**THE EUROPEAN
PHYSICAL JOURNAL D**

Regular Article - Atomic Physics

A FAC potential for AUTOSTRUCTURE

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Abstract. We describe the implementation of the current Flexible Atomic Code (FAC) unique electron central potential within the AUTOSTRUCTURE code. We show that the two codes then give the same atomic data for all practical application purposes. However, AUTOSTRUCTURE has more flexible potential options which can lead to a more accurate description of atomic processes, especially in low-charged ions.

1 Introduction

This paper describes features available in AUTOSTRUCTURE (AS) that require use of the current public version (30.x) which can be found at: http://amdpp.phys.strath.ac.uk/autos/autos-30/. The discussion
below assumes a working knowledge of AS and familiarity with the contents of its current documentation http://amdpp.phys.strath.ac.uk/autos/autos-30/WRITEUP.

1.1 Motivation

The Flexible Atomic Code (FAC) of Gu [7] is in widespread use. As such, users of different atomic codes (e.g., AUTOSTRUCTURE) can encounter the questions:
'Why are you not using FAC?'
and
'Why do your results differ from those of FAC?'
This paper attempts to help you answer these questions.
(Note: we are concerned here only with the calculation of atomic data and not plasma population modeling.)

1.2 Background

AS and FAC have a key common feature—they are both 'distorted-wave' codes, i.e., they solve uncoupled radial equations. This distinguishes them from Hartree–Fock and Dirac–Fock structure codes, which solve coupled radial equations, and, similarly, collision codes such as R-matrix.

FAC is fully relativistic: it solves the four-component Dirac equation. It includes the Breit interaction in the Hamiltonian (+QED).
AS is semi-relativistic: it solves the kappa-averaged Dirac equation (and usually neglects the small component, renormalizing the large component instead). It includes the Breit interaction in the Pauli approximation in the Hamiltonian (+QED).
The K-shell of Uranium aside, these differences are not important, in general.
As always, the configuration interaction (CI) expansion is key—the larger the CI expansion, the more complete our basis.
But, if we use the same CI expansion, what is the main source of difference between AS and FAC then?
The answer lies in the distorted-wave potential(s) used by the two codes.

The key difference between FAC and AS is that FAC uses a unique potential

The use of unique potential gives rise to a unique set of orthogonal orbitals. But, no matter whether they be bound, continuum, or are used to represent both N- and $(N-1)$-electron atoms and ions in describing bound-free atomic processes (e.g., autoionization, photoionization), all orbitals are described by the same single distorting potential within FAC.
In contrast, while AS can use a unique potential such as Thomas–Fermi, it is free to use different potentials as it or the user sees fit: for bound vs continuum or different charge states. The use of such potentials gives rise to both non-orthogonal and/or non-unique orbitals. This (apparently) gives rise to a much more complicated atomic structure problem which needs to take account of all the overlap integrals, and which disappears on using a unique potential.
However, we follow the approach of Cowan [4] whose Hartree–Fock relativistic (HFR) approach is inherently

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non-orthogonal (which follows directly from solving the kappa-averaged HFR equations). This approach involves taking all bound orbital overlap integrals to be zero or unity based on whether $n \neq n'$ or $n = n'$, for $l = l'$. AS includes the resulting exchange overlap integrals for the continuum as well. It is justified by the long experience with HFR (and AS) in comparison of their results with those from HF and DF codes, as well as experiment.

The flexibility of AS with regard to potentials and the orbitals they describe part ways answers the questions raised at the start. However, a more powerful response is to be able to reproduce the unique FAC potential within AS and hence obtain comparable results. One is then free to use such or to argue for a different choice of atomic structure available within AS, but not FAC.

However, constructing the FAC potential within AS requires a little work and understanding.

We first note FAC versions in use. The last official release of FAC is v1.1.4 dated 2016.11.9. Most users make use of the unreleased v1.1.5. Specifically, for this work we used FAC v1.1.5 dated 2023.03.23 from GitHub, while an earlier version of 1.1.5 used is dated 2020.04.20 on GitHub. We refer to these versions unofficially as FAC 2020 and FAC 2023.

