lmf – Questaal's Full Potential LMTO Code

Part 1: Practical introduction and overview of the lmf code

- full-potential implementation & basis
- verification exercise results

Part 2: Using the lmf code

- walk-through of $SrTiO_3$ calculation

Part 3: Hands-on example

- Se relaxation

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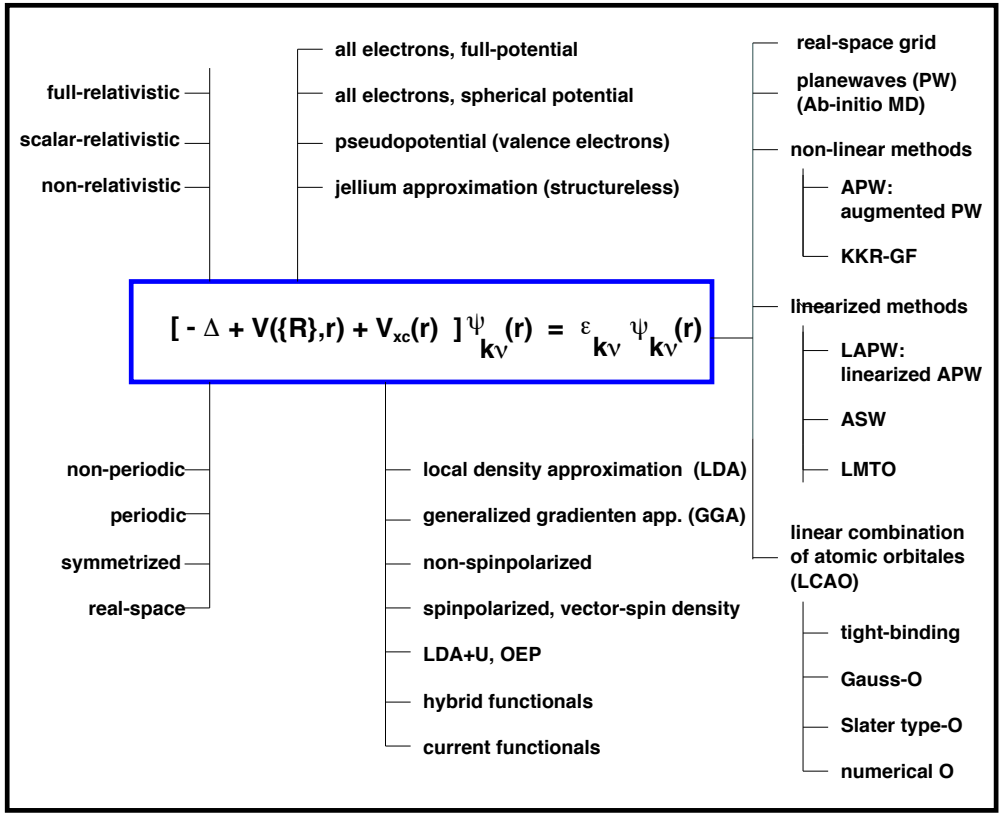

lmf – Questaal's Full Potential LMTO Code

why use lmf?

- simple, powerful user interface (unix style?)
- geometry/system setup straightforward
- default settings are reliable for high accuracy: highly automated
- very fast (small basis)
- spin-orbit coupling, +U, optional APW mode
- huge wealth of features: optics, core-level spectroscopies, external fields, relaxation,...

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Muffin-Tin Orbitals:

$$\Psi_{l,m}(\vec{r},\epsilon) = \Psi_l(r,\epsilon)Y_{l,m}(\hat{r}) \tag{1}$$

$$\Psi_l(r,\epsilon;\kappa) = \begin{cases} R_l(r,\epsilon;\kappa) + P_l(\epsilon;\kappa)\bar{j}_l(\kappa r) & r < r_{mt} \\ \bar{n}_l(\kappa r) & r \geq r_{mt}; \end{cases} \tag{2}$$

- solutions of radial problem R_l within muffin-tin; Hankel envelope ($\bar{n}$) outside
- divergent $r \to \infty$ (KKR) scattering solutions "folded back" into muffin-tin
- potential function P matches radial solution to envelope
- "tail cancellation" simplifies solution in the ASA (no interstitial)
- R_l linearized to remove energy dependence

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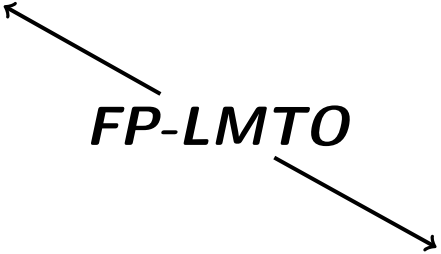
full-potential

- muffin-tin partitioning of space (`R`)
- additive augmentation (`lmxa`)
- G-space mesh (`GMAX`)



linearized muffin-tin orbital

- maximum l for basis (`lmx`)
- number of basis functions per l, m (1 or 2)
- basis "shape" (`EH`,`RSMH`)

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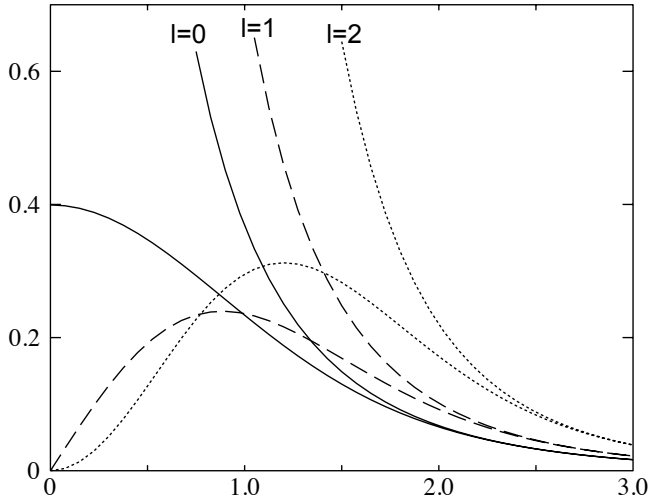
FP-basis:

- envelope functions are *smoothed*-Hankel functions
- combination of Gaussian (width `RSMH`) with a Hankel function (energy `EH`)



- no $1/r^{l+1}$ divergence at the origin; "more physical" form
- augment continuously with radial solutions and energy derivatives at r_{mt} (explicit interstitial)

Dreyssé (ed.) *The Uses of the LMTO Method* Springer, 2000
Bott, Methfessel, Krabs, Schmidt J.Math.Phys., 39, 3393–3425, 1998

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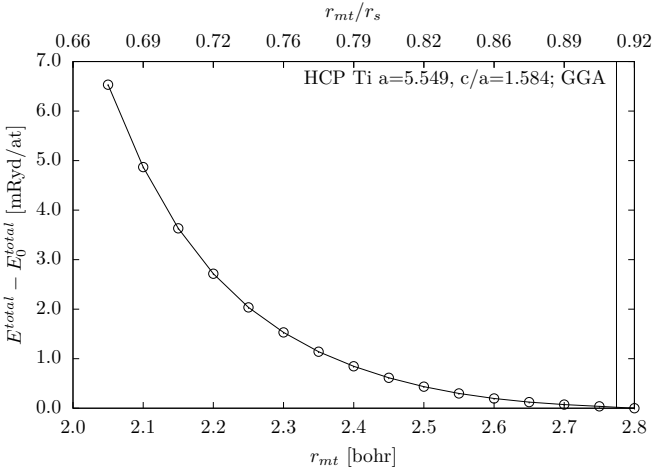
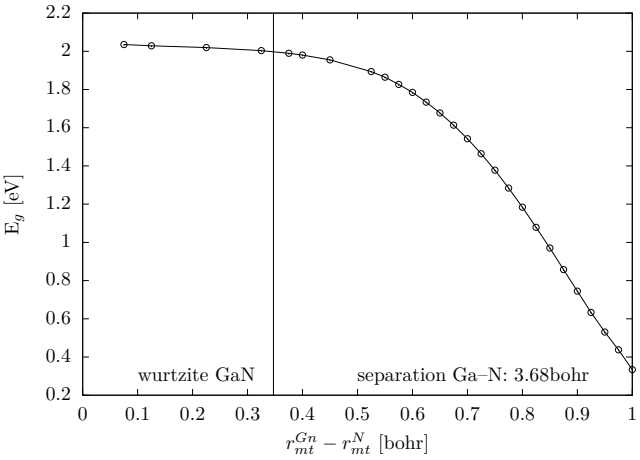
- augmentation with non-overlapping muffin-tin spheres with radius `R`
- within `R`, the solution is essentially exact: try to maximise
- quality of solution depends sensitively on relative `R` for multi-component systems
- `R` estimate given by first maximum in $V(r)$ is generally close to optimal





