LUND UNIVERSITY
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GRASP2k

A General Relativistic Atomic Structure Package

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Description Grasp2k [1] is a general system for the calculation of relativistic atomic structure and properties, based upon Multiconfiguration Dirac-Hartee-Fock (MCDHF) theory as outlined by for example I.P. Grant [2].

The starting point for our approach is to describe the atom by an independent particle and central field model, corrected by a configuration state function (CSF) expansion to treat electron correlation

$$\psi(\Gamma, J, M_J) = \sum_i c_i \Phi(\gamma_i, J, M_J)$$

Each of these CSF's are constructed as a coupled antisymmetric sum of products of one-electron Dirac-orbitals,

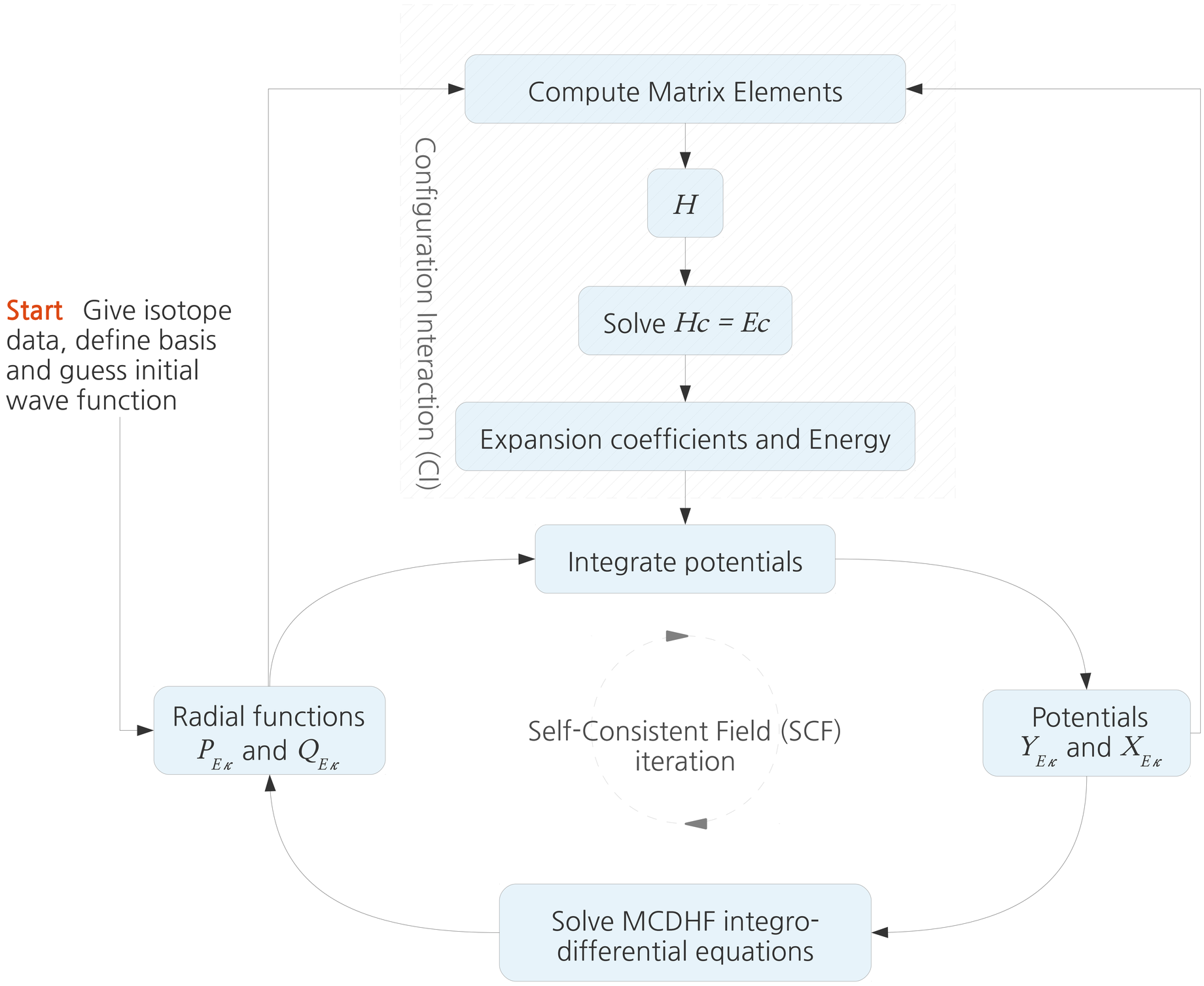
$$\Phi(r, \theta, \varphi, \sigma) = \frac{1}{r} \begin{pmatrix} P_{E\kappa}(r)\chi_{\kappa m}(\theta, \varphi, \sigma) \\ iQ_{E\kappa}(r)\chi_{-\kappa m}(\theta, \varphi, \sigma) \end{pmatrix}$$

according to angular momentum coupling theory. The spin-angular part is assumed to be known, the radial functions $P_{E\kappa}$ and $Q_{E\kappa}$ and the expansion coefficients, c_i remain to be determined.

Advantages A general ab-initio and fully relativistic method on QED level, applicable to in principle any atomic system, ranging from negative to highly positively charged ions.

Limitations Truncation of basis is necessary, QED-effects are only included as perturbation.

Numerical Methods Eigenvalue problem, Self-Consistent Fields, ODE's solved with finite difference, B-splines (in progress)



[1] Jönsson P, He X, Froese Fischer C and Grant I.P. 2007 *Comput. Phys. Commun.* 177 597
[2] Grant I P 2007 *Relativistic Quantum Theory of Atoms and Molecules: Theory and Computation* (Springer Series on Atomic, Optical and Plasma Physics) (Berlin: Springer)

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