ADAS and fundamental data generation

Martin O'Mullane, Nigel Badnell, Hugh Summers and Alessandra Giunta
Department of Physics
University of Strathclyde

Fundamental data production and ADAS

One of the philosophies of ADAS is to provide baseline quality data for atomic processes of any ion stage of an arbitrary element.

These are selectively updated with higher quality data.

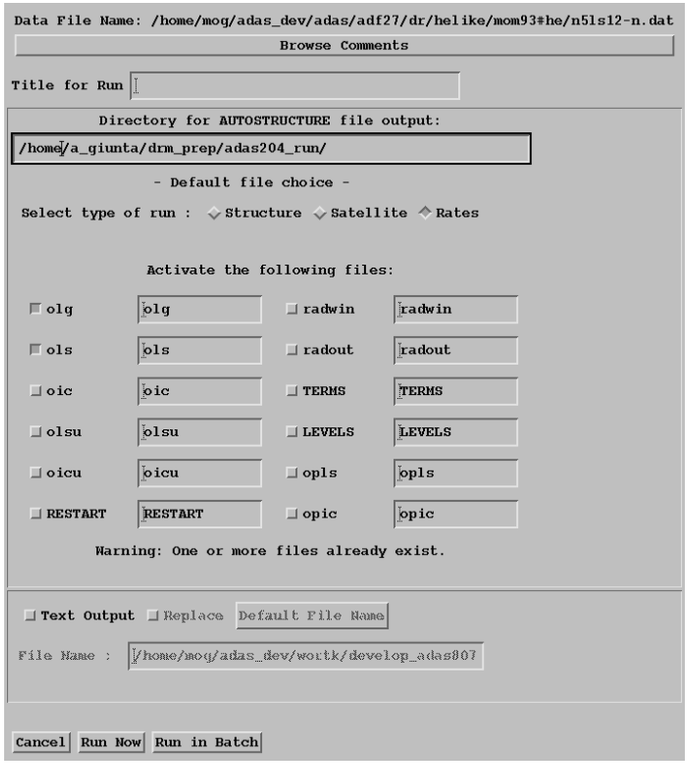
Fundamental data production codes available within ADAS:

- Cowan code to produce *adf04* data.
- AUTOSTUCTURE for dielectronic recombination.*
- CADW ionisation rate generation.
- R-matrix for electron impact excitation data.*
- IDL and FORTRAN routines for ECIP, Lodge ion impact and others.
- For charge exchange data extraction from a universal formula.

* It is a little modest to class these as a baseline quality code.

adas701 — AUTOSTRUCTURE (for dielectronic recombination)

Developed by Nigel Badnell the `adas701` implementation is tuned to produce state selective dielectronic data.



For larger problems (and systematic production) use the offline version, `adas7#1` or AS direct from Nigel.

Data from adas701

- AUTOSTRUCTURE produces the data for the DR Project.
- 13 isoelectronic sequences, elements up to Zn, IC and LS resolutions.
- 1.5Gb data in *adf09* collection.
- Sets a very high bar for 'baseline' data.
- See N R Badnell *et al*, 'Dielectronic recombination data for dynamic finite-density plasmas', Astron & Astrophys., 406, 1151–1165 (2003).
- Other papers for each iso-electronic sequence.
- Extended for photo-excitation and ionisation *(adf38* and *adf39)*.

Input to adas701

A little daunting so reading the manual is essential.

