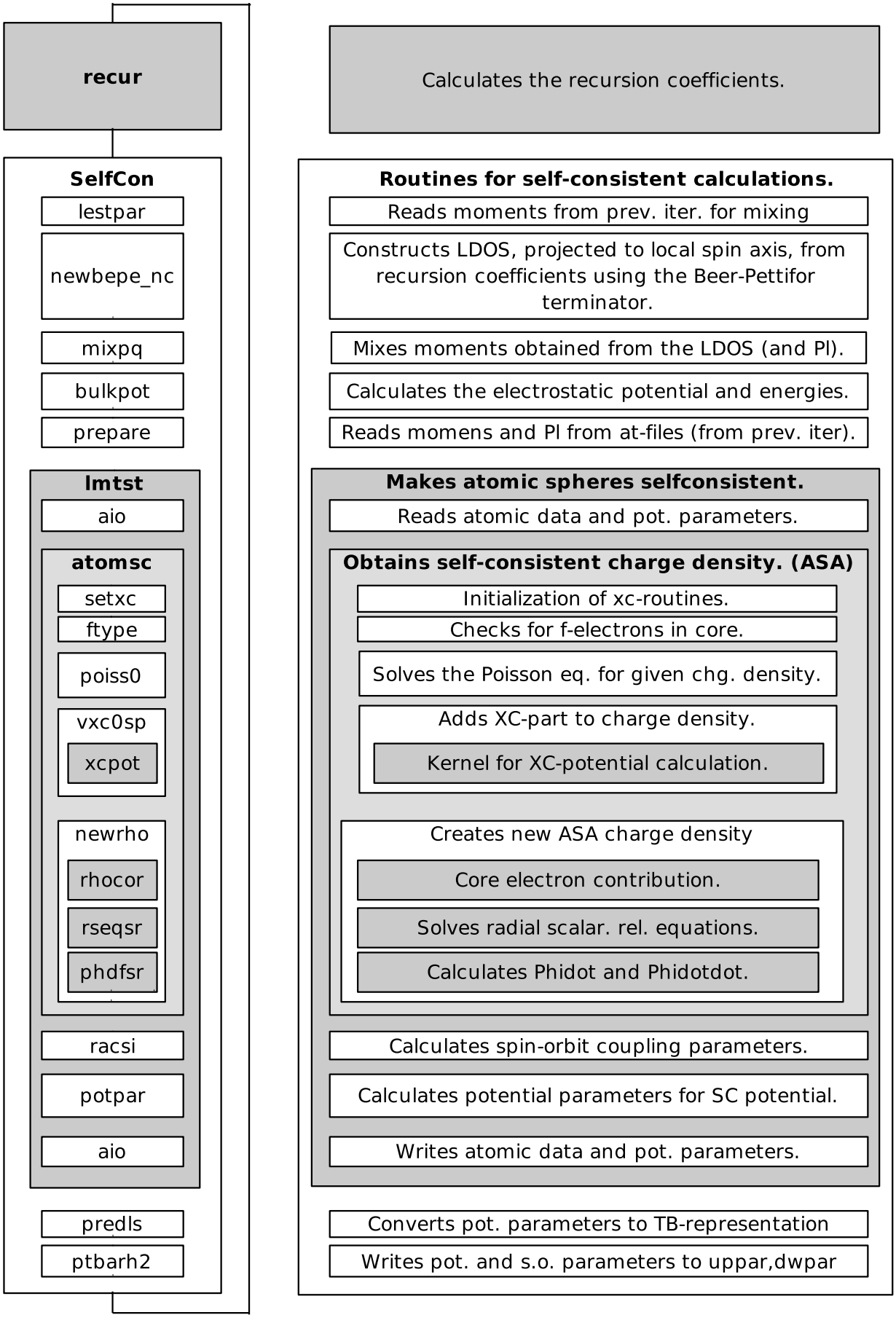
recur
Calculates the recursion coefficients.
SelfCon
Routines for self-consistent calculations.
lestpar
Reads moments from prev. iter. for mixing
newbepe_nc
Constructs LDOS, projected to local spin axis, from recursion coefficients using the Beer-Pettifor terminator.
mixpq
Mixes moments obtained from the LDOS (and Pl).
bulkpot
Calculates the electrostatic potential and energies.
prepare
Reads momens and Pl from at-files (from prev. iter).
lmtst
Makes atomic spheres selfconsistent.
aio
Reads atomic data and pot. parameters.
atomsc
Obtains self-consistent charge density. (ASA)
setxc
Initialization of xc-routines.
ftype
Checks for f-electrons in core.
poiss0
Solves the Poisson eq. for given chg. density.
vxc0sp
Adds XC-part to charge density.
xcpot
Kernel for XC-potential calculation.
newrho
Creates new ASA charge density
rhocor
Core electron contribution.
rseqsr
Solves radial scalar. rel. equations.
phdfsr
Calculates Phidot and Phidotdot.
racsi
Calculates spin-orbit coupling parameters.
potpar
Calculates potential parameters for SC potential.
aio
Writes atomic data and pot. parameters.
predls
Converts pot. parameters to TB-representation
ptbarh2
Writes pot. and s.o. parameters to uppar,dwpar