2 Constructing a FAC potential for AS—part 1 (a history lesson)

Like the Slater–Type–Orbital (STO) potential (Burgess et al, [3]) available in AS for some time, the FAC potential is based on a shell-structure description of the ion in question. It is actually closely related to the average energy of a configuration.

We start off by detailing the potential V_α seen by an electron (of orbital) α, in a configuration of an N-electron ion due to the other $N-1$ electrons in the same configuration. Let ω_α denote the occupation numbers which define the configuration. Then $\sum_\alpha \omega_\alpha = N$. In the configuration-average approximation [4]

$$
\begin{aligned}
V_\alpha(r) = & \sum_\beta (\omega_\beta - \delta_{\alpha\beta}) Y_{\beta\beta}^0(r) \\
& - \sum_\beta (\omega_\beta - 1) \delta_{\alpha\beta} \sum_{\lambda > 0} f_{\beta\beta}^\lambda Y_{\beta\beta}^\lambda(r) \\
& - \sum_\beta (1 - \delta_{\alpha\beta}) \omega_\beta \sum_\lambda g_{\alpha\beta}^\lambda Y_{\alpha\beta}^\lambda(r) \rho_{\alpha\beta}(r)/\rho_{\alpha\alpha}(r)
\end{aligned}
\tag{1}
$$

where the sum over β is over all orbitals (including α) of the configuration in question.

The corresponding interaction energy (E_α) between an electron α and all other electrons is given by

$$
E_\alpha = \int_0^\infty V_\alpha(r) \rho_{\alpha\alpha}(r) \mathrm{dr}.
\tag{2}
$$

Then,

$$
\bar{E} = \frac{1}{2} \sum_\alpha \omega_\alpha E_\alpha
\tag{3}
$$

is the total electron–electron Coulomb average energy of the configuration.

Here,

$$
Y_{\alpha\beta}^\lambda(r) = \int \frac{r_<^\lambda}{r_>^{\lambda+1}} \rho_{\alpha\beta}(r') \mathrm{dr}'
\tag{4}
$$

where $r_<, r_> = \min, \max(r, r')$, respectively, and $\rho_{\alpha\beta}$ is the probability density, given by

$$
\rho_{\alpha\beta}(r) = P_\alpha(r) P_\beta(r) + \{Q_\alpha(r) Q_\beta(r)\}
\tag{5}
$$

(and where the small component Q_α may, or may not, be included.)

Finally, if α represents $n_\alpha l_\alpha$ (e.g., in AS), then

$$
f_{\alpha\alpha}^\lambda = \frac{2l_\alpha + 1}{4l_\alpha + 1} \begin{pmatrix} l_\alpha & \lambda & l_\alpha \\ 0 & 0 & 0 \end{pmatrix}^2
\tag{6}
$$

and

$$
g_{\alpha\beta}^\lambda = \frac{1}{2} \begin{pmatrix} l_\alpha & \lambda & l_\beta \\ 0 & 0 & 0 \end{pmatrix}^2
\tag{7}
$$

while if α represents $n_\alpha l_\alpha j_\alpha$ (e.g., in FAC) then

$$
f_{\alpha\alpha}^\lambda = \frac{1}{2j_\alpha + 1} \begin{pmatrix} j_\alpha & \lambda & j_\alpha \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}^2
\tag{8}
$$

and

$$
g_{\alpha\beta}^\lambda = \begin{pmatrix} j_\alpha & \lambda & j_\beta \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}^2.
\tag{9}
$$

We note that line 1 in equation (1) is just the static potential term used by the STO potential of Burgess et al [3] which is incorporated into AS. It can be evaluated analytically when the $P_\alpha(r)$ are STOs. The introduction of adjustable scaling parameters (λ_α) in this analytic potential combined with the minimization of $< H >$ means the remaining two lines (due to equivalent electrons and exchange, respectively) can be neglected.[1]

