The OPEN-ADAS approach to atomic data provision

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Brief history of the ADAS view of atomic data

- ADAS has focused its efforts in providing atomic data to model and interpret emission from hot, confined plasmas.
- Historical roots are in fusion (JET) and so are the bulk of the users.
- Has also been extensively applied to astrophysics.
- This background lead to the ADAS Project becoming a self-funding consortium of mostly fusion laboratories and its governance is by a steering committee of these members.
- OPEN-ADAS was championed (and funded) by IAEA to make the data more widely available.
- The delivery of this data is via the web but the data is returned as ADAS datasets rather than the more traditional individual cross sections.

Why is ADAS being different? Are we just contrarians?

Derived, fundamental and driver data

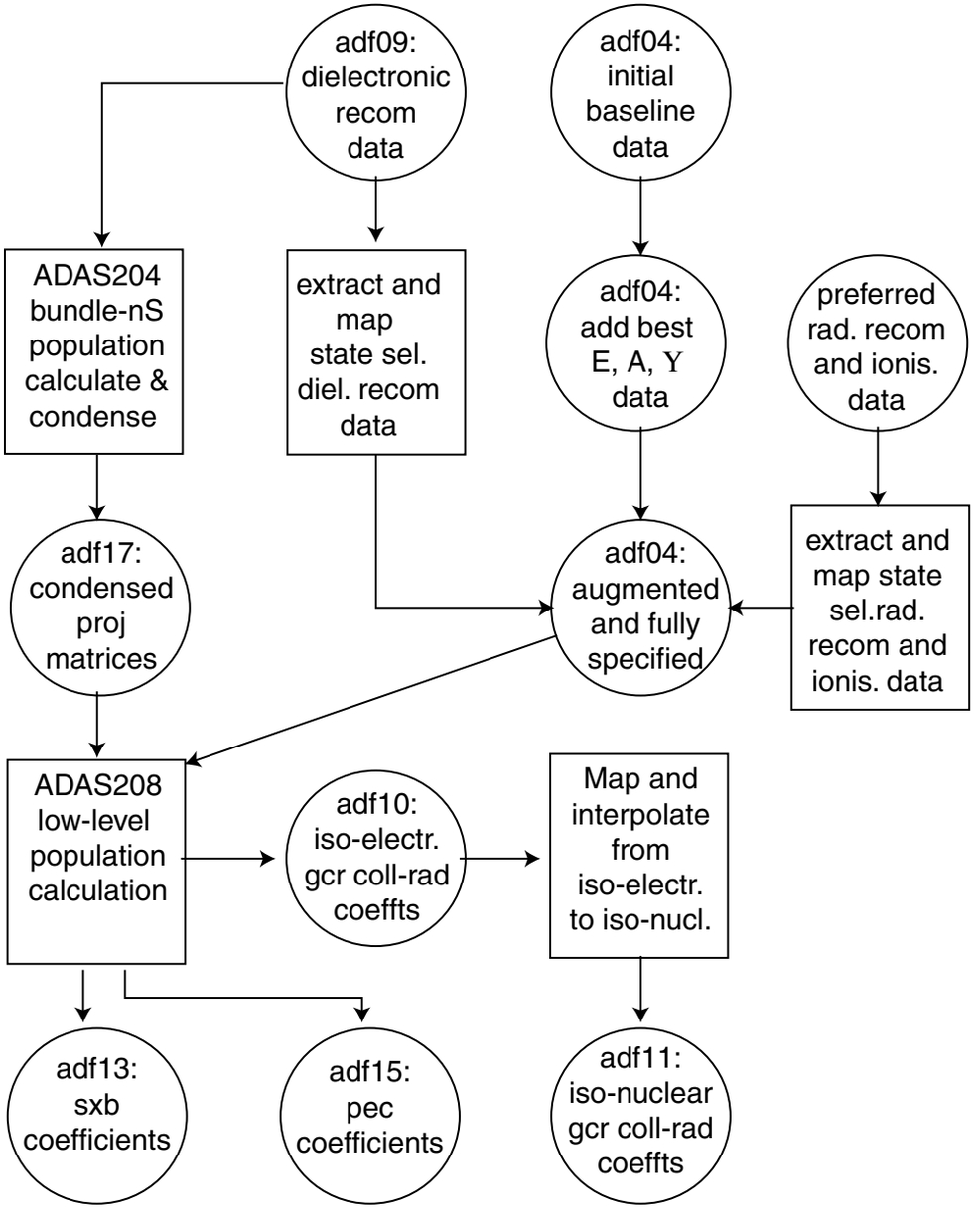
ADAS data falls into 3 broad classes:

- **Derived data** are data tailored for modelling: electron temperature and density dependent effective emission coefficients, effective ionisation/recombination rates, radiated power, spectral emissivities etc.,
  - Fundamental data processed via population models.
  - Most of these data are ***not*** catalogued in data centres.

