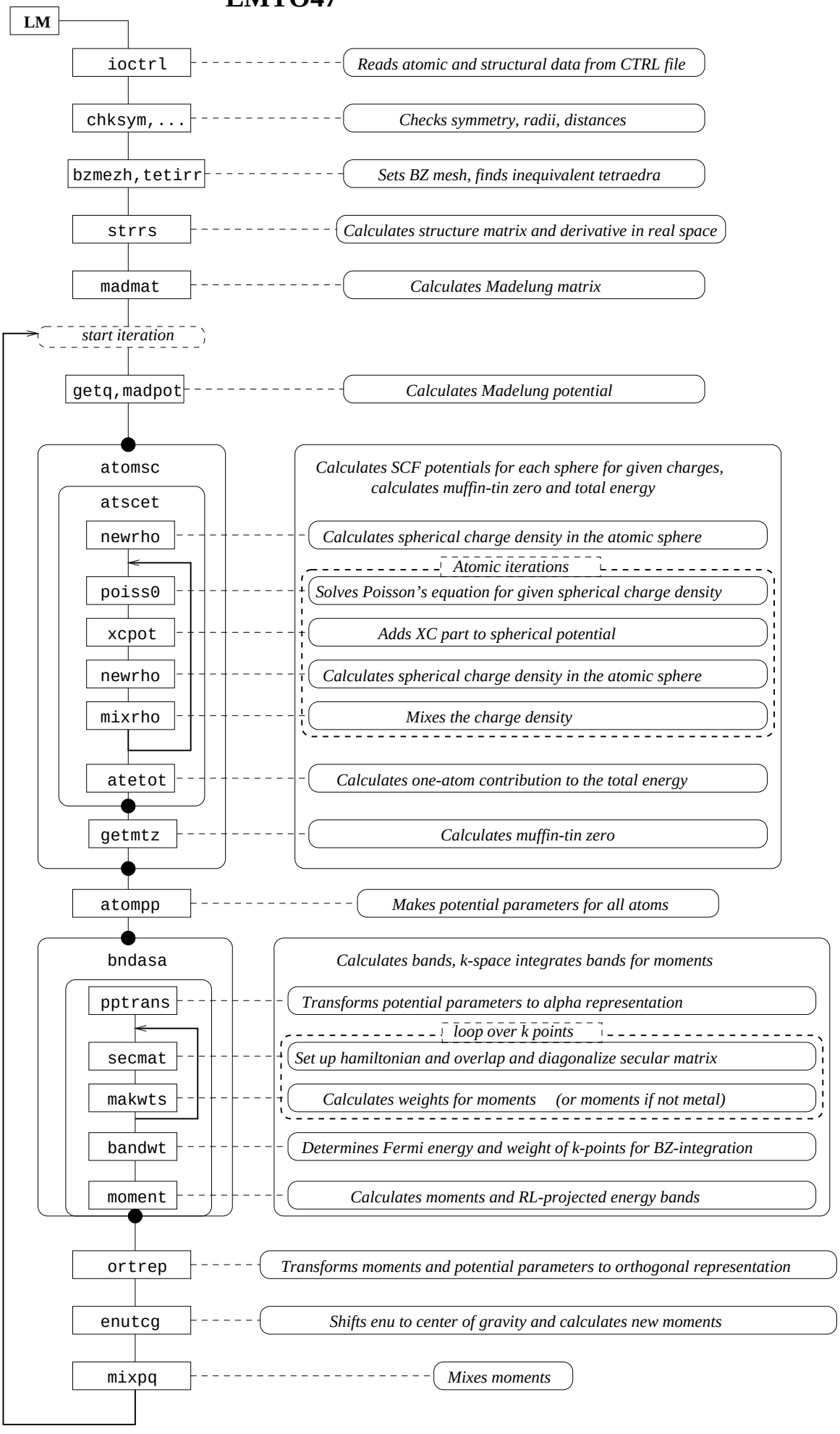
LMTO47


LM
ioctrl
Reads atomic and structural data from CTRL file
chksym,...
Checks symmetry, radii, distances
bzmezh,tetirr
Sets BZ mesh, finds inequivalent tetraedra
strrs
Calculates structure matrix and derivative in real space
madmat
Calculates Madelung matrix
start iteration
getq,madpot
Calculates Madelung potential
atomsc
atscet
Calculates SCF potentials for each sphere for given charges, calculates muffin-tin zero and total energy
newrho
Calculates spherical charge density in the atomic sphere
Atomic iterations
poiss0
Solves Poisson's equation for given spherical charge density
xcpot
Adds XC part to spherical potential
newrho
Calculates spherical charge density in the atomic sphere
mixrho
Mixes the charge density
atetot
Calculates one-atom contribution to the total energy
getmtz
Calculates muffin-tin zero
atompp
Makes potential parameters for all atoms
bndasa
Calculates bands, k-space integrates bands for moments
pptrans
Transforms potential parameters to alpha representation
loop over k points
secmat
Set up hamiltonian and overlap and diagonalize secular matrix
makwts
Calculates weights for moments (or moments if not metal)
bandwt
Determines Fermi energy and weight of k-points for BZ-integration
moment
Calculates moments and RL-projected energy bands
ortrep
Transforms moments and potential parameters to orthogonal representation
enutcg
Shifts enu to center of gravity and calculates new moments
mixpq
Mixes moments