original Code
  - Modular executables
  - Fortran90
    - dynamical memory allocation
  - BLAS and LAPACK libraries
  - PSP : postscript plot routines
  - MPI parallelization

HiLAPW - Executables

executables	contents
xsets	initialization
xlapw	SCF calculation
xdoss	DOS
xnewa	modification k-point data
xwbox	electron density on 3D mesh
xpbox	potential on 3D mesh
xspin	addition of spin polarization
xsymm	irreducible representation extract
xrept	rearrangement of eigenvalues

HiLAPW - Executables



*:spgrdata_alt: spgrdata is used in old versions

GETTING STARTED 1

- Login Linux server with “ssh –Y rl”
- Copy the HiLAPW package onto your home directory

```
# cd
# tar zxvf ~teac03/hilapw.tar.gz
```

prompt

My home directory:
Some other files can be obtained here
as I shall show it later.

GETTING STARTED 2

- Set PATH and HiLAPW link

```
# cd hilapw
# ./configure.sh
```

- Activate the setting (only when you update)

```
# source ~/.bashrc          ← if bash is used
# source ~/.cshrc           ← if csh or tcsh is used

# echo $PATH                ← to check
```

GETTING STARTED 3

- **Create working directories and get example data**

  # cd

  # mkdir hilapw1

  # cd hilapw1

  # mkdir Cu

  # cd Cu

  # tar xvf ~/hilapw/data/Cu.tar

Please keep the directory ~/hilapw you installed package untouched.

RUNS

- fcc Cu
  - total and partial density of states
  - band structure
- Ferromagnetic bcc Fe
  - total and partial density of states
  - band structure
- Diamond-type Si
  - total energy
- Ferroelectrics
  - electric polarization
  - structure optimization

fully prepared

JOB SUBMISSION

- **Batch Job Commands**

  # qsub JOB.sh — **submit a batch job**

  # qstat — **show the job status with ID**

  # qdel "job-ID" — **delete the job from queue**

  – **Script-file: JOB.sh**

```
#$ -S /bin/bash
#$ -cwd
#$ -pe smp 6
#$ -N HiLAPW
./JOB-SCF
```

OUTPUT GRAPH

- Get a post-script graphic file

total DOS plot

PSP < psp_tdos > tdos.ps

- PS file processes

to view

gs tdos.ps

evince tdos.ps

to convert to pdf format

ps2pdf tdos.ps

to convert to eps format

ps2epsi tdos.ps

LAcopy

- The executable "xlapw" is often run several times, outputting the same files such as dis, ekn, foa, lapw.out, ten, wavout, and etc.
- To (re)name the files generated at each xlapw run, a command "LAcopy" can be used.

LAcopy A1

ekn → eknA1

foa → foaA1

lapw.out → outA1

ten → tenA1

wavout → wavA1 and wavin

Don't use it before the job ends !

Total Energy Calculation of Si

1st STEP

```
# cd hilapw1
# mkdir Si
# cd Si
# tar xvf ~/hilapw/data/Si.tar
# qsub JOB.sh

# ./GET-TEN > TEN
# xefitm < TEN > fit_TEN
# tail -103 fit_TEN > TEN2
# PSP < psp_TEN > TEN.ps
```

Total Energy Calculation of Si

1st STEP

cd hilapw1

mkdir Si

cd Si

tar xvf ~/hilapw/data/Si.tar

qsub JOB.sh

./GET-TEN > TEN

xefitm < TEN > fit_TEN

tail -103 fit_TEN > TEN2

PSP < psp_TEN > TEN.ps

2nd STEP

vi excodata

LDA MJW → GGA PBE

vi JOB.sh

./JOB-TEN → ./JOB-TEN_G

qsub JOB.sh

./GET-TEN_G > TEN_G

xefitm < TEN_G > fit_TEN_G

tail -103 fit_TEN_G > TEN2_G

PSP < psp_TEN_G > TEN_G.ps

gs TEN_G.ps