- **Fundamental data** are core atomic data necessary for modelling: A-values, cross sections, effective collision strengths etc.,
  - Many sources: collaborators, literature, data centres etc.
  - Many resolutions: from simplistic to the forefront of computational physics.

- **Driver data** allow complete regeneration of all ADAS derived data (and some fundamental data) in conjunction with the various ADAS codes,are core atomic data necessary for modelling:
  - unique to ADAS and of no use/interest to non-ADAS users.

Workflow to generate derived data



□ : codes and hand-editing / scripting.

◯ : *adf* datasets.

The production of the fundamental data is not shown!

Purity of data within ADAS

Population models require a complete set of data

A primary goal of ADAS is to 'transform' fundamental data into a form suitable for diagnostic interpretation and plasma modelling. If high quality data does not exist, *baseline* quality data is used in its place.

Sources of (vast quantities) of fundamental data — delivered in *adf* formats:

- Baseline data generation of structure and electron driven processes.
- DR Project and BBGP developments.
- Heavy species activities.
- Photo-ionisation/excitation APAP network.
- R-matrix — is now highly automated.
- CADW ionisation.
- The literature — occasionally comes in ADAS formats.

There is a steady movement of leading edge codes into a 'workhorse' mode which lifts the quality of the baseline.

How is ADAS data used?

Mostly the data is embedded in codes and the ‘user’ is either unaware or does not want to know about the (wonderful) intricacies of atomic data.

eg EDGE-2D post-processing file:

```
C
 'PS6 ' 'C5A '  1  6  5  '/u/sim/cmg/data/adas/ldh'        96  'pju'   1  22   0     33.8     33.8      0.0
C
 'PS3 ' 'H0H '  1  1  0  '*'                               96  'pju'   3  69   0   6561.9   6561.9      0.0
 'PS3 ' 'C2H '  1  6  2  '*'                               96  'vsu'   2  52   0   4650.1   4650.1      0.0
 'PS3 ' 'BE1H'  1  4  1  '*'                               -1  'pec'   2   0   0   5270.7      0.0      0.0
 'PS3 ' 'H0V '  2  1  0  '*'                               96  'pju'   3  69   0   6561.9   6561.9      0.0
 'PS3 ' 'C2V '  2  6  2  '*'                               96  'vsu'   2  52   0   4650.1   4650.1      0.0
```

- Can be very specific — here PS3 refers to a JET visible spectrometer.
- The post-processing driving scripts are originally written by experts but updating is problematic.
- Often use private copies/versions of data — but “it’s from ADAS” when asked.

Reading ADAS dataset from fortran

If the plasma simulation code users are isolated/insulated from handling atomic data by expert written post-processing scripts it does not matter than the code internals need to know where to find the atomic database, which data to draw or which extrapolation method is best.

```
      call xxdata_15( iunit   , dsname ,
     &                nstore , ntdim  , nddim  ,
     &                ndptnl , ndptn  , ndptnc , ndcnct ,
     &                ndstack, ndcmt ,
     &                iz0    , is     , is1    , esym   ,
     &                nptnl  , nptn   , nptnc  ,
     &                iptnla , iptna  , iptnca ,
     &                ncnct  , icnctv ,
     &                ncptn_stack     , cptn_stack      ,
     &                lres   , lptn   , lcmt   , lsup   ,
     &                nbsel  , isela  ,
     &                cwavel , cfile  , ctype  , cindm  ,
     &                wavel  , ispbr  , isppr  , isstgr , iszr  ,
     &                ita    , ida    ,
     &                teta   , teda   ,
     &                pec    , pec_max,
     &                ncmt_stack      , cmt_stack
     &              )
```

But this approach demands that the ADAS data supplied is appropriate for the modelling / diagnostic interpretation task.

FORTRAN code to read OPEN-ADAS data is supplied

OPEN-ADAS

Atomic Data and Analysis Structure

OPEN-ADAS Version 1.2
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Documentation

ADAS consists of around one million lines of source code. These codes are available to members of the ADAS Project and are not relased as part of OPEN-ADAS. Collected here are subroutines used to read data supplied via OPEN-ADAS.

Reading routines

Below are links to compressed tar files (.tar.gz) containing subroutines to read each of the ADAS data formats released by OPEN-ADAS.