- (use **blm** or `lmchk --getwsr`)

lmf – Questaal's Full Potential LMTO Code

- combination of real-space mesh extending over all space and atomic radial contributions

$$V(\vec{r}) = V^{\text{smooth grid}}(\vec{r}) + \sum_{atoms} \left[V_i^{\text{radial}}(\vec{r}) - V_i^{\text{radial evaluated on grid}}(\vec{r}) \right]$$

- $V^{\text{radial}}(\vec{r})$ expanded in spherical harmonics

- higher l contributions carried effectively by smooth grid component

- similarly for augmented envelope functions: generally $l_{max} \leq 3$ required

- similar to pseudopotential/PAW methods (unlike APW)

lmf – Questaal's Full Potential LMTO Code

Local orbitals:

- enables inclusion of higher or lower n
- unoccupied ("high-lying local orbitals") and semi-core states
- improved by adding own basis functions for semi-core states: "extended local orbitals"

Core Treatment:

- self-consistent or "frozen"
- frozen core can extend into interstitial – much more accurate
- use local orbitals when in doubt
- scalar/fully-relativistic solvers available

APW component:

- plane-wave component in addition to (or instead of) LMTO basis
- effective for open systems (eg, molecular crystals)
- improves description of unoccupied states

lmf – Questaal's Full Potential LMTO Code

DeltaCodes exercise:

- community driven effort to compare solid-state codes
- lead by K. Lejaeghere and S. Cottenier (Uni. Ghent)
- first publication 2014 (VASP, WIEN2k, GPAW)

TABLE 8
Comparison between codes for two extreme situations: large (Tc an Ru) and small (Ar) numerical errors Δ_i. V_0 is given in Å^3/atom, B_0 in GPa, and Δ_i in meV/atom. B_1 is dimensionless

		V_0	B_0	B_1	Δ_i
Tc	APW+lo$_{(WIEN2k)}$	14.47	301.4	4.56	0
	PAW$_{(VASP)}$	14.60	298.5	4.55	8.3
Ru	APW+lo$_{(WIEN2k)}$	13.81	315.4	4.96	0
	PAW$_{(GPAW)}$	14.09	310.9	4.87	20.9
Ar	APW+lo$_{(WIEN2k)}$	52.21	0.7	7.84	0
	PAW$_{(VASP)}$	52.65	0.8	7.35	0.1
	PAW$_{(GPAW)}$	52.66	0.8	3.27	0.1

- 2016 > 40 codes/pseudopotential schemes
- 71 elemental solids (no f-electron systems); ranging from close packed to molecular crystals

lmf – Questaal's Full Potential LMTO Code

- integrated difference of GGA $E(V)$ curves (in meV/atom)
- total energy offsets ignored; fits to Birch-Murnagham, averaged over the periodic table
- good agreement between methods, FP-LAPW and PAW in particular: differences in $V_0 < 1\%$.
- (no expense spared ☺)

		AE												PAW									USPP						NCPP							
		Elk	exciting	FHI-aims/tight	FHI-aims/really_tight	FHI-aims/tier2	FLEUR	FPLO/default	FPLO/T+F	FPLO/T+F+s	RSPt	WIEN2k/default	WIEN2k/enhanced	WIEN2k/acc	GBRV12/ABINIT	GPAW06/GPAW	GPAW09/ABINIT	GPAW09/GPAW	JTH01/ABINIT	JTH02/ABINIT	PSlib031/QE	PSlib100/QE	VASP2007/VASP	VASP2012/VASP	VASPGW2015/VASP	GBRV12/QE	GBRV14/CASTEP	GBRV14/QE	OTFG7/CASTEP	OTFG9/CASTEP	SSSP/QE	Vdb/CASTEP	Vdb2/DACAPO	FHI98pp/ABINIT	HGH/ABINIT	HGH-NLCC/BigDFT	MBK2013/OpenMX	ONCVPSP(PD0.1)/ABINIT	ONCVPSP(SG15)1/CASTEP	ONCVPSP(SG15)1/QE	ONCVPSP(SG15)2/CASTEP
AE	Elk		0.3	0.6	0.6	0.3	0.6	3.9	1.0	1.0	0.9	1.7	1.8	0.3	0.9	3.8	1.3	1.5	1.2	0.6	1.6	0.9	2.1	0.7	0.4	1.1	1.1	1.0	2.5	0.4	0.4	6.4	6.3	13.5	2.2	1.1	2.1	0.7	1.5	1.4	1.4
	exciting	0.3		0.5	0.5	0.1	0.5	3.9	1.0	0.9	0.8	1.7	1.8	0.2	0.8	3.8	1.3	1.5	1.2	0.6	1.6	0.8	2.1	0.6	0.4	1.0	1.1	1.0	2.5	0.5	0.3	6.4	6.3	13.4	2.2	1.1	2.1	0.7	1.4	1.3	1.4
	FHI-aims/tight	0.6	0.5		0.0	0.5	0.7	3.8	0.9	1.1	0.7	1.8	1.8	0.5	1.0	3.8	1.3	1.6	1.3	0.7	1.7	1.0	2.2	0.8	0.6	1.1	1.2	1.1	2.6	0.7	0.6	6.4	6.3	13.6	2.2	1.2	2.0	0.8	1.5	1.4	1.5
	FHI-aims/really_tight	0.6	0.5	0.0		0.5	0.7	3.8	0.9	1.1	0.8	1.8	1.8	0.5	1.0	3.8	1.3	1.6	1.3	0.7	1.7	1.0	2.2	0.8	0.6	1.1	1.2	1.1	2.6	0.7	0.6	6.5	6.3	13.6	2.2	1.2	2.0	0.8	1.5	1.4	1.5
	FHI-aims/tier2	0.3	0.1	0.5	0.5		0.5	3.9	0.9	0.9	0.8	1.7	1.8	0.2	0.8	3.8	1.3	1.5	1.2	0.6	1.6	0.8	2.0	0.6	0.4	0.9	1.0	0.9	2.5	0.5	0.3	6.4	6.3	13.4	2.2	1.1	2.1	0.7	1.4	1.3	1.4
	FLEUR	0.6	0.5	0.7	0.7	0.5		3.6	0.8	0.8	0.6	1.4	1.5	0.4	0.9	3.5	1.3	1.5	1.0	0.6	1.5	0.8	1.9	0.7	0.6	1.0	1.0	1.0	2.6	0.7	0.5	6.5	6.3	13.2	2.0	1.0	1.9	0.6	1.3	1.3	1.3
	FPLO/default	3.9	3.9	3.8	3.8	3.9	3.6		3.1	3.6	3.3	2.9	2.5	3.9	4.0	3.1	4.1	4.1	3.4	3.6	3.3	3.9	2.8	3.9	4.0	4.0	4.0	4.1	5.8	4.1	3.9	7.9	7.2	13.0	4.9	3.6	3.2	3.7	4.1	4.1	4.1
	FPLO/T+F	1.0	1.0	0.9	0.9	0.9	0.8	3.1		0.8	0.7	1.4	1.4	0.9	1.3	3.4	1.7	1.9	1.0	0.9	1.5	1.3	1.9	1.2	1.0	1.3	1.3	1.3	3.1	1.1	1.0	6.6	6.4	13.7	2.4	1.2	1.8	1.0	1.6	1.6	1.6
	FPLO/T+F+s	1.0	0.9	1.1	1.1	0.9	0.8	3.6	0.8		0.9	1.5	1.5	0.9	1.3	3.5	1.7	1.8	1.2	0.9	1.4	1.3	1.9	1.2	1.0	1.4	1.4	1.4	2.9	1.0	0.9	6.4	6.4	13.0	2.3	1.2	1.8	1.0	1.6	1.6	1.6
	RSPt	0.9	0.8	0.7	0.8	0.8	0.6	3.3	0.7	0.9		1.3	1.3	0.8	1.1	3.4	1.5	1.7	0.9	0.7	1.6	1.1	1.9	1.0	0.8	1.2	1.3	1.3	3.0	1.0	0.8	6.7	6.5	13.2	2.2	1.1	1.8	0.8	1.5	1.5	1.5
	WIEN2k/default	1.7	1.7	1.8	1.8	1.7	1.4	2.9	1.4	1.5	1.3		0.9	1.7	1.9	3.2	2.2	2.3	1.3	1.5	1.8	1.8	1.7	1.8	1.8	1.9	1.9	1.9	3.8	1.8	1.6	7.1	7.0	13.0	2.8	1.7	1.9	1.6	2.1	2.1	2.1
	WIEN2k/enhanced	1.8	1.8	1.8	1.8	1.8	1.5	2.5	1.4	1.5	1.3	0.9		1.8	2.0	2.6	2.1	2.2	1.1	1.5	1.6	1.8	1.4	1.9	2.0	2.0	2.0	2.0	3.8	2.0	1.7	6.9	6.9	12.3	2.8	1.6	1.5	1.7	1.9	1.9	1.9
	WIEN2k/acc	0.3	0.2	0.5	0.5	0.2	0.4	3.9	0.9	0.9	0.8	1.7	1.8		0.8	3.8	1.3	1.5	1.2	0.5	1.6	0.8	2.0	0.7	0.3	0.9	1.0	1.0	2.5	0.5	0.3	6.4	6.2	13.4	2.1	1.0	2.0	0.6	1.4	1.3	1.4
	GBRV12/ABINIT	0.9	0.8	1.0	1.0	0.8	0.9	4.0	1.3	1.3	1.1	1.9	2.0	0.8		4.1	1.5	1.6	1.5	1.1	2.0	1.1	2.3	1.0	0.9	0.7	0.8	0.7	2.8	1.0	0.7	6.4	6.3	15.1	2.5	1.5	2.4	1.1	1.8	1.7	1.8
	GPAW06/GPAW	3.8	3.8	3.8	3.8	3.8	3.5	3.1	3.4	3.5	3.4	3.2	2.6	3.8	4.1		3.6	3.5	3.2	3.5	3.0	3.8	2.8	3.7	3.8	4.0	3.8	4.0	5.6	3.9	3.6	7.4	7.6	12.3	4.5	3.0	3.0	3.6	3.7	3.8	3.7

