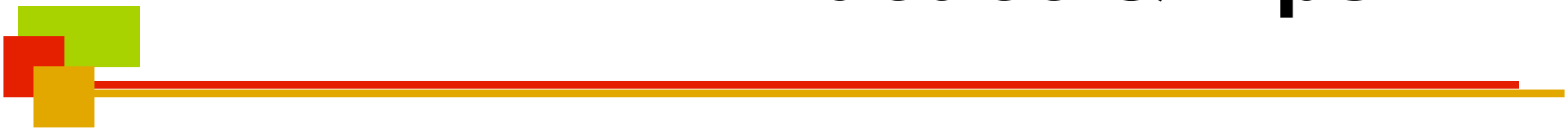
HiLAPW – Practice & Tips



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, dielectric function, ...

optional functionalities

HiLAPW – Specifications

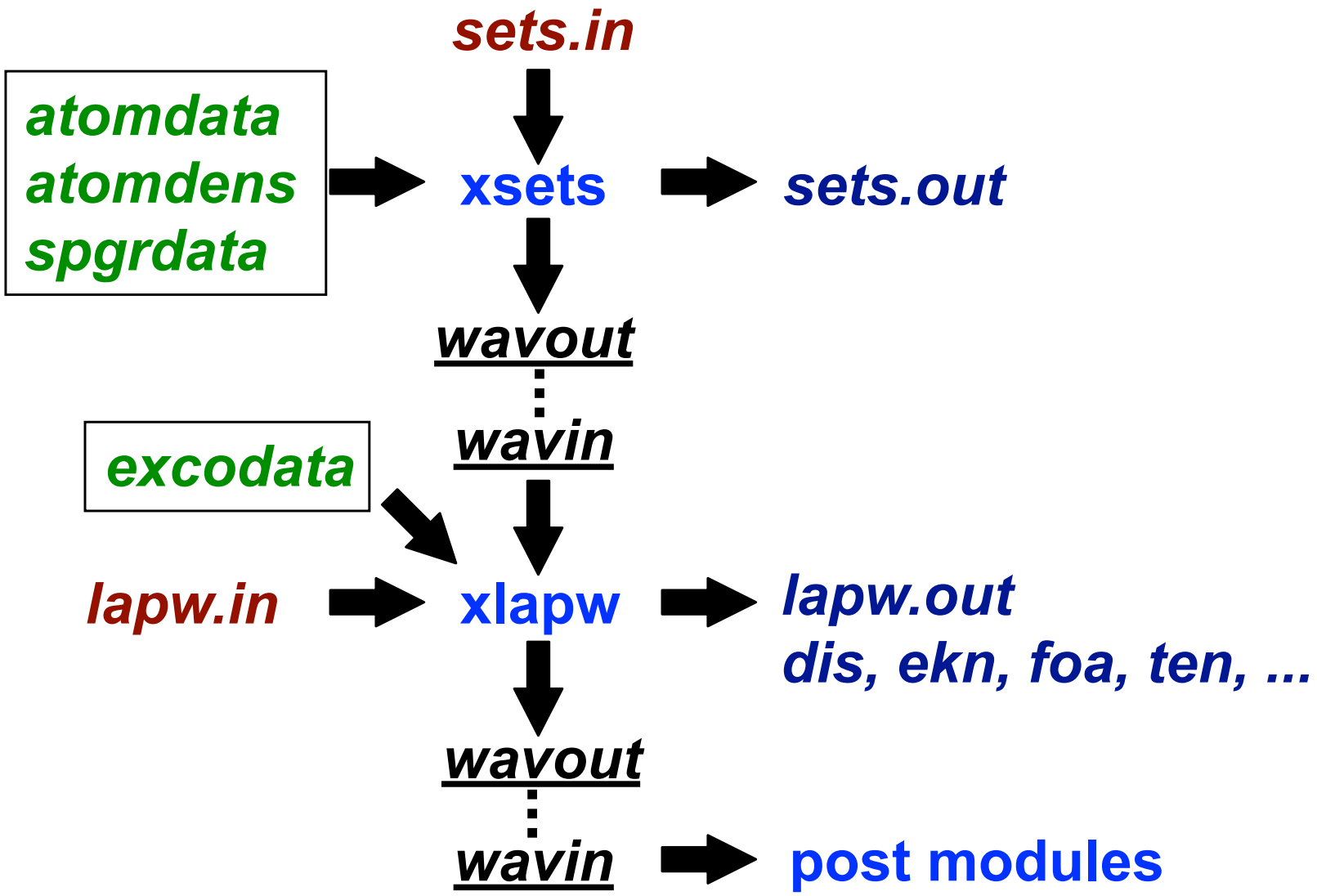
- 100% Original Code
  - Modular executables
  - Fortran90
    - dynamical memory allocation
  - BLAS and LAPACK libraries
  - PSP : postscript plot routines
  - MPI parallelization

- 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



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_1.13_tar.gz .

  14
- Extract the package

  # tar zxvf hilapw_1.13_tar.gz

  14

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

  # getdata

  # 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**

```
#!/bin/csh
#$ -cwd
#$ -N HiLAPW
cd ~/hilapw1/Cu
./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 !