A FAC potential for AUTOSTRUCTURE

Nigel Badnell & Chunyu Zhang

Department of Physics
University of Strathclyde
Glasgow, UK

Motivation

The Flexible Atomic Code (FAC) of Gu (2008) is in widespread use.

As such, one can encounter the questions:

  'Why are you not using FAC?'

and

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

This talk attempts to answer these questions.

(Note: we are concerned here only with the calculation of atomic data and not plasma population modelling.)

Background

AUTOSTRUCTURE (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 two-component Dirac radial equation. It includes the Breit interaction in the Hamiltonian (+QED).

AS is semi-relativistic: it solves the kappa-averaged two-component Dirac radial equation. It includes the Breit interaction in the Pauli approximation[1] in the Hamiltonian (+QED).

For many applications, these differences are not important.

---

[1] Some of Pauli's original approximations have been reversed in AS.

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 a unique potential gives rise to a unique set of orthonormal 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 flexibility of AS with regards to potentials and the orbitals they describe partways answers the questions raised at the beginning of the talk.

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 that is available within AS but not FAC.

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

We first note different versions of FAC in common 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 last two versions unofficially as FAC2020 and FAC2023.

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

The historic FAC potential is based on a shell-structure description of the ion in question.

It is actually closely related to the electron-electron Coulomb 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

$$\sum_\alpha \omega_\alpha = N \, . \tag{1}$$

In the configuration-average approximation (Cowan, 1981)

$$
\begin{aligned}
V_\alpha(r) \;=\; & \sum_\beta (\omega_\beta - \delta_{\alpha\beta}) Y^0_{\beta\beta}(r) \\
& - \sum_\beta (\omega_\beta - 1)\delta_{\alpha\beta} \sum_{\lambda>0} f^\lambda_{\beta\beta} Y^\lambda_{\beta\beta}(r) \\
& - \sum_\beta (1 - \delta_{\alpha\beta})\omega_\beta \sum_\lambda g^\lambda_{\alpha\beta} Y^\lambda_{\alpha\beta}(r)\rho_{\alpha\beta}(r)/\rho_{\alpha\alpha}(r) \quad (2)
\end{aligned}
$$

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

$$
E_\alpha = \int_0^\infty V_\alpha(r)\rho_{\alpha\alpha}(r)\mathrm{d}r \,. \qquad (3)
$$

Then,

$$\bar{E} = \frac{1}{2} \sum_{\alpha} \omega_{\alpha} E_{\alpha} \tag{4}$$

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

Here,

$$Y_{\alpha\beta}^{\lambda}(r) = \int \frac{r_<^{\lambda}}{r_>^{\lambda+1}} \rho_{\alpha\beta}(r') \mathrm{d}r' \tag{5}$$

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

$$\rho_{\alpha\beta}(r) = P_{\alpha}(r)P_{\beta}(r) + Q_{\alpha}(r)Q_{\beta}(r) \tag{6}$$

in terms of the large (P_{α}) and small components (Q_{α}).

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

$$f_{\alpha\alpha}^\lambda = \frac{2l_\alpha + 1}{4l_\alpha + 1} \left(\begin{array}{ccc} l_\alpha & \lambda & l_\alpha \\ 0 & 0 & 0 \end{array} \right)^2 \tag{7}$$

and

$$g_{\alpha\beta}^\lambda = \frac{1}{2} \left(\begin{array}{ccc} l_\alpha & \lambda & l_\beta \\ 0 & 0 & 0 \end{array} \right)^2 \tag{8}$$

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

$$f_{\alpha\alpha}^\lambda = \frac{1}{2j_\alpha + 1} \left(\begin{array}{ccc} j_\alpha & \lambda & j_\alpha \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{array} \right)^2 \tag{9}$$

and

$$g_{\alpha\beta}^\lambda = \left(\begin{array}{ccc} j_\alpha & \lambda & j_\beta \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{array} \right)^2 . \tag{10}$$

Existing implementations with AS:

Option 1/ Line 1 in equation (2) is just the static potential term used by the STO potential of Burgess *et al* (1989) which is incorporated into AS. It can be evaluated analytically when the $P_\alpha(r)$ are STOs.