lmf – Questaal's Full Potential LMTO Code

- "large" LMTO basis
- PW component needed for molecular crystals (eg, N_2)

LMF: PMT+LO

Δ^{WIEN2k} (mean=0.58meV/at)

PWEMAX=2Ryd (N,O,F:7.5Ryd),OVEPS=1e-10,RMT_MAX=2.6bohr

	1 IA	2 IIA	3 IIIA	4 IVB	5 VB	6 VIB	7 VIIB	8 VIIIB	9 VIIIB	10 VIIIB	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	0.027 H Hydrogen,1																	0.084 He Helium,2
2	0.031 Li Lithium,3	0.158 Be Beryllium,4											0.308 B Boron,5	0.556 C Carbon,6	0.928 N Nitrogen,7	0.963 O Oxygen,8	0.646 F Flourine,9	0.060 Ne Neon,10
3	0.630 Na Sodium,11	0.389 Mg Magnesium,12											0.526 Al Aluminium,13	0.749 Si Silicon,14	0.264 P Phospho-rus,15	1.443 S Sulphur,16	0.538 Cl Chlorine,17	0.046 Ar Argon,18
4	0.025 K Potassium,19	0.417 Ca Calcium,20	0.189 Sc Scandium,21	0.402 Ti Titanium,22	0.867 V Vanadium,23	0.871 Cr Chromium,24	0.410 Mn Manganese,25	0.322 Fe Iron,26	1.273 Co Cobalt,27	1.169 Ni Nickel,28	0.364 Cu Copper,29	0.330 Zn Zinc,30	0.224 Ga Gallium,31	0.151 Ge Germa-nium,32	2.003 As Arsenic,33	1.473 Se Selenium,34	0.960 Br Bromine,35	0.076 Kr Krypton,36
5	0.158 Rb Rubidium,37	0.319 Sr Strontium,38	0.077 Y Yttrium,39	0.368 Zr Zirconium,40	0.617 Nb Niobium,41	0.171 Mo Molybde-num,42	1.630 Tc Tech-netium,43	0.214 Ru Ruthenium,44	0.631 Rh Rhodium,45	0.284 Pd Palladium,46	0.497 Ag Silver,47	1.983 Cd Cadmium,48	0.198 In Indium,49	0.659 Sn Tin,50	0.586 Sb Antimony,51	0.431 Te Tellurium,52	0.809 I Iodine,53	0.094 Xe Xenon,54
6	0.018 Cs Caesium,55	2.114 Ba Barium,56	0.108 Lu Lutetium,71	0.309 Hf Halfnium,72	1.273 Ta Tantalum,73	3.520 W Tungsten,74	1.437 Re Rhenium,75	0.799 Os Osmium,76	0.782 Ir Iridium,77	0.204 Pt Platinum,78	0.177 Au Gold,79	0.027 Hg Mercury,80	0.129 Tl Thallium,81	0.052 Pb Lead,82	0.340 Bi Bismuth,83	0.040 Po Polonium,84		0.075 Rn Radon,86

- comparable with other "all-electron" methods
- "general purpose" DFT code

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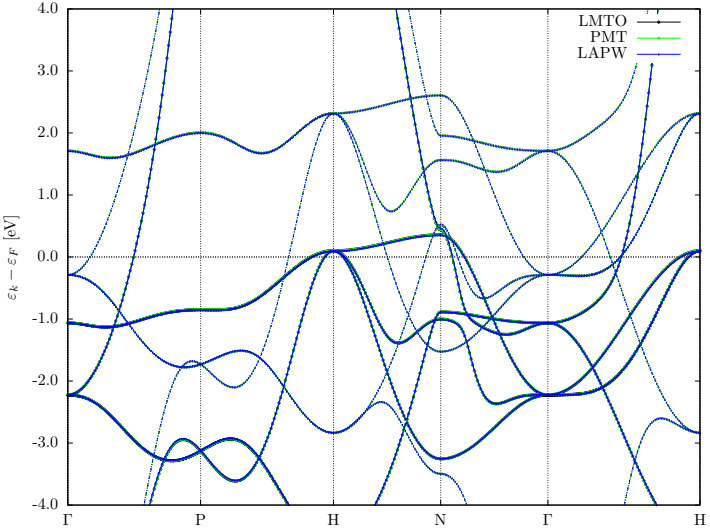

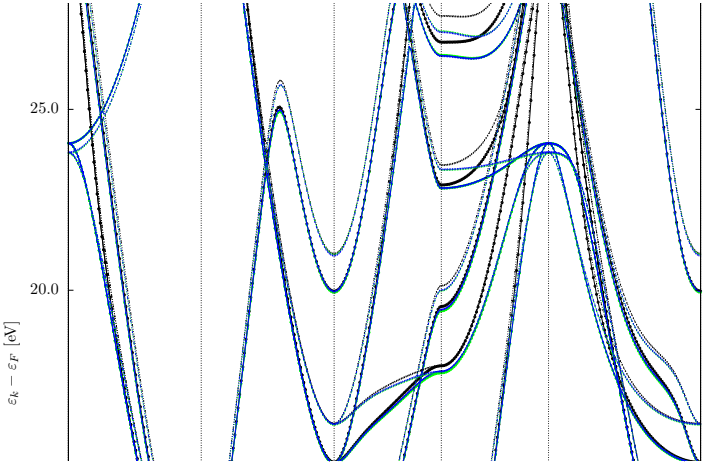

- BCC Fe bands@GGA: LMTO, LMTO+PW
- comparison with LAPW (`elk` code)
- excellent agreement for the occupied bands (variation over occupied eigenvalues < 1mRyd)
- unoccupied improved by a small PW component (error ~ 40mRyd over 20 empty bands)

lmf – Questaal's Full Potential LMTO Code

Basis setup:

current strategy:

1. fit `EH` and `RSMH` for each l to free-atom solutions
2. apply minimum/maximum limits to these, depending upon r_{mt}
3. add second set (if requested) at a deeper (more negative) `EH` (same `RSMH`)

alternative strategy:

