Module 7

Calculating fundamental atomic structure and electron impact cross-section data – Autostructure and R-Matrix.

Lecture viewgraphs

Hugh Summers, Nigel Badnell, Martin O'Mullane and Alessandra Giunta

University of Strathclyde

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1.1 Atomic structure codes in general use

Code	Method	Usual application	Precision (E%, A%)	Comments
AUTOSTRUCTURE	Multi-config, Breit-Pauli, Thomas-Fermi and Slater-type parametric potential	General + Auger rates + Born integrals	(~2, ~5) typically dependent on CI scope.	Recently extended to multiply- occupied f-shells. Extended experience of use up to M-shell. Limited coupling scheme information. Specially tuned for dielectronic and radiative recombination. Can separate term, level and configuration average resolution calculations. A preferred code for ADAS.
COWAN	Multi-config, Breit-Pauli, Hartree-Fock potential.	General + Auger rates + Born	(~2, ~5) typically dependent on CI scope and tuning.	Handles multiply-occupied f-states. Extended experience in many complex systems. Flexible coupling scheme information. Easy access to configuration average information. Executes level resolution calculation and averages to terms. A preferred code for ADAS.
HULLAC	Multi-configuration, Dirac Hamiltonian; j-j coupled basis, Breit and QED	General, but extensive use with EBIT measurements.	(~2, ~5) typically dependent on CI scope.	Proprietary code package; structure code part matched to distorted wave collision code and collisional-radiative modelling.
FAC	As for HULLAC	General, but mostly astro-physics.	(~2, ~5) typically dependent on CI scope and tuning.	Public domain variant of HULLAC. Use increasing and experience building up.
GRASP	Multi-configuration, Dirac/ Breit Hamiltonian; MCDHF or parametric potential; various couplings and optimizations.	General.	(<1, <3) with extensive core/ valance CI.	High grade code, but MCDHF not always able to converge on potential. Tuned to DARC fully relativistic version of R-matrix collision code. A preferred code for ADAS level 2 in relativistic region.

1.2 Electron impact collision codes in general use

Code	Method	Usual application	Precision (%)	Comments
AUTOSTRUCTURE/ COWAN	Born with modified threshold region.	Low - medium/ high z.	(<40%)	Very general, stable and enabled by all structure codes with a free electron wave-function generator. No spin change. CA, LS and IC coupling. Suitable for ADAS baseline.
CCC / CCC-R	Convergent close-coupling.	Low - medium/ high z; 1-2 valence electrons	(<5%)	Highest precision, inefficient for very many energies and delimiting resonances. Limited ion scope. Currently being extended to Dirac relativistic.
DARC/ DRMPS	Relativistic R-matrix close-coupling / with pseudo-states.	Low - high z.	(~ 5-10%)	Very high precision, tuned to GRASP structure and shared algebra. Resonances included. Recent pseudo-state extension increases heavy element near neutral scope. Use also for ionization. Intermediate coupling. Suitable for ADAS level 2 at low and high z.
HULLAC / FAC	Distorted wave.	Medium - high z.	(~20%)	Intermediate coupling, includes spin change, no resonances. Efficient algebra – but now used universally. Matched to HULLAC structure part.
AUTOSTRUCTURE	Distorted wave	Medium - high z with some use at low z	(~20%)	Very stable. In continuing development. CA, LS and IC coupling. Integrated in ADAS and suitable for level 1 increase from baseline.

