Software Spec – Atom Class

This class solves the radial Schrodinger equation for all electrons to obtain the wave functions Pnl(r), energy eigenvalues Enl, and total potential V(r) for an atom of given atomic number Z and electronic configuration.

The main solve routine uses the BoundRSESolver class to solve the radial schrodinger equation for a single orbital.

# Background

Inputs:

* Atomic number Z
* Electronic configuration

Outputs:

* The total atomic potential V(r)
* All atomic orbitals (including Pnl(r) and Enl)
* The radial mesh

Program Flow:

1. Vtrial = a starting potential V
   1. Take from Herman & Skillman tables
   2. Create from basic functional form (Thomas-Fermi function)
2. For each orbital in the configuration
   1. Call BoundRSESolver with Vtrial
3. Vnew = HermanSkillmanPotential(orbitals)
4. If Vnew – Vtrial < tolerance, then done
   1. Criteria is that maximum % difference in the potential is less than tol.
5. Create new trial potential.
   1. Herman and Skillman recommend using the average of Vnew and the old Vtrial.
6. Loop to (2)