Instead, let us consider using the STO potential (flagged by NZION< 0 in the AS NAMELIST SMINIM input—see WRITEUP) to start off a self-consistent iteration (PPOT='SCCA' in SMINIM) using the full expression in (1). The occupation numbers ω_α are defined as in the STO case. For example, for each orbital α the user flags (via MCFMX in SMINIM) the

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[1] The addition of a local exchange STO potential to the static one is an option in AS.

configuration to be used by AS to define the occupation numbers to be used in (1) for that orbital. In the case of fully relaxed orbitals (BASIS='RLX' in the AS NAMELIST SALGEB input) the occupation numbers are trivially known by AS. In all instances described so far, the potential is orbital dependent due to (1) taking account of self-screening, i.e., if $\sum_\alpha \omega_\alpha = N$ then $rV_\alpha(r) \to N - 1$ as $r \to \infty$.

A unique potential $V_\alpha = V$ can be imposed by the user defining (NOCC via SMINIM) occupation numbers such that $\sum_\alpha \omega_\alpha = N - 1$ and the account of self-interaction in (1) is then switched off. The usual choice for the occupation numbers ω_α in this instance is those of the ground configuration of the next ionization stage—see the discussion in Tanaka *et al* [14] in relation to HULLAC [2] and AS Working Notes No. 1 [1] in relation to AS.

FAC takes an alternative approach [7]. It forms a unique potential by averaging the V_α of (1) over the probability densities $\rho_{\alpha\alpha}$ (and occupation numbers ω_α), viz.

$$V(r) = \frac{\sum_\alpha \omega_\alpha V_\alpha(r)\rho_{\alpha\alpha}(r)}{\sum_\alpha \omega_\alpha \rho_{\alpha\alpha}(r)} \qquad (10)$$

and

$$\frac{1}{2}\int_0^\infty V(r)\sum_\alpha \omega_\alpha \rho_{\alpha\alpha}(r)\mathrm{d}r = \frac{1}{2}\sum_\alpha \omega_\alpha \mathrm{E}_\alpha = \bar{\mathrm{E}} \quad (11)$$

is again the electron–electron Coulomb average energy of the configuration defined by ω_α.

If the user supplies a unique set of occupation numbers ω_α such that $\sum_\alpha \omega_\alpha = N$ then again $rV(r) \to N - 1$ as $r \to \infty$, by inspection of (1) and (10).

The choice as to whether N corresponds to the recombined or recombining ion in bound-free problems is not set by FAC, the user must choose—Gu [7] recommends the use of N rather than $N - 1$. In contrast, if the user does not specify the occupation numbers, then FAC uses the mean of the subconfiguration occupation numbers meant over all subconfigurations.

This completes the detailing of the original unique FAC potential described by Gu [7] now available in v30.x of AS. It can be switched on by adding FAC='OLD'[2] to SMINIM, together with NOCC occupation numbers[3] such that $\sum_\alpha \omega_\alpha = N$, so as to obtain screening by $N - 1$ electrons.

Although NZION< 0 and PPOT='SCCA' are implicitly required, the flagging of FAC operation by the user is sufficient. AS automatically switches them on necessarily so. In addition, AS also automatically sets all flags necessary to align its operation with those of the FAC default operation. Note, the default user cannot accidentally reset such to conflict with FAC. An expert

flag is available for developers to override this operation.

3 Constructing a FAC potential for AS—part 2 (the present day)

Despite Gu [7], the FAC potential just described has not been used by FAC since its early days [9]. Gu [6] already noted the use by FAC of a Dirac–Hartree–Slater (DHS) potential. The basic DHS potential (or Dirac–Fock–Slater, DFS) is the same as that described in detail by Cowan (1981, Sec 7.11) under the Hartree–Fock–Slater (HFS) method. The analogous Dirac form is described by Sampson *et al* [12].