1.3 Electron impact collision codes in general use (contd)

Code	Method	Usual application	Precision (%)	Comments
RM / RMPS	R-matrix close-coupling / with pseudo-states.	Low - med		High precision, tuned to AUTOSTRUCTURE and shared algebra. Resonances included. Use also for ionization. Implemented for isoelectronic sequences with scripts. LS coupling. Parallelized versions. Suitable for ADAS level 1, 2 medium-scale mass production.
RM – ICFT /RM-II	R-matrix close-coupling with interrnediate-coupling frame transformations/ R-matrix close-coupling with IC inner region.	Medium - medium/ high z.	(~ 5-10%)	As for RM, but extends to higher z ions in intermediate coupling. Suitable for ADAS level 1, 2 medium-scale mass production. R-matrix inner region IC gives improved higher z treat-ment. Suitable for ADAS level 2 and bench-marking of RM-ICFT.
RM-RD / DARC-RD	R-matrix close-coupling with radiation damping.	Medium - high z.	(~ 5-10%)	As for RM, but extends to high z ions with significant radiative/ Auger branching of resonances. Suitable for ADAS level 1, 2.
TDCC	Time-dependent close coupling.	Low z; 1-2 valence electrons.	(<5%)	Highest precision. Benchmark for low-z ionization. Used for ADAS level 2.
UCL-DW / JAJOM	LS distorted wave with IC transformation.	Medium -medium/ high z.	(~20%)	Matched to AUTOSTRUCTURE. Extension to IC via algebraic transformation. Includes spin change. No resonances. Can isolate calculation of cross-sections starting with selected metastables. Now inefficient and falling out of use in comparison with RM.

* depends on precision of multi-configuration multi-electron structure calculation and/or close-coupled set and/or pseudo-state span and completeness.

2.1 Driving the Cowan code for ADAS

adf34 config. file:

```
2  -5    2   10  1.0    5.d-09    5.d-11-2  0130    1.0 0.65  0.0  0.5
    4    2   Be  2s1             1s2  2s1
    4    2   Be  3s1             1s2  3s1
    4    2   Be  4s1             1s2  4s1
    .    .   .
    4    2   Be  4f1             1s2  4f1
    4    2   Be  5f1             1s2  5f1
   -1
```

contol parameters

config. list, 1st parity then 2nd partity

RCN2 instruction file:

```
z0 74
zi  0
parity-1 11 : 2  1  2
parity-2  9 : 2  1  7
E2 3
M1 3
scale 85 95 85 85 50
temperature 25
 1.00e+03 1.47e+03 2.15e+03 3.16e+03 4.64e+03 6.81e+03 1.00e+04 1.47e+04
 2.15e+04 3.16e+04 4.64e+04 6.81e+04 1.00e+05 1.47e+05 2.15e+05 3.16e+05
 4.64e+05 6.81e+05 1.00e+06 1.47e+06 2.15e+06 3.16e+06 4.64e+06 6.81e+06
 1.00e+07
```