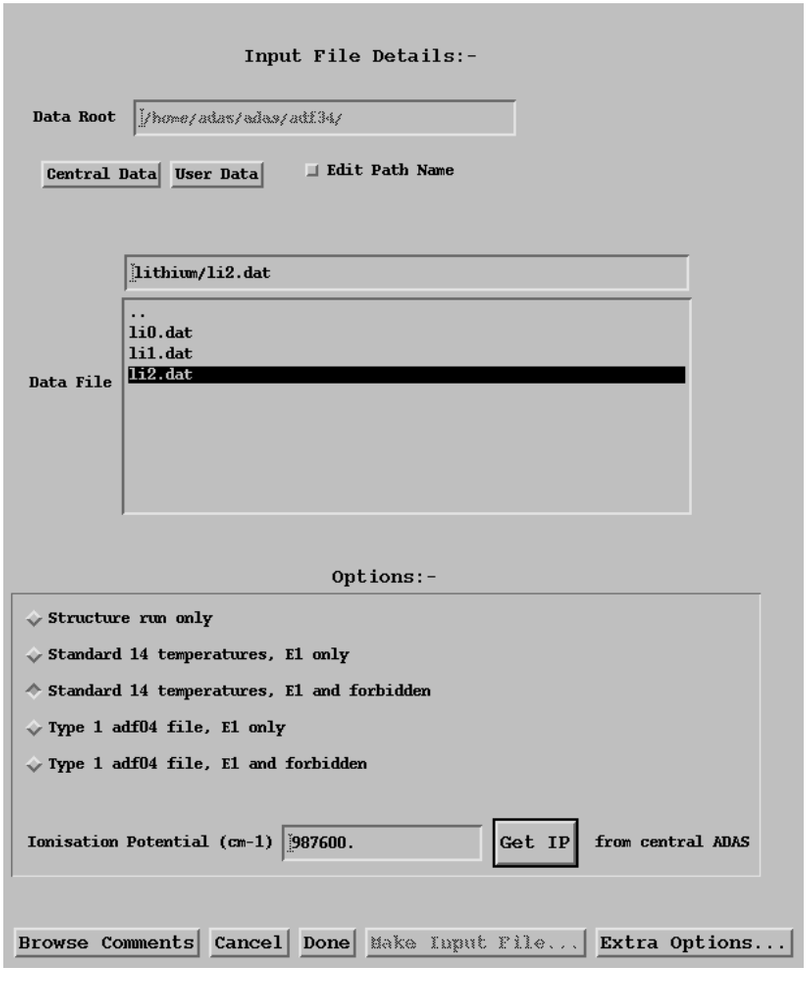
From `/home/adas/adas/adf27/dr/olike/oiz00#o/cu12ic23-n.dat`:

```
S.S.
123456789 22533514517 22533515517 22533516517
          12543514517 12543515517 12543516517
          22543518 22543519 2254351A 2254351B 2254351C
          12553518 12553519 1255351A 1255351B 1255351C
          22533514518 22533514519 2253351451A 2253351451B 2253351451C
          22533515518 22533515519 2253351551A 2253351551B 2253351551C
          22533516518 22533516519 2253351651A 2253351651B 2253351651C
          12543514518 12543514519 1254351451A 1254351451B 1254351451C
          12543515518 12543515519 1254351551A 1254351551B 1254351551C
          12543516518 12543516519 1254351651A 1254351651B 1254351651C
          22543514 22543515 22543516 22543517
          12553514 12553515 12553516 12553517
          22553 12563
               7107207217307317328029009019029039 04

 &SALGEB  RUN='DR' RAD='YES' CUP='IC' KORB1=1 KORB2=1 MSTART=4 &END
 &DRR     NMIN=4 NMAX=15 JND=14 LMIN=0 LMAX=6 LCON=5 &END
    16   20   25   35   45   55   70  100  150  200  300  450  700  999
 &SMINIM  NZION=29 PRINT='UNFORM'   &END
 &SRADWIN  KEY=-9  &END
 &SRADCON MENG=-15 &END
    0.0000 160.0000
```

adas801 — Cowan code for adf04 production

This was the first fundamental data generation code added as an ADAS interactive series code and forms the basis of series 8.



adas8#1 — Cowan code for adf04 production

The # indicates an offline code.

- Designed to be independent of the interactive system (and hence IDL).
- Self-contained to be portable to large computer systems.
- Workhorse code for the heavy species project.
- Recently modified to use the U Mons improved structure correctiosn as an optional, extra input.

```
/home/adas/offline_adas/adas8#1/scripts/run_adas8#1 c2.in c2.inst c2.pp
```

The input file can be crafted by hand or IDL based tools from the heavy species project can be used.

As an example consider Sn^{13+}

- What is its ground state configuration?
- What configurations contribute to spectral emission?
- And to radiated power?
- How do we choose which ones to include?

The *adf00* set archives ionisation potential and ground configurations:

```
tin                  -50
 0 7.343d+00 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f0  5s2  5p2
 1 1.463d+01 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f0  5s2  5p1
                           ..
                           ..
12 2.744d+02 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d2
13 2.995d+02 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d1
14 3.959d+02 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6
                              ..
```

What configurations should be considered?