Using the notation introduced in part 1, the unique DHS potential is given in terms of the direct static term again plus a *local* exchange potential

$$V(r) = \sum_\beta \omega_\beta Y_{\beta\beta}^0(r) - a\frac{3}{2}\left[\frac{24}{\pi}\rho(r)\right]^{1/3}. \qquad (12)$$

The term in $\rho(r)$ without subscripts is the total spherically averaged electron number density, viz.

$$\rho(r) = \frac{1}{4\pi r^2}\sum_\alpha \omega_\alpha \rho_{\alpha\alpha}, \qquad (13)$$

such that (dV is the volume element here)

$$\int \rho(r)\mathrm{d}V = N. \qquad (14)$$

The coefficient $a = 1/2$ a.u. in equation (12) gives the original Slater derivation. Subsequently, the Kohn–Sham [10] value of $a = 1/3$ a.u. was found to give better agreement with Hartree–Fock—see Cowan [4] for a detailed discussion. Sampson *et al* [12] adopt $a = 1/3$ a.u. as well in the Los Alamos Relativistic ATomic Structure (RATS) code suite.

More generally, a can be treated as an optimizable parameter. Indeed, FAC uses a look-up table of values for a which were pre-optimized on the ground configuration of the ion defined by Z and N. Actually, FAC collects all the numerical factors together in terms of a variable AHX a.u. (i.e., AHX $= (1/3)(3/2)(6/\pi^2)^{1/3} = 0.4235$ a.u. for the above) and it is this rather than a which is held in the look-up table.

The FAC look-up table has been ported into AS

It is also possible for the user to set their own value of AHX directly, using the AS variable FAC_AHX in SMINIM.[4]

---

[2] FAC='NO' is the default for PPOT='SCCA', which then uses the V_α potentials of equation (1).
[3] Only the occupation numbers for the valence orbitals should be supplied.

---

[4] TBD: allow AS to optimize FAC_AHX itself using the usual AS optimization flags save that there is a single scaling and variational parameter (so NLAM/NVAR are ignored.)
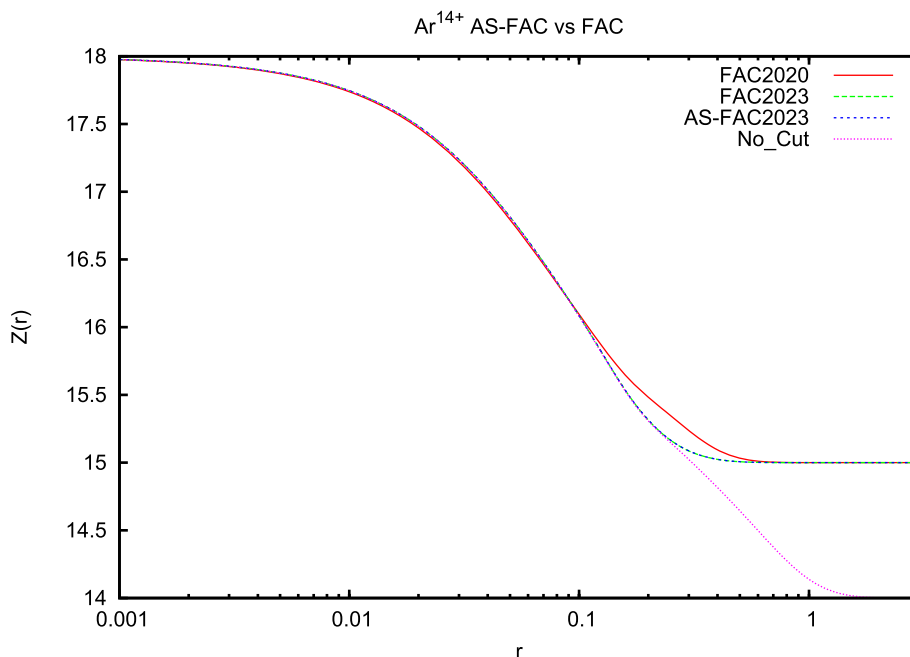
Fig. 1 Effective charges for be-like Ar^{14+}

As is well known, the drawback with 'Hartree–Slater' methods is that for $\sum_\alpha \omega_\alpha = N$

$$rV(r) \to N \qquad \text{as} \qquad r \to \infty, \qquad (15)$$

instead of the desired value of $N-1$.