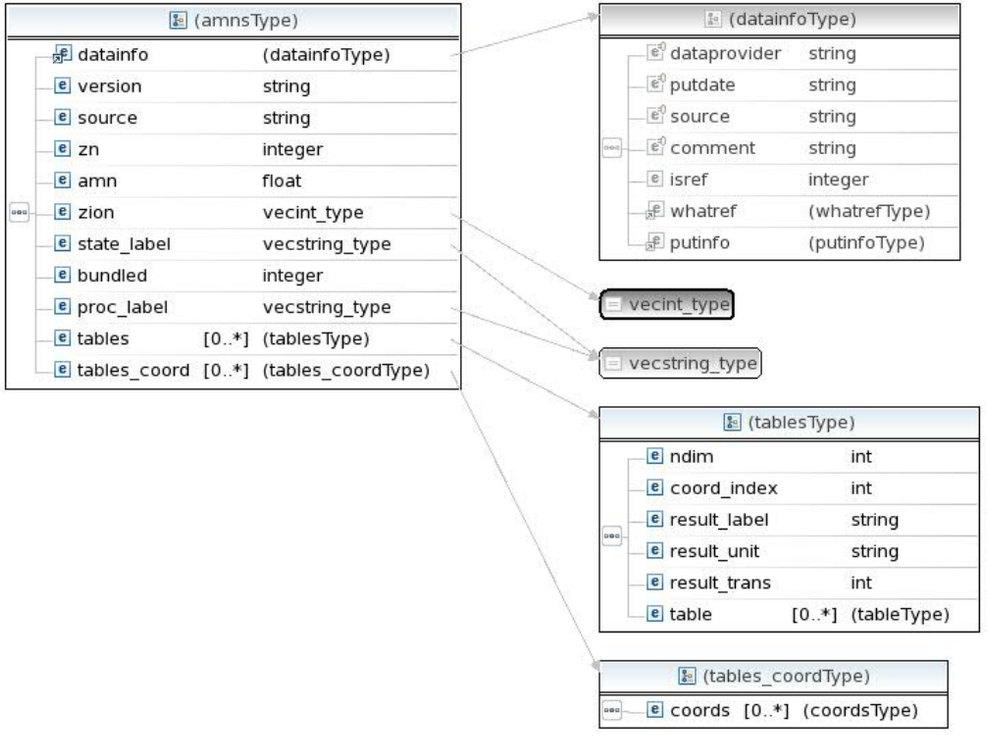
- **xxdata_01.tar.gz** - Reading routine for ADF01 files.
- **xxdata_04.tar.gz** - Reading routine for ADF04 files.
- **xxdata_07.tar.gz** - Reading routine for ADF07 files.
- **xxdata_08.tar.gz** - Reading routine for ADF08 files.
- **xxdata_09.tar.gz** - Reading routine for ADF09 files.
- **xxdata_11.tar.gz** - Reading routine for ADF11 files.
- **xxdata_12.tar.gz** - Reading routine for ADF12 files.
- **xxdata_13.tar.gz** - Reading routine for ADF13 files.
- **xxdata_15.tar.gz** - Reading routine for ADF15 files.
- **xxdata_21.tar.gz** - Reading routine for ADF21 files.
- **xxdata_22.tar.gz** - Reading routine for ADF22 files.

Compilation and licensing

The codes are designed to work in a UNIX environment and have been tested against various Fortran compilers, full details are contained inside the compressed tar archives.

The EFDA ITM AMNS CPO approach

Atomic, Molecular, Nuclear and Surface (**AMNS**) data is required for the activities of the Integrated Tokamak Modelling (**ITM**) task-force of the European Fusion Development Agreement (**EFDA**) where all data interchange between all codes is via Consistent Physical Objects (**CPO**s).



Again this is shielding the end user from the details of the atomic data.