The introduction of adjustable radial scaling parameters (λ_α) within this analytic potential combined with the minimization of $< H >$ means the remaining two lines (due to equivalent electrons and exchange, respectively) can be neglected. The addition of a local exchange STO potential to the static one is an option in AS.

Option 2/ Alternatively, let us consider using the STO potential to start-off a self-consistent iteration using the full expression in (2). The occupation numbers ω_α can be flagged by the user to AS in several ways. But, in all instances, the potential is orbital dependent due to (2) taking account of self-screening, i.e., if $\sum_\alpha \omega_\alpha = N$ then $rV_\alpha(r) \rightarrow N - 1$ as $r \rightarrow \infty$.

Option 3/ A unique potential $V_\alpha = V$ can be imposed by the user defining a set of occupation numbers such that $\sum_\alpha \omega_\alpha = N - 1$ and the account of self-interaction in (2) is then switched-off.

The usual choice for the occupation numbers ω_α in this instance of a unique potential is those of the ground configuration of the next ionization stage — see the discussion in Tanaka *et al* (2020) in relation to HULLAC (Bar-Shalom *et al* 2001) and AS Working Notes No. 1 (Badnell 2022) in relation to AS.

FAC historic implementation:

FAC took an alternative approach (Gu, 2008). It formed a unique potential by averaging the V_α of (2) over the probability densities $\rho_{\alpha\alpha}$ (and occupation numbers ω_α) viz.

$$V(r) = \frac{\sum_\alpha \omega_\alpha V_\alpha(r) \rho_{\alpha\alpha}(r)}{\sum_\alpha \omega_\alpha \rho_{\alpha\alpha}(r)} \qquad (11)$$

and then

$$\frac{1}{2} \int_0^\infty V(r) \sum_\alpha \omega_\alpha \rho_{\alpha\alpha}(r) \mathrm{d}r = \frac{1}{2} \sum_\alpha \omega_\alpha E_\alpha = \bar{E} \qquad (12)$$

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

If the user supplied 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 (2) and (11).

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 (2008) recommends the use of $N + 1$ rather than N.

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 (2008).

It is frequently referenced in the current literature, with some authors even detailing these as the 'working' equations of FAC...

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

Despite Gu (2008) the FAC potential just described has not been used by FAC since its early days (Gu, 2023). Gu (2003) 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 analagous Dirac form is described by Sampson *et al* (2009).

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

$$
V(r) \quad = \quad \sum_\beta \omega_\beta Y_{\beta\beta}^0(r) - a \frac{3}{2} \left[\frac{24}{\pi} \rho(r) \right]^{1/3} . \tag{13}
$$

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

$$\rho(r) = \frac{1}{4\pi r^2} \sum_\alpha \omega_\alpha \rho_{\alpha\alpha} , \qquad (14)$$

such that (dV is the volume element here)

$$\int \rho(r) dV = N . \qquad (15)$$

The coefficient $a = 1/2$ a.u. in equation (13) gives the original Slater derivation. Subsequently, the Kohn-Sham (1965) value of $a = 1/3$ a.u. was found to give better agreement with Hartree-Fock — see Cowan (1981) for a detailed discussion. Sampson et al (2009) adopt $a = 1/3$ a.u. as well.

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. $\text{AHX} = (1/3)(3/2)(6/\pi^2)^{1/3} = 0.4235$ 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 in both AS and FAC.

As is well known, the drawback with 'Hartree-Slater' methods is that for

$$\sum_\alpha \omega_\alpha = N \, , \tag{16}$$

$$rV(r) \to N \qquad \text{as} \qquad r \to \infty \, , \tag{17}$$

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 (1955) cut-off:

$$V(r) = \min\left(V(r), \frac{N-1}{r}\right), \tag{18}$$

which is only problematic accuracy-wise for near neutrals (Cowan, 1981).

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 between different versions of FAC because of the way the Latter cut-off in equation (18) was originally (e.g. to at least 2020) implemented. It was revised subsequently (e.g. by 2023 — Gu, 2023).

