General LAPW Notes

Compiling:

- Make fiel doesn't understand dependencies – erase objects files before recompiling.
- Parameter statements are contained in the 17 files: P1, P2, … P17.
- Make_maz made load subroutines that work better for GGA calculations.
- Use subroutines that end in .noessl.f for SUN's. CRAY version is different.

Running Code:

- It is necessary to set a "SCRATCH" variable in the UNIX system. For C-SHELL, use the setenv command to set SCRATCH. This variable should be set to a directory where scratch files can be placed during the running of the program.
- Be sure to remove any BRH files after any change in basis or substantial change in running.

File Names and Usage:

- ATOMCG = results of atomic calculation – needed when starting up for first run
- BRH1, BRH2 = Broyden files (erase to restart Broyden procedure).
- CDN1, CDN2, … = converged self-consistent decks (one for each iteraction).
  To restart the next set of calculations with one of these decks, rename the file to be CDN1.
- CORECG = scratch file (work space)
- EIG-files = scratch space [NOTE: erase these files before starting a run]
  NOTE: do one last iteration erasing these files to make sure run is converged with no funny business.
- INFILE = input file
- OUTFILE = redirect to /dev/null on UNIX systems
- INFO = real output file
- IOSTEP = scratch file
- PLFILE = dump file – contains charge density, etc. in binary – useful for plotting
- POT = scratch file
- QLMT = has eigenvalues
- RECIP = scratch file
- SPCGRP = symmetry file – must be copied or created
- WORK-files = work files
- fort43 = scratch file

General Comments:

- Local orbitals reduce dependency on linearization parameters.
- For compounds, sphere ratio = RKMAX ratio
  For example, 7 is good for simple metals and oxygen, 9 for transition metals, hence:
  $RMT_O / RMT_{Ba} = 7/9$
- Time for running ~ (# of plane waves)^3
  ~ $[RKMAX/(RMT)_{MIN}]^9(\Omega)^3$
- Whenever possible, always choose origin of unit cell to get inversion symmetry.
- Ultimate test of LAPW: change sphere radii slightly – do results depend on this?

LAPW Output:

- RNOT= gives first radial mesh point
- GKI GKJ GKK gives minimum box
  Note: however, input deck will always require an even number.
  This effects LOOSID etc in file P2.
- "USING LOCAL ORBITALS FOR L LE 2 ON ATOM 1"
  First line gives E_ℓ and second line $E_\ell^{(2)}$
- RMS values should always be 10^{-3} or 10^{-4} or calculation may be bad
  (except for GGA where it will always be less good, maybe 10^{-2}).
- "EXTENDED BASIS: NV, NVDIFF" gives basis size and number of local orbitals.
- "FERMI ENERGY IS" gives an estimate of the Fermi energy.
  "NEW FERMI ENERGY" gives the correct value (including temperature corrections) – use this one.
- Q(ATOM,L) values are only given for occupied states.
- TOTAL CHARGE only gives total valence charge.
- ELECTRONS LOST FROM CORE should be less than 0.02 or 0.03 per atom for a safe calculation.
- DISTANCE OF CHARGE DENSITIES should be less than 0.2 for convergence and less than 0.003 for forces.

$$\frac{\left[\int d^3r\left(\rho_{in}-\rho_{out}\right)^2\right]^{1/2}}{\Omega}$$

GGA:

- Need to increase FFT by one
  Interstitial region is problematic (not muffin-tin spheres)
  Make_maz may have better subroutines for GGA (perhaps more stable interpolation)
- GGA potential will never be as continuous as LDA due to noise from interstitial mesh.
- GGA will probably require more interstitial points.
- GGA often seems to be more sensitive – may need to cut mixing down and iterate longer.

Atomic Calculations:

- ATOMIN = input file
- ATOMOUT = output file
- CDINATOM = file needed for LAPW code – rename this to be ATOMCG
- For LAPW compound calculations, you need to concatenate the different atomic files (in the order specified by the LAPW code)– there is one comment line at the very beginning of the file (after that remove the first comment line when concatenating subsequent atomic files).
- The atomgen.f fortran code usually has the MSH parameter set to be 499.
  You may need to occasionaly change this to MSH=850.
  This value must be only slightly larger (100-150 larger) than the actual number of mesh points used.

Spin-Orbit

- Keep all relevant energy states, make sure that you go far enough above the Fermi energy.
- $p^{1/2}$ not accurately represented by scalar-relativistic
  To fix, would try to add $p^{1/2}$ states during 2nd variation stage.
- Set window and number of bands.
  Set band number to equal the total number of bands.
  Use window constraint to cut things down.
- Don't partially turn-off spin-orbit for atoms.
- Blanks read as FALSE; hence be carefully not to accidentally turn off spin-orbit for large unit cell
- LSPNOR = T for spin-orbit
- 180 = MAX number of bands -> set to a large number, cut off with window
- LNCLSLO = TTT (first T for atom-1, second T for atom-2, etc)
  Add more T's for more atoms
- Energy window – applies to scalar-relativistic states
- Comdecks:
  P5:
  NOBD= increase because spin-orbit doubles bands
  NOBD = total number of bands
  P9:
  NSOBND = maximum number of non-relativistic bands

DOS Calculations:

- QLMT is the file produced by the LAPW code that you need to use for DOS calculations.
- dos501.f is the code that calculates the DOS.
- Requires interpolation of k-point eigenvalues – used star of plane waves and smoothness
- Redimension tetrahedrons
  NEMAXD -> # of energies (e.g., 2001)
  KREAD -> # of k-points in QLMT code, how many to read (e.g., 100)
- Move P1, P2, … into directory where DOS calculations will be done.
- Run COMP.SCRIPT (or source COMP.SCRIPT).
- Rename executable DOS501
- cp INFILE DOSINP
- Edit DOSINP file (change last few lines):
  Interpolation: 8 8 8 -> bigger number
  At bottom of file, put energy range, grid spacing
  Cut off for interpolation: 75
    (depends on size of unit cell)
  Use twice as many plane waves as k-points
  FIT=1 to do fit.
  DOS=1 to do DOS.
  FMSF to do Fermi surface
    Input down below has to do with Fermi surface plot
  N3D = number of stars

QLMT2 = where DOS resides
  Format:
  Energy, Total-DOS, spdf (atom1), spdf (atom2) … ,(# of electrons)
  Units for Total-DOS is in $Ry^{-1}cell^{-1}$
  Units for partials (s,p,d,f) are in $Ry^{-1}atom^{-1}$
  The number of electrons is a rough interpolation.

- Interpolation is pretty safe
- If the the matrices are symmetric or not, may require a change of subroutines:
  Call DPPS or DPPF (“solve the linear equation)