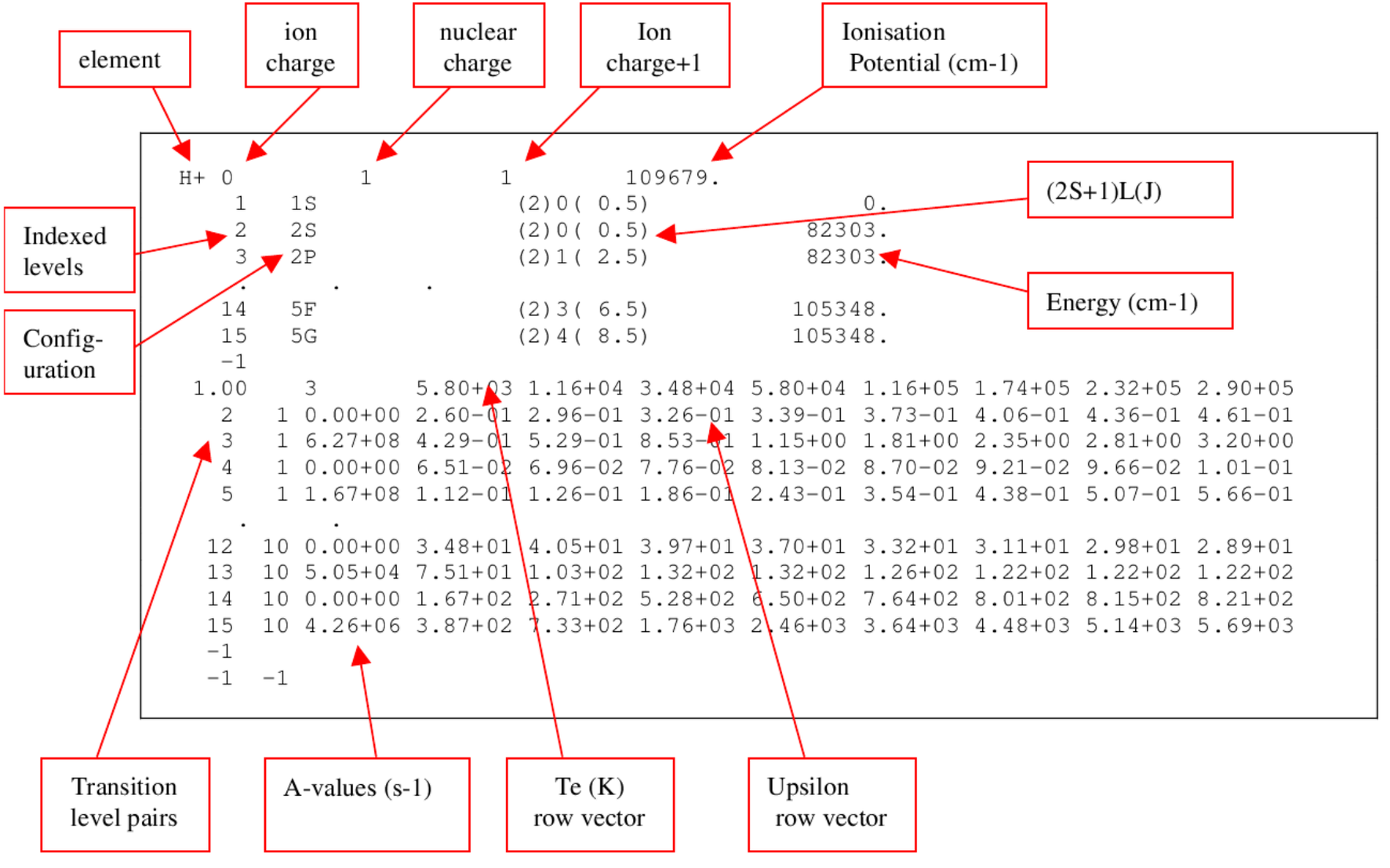
AMNS CPOs

The goal is to separate the use of AMNS data from the details of how it is provided.

```
  call ITM_AMNS_SETUP(amns)                                          ! initialize system
  query%string='version'
  call ITM_AMNS_QUERY(amns,query,answer)
...
  call ITM_AMNS_SETUP_TABLE(amns, lr_rx, species_lr, amns_lr) ! setup space for data
  query%string='source'
  call ITM_AMNS_QUERY_TABLE(amns_lr,query,answer)
...
  set%string='nowarn'                                                ! set options
  call ITM_AMNS_SET_TABLE(amns_lr,set)
...
  call ITM_AMNS_RX(amns_lr,rate(:,:,0),ne,te)                        ! read/interpolate data
...
  call ITM_AMNS_FINISH_TABLE(amns_lr))                               ! finish up
  call ITM_AMNS_FINISH(amns)
```

We have supplied code to write CPOs from ADAS data.