1. choose `EH` for all l
2. specify energies corresponding to wealky and strongly bound states
3. setup two separated `RSMH` corresponding to states at those energies in $V(r)$
4. try with: `AUTOBAS[MTO=12 EIN=-2.0 EOUT=-0.5]`

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- full-potential implementation & basis
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Part 2: Using the lmf code

- walk-through of $SrTiO_3$ calculation

Part 3: Hands-on example

- Se relaxation

Ctrl file for SrTiO3

- Pm-3m (space group 221); ICSD ref 80872: $a = 3.8996(5)$Å

spec	Wyckoff	positions
Sr	(1a)	$(0, 0, 0)$
Ti	(1b)	$(1/2, 1/2, 1/2)$
O	(3c)	$(0, 1/2, 1/2)$

```
# cubic perovskite SrTiO3
STRUC
 NSPEC=3      # number of different species
 NBAS=5       # number of occupied sites
 ALAT=7.3692  # expt lattice constant (bohr) (3.8996AA)
 PLAT=1 0 0
      0 1 0
      0 0 1   # lattice vectors

SITE
 ATOM=Sr XPOS=0 0 0
 ATOM=Ti XPOS=1/2 1/2 1/2
 ATOM=O  XPOS=0 1/2 1/2
 ATOM=O  XPOS=1/2 1/2 0
 ATOM=O  XPOS=1/2 0 1/2

SPEC          # definitions for individual species
 ATOM=Sr Z=38 R=2.6 LMX=2 # R_mt and LMX key in LMTO
 ATOM=Ti Z=22 R=2.2 LMX=2
 ATOM=O  Z=8  R=1.6 LMX=2

VERS          # ctrl file format version
 LMF=7 FP=7 LM=7
```

SrTiO3 – lmchk output

great! Can we check that it makes sense?

```
run > ls -l
total 8
-rw-r--r--  1 jerome  staff  571 May 12 11:32 ctrl.srtio3
run > lmchk ctrl.srtio3
 ----------------------  START LMCHK ----------------------

 LMCHK:    nbas = 5  nspec = 3  vn 7.11.i  verb 35
 special
 pot:      XC:BH
 float:    float P LDA-style
 autoread: none

                Plat                                  Qlat
   1.000000   0.000000   0.000000        1.000000   0.000000   0.000000
   0.000000   1.000000   0.000000        0.000000   1.000000   0.000000
   0.000000   0.000000   1.000000        0.000000   0.000000   1.000000
   alat = 7.3692  Cell vol = 400.185207

 LATTC:  as= 2.000   tol=1.00E-08   alat= 7.36920   awald= 0.271
         r1=  2.885   nkd= 93       q1=  3.426   nkg= 171

 SGROUP: 1 symmetry operations from 0 generators
 SYMLAT: Bravais system is cubic with 48 symmetry operations.
 SYMCRY: crystal invariant under 48 symmetry operations for tol=1e-5
 GROUPG: the following are sufficient to generate the space group:
         i*r3d r2(0,1,1)
         i*r3d r2(0,1,1)
 MKSYM:  found 48 space group operations ... includes inversion
 Use default rmaxs = 7.218 a.u. = 2.7*avw = 0.98*alat
```

SrTiO3 – lmchk output

```
   Site     Class            Rmax        Hcr                 Position
    1       1  Sr          2.600000    1.820000    0.00000    0.00000    0.00000
    2       2  Ti          2.200000    1.540000    0.50000    0.50000    0.50000
    3       3  O           1.600000    1.120000    0.00000    0.50000    0.50000
    4       3  O           1.600000    1.120000    0.50000    0.50000    0.00000
    5       3  O           1.600000    1.120000    0.50000    0.00000    0.50000

 Cell volume= 400.18521   Sum of sphere volumes= 169.69627 (0.42404)

 ib jb  cl1     cl2        Pos(jb)-Pos(ib)      Dist  sumrs   Ovlp    %    summt   Ovlp   %
  2  3  Ti      O        -3.685  0.000  0.000   3.685  3.800   0.12   3.1*  2.660  -1.02 -27.8
  2  4  Ti      O         0.000  0.000 -3.685   3.685  3.800   0.12   3.1*  2.660  -1.02 -27.8
  2  5  Ti      O         0.000 -3.685  0.000   3.685  3.800   0.12   3.1*  2.660  -1.02 -27.8

 OVMIN, 81 pairs:  fovl = 9.43828e-10   <ovlp> = 3.1%   max ovlp = 3.1%
 Exit 0 LMCHK
 CPU time:    0.031s   Wall clock    0.062s   11:33:00 12.05.2017        on

 Wall-clock time: 0.063s. Resolution 0.000001s

run >
```

- overlap $\sim 3\%$ is maybe ok: we will learn later how to improve upon this using **blm**
- for more information, increase the verbosity from the command line, eg:

  `lmchk --pr50 srtio3`
- lots of information: also neighbour tables, bond angles, ... (see Se example)

Ctrl file for SrTiO3

Before running a DFT calculation we must:

1. specify the exchange-correlation functional
2. run the atom solver **lmfa** to generate free-atom densities and setup basis
3. identify any semicore states
4. specify the smooth grid (plane-wave cut-off) for representing n and V (`GMAX`)
5. specify the $\vec{k}$-sampling
6. specify the maximum number of iterations to self-consistency

SrTiO3 – Basis

specify the exchange-correlation functional and LMTO basis:

```
VERS          # ctrl file format version
 LMF=7 FP=7 LM=7

HAM           # options relating to the Hamiltonian
  XCFUN=1     # LDA (VWN)
# XCFUN=0 101 130 #PBE-GGA using LibXC interface
  AUTOBAS[MTO=2 LMTO=5] # MTO=2: read from "basp" file
                        # LMTO=5: use BIG basis
  GMAX=0      # smooth grid cut-off
              # use the recommendation from lmfa
```

`AUTOBAS` introduces options for automatic basis:

lmfa: (radial) atom solver, *writes* core density and basis definitions to `basp` file

lmf: (full potential) band program, *requires* atom density and basis definitions in `basp` file
– *must always execute `lmfa` to start a new calculation: run* "`lmfa ctrl.srtio3`"

SrTiO3 – lmfa output (1)

output of running **lmfa**:

```
 Species Sr:  Z=38  Qc=36  R=2.600000  Q=0
 mesh:   rmt=2.600000  rmax=49.676653  a=0.025  nr=425  nr(rmax)=543
  Pl=  5.5     5.5     4.5     4.5
  Ql=  2.0     0.0     0.0     0.0

  iter      qint         drho          vh0          rho0          vsum      beta
    1    38.000000   6.880E+03      190.0000    0.1890E+03     -76.3617   0.30
   52    38.000000   4.253E-05      403.4924    0.8727E+05    -286.9181   0.30


 sumev=-0.535008  etot=-6351.658531  eref=0.000000

 Free-atom wavefunctions:
 valence:       eval        node at       max at        c.t.p.    rho(r>rmt)
   5s        -0.26750          1.649        3.616        5.425      0.892875
   5p        -0.09680          1.962        4.862        8.333      0.965189
   4d        -0.10320          0.652        2.151        8.148      0.611161
   4f         0.01876          0.000       35.936       49.677*     1.000000

 core:          ecore        node at       max at        c.t.p.    rho(r>rmt)
   1s     -1169.16523          0.000        0.026        0.052      0.000000
   2s      -158.32529          0.052        0.145        0.227      0.000000
   2p      -140.77626          0.000        0.116        0.244      0.000000
   3s       -24.44466          0.210        0.436        0.632      0.000000
   3p       -18.78747          0.188        0.431        0.721      0.000000
   3d        -9.42158          0.000        0.376        1.008      0.000003
   4s        -3.00733          0.594        1.187        1.701      0.017430
   4p        -1.68003          0.613        1.324        2.193      0.059807
```

