ctrl

ctrl contains basis inputs to invoke lmf,lmfa, and lmchk.
ctrl has `Category_Token` structures. It is easier to understand it by examining the ctrl files generated by ctrlgenM1.py.

ctrl is the basic input file. It is better to look into template of ctrl file generated by ctrlgenM1.py.
Generated ctrl file is self-documented. See Tutorial.

> When we run fortran programs (lmf, lmfa, and lmchk),
> we run ecalj/SRC/exec/ctrl2ctrlp.py (at your BINDIR) from the fortran program in order
> to convert ctrl.foobar to ctrlp.foobar. See ~/ecalj/SRC/main/lmf.f90 for example.
> Then we read ctrlp.foobar by SRC/subroutines/m_lmfinit.f90.

Here is the list of Categoy_Token. Note that those with `.` at top is only for developers.
To see full list, look into `m_lmfinit.f90` which reads in ctrlp file.

```
 Categoy_Token    Input   cast  (size,min) --------------------------
 IO_VERBOS         opt    i4       1,  1          default= 30
    Verbosity for printout. Set from the command-line with --pr=xxx

 IO_TIM            opt    i4v      2,  1          default= 1 1
    Turns CPU timing log. Value sets tree depth.
    Optional 2nd arg prints CPU times as routines execute.
    Args may be set through command-line: --time=#1,#2  --time=5,3 for
example.

 . OPTIONS_HF        opt    lg       1,  1      default= F   T for non-
self-consistent Harris
```

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```
 STRUC_PLAT        reqd   r8v      9,  9      Primitive lattice vectors

 STRUC_ALAT        reqd   r8       1,  1      Units of length (atomic
unit, a.u.)
 STRUC_DALAT       opt    r8       1,  1      default= 0   added to alat
after reading inputs (only affecting to SPEC_ATOM_R/A case)
```

```
 HAM_NSPIN         opt    i4       1,  1      default= 1   Set to 2 for
spin polarized calculations

 HAM_REL           opt    i4       1,  1      default= 1
   relativistic switch
   0 for nonrelativistic Schrodinger equation
   1 for scalar relativistic Schrodinger equation
```

```
 For SO=1 or 2, HAM_NSPIN must be 2
 HAM_SO            opt    i4       1,  1          default= 0
   Spin-orbit coupling (for REL=1)
   0 : no SO coupling
   1 : Add L.S to hamiltonian
   2 : Add Lz.Sz only to hamiltonian
 HAM_SOCAXIS       opt    r8v      3,  3          default= 0 0 1
    SOC axis! Currently 0,0,1 (default) or 1,1,0 are effective for
HAM_SO=1
    I think this works but not fully tested.
```

```
 . HAM_GMAX          reqd   r8       1,  1
    Energy cutoff for plane-wave mesh
    * If HAM_GMAX is not parsed, attempt to read HAM_FTMESH:
    HAM_FTMESH        reqd   i4v      3,  1
       No. divisions for plane-wave mesh along each of 3 lattice
vectors.
       Supply one number for all vectors or a separate number for each
vector.
 . HAM_TOL           opt    r8       1,  1          default= 0.100D-05
    wave function tolerance for FT mesh

 . HAM_FRZWF         opt    lg       1,  1          default= F
    Set to freeze augmentation wave functions for all species

 HAM_FORCES        opt    i4       1,  1          default= 0
    Controls the ansatz for density shift in force calculation.
   -1 no force: no shift
    1 free-atom shift  12 screened core+nucleus

 HAM_XCFUN         opt    i4       1,  1          default= 2
    Specifies local exchange correlation functional:
   1 for Ceperly-Alder (VWN)
   2 for Barth-Hedin (ASW fit)
   103 for PBE-GGA (use xcpbe.F in ABINIT

 HAM_ScaledSigma   opt    r8       1,  1          default= 1
    =\alpha_Q for QSGW-LDA hybrid. \alpha \times (\Sigma-Vxc^LDA) is
added to LDA/GGA Hamiltonian.