ADAS data formats — *adf* — are precisely defined




```
H+ 0          1          1         109679.
   1   1S               (2)0( 0.5)              0.
   2   2S               (2)0( 0.5)          82303.
   3   2P               (2)1( 2.5)          82303.
   .    .      .
  14   5F               (2)3( 6.5)         105348.
  15   5G               (2)4( 8.5)         105348.
  -1
1.00    3       5.80+03 1.16+04 3.48+04 5.80+04 1.16+05 1.74+05 2.32+05 2.90+05
  2   1 0.00+00 2.60-01 2.96-01 3.26-01 3.39-01 3.73-01 4.06-01 4.36-01 4.61-01
  3   1 6.27+08 4.29-01 5.29-01 8.53-01 1.15+00 1.81+00 2.35+00 2.81+00 3.20+00
  4   1 0.00+00 6.51-02 6.96-02 7.76-02 8.13-02 8.70-02 9.21-02 9.66-02 1.01-01
  5   1 1.67+08 1.12-01 1.26-01 1.86-01 2.43-01 3.54-01 4.38-01 5.07-01 5.66-01
  .     .
 12  10 0.00+00 3.48+01 4.05+01 3.97+01 3.70+01 3.32+01 3.11+01 2.98+01 2.89+01
 13  10 5.05+04 7.51+01 1.03+02 1.32+02 1.32+02 1.26+02 1.22+02 1.22+02 1.22+02
 14  10 0.00+00 1.67+02 2.71+02 5.28+02 6.50+02 7.64+02 8.01+02 8.15+02 8.21+02
 15  10 4.26+06 3.87+02 7.33+02 1.76+03 2.46+03 3.64+03 4.48+03 5.14+03 5.69+03
 -1
 -1  -1
```

See http://www.adas.ac.uk/man/appxa-04.pdf

Reading ADAS for interactive manipulation

IDL is widely used in the fusion and astrophysics communities

```
IDL> read_adf40,file='adf40_ca_sn13.dat', fulldata=all

IDL> help, all, /st
   ESYM            STRING    'Sn'
   IZ0             LONG                50
   IS              LONG                13
   IS1             LONG                14
   NBLOCK          LONG                 2
   NPIX            LONG      Array[2]
   WAVE_MIN        DOUBLE    Array[2]
   WAVE_MAX        DOUBLE    Array[2]
   NTE             LONG      Array[2]
   TE              DOUBLE    Array[8, 2]
   NDENS           LONG      Array[2]
   DENS            DOUBLE    Array[4, 2]
   FPEC            DOUBLE    Array[256, 8, 4, 2]
   TYPE            STRING    Array[2]
```

ADAS data and discoverability

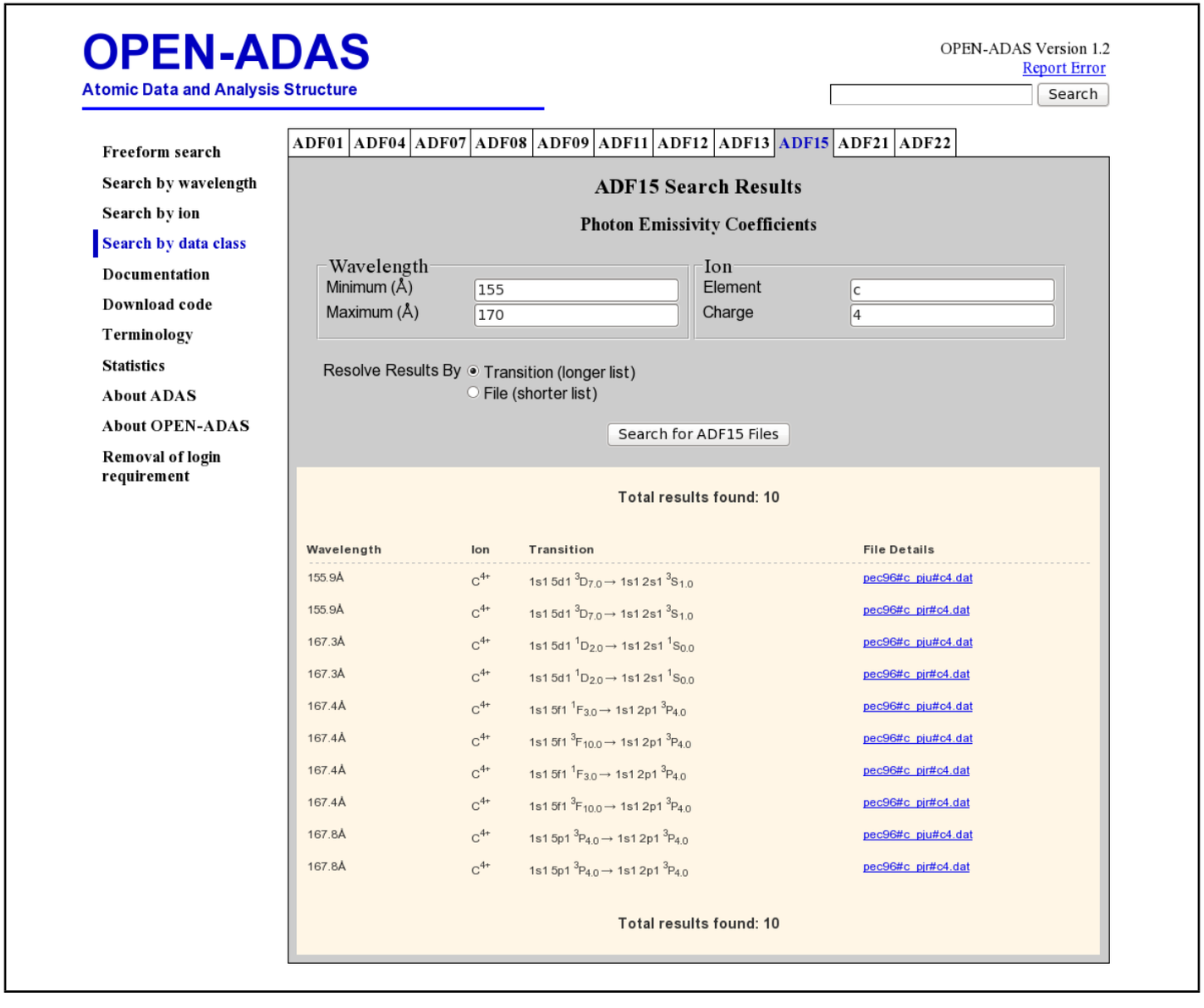
- ADAS data is highly structured and is routinely read into computer code structures and objects.
- Yet there is a perceived difficulty of finding stuff within ADAS.