Rather than the user supplying occupation numbers $\sum_\alpha \omega_\alpha = N-1$, the FAC default is to make use of the Latter [11] cut-off:

$$V(r) = \min\left(V(r), \frac{N-1}{r}\right), \qquad (16)$$

which is only problematic accuracywise for near neutrals [4]. Note: FAC additionally smooths $V(r)$ around the switch-over r—the same smoothing has been adopted by AS.

Aside, slight differences in the FAC DHS potential arise because the Latter cut-off in equation (16) was originally (e.g., to at least 2020) applied to the direct potential only. Subsequently (e.g., by 2023), it was applied to the total (direct-plus-exchange), Gu [9].

This is likely of no consequence to the general user, given that AS ultimately uses kappa-averaged orbitals, but it is possible for the expert user to recover this earlier operation if necessary. Note the look-up table and smoothing are unchanged between '2020' and '2023' operation.

In Fig. 1, we plot above various effective charges

$$Z(r) = Z_0(r) - rV(r), \qquad (17)$$

where $Z_0(r)$ is the finite nucleus charge, for Be-like Ar^{14+} to illustrate.

We see that the AS-FAC2023 and FAC2023 curves are indistinguishable.

This completes the detailing of the **current** unique FAC potential described by Gu [9] now available in v30.x of AS. It can be switched on by adding FAC='YES'[5] to SMINIM again together with the NOCC valence occupation numbers such that $\sum_\alpha \omega_\alpha = N$ still, so as to obtain screening by $N-1$ electrons. Again, **AS itself sets all flags necessary to align its operation with that of FAC.**

The default AS implementation follows the FAC v1.1.5 2023.03.23 Dirac–Hartree–Slater implementation.

4 Detailed benchmarking of AS-FAC against FAC

We consider a model problem, involving only s-orbitals; then we should be solving the same Dirac equation and thus obtain the same epsilon orbital energies. We compare AS results obtained by 1/ calculating the FAC potential within AS, 2/ reading the FAC potential written by FAC GetPotential, and 3/ running FAC itself. The same physical occupation numbers are used in AS and FAC (via AvgConfig & OptimizeRadial). All potentials use the FAC2023 Dirac–Hartree–Slater local exchange form.

AS-FAC vs FAC epsilons (Ryd) for H-like, He-like & Be-like Ar, ground configs only.

---

[5] FAC='NEW' is also supported to contrast with 'OLD'.

```
H-like:    AS-FAC           FAC2023        Diff
1s:        -325.408963      -325.408872    0.00011
           ASreadFACpot
           -325.408954
```

There is nothing to iterate here since there is just the nuclear potential. We both appear to use a similar Fermi finite nucleus. The difference between AS-FAC and FAC epsilons is likely down to numerics. (The AS radial mesh accurate to a few e-6 Ryd here.)

```
He-like:   AS-FAC           FAC2023        Diff
1s^2:      -302.23469       -302.235963    0.00127
           ASreadFACpot : recommended 8 s.f.
           -302.23604
           ASreadFACpot : FAC2023 default 6 s.f.
           -302.22828
```

The AS-FAC epsilons here are converged to 1.d-5 Ryd.
AS-FAC is not sensitive to the starting potential.
(The AS radial mesh here is accurate to a few e-5 Ryd.)

```
Be-like:   AS-FAC           FAC2023        Diff
1s^2 2s^2: -283.58005       -283.580272    0.00022
           -62.13629        -62.139234     0.00294
           ASreadFACpot : recommended 8 s.f.
           -283.58031
           -62.13925
           ASreadFACpot : FAC2023 default 6 s.f.
           -283.57717
           -62.13889
```

When we read the FAC potential produced by GetPotential into AS then the AS epsilons are in very close agreement with the original FAC ones. (This is provided we add more significant figures to the GetPotential output file, FAC 2020.04.20 only uses 4 s.f., while FAC 2023.03.23 uses 6 s.f., but 8 s.f. is recommended for AS to achieve closest agreement with the native FAC epsilons.)

Differences in epsilon (e.g., for non s-orbitals) should not translate into as large differences in level energies of course since we are just playing with perturbation theory. It appears that epsilons are not the main source of differences in level energies.