 . HAM_EWALD         opt    lg       1,  1          default= F
    Make strux by Ewald summation

 HAM_OVEPS         opt    r8       1,  1          default= 0.100D-06
    Diagonalize hamiltonian in reduced hilbert space,
    discarding part with evals of overlap < OVEPS
 HAM_PWMODE        opt    i4       1,  1          default= 0
    Controls APW addition to LMTO basis. Use 11 usually.
   1s digit:
```

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```
     LMTO basis only
     Mixed LMTO+PW
     PW basis only
   10s digit:
     PW basis G is given at q=0
     PW basis q-dependent. |q+G| cutoff
   (for jobgw=1, lmf automatically set PWMODE=11)
```

```
 HAM_PWEMAX        opt    r8       1,  1          default= 0
    Include APWs with energy E < PWEMAX (Ry) ctrlgenM1.py set pwemax=3
 . HAM_READP         opt    lg       1,  1          default= F !but =T
in ctrlgenM1.py
    Read Pnu and PZ (b.c. of radial func) from atmpnu.*(by lmfa) when we
have no rst file

 . HAM_V0FIX         opt    lg       1,  1          default= F
    Fix potential of radial functions-->Fix radial func. if READP=T
together
 . HAM_PNUFIX        opt    lg       1,  1          default= F
    Fix b.c. of radial functions
```

```
 SYMGRP            opt    chr      1,  0
    Generators for symmetry group
 SYMGRPAF          opt    chr      1,  0
    One (or multiple) Extra Generator for adding anti ferro symmetry
```

SPEC_ATOM

The following tokens are input for each species. See examples.

PROF

```
  SPEC_ATOM         reqd   chr      1,  0
    Species label
  SPEC_ATOM_Z       reqd   r8       1,  1
    Atomic number
.  SPEC_ATOM_R       reqd   r8       1,  1
    Augmentation sphere radius rmax
   * If token is not parsed, attempt to read the following:
    SPEC_ATOM_R/W     reqd   r8       1,  1
    rmax relative to average WS radius
   * If token is not parsed, attempt to read the following:
    SPEC_ATOM_R/A     reqd   r8       1,  1
    rmax ratio to alat
.  SPEC_ATOM_A       opt    r8       1,  1          default depends on
other input
    Radial mesh point spacing parameter
.  SPEC_ATOM_NR      opt    i4       1,  1          default= 51
```

```
    Number of radial mesh points
.  SPEC_ATOM_RSMH    reqd   r8v     10,  1
    Smoothing radii for basis. Gives l-cut max for base. We set =1/2*R
in ctrlgenM1.py
.  SPEC_ATOM_EH      reqd   r8v     10,  0
    Kinetic energies for basis            We set EH=-1 in ctrlgenM1.py
.  SPEC_ATOM_RSMH2   opt    r8v     10,  1
    Basis smoothing radii, second group
.  SPEC_ATOM_EH2     opt    r8v     10,  0
    Basis kinetic energies, second group  We set EH=-2in ctrlgenM1.py

.  SPEC_ATOM_LMX     opt    i4       1,  1          default= 10
    optional l-cutoff for basis. Convenient for debugging or tests.

 SPEC_ATOM_LMXA    opt    i4       1,  1          default depends on
other input
    l-cutoff for augmentation
    We use lmxa=4 mainly but lmax=6 for 4f,5f atoms.

 SPEC_ATOM_MMOM    opt    r8v      1,  1          default= 0
    Starting mag. moms for each l channel.
   For a chanel with PZ, this is enforced to be zero.
   See explanation for SPEC_ATOM_Q.
 SPEC_ATOM_PZ      opt    r8v      1,  1          default= 0
    Starting semicore log der. parameters
     Add 10 to attach Hankel tail

. SPEC_ATOM_LMXL    opt    i4       1,  1          default depends on
other input
    lmax for which to accumulate rho,V in sphere
. SPEC_ATOM_P       opt    r8v      1,  1          default= 0
    Starting log der. parameters for each l
. SPEC_ATOM_Q       opt    r8v      1,  1          default= 0
    Starting valence charges for each l channel.
   Q do not include semicore(PZ) electrons.
   Charge configuration is shown by lmfa
   WARN: This version cannot treat two valence channels
   per l (Q for a l-channl is zero if the l is with PZ).
   This causes a problem typically in Li; then we
   can not treat both of PZ=1.9 and P=2.2 as valence.
   To avoid this, use Q=0,1 together. This trick supply an
   electron to 2p channel; this trick works fine.
. SPEC_ATOM_NMCORE  opt    i4       1,  1          default= 0
    spin-averaged core: jun2012takao
   0(default): spin-polarized core
   1         : spin-averaged core density is from spin-averaged
potential
. SPEC_ATOM_LFOCA   opt    i4       1,  1          default depends on
other input
    FOCA switch 0(within MT):=1(frozenCore). Default: 1 for z>8;0 for
z<=8
. SPEC_ATOM_KMXA    opt    i4       1,  1          default= 3
    k-cutoff for projection of wave functions in sphere.
```

```
. SPEC_ATOM_RSMA    opt    r8       1,  1          default depends on
other input
    Smoothing for projection of wave functions in sphere.
   input<0 => choose default * -input
. SPEC_ATOM_IDMOD   opt    i4v      1,  1          default= 0
    idmod=0 floats P to band CG, 1 freezes P, 2 freezes enu
. SPEC_ATOM_CSTRMX  opt    lg       1,  1          default= F
    Set to exclude this species when automatically resizing sphere radii
(SCLWSR>0)
. SPEC_ATOM_FRZWF   opt    lg       1,  1          default= F
    Set to freeze augmentation wave functions for this species
```