occupancy and eigenvalues for atomic states of each species

SrTiO3 – lmfa output (2)

```
Optimise free-atom basis for species Sr, rmt=2.6
l  it     Rsm       Eh      stiffR    stiffE       Eval       Exact      Pnu     Ql
0  50    5.014   -1.324       34.7       1.2    -0.25087   -0.26750     5.32    2.00
... rsm exceeded rmt .. repeat with rsm=rmt
0  14    2.600   -0.100       34.7    2365.1    -0.21210   -0.26750     5.32    2.00
1  21    3.783   -0.100       32.7    1011.9    -0.10503   -0.09680     5.12    0.00
... rsm exceeded rmt .. repeat with rsm=rmt
1   1    2.600   -0.100       32.7    -612.9    -0.07161   -0.09680     5.12    0.00
2  11    1.658   -0.100      576.5    -114.9    -0.08060   -0.10320     4.79    0.00
eigenvalue sum:  exact   -0.53501    opt basis   -0.42419    error 0.11081

Make LMTO basis parms for species Sr to lmxb=3, rmt=2.6  vbar=0
l  it     Rsm        Eh         Eval       Exact      Pnu     Ql    Gmax
0  11    1.733*   -0.100*    -0.13053   -0.26750     5.32    2.00    4.0
1  42    0.300    -5.000     -1.01117   -0.09680     5.12    0.00   26.2
... l=1  fit parms out of range ... revert to defaults
1  42    1.733+   -0.100+    -0.05603   -0.09680     5.12    0.00
2  11    1.658    -0.100*    -0.08060   -0.10320     4.79    0.00    4.7
3   1    1.733+   -0.100+     0.30532    0.01876     4.19    0.00
```

basis construction ... for all species. Lastly:

```
   rho: r>rmt   1.368046   r<rmt   4.631954   qtot   6.000000

FREEAT:  writing file basp0

FREEAT:  estimate HAM_GMAX from RSMH:  GMAX=9.4

Sum of reference energies: 0
Exit 0 LMFA
CPU time:    0.177s   Wall clock    0.205s   13:27:25 12.05.2017        on

Wall-clock time: 0.206s. Resolution 0.000001s
```

we use this recommendation for the smooth mesh grid

SrTiO3 – lmfa output (3)

lmfa also generates the "basp" file, containing the automatically fitted basis:

```
BASIS:
 Sr RSMH= 1.733 1.733 1.658 1.733 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.733 1.733 1.658 EH2= -0.9 -0.9 -0.9
 Ti RSMH= 1.467 1.467 1.091 1.467 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.467 1.467 1.091 EH2= -0.9 -0.9 -0.9
 O RSMH= 0.851 0.813 1.067 1.067 EH= -0.465 -0.1 -0.1 -0.1 RSMH2= 0.851 0.813 1.067 EH2= -1.265 -0.9 -0.9
```

- `AUTOBAS_LMTO=5` gives a large *spdf,spd* basis (but, remember `LMX`)
- the generated basis definition is written to **`basp0.ext`**
- `EH` and `EH2`: Hankel energies, here in "LDA" style
- `RSMH` and `RSMH2`: smoothing radii optimised by **lmfa**
- to use the basis, we **need to copy `basp0.ext`** to **`basp.ext`**

SrTiO3 – ready to go

```
# cubic perovskite SrTiO3
STRUC
 NSPEC=3       # number of different species
 NBAS=5        # number of occupied sites
 ALAT=7.3692   # expt lattice constant (bohr) (3.8996AA)
 PLAT=1 0 0
      0 1 0
      0 0 1    # lattice vectors

SITE
 ATOM=Sr XPOS=0 0 0
 ATOM=Ti XPOS=1/2 1/2 1/2
 ATOM=O  XPOS=0 1/2 1/2
 ATOM=O  XPOS=1/2 1/2 0
 ATOM=O  XPOS=1/2 0 1/2

SPEC           # definitions for individual species
 ATOM=Sr Z=38 R=2.6 LMX=2 # R_mt and LMX key in LMTO
 ATOM=Ti Z=22 R=2.2 LMX=2
 ATOM=O  Z=8  R=1.6 LMX=2

VERS           # ctrl file format version
 LMF=7 FP=7 LM=7

HAM            # options relating to the Hamiltonian
 XCFUN=1       # LDA (VWN)
# XCFUN=0 101 130 #PBE-GGA using LibXC interface
 AUTOBAS[MTO=2 LMTO=5] # MTO=2: read from "basp" file
                       # LMTO=5: use BIG basis
 GMAX=9.5      # smooth grid cut-off from LMFA

BZ
 NKABC=10 10 10 # k-mesh divisions

ITER
 NIT=50        # max scf iterations
```

SrTiO3 – run lmf (1)

```
run > clear
run > ls
ctrl.srtio3
run > lmfa srtio3 > atomlog
run > mv basp0.srtio3 basp.srtio3
run > mpirun -np 4 lmf srtio3 > scflog
run > cat save.srtio3
h ehf=-8505.8980933 ehk=-8504.4915374
i ehf=-8507.0104948 ehk=-8492.1939833
i ehf=-8505.7239925 ehk=-8504.9668352
i ehf=-8505.5817481 ehk=-8505.2006142
i ehf=-8505.4880124 ehk=-8505.417938
i ehf=-8505.4825994 ehk=-8505.4432019
i ehf=-8505.4728415 ehk=-8505.4631945
i ehf=-8505.4721799 ehk=-8505.4721639
i ehf=-8505.47202 ehk=-8505.4720064
c ehf=-8505.4720245 ehk=-8505.4720211
run > tail scflog

   it 10  of 50    ehf=   -8505.472024   ehk=   -8505.472021
 From last iter    ehf=   -8505.472020   ehk=   -8505.472006
 diffe(q)= -0.000004 (0.000026)    tol= 0.000010 (0.000030)   more=F
c ehf=-8505.4720245 ehk=-8505.4720211
 Exit 0 LMF      on vpn-3-063
 CPU time:   63.127s   Wall clock   63.196s   14:38:46 12.05.2017        on

 Wall-clock time: 63.195s. Resolution 0.000001s

run >
```

- mpi parallelised over $\{\vec{k}\}$: use nproc less than/equal to NKIBZ
- remember: energies in Rydberg

SrTiO3 – run lmf (2)

main reporting via stdout:

- version, special features
- header, lattice, symmetry, BZ sampling, species data
- Hamiltonian info, charges
- for each scf step:
  - energy contributions
  - E_f, VBM/CBM/E_g
  - eigenvalues at some selected $\vec{k}$
  - update augmentation: $\bar{e}$, logarithmic derivatives
  - local orbital setup
  - info on (charge) mixing

varies depending upon setup/code

verbosity can be changed: `lmf --pr10` **(spartan) or** `--pr60` **(hefty)**

SrTiO3 – run lmf (3)

`STDOUT`	stdout from **lmfa**, **lmf**, etc., is the main output mechanism
`atm.srtio3`	core and valence density and potential for atom (ASCII)
`basp.srtio3`	basis definition (essentially ctrl file data)
`ctrl.srtio3`	main input file
`log.srtio3`	slightly cryptic log info
`mixm.srtio3`	scf mixing history (binary)
`moms.srtio3`	weights of overlap matrix (binary)
`rst.srtio3`	full restart information (binary, can ask for ASCII)
`save.srtio3`	total energy (and possibly spin): for monitoring convergence
`wkp.srtio3`	$\vec{k}$-point weights (binary)

–plus other files generated for different tasks

SrTiO3 – run lmf (4)

`lmf --input|less` very useful quick-reference for input tokens!

```
run > lmf --input
...

 DYN_MD                 opt    ---
   Parameters for molecular dynamics
 DYN_MD_MODE            reqd   i4       1,  1     default = 0
   0: no MD 1: NVE 2: NVT 3: NPT
 DYN_MD_TSTEP           opt    r8       1,  1     default = 20.671
   Time step (a.u.)
 DYN_MD_TEMP            opt    r8       1,  1     default = 0.00189999
   Temperature (a.u.)
 DYN_MD_TAUP            opt    r8       1,  1     default = 206.71
   Thermostat relaxation time (a.u.)
 DYN_MD_TIME            reqd   r8       1,  1     default = 20671000
   Total MD time (a.u.)
 DYN_MD_TAUB            opt    r8       1,  1     default = 2067.1
   Barostat relaxation time (a.u.)
 DYN_MD_P               opt    r8       1,  1     default = 0
   External pressure
 NB: 1 deg.K = 6.3333e-6 a.u.; 1 fs = 20.67098 a.u.

 --- Parameters for GW ---
 GW_NKABC               opt    i4v      3,  1
   No. qp along each of 3 lattice vectors.
   Supply one number for all vectors or a separate number for each vector.
 GW_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.
run >
```

each of the codes **lmf**,**blm**,**lmgf**,**lmfgwd**, etc ... provide this

SrTiO3 – run lmf (5)