With a ground state of $3\mathrm{d}^{10}4\mathrm{s}^{2}4\mathrm{p}^{6}4\mathrm{d}^{1}$ we can

- promote the valence 4d electron to any higher nl shell
- allow 4s or 4p electrons to be excited
- or any other electron — from 2p perhaps?
- however where do we stop in Δn or Δl?
- and how many configurations should we consider?

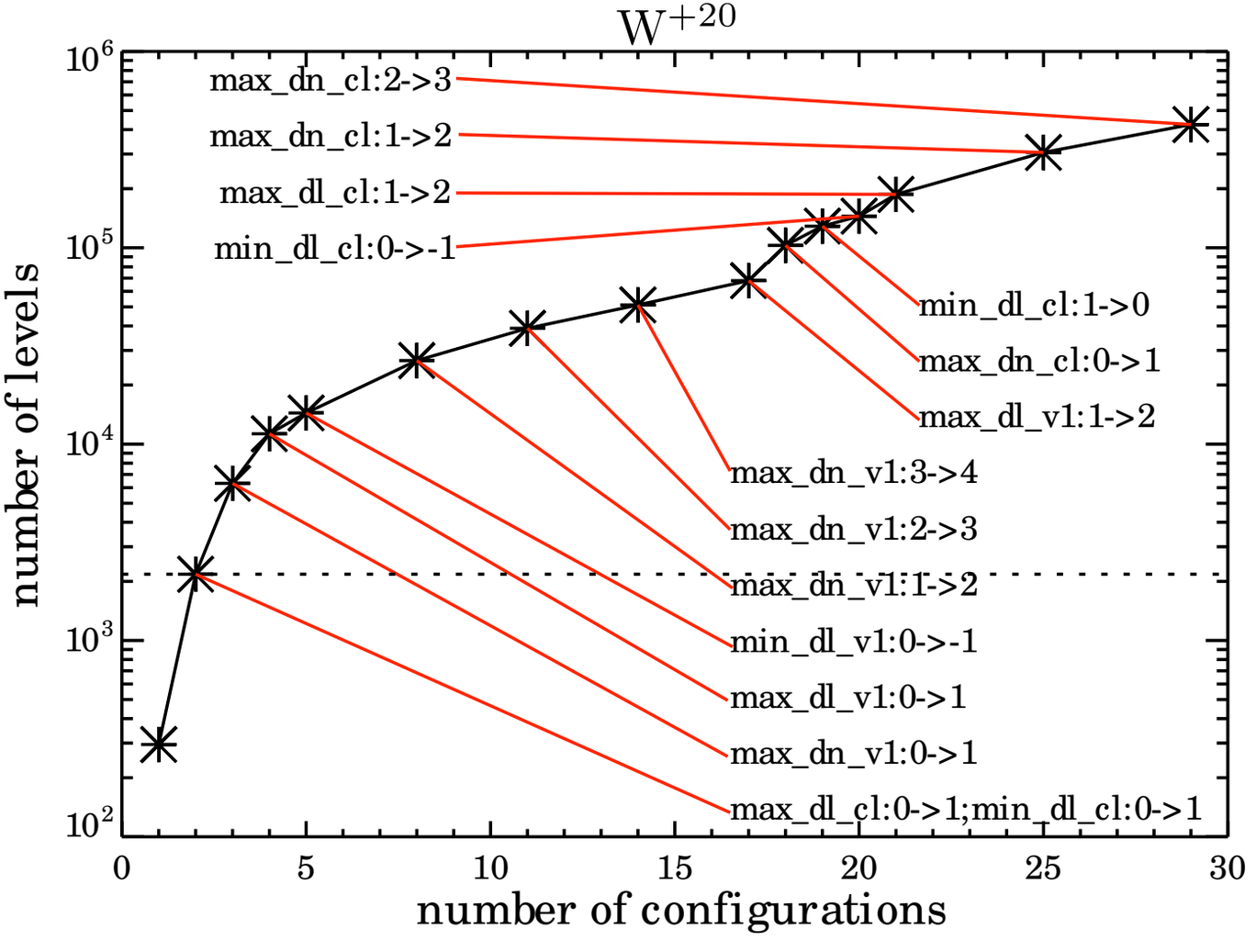
There are 180 distinct ground configurations (for elements up to Radon)

A rule based method is desirable (essential!)