OPEN-ADAS introduced ADAS *.tag* files. Consider the photon emissivity coefficient of CV or C^{+4}.

```
<adf15>
        <file>
                <type>ADF15</type>
                <filename>pec96#c_pju#c4.dat</filename>
                <directory>adf15/pec96#c</directory>
                <filesize>1003454</filesize>
                <tagged_on>2011-09-02</tagged_on>
                <tagged_by>Martin O'Mullane</tagged_by>
                <md5sum>0c9903fb467e4fd5de16561cc02ba5c6</md5sum>
        </file>
        <ion>
                <z0>6</z0>
                <z>4</z>
        </ion>
        <limits>
                <density>
                        <min units="cm-3">7.81E+05</min>
                        <max units="cm-3">7.81E+19</max>
                </density>
```

```
                <temperature>
                        <min units="eV">1.08E+00</min>
                        <max units="eV">6.46E+03</max>
                </temperature>
                <wavelength>
                        <min units="A">32.8</min>
                        <max units="A">2274.7</max>
                </wavelength>
        </limits>
        <contributors>
                <contributor>Martin O'Mullane</contributor>
        </contributors>
        <transitions>
                <transition>
                        <z>4</z>
                        <lambda units="A">40.7</lambda>
                        <upper>
                                <level>3</level>
                                <cfg>1S1 2S1</cfg>
                                <m>1</m>
                                <l>0</l>
                                <j>.0</j>
                        </upper>
                        <lower>
                                <level>1</level>
                                <cfg>1S2</cfg>
                                <m>1</m>
                                <l>0</l>
                                <j>.0</j>
                        </lower>
                        <type>Excitation</type>
                </transition>
        </transitions>
</adf15>
```

The *.tag* files index OPEN-ADAS searching



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ADF01 | ADF04 | ADF07 | ADF08 | ADF09 | ADF11 | ADF12 | ADF13 | ADF15 | ADF21 | ADF22

ADF15 Search Results

Photon Emissivity Coefficients

Wavelength — Minimum (Å): 155; Maximum (Å): 170

Ion — Element: c; Charge: 4

Resolve Results By: (•) Transition (longer list); ( ) File (shorter list)