`lmf --help` print quick information about command line arguments

```
run > lm --help
 usage:  lm [--OPTION] [-var-assign] [ext]

 --h
 --help          Print this message, and quit
 --input         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
 --showp         Same as --show, but quit after input parsed
 --iactiv        (--no-iactiv) Turn on (off) interactive mode
                 This switch overrides input file setting
 --pr#1[,#2...] Set the verbosity (stack) to values #1,#2, ...
 --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'
 -cnam=strn      Define character variable "nam"; set to 'strn'

 --rpos=filnam  After reading input file, read site positions from "filnam"
 --fixlat        Adjust lattice vectors and point group ops, attempt to
                 render them internally consistent
 --fixpos[:tol=#] Adjust positions slightly, rendering them
                 as consistent as possible with the symmetry group
 --nosym         Suppress symmetry operations

 lm-specific options:

 --rs=#1,#2 --band[~option...] --pdos[~option...] -mix=#1[,#2] --onesp --weula --rsedit --efrnge
 For --band mode options, see doc/generating-energy-bands.html

 lm v 7.11.i

 Wall-clock time: 0.001s. Resolution 0.000001s

run >
```

SrTiO3 – a little ctrl file magic

```
1  -vnam=expr      Define numerical variable "nam"; set to result of 'expr'
```

- access from the command line to variables defined in the ctrl file!
- preprocessor variables in **`ctrl`** file introduced by "% const var=exp"
- evaluated before being passed to the code
- variables which are changed from their defaults are echoed in the **`save.ext`** file
- quite a rich syntax/grammar with many features
- used extensively by **blm** and demo cases

SrTiO3 – a little ctrl file magic

- example: converging the $\vec{k}$ mesh:

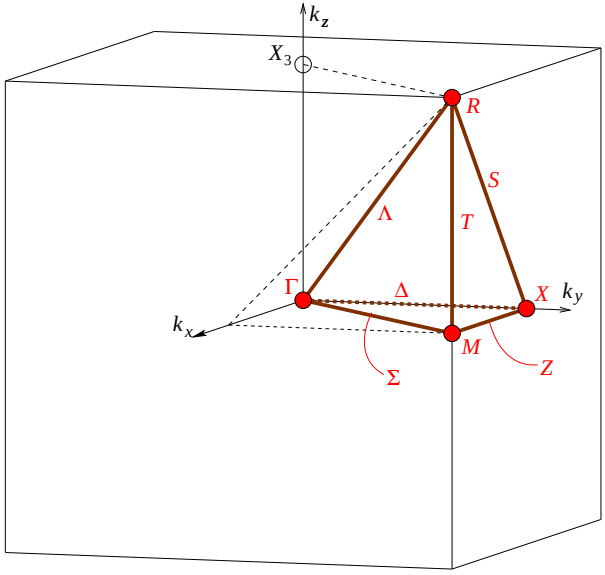
```
 GMAX=9.5      # smooth grid cut-off from LMFA

% const nk=10
BZ
 NKABC={nk} # k-mesh divisions

ITER
 NIT=50        # max scf iterations
```

- **NKABC**: can take three arguments (a,b,c) or one (all the same)
- **NKABC**: when one negative value given, value relates to full BZ, (a,b,c) are scaled according to reciprocal cell vector lengths

```
run > vi ctrl.srtio3
run > for i in -50 -100 -200 -500 -1000 -1e4
> do
> lmf -vnk=$i srtio3 >scflog_$i
> done
run > grep ^c save.srtio3
c nk=-50 ehf=-8505.4706686 ehk=-8505.4706653
c nk=-100 ehf=-8505.4717582 ehk=-8505.4717562
c nk=-200 ehf=-8505.4719586 ehk=-8505.471957
c nk=-500 ehf=-8505.4720141 ehk=-8505.4720126
c nk=-1e3 ehf=-8505.4720129 ehk=-8505.4720116
c nk=-1e4 ehf=-8505.4720128 ehk=-8505.4720116
run >
```

SrTiO3 – plot the band structure (simple)

- require path in $\vec{k}$



©bilbao crystallographic server
http://www.cryst.ehu.es

setup a file **qp.srtio3** describing the path...

```
68   0.5 0.0 0.0   0.0 0.0 0.0 # X--G
96   0.0 0.0 0.0   0.5 0.5 0.0 # G--M
68   0.5 0.5 0.0   0.5 0.5 0.5 # M--R
118  0.5 0.5 0.5   0.0 0.0 0.0 # R--G
0    0.0 0.0 0.0   0.0 0.0 0.0 # terminates
```

Cartesian $\vec{k}$ coordinates

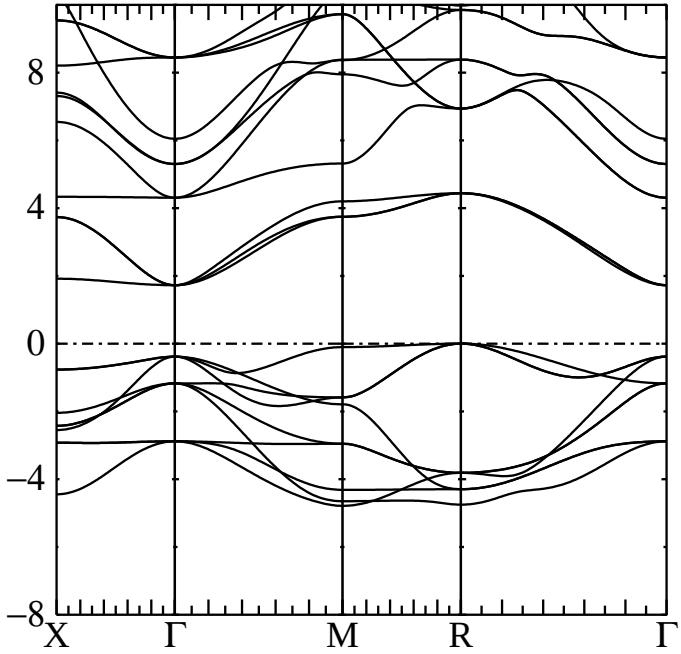
try to get reasonably equal spacing

rerun: **`lmf --band srtio3`**
(using converged potential contained in **rst** file)

gives new file: **bnds.srtio3** (ASCII $\varepsilon_{i,\vec{k}}$)

SrTiO3 – plot the band structure (simple)

- `echo -8,10,8,6 | plbnds -fplot -ef=0 -scl=13.6 -lbl=X,G,M,R,G bnds.srtio3`
- **`fplot`** – general plotting utility
- **`plbnds`** – bnds to plot tool
- options: emin, emax, width(cm), height(cm)
- **`fplot -disp -f plot.plbnds`**
  – gives you a .ps figure:
- lots of information:
  https://www.questaal.org/docs/misc/fplot/

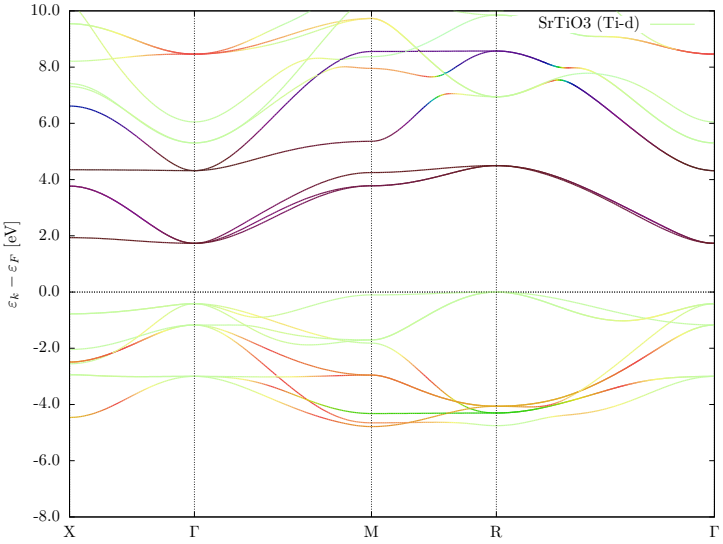


SrTiO3 – band structure with character

- first ask **lmf** for details of the order of the basis:
  `lmf --quit=ham --pr60 srtio3`

```
Orbital positions in hamiltonian, resolved by l:
 Site  Spec  Total    By l ...
   1    Sr     1:18   1:1(s)   2:4(p)   5:9(d)   10:10(s) 11:13(p) 14:18(d)
   2    Ti    19:36   19:19(s) 20:22(p) 23:27(d) 28:28(s) 29:31(p) 32:36(d)
   3    O     37:54   37:37(s) 38:40(p) 41:45(d) 46:46(s) 47:49(p) 50:54(d)
   4    O     55:72   55:55(s) 56:58(p) 59:63(d) 64:64(s) 65:67(p) 68:72(d)
   5    O     73:90   73:73(s) 74:76(p) 77:81(d) 82:82(s) 83:85(p) 86:90(d)
suham :  80 augmentation channels, 80 local potential channels  Maximum lmxa=3
```

- want the 10 Ti-d components (2-κ basis)
- run **lmf** again with options to the –band flag:
  `lmf --band col=23:27,32:36 srtio3`
- fplot does colouring well, also!



