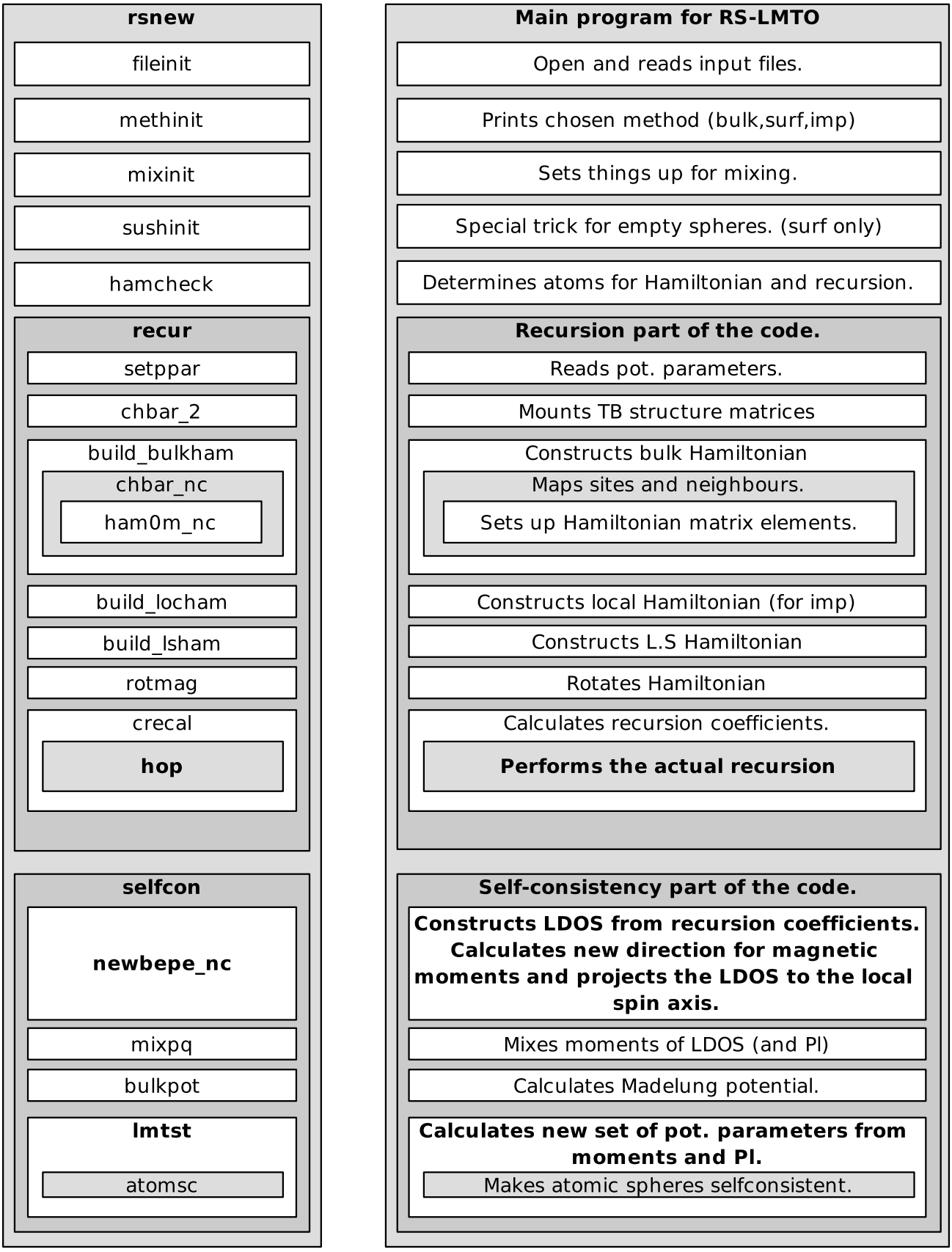
rsnew
fileinit
methinit
mixinit
sushinit
hamcheck
recur
setppar
chbar_2
build_bulkham
chbar_nc
ham0m_nc
build_locham
build_lsham
rotmag
crecal
hop
selfcon
newbepe_nc
mixpq
bulkpot
lmtst
atomsc
Main program for RS-LMTO
Open and reads input files.
Prints chosen method (bulk,surf,imp)
Sets things up for mixing.
Special trick for empty spheres. (surf only)
Determines atoms for Hamiltonian and recursion.
Recursion part of the code.
Reads pot. parameters.
Mounts TB structure matrices
Constructs bulk Hamiltonian
Maps sites and neighbours.
Sets up Hamiltonian matrix elements.
Constructs local Hamiltonian (for imp)
Constructs L.S Hamiltonian
Rotates Hamiltonian
Calculates recursion coefficients.
Performs the actual recursion
Self-consistency part of the code.
Constructs LDOS from recursion coefficients. Calculates new direction for magnetic moments and projects the LDOS to the local spin axis.
Mixes moments of LDOS (and Pl)
Calculates Madelung potential.
Calculates new set of pot. parameters from moments and Pl.
Makes atomic spheres selfconsistent.