KKRimp subroutines

amn2010.f90:
Module handling the structure constants for the intersite potential
Category: electrostatics, potential, KKRimp

amngaunt.f:
Module handling the Gaunt coefficients for the structure constants used in the intersite potential
Category: electrostatics, potential, special-functions, KKRimp

arrayparams.f90:
Module handling common array dimensions
Category: initialization, KKRimp

averagewldau.f:
Module handling the averaged LDA+U potential
Category: potential, lda+u, KKRimp

beshan.f:
Module handling spherical bessel, hankel and neumann functions
Category: special-functions, single-site, reference-system, KKRimp

beshank.f:
Module handling spherical bessel, hankel and neumann functions for SRA
Category: special-functions, single-site, KKRimp

beshanksra.f90:
Seems to be a partial copy of beshank.f, not used anywhere
Category: special-functions, KKRimp

bessel1.f:
Module handling spherical bessel, hankel and neumann functions
This version is used by the routine that constructs the transformations for shifted positions
Category: special-functions, single-site, KKRimp
*** Could make the intents and variable comments appear in the right place ***

calcJij.f90:
Subroutine that computes the exchange interactions using the non-relativistic collinear formula
Not used anywhere, unfinished
Category: physical-observables, potential, KKRimp

calccouplingconstants.f90:
Module handling the relativistic exchange interactions
Category: physical-observables, input-output, KKRimp

calcforce.f90:
Module handling the calculation of the forces
Category: physical-observables, KKRimp