SrTiO3 – using local orbitals (1)

- **lmf** offers several ways of including semicore states in the valence: traditional local orbitals and extended local orbitals (their own $h(z)$)
- generally qualitative difference, sometimes significant
- when to include semicore-states?
  - reasonably shallow atomic states ($\varepsilon_i > -2.5 Ryd$)
  - atomic states that leak ($Q(r > r_{mt}) > 0.002e$)
- this is a change in the basis: re-run the atom solver **lmfa**
- a couple of new ctrl parameters

```
1
2  HAM            # options relating to the Hamiltonian
3   XCFUN=1       # LDA (VWN)
4  # XCFUN=0 101 130 #PBE-GGA using LibXC interface
5   AUTOBAS[MTO=2 LMTO=5 LOC=1 ELOC=-2.5 QLOC=0.002]
6                           # MTO=2: read from "basp" file
7                           # LMTO=5: use BIG basis
8                           # LOC=1: search for semicore states
9               # ELOC: atomic eigenvalue condition
10              # QLOC: semicore leakage condition
11  GMAX=9.5      # smooth grid cut-off from LMFA
```

SrTiO3 – using local orbitals (2)

```
1
2  HAM            # options relating to the Hamiltonian
3   XCFUN=1       # LDA (VWN)
4  # XCFUN=0 101 130 #PBE-GGA using LibXC interface
5   AUTOBAS[MTO=2 LMTO=5 LOC=1 ELOC=-2.5 QLOC=0.002]
6                           # MTO=2: read from "basp" file
7                           # LMTO=5: use BIG basis
8                           # LOC=1: search for semicore states
9              # ELOC: atomic eigenvalue condition
10             # QLOC: semicore leakage condition
11  GMAX=9.5      # smooth grid cut-off from LMFA
```

- **lmfa** finds Sr 4p ($-1.680 Ryd$) and Ti 3p ($Q(r > r_{mt}) = 0.0220$)

```
1  run > ls
2  ctrl.srtio3_5
3  run > lmfa ctrl.srtio3_5 >atomlog
4  run > grep -A5 "Find local" atomlog
5   Find local orbitals which satisfy E > -2.5 Ry  or  q(r>rmt) > 2e-3
6   l=1   eval=-1.680  Q(r>rmt)=0.0598  PZ=4.915  Use: PZ=14.915
7   l=2   eval=-9.422  Q(r>rmt)=3e-6  PZ=3.964  Use: PZ=0.000
8
9   tailsm: fit tails to 6 smoothed hankels, rmt= 2.60000, rsm= 1.30000
10  HNSMFT: 103 points in interval  2.60000  33.29923;  q=  1.785753
11 --
12  Find local orbitals which satisfy E > -2.5 Ry  or  q(r>rmt) > 2e-3
13  l=1   eval=-2.851  Q(r>rmt)=0.0220  PZ=3.926  Use: PZ=13.926
```

- syntax for local orbitals: `PZ` (l)
- +10 for extended local orbital (default and best)

SrTiO3 – using local orbitals (3)

- new basis file:

```
BASIS:
 Sr RSMH= 1.733 1.733 1.658 1.733 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.733 1.733 1.658 EH2= -0.9 -0.9 -0.9
     PZ= 0 14.915
 Ti RSMH= 1.467 1.467 1.091 1.467 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.467 1.467 1.091 EH2= -0.9 -0.9 -0.9
     PZ= 0 13.926
 O RSMH= 0.851 0.813 1.067 1.067 EH= -0.465 -0.1 -0.1 -0.1 RSMH2= 0.851 0.813 1.067 EH2= -1.265 -0.9 -0.9
```

- after running **lmfa**, copy `basp0.ext`→`basp.ext`

- the core Q has now changed as we move the semicore into the valence: **must rerun lmfa**

  – note that `GMAX` requirement may be now increased!

  (otherwise: "Exit -1 problem in locpot – possibly low LMXA, or orbital mismatch, species Sr")

- transition elements, high-lying (higher n than occupied) local orbitals are useful, too:
  - for Ti: `PZ= 0 13.926` becomes `PZ= 0 13.926 4.3`
  - high-lying local orbitals are of conventional type

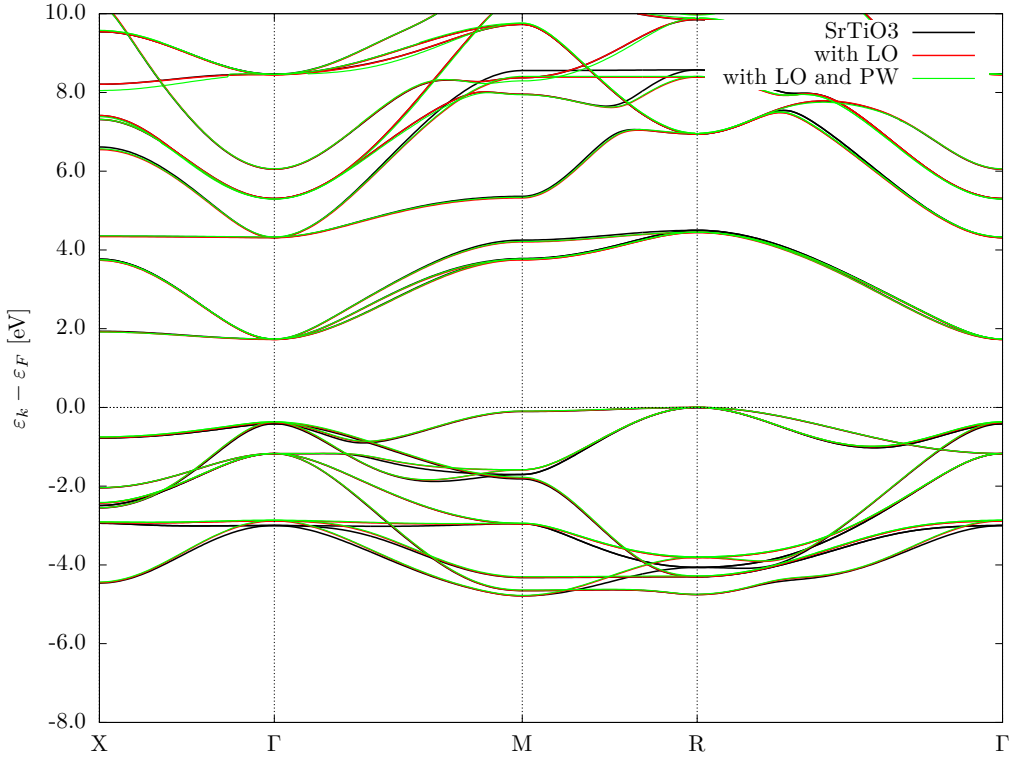
SrTiO3 – improving the basis with plane waves

- pretty easy to specify: cut-off energy
- necessary for more open structures
- remedies LMTO deficiencies

```
                        # LMTO=5: use BIG basis
                        # LOC=1: search for semicore states
             # ELOC: atomic eigenvalue condition
             # QLOC: semicore leakage condition
 GMAX=9.5      # smooth grid cut-off from LMFA
 PWMODE=11 PWEMIN=0.0 PWEMAX=2.0

BZ
 NKABC=10 10 10 # k-mesh divisions
```

- prefer **PWMODE=11**: cut-off relates to $(\vec{k} + \vec{G})$
- reduce r_{mt} if a large PW set is desired
- avoid over-completeness in difficult cases with **HAM_OVEPS=1e-10**
- beware that expense increases with **PWEMAX**
  (here, 2Ryd amounts to ~ 30 extra basis functions)