We show next various effective charges

$$Z(r) = Z_0(r) - rV(r), \tag{19}$$

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

Ar^{14+} AS-FAC vs FAC
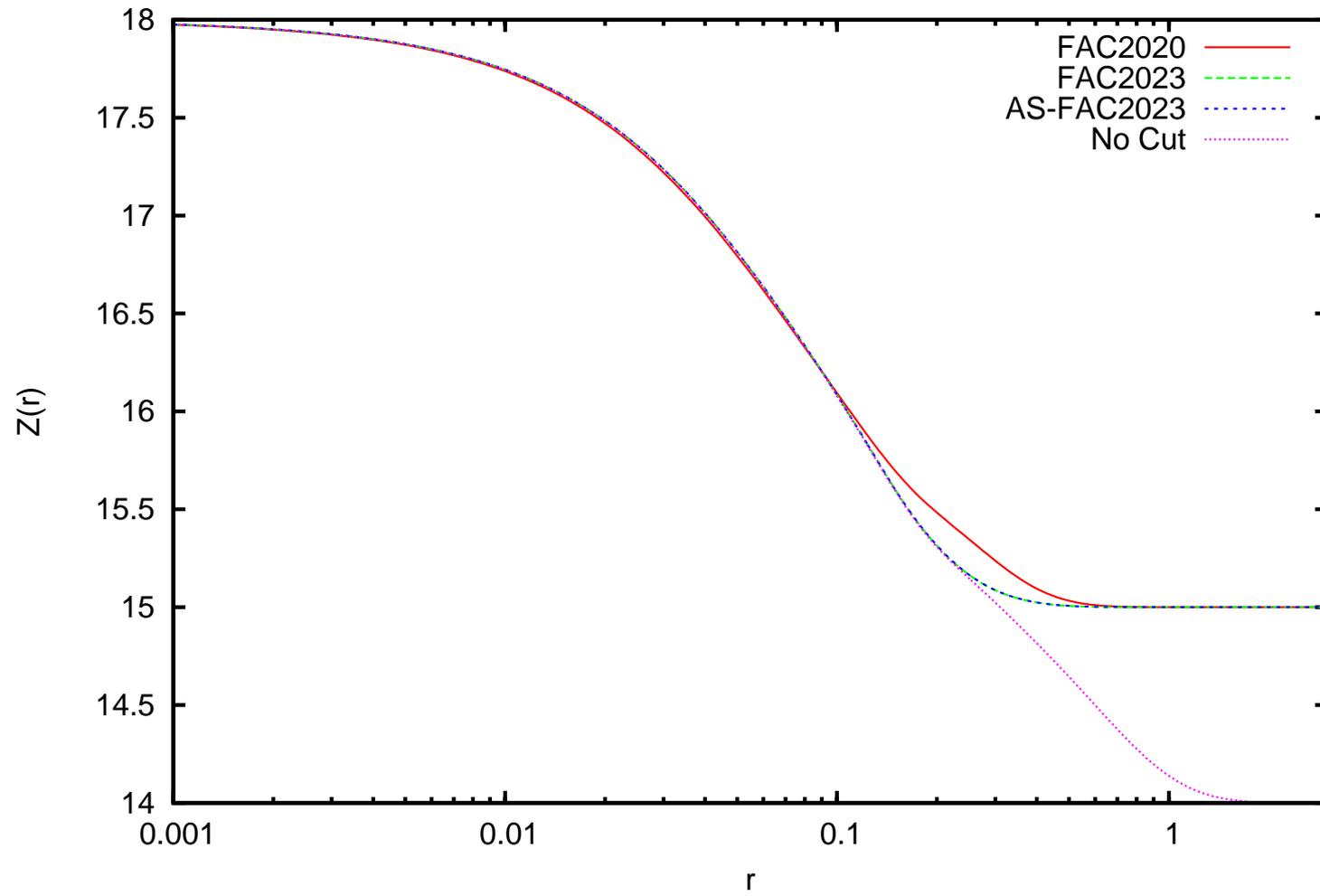
This completes the detailing of the **current** unique FAC potential described by Gu (2023) and now available in v30.x of AS.

It can be switched-on by a simple NAMELIST flag in the usual AS input (FAC='YES' in &SMINIM).

The user still needs to specify the occupation numbers ω_α such that $\sum_\alpha \omega_\alpha = N$, so as to obtain screening by $N - 1$ electrons.

The choice as to whether N corresponds to the recombined or recombining ion for bound-free processes remains the the users'.

AS itself sets all flags necessary to align its operation with that of FAC then.