ADAS rules for choosing where to promote electrons

index[]	:	index of ground configuration of each ion of element in *adf54* file
config[]	:	ground configuration for each ion of element
n_el[]	:	number of electrons for each ion of element
no_v_shl[]	:	number of open (valence) shells. Include outer-most shell even if closed.
max_dn_v1[]	:	maximum Δn promotion for first (outer-most) valence shell.
min_dn_v1[]	:	minimum Δn promotion for first (outer-most) valence shell.
		Negative value allows access to inner unoccupied or open shells
max_dl_v1[]	:	maximum delta Δl promotion for first (outer-most) valence shell.
min_dl_v1[]	:	minimum delta Δl promotion for first (outer-most) valence shell.
max_dn_v2[]	:	maximum Δn promotion for second (inner-most) valence shell.
min_dn_v2[]	:	maximum Δn promotion for second (inner-most) valence shell.
max_dl_v2[]	:	maximum delta Δl promotion for second (inner-most) valence shell.
min_dl_v2[]	:	minimum delta Δl promotion for second (inner-most) valence shell.
prom_c1[]	:	promote from inner shell closed shells (1=yes,0=no).
max_n_c1[]	:	maximum inner shell *n* from which promotions are permitted.
min_n_c1[]	:	minimum inner shell *n* from which promotions are permitted.
max_l_c1[]	:	maximum inner shell *l* from which promotions are permitted.
min_l_c1[]	:	minimum inner shell *l* from which promotions are permitted.
max_dn_c1[]	:	maximum Δn promotion from a permitted inner shell.
min_dn_c1[]	:	minimum Δn promotion from a permitted inner shell.
		Negative values of Δn allow access to inner unoccupied or open shells.
max_dl_c1[]	:	maximum Δl promotion from a permitted inner shell.
min_dl_c1[]	:	minimum Δl promotion from a permitted inner shell.
fill_n_v1[]	:	add all *nl* configurations of outer valence shell n (1=yes,0=no).
fill_par[]	:	if *n_fill* only add opposite parity to valence shell else add both parities (1=yes, 0=n0).
for_tr_sel[]	:	Cowan option for radiative transitions 1 - first parity, 2 or 3(default).
last_4f[]	:	shift an electron valence shell to unfilled 4f as extra ground.
grd_cmplx[]	:	include configurations of same complex as ground configuation for valence n-shell.

adf54 : rules for automatic data generation



Care needed!! resolved calculations (ic or LS) can overwhelm computers.

Limitations of adas801/adas8#1

- The Cowan code is well integrated into ADAS workflows.
- However.... spin changing transitions are absent.
- and no resonance effects.
- But it produces good structure so work is underway to use AS for the collisional part.

- AUTOSTRUCTURE has a distorted wave module and can generate *adf04* datasets.
- Auto-generation of input files is part of the heavy species rules-based routines.
- Under active development with data already produced and waiting for next ADAS release (Hugh Summers & Alessandra Giunta).

adas8#2 — CADW Ionisation (collaboration with Auburn)

Very similar specification probelm as excitation — driven by *adf56* set of rules

index[]	:	index of ground configuration of each ion of element in *adf56* file
config[]	:	ground conf[]iguration for each ion of element
n_el[]	:	number of electrons for each ion of element
no_v_shl[]	:	number of shells to treat as valence shells. Max. 2 relevant to relating ion and parent.
v1_shl[]	:	first valence shell position in adf56 configuration specifications.
v2_shl[]	:	second valence shell position in adf56 configuration specifications. zero if none defined.
drct_eval_v[]	:	evaluate direct ionisation from the valence shell(s).
drct_eval_cl[]	:	evaluate direct ionisation from other non-valence (closed) shells.
min_shl_cl[]	:	lowest closed shell to include (position in adf56 configuration specifications).
exca_eval_v2[]	:	evaluate excitation/autoionisation from second valence shell if identified.
max_dn_v2[]	:	maximum change in v2 n-shell to be included.
min_dn_v2[]	:	minimum change in v2 n-shell to be include.
max_dl_v2[]	:	maximum change in v2 l-shell to be included.
min_dl_v2[]	:	minimum change in v2 l-shell to be include.
exca_eval_cl[]	:	evaluate excitation/autoionisation from other non-valence (closed) shells.
max_dn_cl[]	:	maximum change in closed n-shell to be included.
min_dn_cl[]	:	minimum change in closed n-shell to be included.
max_dl_cl[]	:	maximum change in closed l-shell to be included.
min_dl_cl[]	:	minimum change in closed l-shell to be included.
exst_eval[]	:	evaluate ionisation from excited states.
exst_adf00_prt[]	:	assume parent for building excited states is as present in the adf00 data set for the ion.
exst_prt_hole_shl[]	:	specify position of shell in ground configuration to form parent if not from adf00 above.
max_n_exst[]	:	maximum n-shell for excited states to be included.
max_l_exst[]	:	maximum l-shell for excited states to be included.
drct_eval_exst_v[]	:	evaluate direct ionisation from excited state valence shells.
drct_eval_exst_cl[]	:	evaluate direct ionisation from excited state non-valence (closed) shells.
exca_eval_exst_v[]	:	evaluate excitation/autoionisation for excited states from valence shells (v1 and v2 above).
exca_eval_exst_cl[]	:	evaluate excitation/autoionisation for excited states from non-valence (closed) shells.