SrTiO3 – improving the basis with plane waves



- LMTO basis is already excellent (PW are not needed)
- the semi-core states are significant

automatic ctrl generator: blm (1)

- a lot of options and settings in the control file
- basis choices, particularly r_{mt}, can be difficult
- different variables needed for different kinds of calculations
- **blm** provides easy automated interface
- common choices represented by command line flags (see: `blm --help`)
- higher level interface to the code

automatic ctrl generator: blm (2)

workflow: **cif→init** using **cif2cell** (community python utility)

init→ctrl using **blm**

```
run > ls
MyBaseFileName_80872.cif
run > /opt/cif2cell-1.2.10/cif2cell MyBaseFileName_80872.cif > cif2cell.stdout
run > ls
MyBaseFileName_80872.cif cif2cell.stdout
run > cif2init cif2cell.stdout >cif2init.stdout
run > ls
MyBaseFileName_80872.cif cif2cell.stdout          cif2init.stdout          init
run > mv init init.srtio3
run > cat init.srtio3
HEADER Sr (Ti O3) (Strontium titanate)
LATTICE
#        SPCGRP=221
#        A=3.8996  B=3.8996  C=3.8996   ALPHA=90  BETA=90  GAMMA=90
% const a=3.8996
         ALAT={a}  UNITS=A
         PLAT=     1.0000000     0.0000000     0.0000000
                   0.0000000     1.0000000     0.0000000
                   0.0000000     0.0000000     1.0000000
SITE
      ATOM=Sr        X=      0.0000000     0.0000000     0.0000000
      ATOM=Ti        X=      0.5000000     0.5000000     0.5000000
      ATOM=O         X=      0.0000000     0.5000000     0.5000000
      ATOM=O         X=      0.5000000     0.5000000     0.0000000
      ATOM=O         X=      0.5000000     0.0000000     0.5000000
run > blm init.srtio3 >blmlog
run > ls
MyBaseFileName_80872.cif blmlog                   cif2init.stdout          log.srtio3
actrl.srtio3             cif2cell.stdout          init.srtio3              site.srtio3
```

automatic ctrl generator: blm (3)

output from **blm**:

```
makrm0: initial MT radii from first estat potential maximum
 site    spec             rmt       rmt-       rmt-       rold    lock
                                   <spec avg>  spec-min
   1     1:Sr            3.1085      0.0000     0.0000     0.0000
   2     2:Ti            2.0893      0.0000     0.0000     0.0000
   3     3:O             1.5945      0.0000     0.0000     0.0000
   4     3:O             1.5945      0.0000     0.0000     0.0000
   5     3:O             1.5945      0.0000     0.0000     0.0000
SCLWSR:  mode = 0  vol = 400.182 a.u.   Initial sphere packing = 53.7%  scaled to 71.8%
constr omax1=   0.0   0.0   0.0 %    omax2= 100.0 100.0 100.0 %
actual omax1=   0.0   0.0   0.0 %    omax2=   0.0   0.0   0.0 %

... Create input file actrl.dat (express mode 3)
IOSITE: wrote to file 'site', 5 sites

Wall-clock time: 0.148s. Resolution 0.000001s
```

- automatic scheme for finding r_{mt} based on potential landscape
- structure is placed in "site.dat" file – separates structure from ctrl variables
- EXPRESS category provides alias to common options

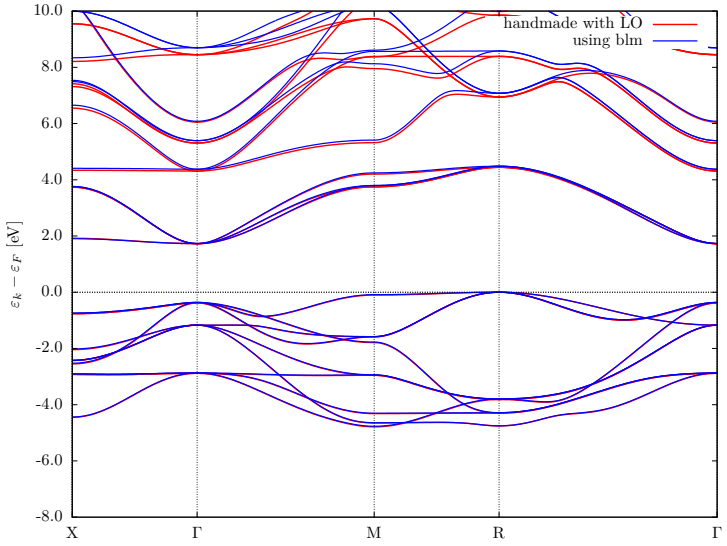
automatic ctrl generator: blm (4)

the generated **ctrl** file:

```
# Autogenerated from init.dat using:
# blm

# Variables entering into expressions parsed by input
% const nit=10
% const met=5
% const so=0 nsp=so?2:1
% const lxcf=2 lxcf1=0 lxcf2=0      # for PBE use: lxcf=0 lxcf1=101 lxcf2=130
% const pwmode=0 pwemax=3           # Use pwmode=1 or 11 to add APWs
% const nkabc=0 gmax=0

VERS  LM:7 FP:7 # ASA:7
IO    SHOW=f HELP=f IACTIV=f VERBOS=35,35  OUTPUT=*
EXPRESS
# Lattice vectors and site positions
  file=   site

# Basis set
  gmax=   {gmax}                   # PW cutoff for charge density
  autobas[pnu=1 loc=1 lmto=5 mto=4 gw=0]

# Self-consistency
  nit=    {nit}                    # Maximum number of iterations
  mix=    B2,b=.3,k=7              # Charge density mixing parameters
  conv=   1e-5                     # Convergence tolerance (energy)
  convc=  3e-5                     # tolerance in RMS (output-input) density

# Brillouin zone
  nkabc=  {nkabc}                  # 1 to 3 values
  metal=  {met}                    # Management of k-point integration weights in metals

# Potential
  nspin=  {nsp}                    # 2 for spin polarized calculations
```

automatic ctrl generator: blm (5)

```
  nspin=  {nsp}                    # 2 for spin polarized calculations
  so=     {so}                     # 1 turns on spin-orbit coupling
  xcfun=  {lxcf},{lxcf1},{lxcf2}   # set lxcf=0 for libxc functionals

#SYMGRP i*r3d r2(0,1,1)
HAM
      PWMODE={pwmode} PWEMIN=0 PWEMAX={pwemax} OVEPS=0 # For APW addition to basis
      FORCES={so==0} ELIND=-0.7
SPEC
  ATOM=Sr        Z= 38  R= 3.615925  LMX=3  LMXA=3
  ATOM=Ti        Z= 22  R= 2.089718  LMX=2  LMXA=4
  ATOM=O         Z=  8  R= 1.594872  LMX=2  LMXA=3
```



- very good agreement (eg, $\Delta E_g = 8$meV)
- **LMX** increased for Sr
- **LMXA** increased for Ti
  (l cut-off for augmentation)
- difference in empty states due to large
  $r_{mt} = 3.6$bohr on Sr
- **blm** much better than my guess!

Advice

- ctrl file:
  - use the **blm** to setup r_{mt}; use `--gw` for GW setup
  - check the `--help` and `--input` to see if what you want is there
- LDA setup
  - use a large basis (eg, `AUTOBAS_LMTO=5`)
  - the default basis setup (`EH,RSMH`) should be satisfactory "out of the box"
  - (also **`lmf --optbas`**, ..!)
  - semicore local orbitals should be included when present
  - use **lmfa** recommendation for `GMAX`, but test for convergence
  - consider plane waves for tricky open structures (`PWEMAX=2Ryd` goes a long way)
- in general
  - *many* tools and utilities to setup different systems, obtain properties and analyse data
  - just ask us! ☺
  - Se relaxation: https://www.questaal.org/tutorial/lmf/molstat/

lmf – Questaal's Full Potential LMTO Code

Part 1: Practical introduction and overview of the lmf code

- full-potential implementation & basis
- verification exercise results

Part 2: Using the lmf code

- walk-through of $SrTiO_3$ calculation

Part 3: Hands-on example

- Se relaxation

  please navigate to: https://www.questaal.org/tutorial/lmf/molstat/