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

Detailed Benchmarking of AS-FAC against FAC

We consider a model problem, involving only s-orbitals (so a single kappa), then we should be solving the exact same Dirac equation and thus obtain the same ('epsilon') orbital energies.

Of course, we recall that the use of perturbation theory means that even relatively large differences in orbital energies due to use of different potentials does not lead to anywhere near as large a difference in level energies!

We compare results obtained by:

1/ generating the FAC potential within AS, as just described,

2/ reading into AS the FAC potential written by a FAC GetPotential call,

3/ running FAC itself.

The same orbital occupation numbers are used in AS and FAC.

All potentials use the FAC2023 Dirac-Hartree-Slater local exchange form.

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

```
H-like:        AS-FAC              FAC2023          Diff

1s:          -325.408963       -325.408872        0.000091


             ASreadFACpot

             -325.408954
```

There is nothing to iterate here since there is just the nuclear potential.

Both codes 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 10^{-6} Ryd here.)

```
He-like:      AS-FAC              FAC2023           Diff

1s^2:       -302.23469          -302.23596        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 1×10^{-5} Ryd.

AS-FAC is not sensitive to the starting potential.

(The AS radial mesh here is accurate to a few 10^{-5} Ryd.)

Note: FAC 2020.04.20 only uses 4 s.f. while FAC 2023.03.23 uses 6 s.f., but 8 s.f. is needed for AS to achieve closest agreement with the native FAC epsilons.

```
Be-like:      AS-FAC              FAC2023        Diff

1s^2 2s^2: -283.58005          -283.58027         0.00022


              -62.13629          -62.13923      0.00294


          ASreadFACpot : recommended 8 s.f.


      -283.58031


          -62.13925


          ASreadFACpot : FAC2023 default 6 s.f.


      -283.57717


          -62.13889
```

A Case Study: O^{5+} KLn autoionization rates

We compare various AS and FAC results for 3 autoionizing levels which we (Foster et al 2023) have found to be sensitive to the calculational method and which contribute strongly to the He-like (dielectronic recombination) satellite lines in O^{5+}.

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. (Aside: This is a generalization of **Option 1/** which uses a different set of orbitals for each configuration.)

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.

We label the corresponding results AS-FACXX and FACXX, where AS-FACXX denotes an AS calculation using the unique DHS FAC potential given by equation (13), and FACXX denotes a FAC calculation.

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

	AS-RLX0	AS-RLX1	AS-SCCA	Dirac-Hartree-Slater			2023		
				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-RLXn 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.

Recapitulation

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

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 those from FAC, but we argue for the use of a more flexible, physical, set of potentials and orbitals.'

AS code availability

The current Gold version of AS (29.x) is publically available at:

`http://amdpp.phys.strath.ac.uk/autos`

This talk has described features that require use of the current development version (30.x) which can be found at:

`http://amdpp.phys.strath.ac.uk/autos/autos-30/`

but it requires a password to access it (since it can be unstable) — e-mail me, if you are interested in testing it further, at `badnell@phys.strath.ac.uk`

Acknowledgements

References

Badnell N R, ASWN No. 1 http://amdpp.phys.strath.ac.uk/autos/autos/DOCS (2022)

Bar-Shalom A, Klapisch M and Oreg J, JQSRT 71, 169 (2001)

Burgess A, Chidichimo M C and Tully J A, A&A 271, 319 (1989)

Cowan R D *The Theory of Atomic Structure and Spectra* University of California Press, Berkeley, CA (1981)

Foster A R, Badnell N R, Benedek K, Okon H, O Mullane M, Smith R K and Zhang C-Y, ApJS To be submitted (2023)

Gu M F, Ap.J. 589. 1085 (2003)

Gu M F, Can.J.Phys. 68, 675 (2008)

Gu M F, Private Communications (2023)

Kohn W and Sham L J. Phys.Rev. 140, A1135 (1965)

Latter R, Phys.Rev. 99, 510 (1955)

Sampson D H, Zhang H L and Fontes C J, Phys.Rep. 477, 111 (2009)

Slater J C, Phys.Rev. 81, 385 (1951)

Tanaka M, Kato D, Gaigalas G and Kawaguchi K, MNRAS 496, 1369 (2020)

Zhang C-Y *et al* submitted to Phys.Rev.A (2023)

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, see the Poster P13 and the paper recently submitted by Zhang *et al* (2023).