Search for ADF15 Files

Total results found: 10

Wavelength	Ion	Transition	File Details
155.9Å	C^{4+}	1s1 5d1 $^3D_{7.0}$ → 1s1 2s1 $^3S_{1.0}$	pec96#c_pju#c4.dat
155.9Å	C^{4+}	1s1 5d1 $^3D_{7.0}$ → 1s1 2s1 $^3S_{1.0}$	pec96#c_pjr#c4.dat
167.3Å	C^{4+}	1s1 5d1 $^1D_{2.0}$ → 1s1 2s1 $^1S_{0.0}$	pec96#c_pju#c4.dat
167.3Å	C^{4+}	1s1 5d1 $^1D_{2.0}$ → 1s1 2s1 $^1S_{0.0}$	pec96#c_pjr#c4.dat
167.4Å	C^{4+}	1s1 5f1 $^1F_{3.0}$ → 1s1 2p1 $^3P_{4.0}$	pec96#c_pju#c4.dat
167.4Å	C^{4+}	1s1 5f1 $^3F_{10.0}$ → 1s1 2p1 $^3P_{4.0}$	pec96#c_pju#c4.dat
167.4Å	C^{4+}	1s1 5f1 $^1F_{3.0}$ → 1s1 2p1 $^3P_{4.0}$	pec96#c_pjr#c4.dat
167.4Å	C^{4+}	1s1 5f1 $^3F_{10.0}$ → 1s1 2p1 $^3P_{4.0}$	pec96#c_pjr#c4.dat
167.8Å	C^{4+}	1s1 5p1 $^3P_{4.0}$ → 1s1 2p1 $^3P_{4.0}$	pec96#c_pju#c4.dat
167.8Å	C^{4+}	1s1 5p1 $^3P_{4.0}$ → 1s1 2p1 $^3P_{4.0}$	pec96#c_pjr#c4.dat

Total results found: 10

OPEN-ADAS delivery

However it is the complete ADAS file that is returned when downloaded.

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ADF01 | ADF04 | ADF07 | ADF08 | ADF09 | ADF11 | ADF12 | ADF13 | ADF15 | ADF21 | ADF22

ADF15 File: pec96#c_pjr#c4.dat

Photon Emissivity Coefficients

Ion: C^{4+}
Temperature Range: 1.080 eV → 6460 eV
Density Range 7.810 x 10^{5} cm^{-3} → 7.810 x 10^{19} cm^{-3}
Filename: pec96#c_pjr#c4.dat
Full Path: adf15/pec96#c/pec96#c_pjr#c4.dat

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Wavelength	Transition	Type	Driving Population
32.8Å	$1s1\ 5d1\ ^{1}D_{2.0} \rightarrow 1s2\ ^{1}S_{0.0}$	Excitation	$1s2\ ^{1}S_{0.0}$
32.8Å	$1s1\ 5p1\ ^{3}P_{4.0} \rightarrow 1s2\ ^{1}S_{0.0}$	Excitation	$1s2\ ^{1}S_{0.0}$
32.8Å	$1s1\ 5p1\ ^{1}P_{1.0} \rightarrow 1s2\ ^{1}S_{0.0}$	Excitation	$1s2\ ^{1}S_{0.0}$
32.8Å	$1s1\ 5d1\ ^{1}D_{2.0} \rightarrow 1s2\ ^{1}S_{0.0}$	Excitation	$1s1\ 2s1\ ^{3}S_{1.0}$
32.8Å	$1s1\ 5p1\ ^{3}P_{4.0} \rightarrow 1s2\ ^{1}S_{0.0}$	Excitation	$1s1\ 2s1\ ^{3}S_{1.0}$
32.8Å	$1s1\ 5p1\ ^{1}P_{1.0} \rightarrow 1s2\ ^{1}S_{0.0}$	Excitation	$1s1\ 2s1\ ^{3}S_{1.0}$
32.8Å	$1s1\ 5d1\ ^{1}D_{2.0} \rightarrow 1s2\ ^{1}S_{0.0}$	Recombination	
32.8Å	$1s1\ 5p1\ ^{3}P_{4.0} \rightarrow 1s2\ ^{1}S_{0.0}$	Recombination	

Data classes supplied in OPEN-ADAS

OPEN-ADAS is designed to appeal to both plasma modellers and those interested in the detailed atomic physics.