For example, He-like $1s^2 + 1s2s$ (with 1 s and 2 s occ. nos 1.5 and 0.5) gives

5 A case study: O^{5+} KLn autoionization rates

We compare various AS and FAC results for three autoionizing levels which we [5] have found to be sensitive to the calculational method and which contribute strongly to the He-like satellite lines.

The three levels in question are:

1: $1s2p(^1P)3d\,^2F_{7/2}$
2: $1s2p(^1P)4d\,^2F_{7/2}$
3: $1s2p(^1P)4p\,^2D_{5/2}$

Our original calculations with AS made use of the fully relaxed orbital basis and the historic STO model potential and are denoted AS-RLX.

We examined the use of several sets of occupation numbers for the unique FAC potential. We label them by XX = 3, 2A and 2B, where 3 represents the Li-like stage and 2X the He-like, as follows:

```
    1s  2s   2p
3 : 2  1/3  2/3

2A: 1  1/3  2/3

2B: 2   0    0
```

Note, FAC then splits the 2/3 2p occupation number as 1/3 and 1/3 for the $2p_{1/2}$ and $2p_{3/2}$ orbitals.

The AS input file can be found in the Appendix

We label the corresponding results AS-FACXX and FACXX, where AS-FACXX denotes an AS calculation using the unique DHS FAC potential detailed in Sect. 3 and FACXX denotes a FAC calculation.

```
Epsilons                   AS-FAC          FAC2023       Diff
1s:                        -306.08865      -306.09173    0.0031
2s:                        -74.26285       -74.26311     0.0003

Level energies (inc. QED)
2*S+1  L   2J   CF          AS-FAC          FAC2023       Diff
  1    0   0    1          -628.0816091    -628.0882704  0.0067
  3    0   2    2           228.0786505     228.0653256  0.0133
  1    0   0    2           229.6389177     229.6260898  0.0128

Level energies (exc. QED)
2*S+1  L   2J   CF          AS-FAC          FAC2023       Diff
  1    0   0    1          -628.2393362    -628.2476403  0.0083
  3    0   2    2           228.1476417     228.1319116  0.0157
  1    0   0    2           229.7079070     229.6927067  0.0152
```

O^{5+} KLn autoionization rates in units of 10^{13}/s:

			Dirac--Hartree--Slater				2023	
AS-RLX0	AS-RLX1	AS-SCCA	AS-FAC3	AS-FAC2A	AS-FAC2B	FAC3	FAC2A	FAC2B
ID								
1: 0.736	0.791	0.785	0.510	0.810	0.775	0.518	0.833	0.790
2: 0.378	0.473	0.406	0.262	0.459	0.428	0.255	0.460	0.431
3: 0.805	0.973	0.880	0.526	1.110	1.026	0.385	1.108	1.020

Notes:

AS-RLX denotes fully relaxed AS results obtained using non-unique potentials and orbitals, but no iteration, just form the STO potentials and generate a set of orbitals.

0 denotes just a Hartree STO potential.

1 denotes Hartree plus local exchange potential.

AS-SCCA is AS-RLX but iterated to self-consistency.

While the AS-SCCA results would appear to contain the most physics, AS-RLX0 is a robust result which can use optional scaling parameters. Introducing exchange (AS-RLX1) without self-consistency is poorer.

Regarding the AS-FAC and FAC results, using occupation numbers for the recombining ion gives much better agreement with the relaxed results. However, those for the recombined ion are often preferred for dielectronic recombination because of its sensitivity to the radiative rates—see the FAC Manual 1.1.5, Section 4.2, Q5 [8].

Further comparisons between AS-FAC and FAC, for the effect of n-mixing on the dielectronic and trielectronic recombination of Ar^{14+}, and the application of Relativistic Many-Body Perturbation Theory (RMBPT) to both, can be found in the paper by Zhang *et al* [15].

6 Recapitulation

We can now provide answers to the questions raised at the start of this paper:

Q. 'Why are you not using FAC?'

A. 'AS is potentially more flexible than FAC.'

and

Q. 'Why do your results differ from those of FAC?'

A. 'If we use the same potential as FAC then our AS results are in close agreement with FAC's, but we argue for the use of a more flexible, physical, set of potentials and orbitals.'

