`lmf,lmfa,lmchk`

We need ctrl file ctrl.foobar for inputs.

lmfa: spherical atom calculations

Example:`

```
lmfa si
```

It finishes instantaneously.

```
lmfa si |grep conf
```

shows electronic configurations. It gives electron densities of spherical atoms
contained in the primitive cell specified by .
With the superposition of the densities From which, we construct initial electronic density for lmf.
In addition,`lmfa` generates

lmf: solving the Kohn-Sham equation

- **Usage**: `mpirun lmf TARGET [options] > llmf`

Example:

```
mpirun -np 4 lmf si [options] > llmf
```

PROF

This is a case we have ctrl.si.

options

- quit option at some point. `--quit=band`, `--quit=ldau`... We need to do 'grep cmdopt SRC//.f90|grep quit' to know details.
- `--tdos`
  total dos calculation.
- `-vfoobar=xxx` : This overide const foobar=yyy defined in ctrl, and used as {foobar} in ctrl file. This is shown in save file explained below.

We have some kinds of options for electron density plot, boltztrap and so on.
(not yet described).

Input files

- syml.`target`
  symmetry line for band plot (usually `job_band` calls lmf internally)
- sigm.`target`
  a part of QSGW calculation
- Usually (when READP=T in ctrl), we need `atmpnu*` generated by lmfa.

Output files

- rst.`target`
  restart file, containing density and related information.
  Together with the ctrl, atmpnu*, sigm*, and rst*, we can start lmf calculation.
  (dmat* is used for LDA+U) calculation.

- save.`target`
  This contains very minimum history for you to execute lmf, lmf, lmchk, and total energies for each iteration stepsof lmf.

- __mix.`target`
  mixing file for electron density. When you stop iteration at the middle, you may need to delete this.
  mixm retains prior iterations of sets
  of input and output moments. Used by the Anderson or
  Broyden mixing scheme to accelerate convergence towards
  self-consistency. Usually you should delete these when
  starting a new calculation (such as changing the lattice
  constant) so it doesn't get used in subsequent runs.

** Main Source** : `SRC/main/lmf.f90`

lmchk: Check crystal symmetry.

lmchk gives useful information of space group symmetry recognized by lmf. In addition, it determines MT radius.