/home/adas/offline_adas/adas8#2/adas8#2.pl adf32_ca_sn13.dat adf23_ca_sn13.dat

```
elem   = Sn
stage  = 13
ip_z   =    3193147.3
ip_z1  =    2415629.2
seq    = rb
-------------------------------------------------------------------------------
Type = Direct /number=3/
#
200-51 1 2  01.   1.   5.0E-08   1.0E-11-2  0130 0 1.00 0.65   71. 0.5       0.70
   50   14  sn+13 ground     4d1                                    4d
   50   15  sn+14 from 4d    3d10 4s2  4p6                          
   -1
#
200-51 1 2  01.   1.   5.0E-08   1.0E-11-2  0130 0 1.00 0.65   73. 0.5       0.70
   50   14  sn+13 ground     4d1                                    4s
   50   15  sn+14 from 4s    3d10 4s1  4p6  4d1                     
   -1
#
200-51 1 2  01.   1.   5.0E-08   1.0E-11-2  0130 0 1.00 0.65   72. 0.5       0.70
   50   14  sn+13 ground     4d1                                    4p
   50   15  sn+14 from 4p    3d10 4s2  4p5  4d1                     
   -1
-------------------------------------------------------------------------------
Type = InDirect /number=2/
#
20 -51 0 2   10  1.0    5.e-08    1.e-11-2   130    1.0 0.65   66.  0.5       0.7
   50   14  sn+13 ground     4d1                                    4s
   50   14  sn+13 via  4d    3d10 4s1  4p6  4d2                     4d
   50   14  sn+13 via  4f    3d10 4s1  4p6  4d1  4f1                4f
   50   14  sn+13 via  5s    3d10 4s1  4p6  4d1  5s1                5s
                              -
                              -
   50   14  sn+13 via  7h    3d10 4s1  4p6  4d1  7h1                7h
   50   14  sn+13 via  7i    3d10 4s1  4p6  4d1  7i1                7i
   -1
#
20 -51 0 2   10  1.0    5.e-08    1.e-11-2   130    1.0 0.65   66.  0.5       0.7
   50   14  sn+13 ground     4d1                                    4p
   50   14  sn+13 via  4d    3d10 4s2  4p5  4d2                     4d
   50   14  sn+13 via  4f    3d10 4s2  4p5  4d1  4f1                4f
                              -
                              -
   50   14  sn+13 via  7h    3d10 4s2  4p5  4d1  7h1                7h
   50   14  sn+13 via  7i    3d10 4s2  4p5  4d1  7i1                7i
   -1
-------------------------------------------------------------------------------
C--------------------
C  I made this!
C--------------------
```

Uplift of baseline

As codes mature they can transition from the domain of the specialist to routine, unattended mass data generation. Standard R-matrix is now at this stage — adas8#3.

```
/home/adas/offline_adas/adas8#3/scripts/adas8#3.pl input.dat Z
```

```
GENERAL                          SCALING PARAMETERS
2Jmax_ex = 23                    1s = 1.0
2Jmax_nx = 91                    2s = 1.0
maxc = 51                        2p = 1.0
mesh_fine = 0.0025               3s = 1.0
mesh_coarse = 0.01               3p = 1.0
maxe/ionpot = 3                  3d = 1.0
rdamp = 1
adamp = 0

CONFIGURATION LIST
1s2
1s1 2s1
1s1 2p1
1s1 3s1
1s1 3p1
1s1 3d1
```

This is a parallel code so tuning to target architecture and physics problem must be expected.