- The next three tokens are for LDA+U

```
 SPEC_ATOM_IDU     opt    i4v      4,  1          default= 0 0 0 0
    LDA+U mode:  0 nothing, 1 AMF, 2 FLL, 3 mixed; +10: no LDA+U if
sigm.* exist
 SPEC_ATOM_UH      opt    r8v      4,  1          default= 0 0 0 0
    Hubbard U for LDA+U
 SPEC_ATOM_JH      opt    r8v      4,  1          default= 0 0 0 0
    Exchange parameter J for LDA+U
```

Core hole options

```
 SPEC_ATOM_C-HOLE  opt    chr      1,  0
    Channel for core hole
 SPEC_ATOM_C-HQ    opt    r8v      2,  2          default= -1 0
    Charge in core hole.  Optional 2nd entry is moment of core hole:
   Q(spin1) = full + C-HQ(1)/2 + C-HQ(2)/2
   Q(spin2) = full + C-HQ(1)/2 - C-HQ(2)/2

. SPEC_ATOM_EREF    opt    r8       1,  1          default= 0
    Reference energy subtracted from total energy (we use little)
```

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SITE

The following tokens are input for each site. See examples.

```
  SITE_ATOM         reqd   chr      1,  0
    Species label
  SITE_ATOM_POS     reqd   r8v      3,  1
    Atom coordinates, cartesian in alat
    * If token is not parsed, attempt to read the following:
    SITE_ATOM_XPOS    reqd   r8v      3,  1
      Atom POS. fractional(POSCAR direct) coordinates
 SITE_ATOM_AF      opt    i4       1,  1          default= 0
```

```
    antiferro ID:=i and -i should be af-pair, we look for space-group
operation with spin-flip
 SITE_ATOM_RELAX   opt    i4v      3,  1          default= 1 1 1
    relax site positions (lattice dynamics) or Euler angles (spin
dynamics)
```

Parameters for Brillouin zone integration ---

```
  BZ_NKABC          reqd   i4v      3,  1
    No. qp along each of 3 lattice vectors.
   Supply one number for all vectors or a separate number for each
vector.

. BZ_BZJOB          opt    i4v      3,  1          default= 0
    0 centers BZ mesh at origin, 1 centers off origin
   Supply one number for all vectors or a separate number for each
vector.
   QSGW requires the default setting.
. BZ_METAL          opt    i4       1,  1          default= 3
    0 insulator only; 3 for metal (2 is for maintenance)
. BZ_TETRA          opt    lg       1,  1          default= T
    Tetrahedron integration
. BZ_N              opt    i4       1,  1          default= 0
    N>0: Polynomial order for Methfessel-Paxton sampling
    N=0: Conventional Gaussian sampling
    N<0: Broadening by Fermi-Dirac distribution
    To be used in conjunction with W= ; see next
 . BZ_W              opt    r8       1,  1          default= 0.500D-02
    If BZ_N>=0, Line broadening for sampling integratio
    If BZ_N<0,  Temperature for Fermi distribution (Ry)
 BZ_ZBAK           opt    r8       1,  1          default= 0
    Homogeneous background charge
 . BZ_SAVDOS         opt    i4       1,  1          default= 0
    Choose 0(F) or 1(T): Write dos.tot.* file (settings are NPTS and
DOS)
 BZ_NPTS           opt    i4       1,  1          default= 2001
    No. DOS points (sampling integration)
 BZ_DOSMAX         opt    r8       1,  1          default= 2.940
    Maximum energy to which DOS accumulated, relative to Efermi
 . BZ_EFMAX          opt    r8       1,  1          default= 5
    Find evecs up to efmax
 . BZ_NEVMX          opt    i4       1,  1          default= 0
    Find at most nevmx eigenvectors
   If NEVMX=0, program uses internal default
   If NEVMX<0, no eigenvectors are generated
 BZ_FSMOM          opt    r8       1,  1          default depends on
other input
    Fixed-spin moment (fixed-spin moment method)
```

```
 BZ_FSMOMMETHOD    opt    i4       1,  1          default= 0
    Method of Fixed-spin moment 0:original 1:discrete
```