Author contributions

N. R. Badnell developed the AS code to mimic FAC and carried out the AS calculations. C. Y. Zhang carried out the FAC calculations.

Appendix

Here we detail and comment on the AS input files which are fully described in the online documentation: http://amdpp.phys.strath.ac.uk/autos/autos-30/WRITEUP.

The file below is for AS-FAC3. AS-FAC2A and AS-FAC2B can be obtained by moving the required occupation numbers to the top of the list.

The AS-RLX input can be obtained by setting BASIS='RLX' and adding &END after INUKE=1.

A one-off (per NZION) structure run is necessary (set MXCCF=0) to generate the TERMS/LEVELS file necessary for AS to set up the continuum interpolation energy mesh.[6]

---

[6] The approximation method used does not matter for this setup.

```
A.S.                                    He-like  1-2,n: n=2-nxtra
 &SALGEB  RUN=' ' RAD='YES' CUP='ICR' MXVORB=3 MXCONF=3 MXCCF=2 BASIS=''
         ICFG=10 NXTRA=5 LXTRA=4 lcon=6 KUTSO=0 KUTOO=1 KUTSS=999 &END
 1 0 2 0 2 1
  2 0 0   !These are just the usual MXCONF=3 He-like target CFs
  1 1 0
  1 0 1
  1 0 0   !minimum occupation (N+1-electron)
  2 2 2   !maximum occupation (N+1-electron)
  2 1 0  1  !two N+1 base configs (MXCCF=2) plus no. of promotions.
  1 1 1  1  !The choice is not unique. One can get the same set of CFs
            !from a different set of occupation constraints, base CFs,
            !and promotions
 &SMINIM  NZION=-8 PRINT='FORM' QED=1 INUKE=1
         NOCC=3 PPOT='SCCA' FAC='YES' &END

  2.0 0.3333 0.6667     !FAC3
  1.0 0.3333 0.6667     !FAC2A
  2.0 0.0    0.0        !FAC2B
 &SRADCON MENG=-15 &END !Requires a TERMS/LEVELS structure file
   -0.1  -1.0           !(case LS/IC)
```

Notes:

0/ Everything is free-formatted (and case insensitive.)

1/ We use NXTRA and LXTRA to extend the orbital definition list They are discussed in Sec.4a NAMELISTs of the AS WRITEUP file. Update to AS v28.46.9 to avoid having to set the continuum expansion (L=0,..LCON-1) via LCON—prior did not check for LXTRA. Even then AS is too conservative/not clever enough and sets more than we need here because all it looks at are the nl-values, not how they are used in configs. So it sets up to allow for 1s5g+continuum—better safe than sorry. The overkill is not an issue for He-like, but in general...

2/ We use promotion rules (via ICFG=10) to generate the N+1 configs, it is not worth it for the N-electron. We could have flagged use of promotion rules for N-electron as well (ICFG=11), but with zero promotions, to obtain the same effect.

ICFG/10 is gives the MXCCF N+1-electron ICFG value and MOD(ICFG,10) gives the MXCONF N-electron ICFG. So, here ICFG=0 for the N-electron MXCONF spec. (the usual) and ICFG=1 for N+1-electron MXCCF. ICFG is also discussed in Sec.4a NAMELISTs of the AS WRITEUP file.

3/ 'Promotion' also includes 'demotion'.

4/ Two base configs can generate the same new config. Duplicates are dropped, of course!

5/ All possible relativistic interactions have been switched on, except that 2-body fine-structure are restricted to being within a configuration (KUTSS=999) for speed, without loss of accuracy (KUTSS= −999 would include between).

*** It is not necessary to switch on relativistic interactions when FAC='YES'. ***

*** AS will automatically switch them on so as to align its operations with FAC's. ***

*** But they *are* required if BASIS='RLX' because FAC='NO' then. ***

6/ Again, QED and INUKE are required if BASIS= 'RLX' (and PPOT='SCCA', if so desired).

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