

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
- **Manuals and some useful data**
 - www.cmp.sanken.osaka-u.ac.jp/~oguchi/HiLAPW/

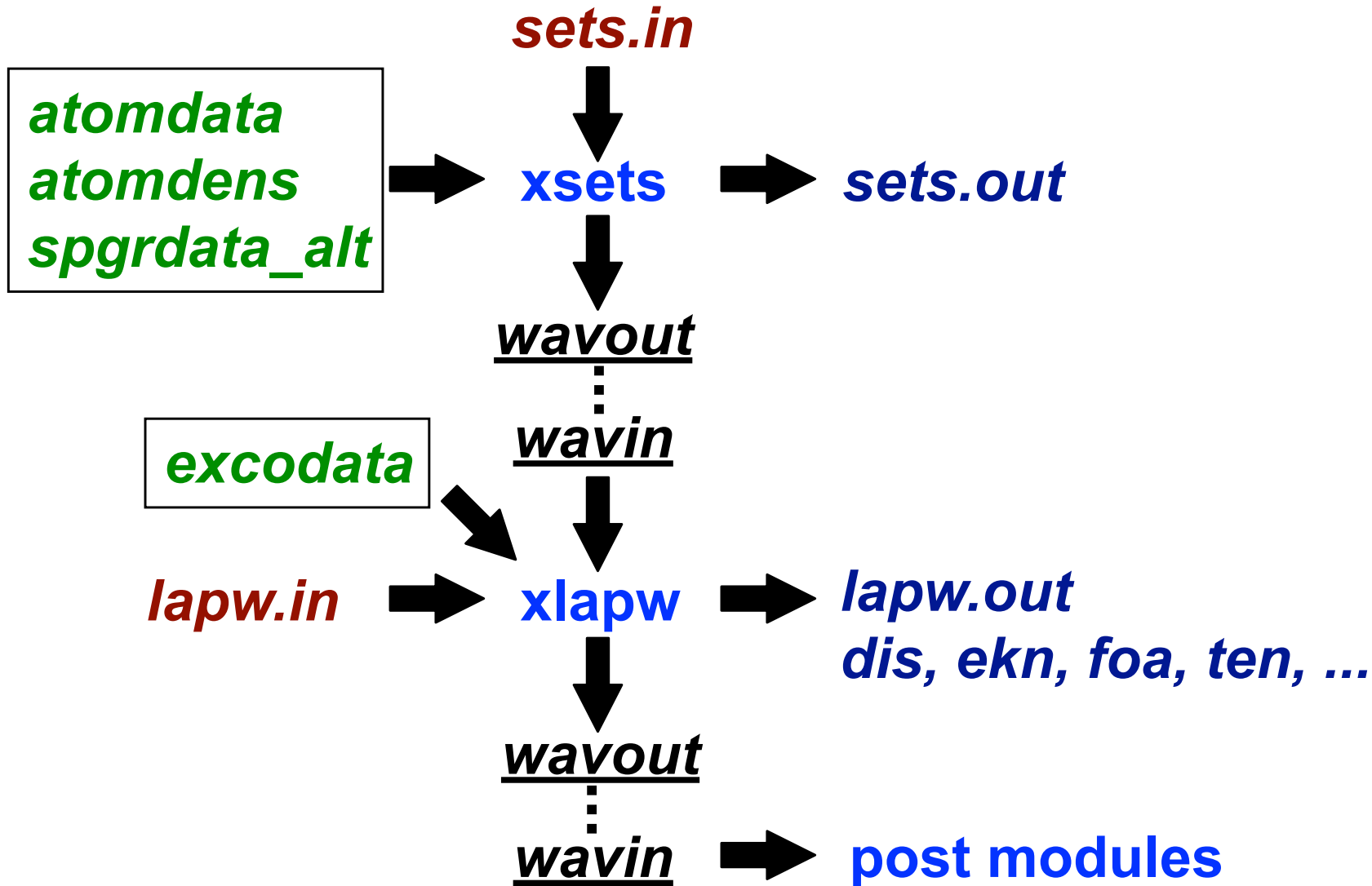


HiLAPW - Executables



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 CMD Machine

- For Advanced Course

- ```
ssh -Y userid@rl.phys.sci.osaka-u.ac.jp
```

- For Beginners Course

- ```
# ssh -Y userid@cmd2.phys.sci.osaka-u.ac.jp
```

- Copy the HiLAPW package onto your home directory

- ```
cd
```

- ```
# cp ~teac03/hilapw.tar.gz .
```

- Extract the package

- ```
tar zxvf hilapw.tar.gz
```

# GETTING STARTED 2



- **Set PATH and HiLAPW link**

```
cd hilapw
```

```
./configure.sh
```

- **Activate the setting**

```
source ~/.cshrc
```

← **when csh or tcsh is used**

```
source ~/.bashrc
```

← **when bash is used**



# GETTING STARTED 3

- **Get example data**

```
cd
```

```
mkdir hilapw1
```

```
cd hilapw1
```

```
mkdir Cu
```

```
cd Cu
```

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



# JOB SUBMISSION



- **Batch Job Commands**

**# qsub JOB**

**submit a batch job**

**# qstat**

**show the job status**

**# 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 PS file**

**total DOS plot**

```
PSP < psp_tdos > tdos.ps
```

- **PS file processes**

**to view**

```
gs tdos.ps
```

```
evince dos.ps
```

**to get pdf file**

```
ps2pdf tdos.ps
```

**to get eps file**

```
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 !**