Parameters for Ewald sums ---

```
. EWALD_TOL         opt    r8       1,  1          default= 0.100D-07
    Ewald tolerance
```

Parameters for iterations ---

```
 ITER_NIT          opt    i4       1,  1          default= 30
    maximum number of iterations in self-consistency cycle
. ITER_NRMIX        opt    i4       1,  1          default= 80
    lmfa rseq max iter
  ITER_MIX          opt    chr      1,  0
    Mixing rules for charge mixing.  Syntax:
   A[nmix][,b=beta][,bv=betv][,n=nit][,w=w1,w2][,nam=fn][,k=nkill][;...]
or
   B[nmix][,b=beta][,bv=betv][,wc=wc][,n=#][,w=w1,w2][,nam=fn][,k=nkill]
 ITER_CONV         opt    r8       1,  1          default= 0.100D-03
    Tolerance in energy change from prior iteration for self-consistency
 ITER_CONVC        opt    r8       1,  1          default= 0.100D-03
    Tolerance in output-input charge for self-consistency
 ITER_UMIX         opt    r8       1,  1          default= 0.500
    Mixing parameter for densmat in LDA+U
 ITER_TOLU         opt    r8       1,  1          default= 0
    Tolerance for densmat in LDA+U
 mmmixing parameters: A/B nmix wt: 0 -1 1.000000  1.000000 -9.000000
beta elin wc killj=  1.000000 -1.000000 0
```

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Parameters for dynamics and statics ---

```
 DYN_MODE          opt    i4       1,  1          default= 0
    0: no relaxation
    4: relaxation: conjugate gradients
    5: relaxation: Fletcher-Powell
    6: relaxation: Broyden
 DYN_NIT           opt    i4       1,  1          default= 1
    maximum number of relaxation steps (statics) or time steps
(dynamics)
. DYN_HESS          opt    lg       1,  1          default= T
    Read hessian matrix
. DYN_XTOL          opt    r8       1,  1          default= 0.100D-02
    Convergence criterion in displacements
   XTOL>0: use length; <0: use max val; =0: do not use
```

```
. DYN_GTOL          opt    r8       1,  1          default= 0
    Convergence criterion in gradients
   GTOL>0: use length;  <0: use max val;  =0: do not use
. DYN_STEP          opt    r8       1,  1          default= 0.015
    Initial (and maximum) step length
. DYN_NKILL         opt    i4       1,  1          default= 0
    Remove hessian after NKILL iter
```

lmf console input

ecalj made from band structure part (lmf), and GW part (plus some additional functionalities such as Wannier).

lmfa (spherical atom for initial condition) and lmchk (crystal structure check) are by single core.

usage: lmf [--OPTION] [-var-assign] [extension]

```
  usage:  lmfgwd [--OPTION] [-var-assign] [extension]

 --help         List categories, tokens, and data program expects, and
quit
 --show         Print control file after parsing by preprocessor,
                and echo input data as read from the control file
 --pr=#1        Set the verbosity (stack) to values #1
 --time=#1[,#2] Print timing info to # levels (#1=summary; #2=on-the-
fly)

 -vnam=expr     Define numerical variable "nam"; set to result of 'expr'
  --jobgw=1 or 2       lmf-MPIK works as the GW driver (previous lmfgw-
MPIK)
  --quit=band,
    Quit after band
  --quit=dmatu
    Quit after initial setup. Convenient for check.
  --quit=band
     Quit after band calculation.
  --quit=mkpot or --quit=dmat: Stop points. Surpress writing rst

  NOTE: Read rst.* prior to atm.* file (No --rs options: 2022-6-20)
  NOTE: Other command-line-options => Search "call cmdopt" in
SRC/*/*.f90
```

Search --quit option in `SRC/*/*.f90`