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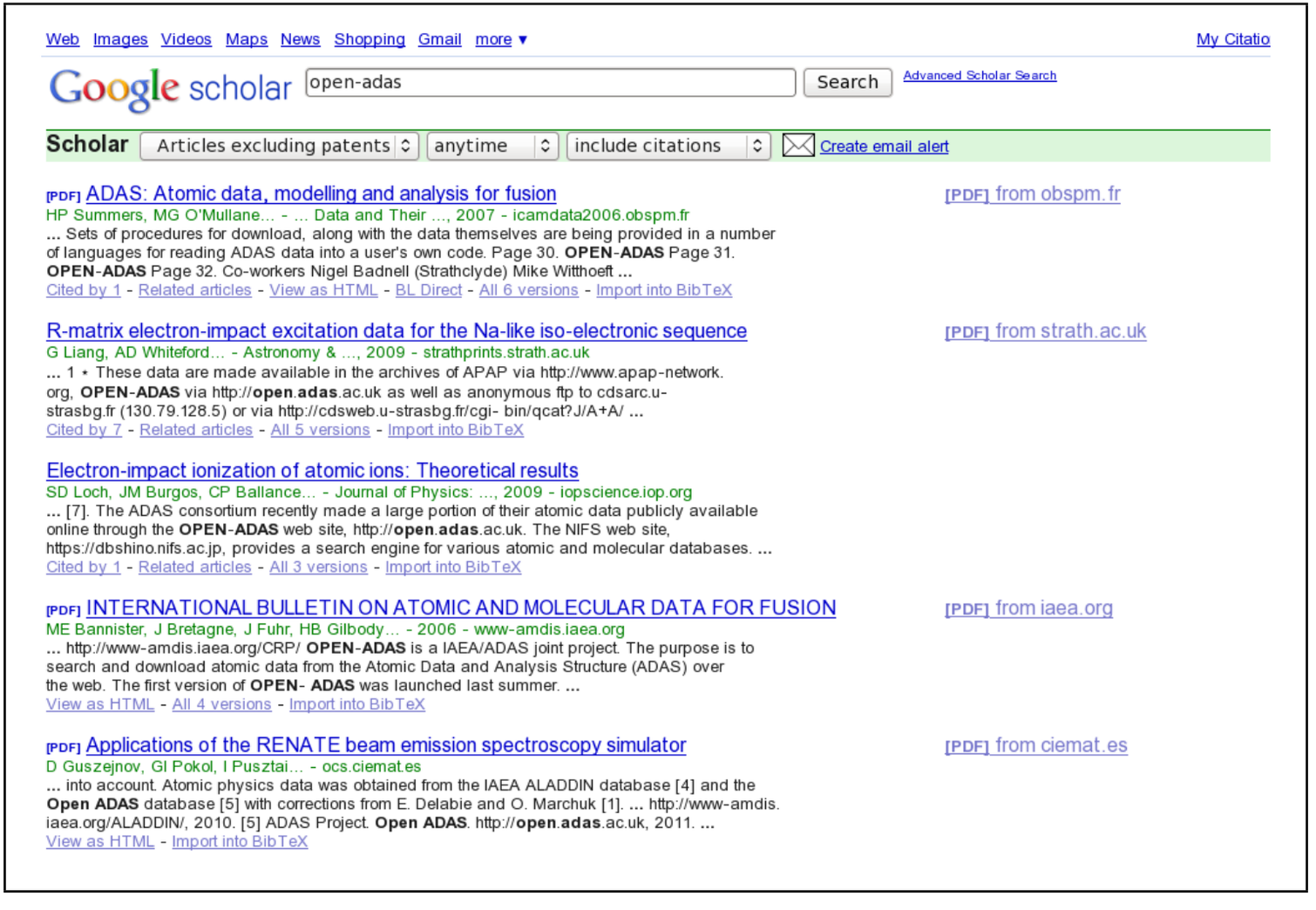
Statistics

Data class	Description	Number of files	Total Size
ADF01	Charge Exchange Cross Sections	127	2 MB
ADF04	Resolved Specific Ion Data Collections	1675	3 GB
ADF07	Electron Impact Ionisation Coefficients	72	645.6 kB
ADF08	Radiative Recombination Coefficients	100	482.5 kB
ADF09	Resolved Dielectronic Recombination Coefficients	1622	1.1 GB
ADF11	Iso-nuclear Master Files	796	111.2 MB
ADF12	Charge Exchange Effective Emission Coefficients	167	4.5 MB
ADF13	Ionisation Per Photon Coefficients	153	35.2 MB
ADF15	Photon Emissivity Coefficients	551	102 MB
ADF21	Effective Beam Stopping/excitation Coefficients	220	1.8 MB
ADF22	Effective Beam Emission/population Coefficients	406	3.4 MB

OPEN-ADAS since the 20th DCN

It is seen as a Google Scholar resource and is appearing in citations, which is welcome as this gives greater visibility and credit to the people who produced the data.



Loss of metrics

Until June 2011 OPEN-ADAS:

- Worked without problems except for minor power outages.
- A steady increase in new users with a wide geographic spread.
- Downloads and file views increased.

Just when one thinks that all is well....

- On 2nd June the OPEN-ADAS website, but not the server, was hacked using a MySQL injection attack.
- Logs showed a large increase in such attacks for the following few weeks.
- June 16, 2011 — hard disk failure on OPEN-ADAS server.

Our response so far:

- A new server was commissioned within a few days.
- Removed the requirement to register in order to download data.
- OPEN-ADAS was off the internet for 8 weeks.
- We have lost the ability to know who our users are but without more resources it the most pragmatic solution.