W^0

contols calculations for each partity

contols radiation multipoles calculated

coulomb integral scaling factors

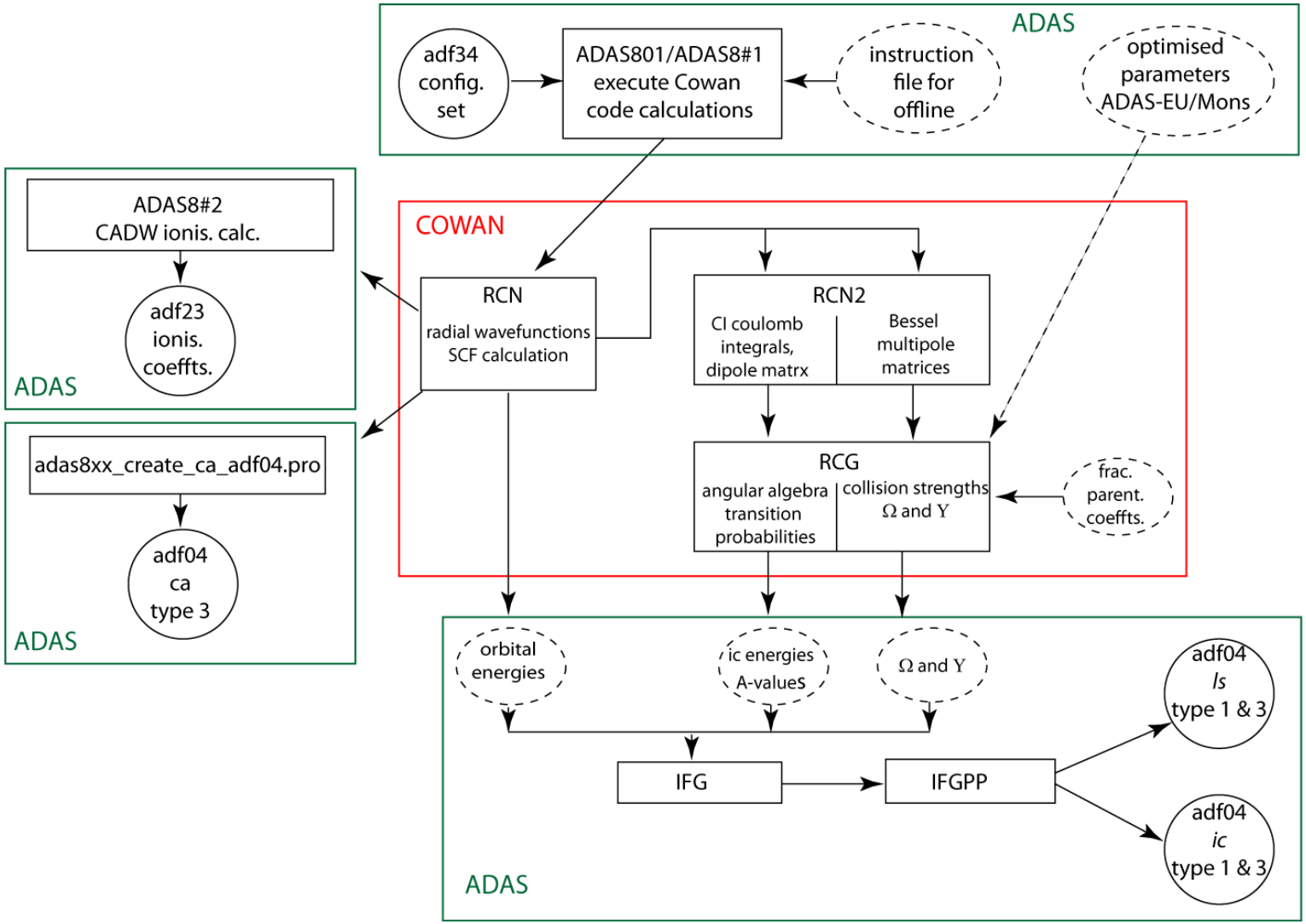
reduced T_e set for adf04

IGFPP instruction file:

```
1
Martin O'Mullane
03-08-2012
5
C
C  Cowan plane wave Born method
C
C  Scale factors 85 95 85 85 50
C
 &FILES ifgfile = 'ifg#w0#a_adf34.dat' , outfile = 'wlike_mons11#w0.dat' &END
 &OPTIONS  ip =  63427.7, coupling = 'IC' ,  aval = 'YES' ,
           isonuclear = 'NO', quantity = 'RATES', lweight = 'NO' ,
           comments = 2,  numtemp = 14 , &END
  1  2  3  5  7  9 11 12 13 14 15 17 19 20
parity-1 11 : 2  1  2
parity-2  9 : 2  1  7
```

comments to be appended to adf04 dataset

2.2 Cowan code schematic and ADAS utilisation



3.1 Basis atomic structure using AUTOSTRUCTURE

At the command line, the AUTO-STRUCTURE code requires a driver dataset. Results are returned to the initial directory as for example:

> *../../bin/as25lm_hps.x < das_2*

The main summary results are returned in the dataset called *olg*.

das_2

```
A.S. Be-like C structure - energies + radiative rates
 &SALGEB CUP='IC' RAD='E1' MXCONF=3 MXVORB=3  &END
 1 0  2 0  2 1
  2    2    0
  2    1    1
  2    0    2
 &SMINIM NZION=6  &END
```

- intermediate coupling
- electric dipole transition probabilities
- 1s orbital
- valence orbitals
- number of valence orbitals
- configs.
- configuration occupation numbers
- number of configurations
- nuclear charge

olg (last part)

quantum numbers

K	LV	T	K*CM	2*S+1	L	2J	CF	(EK-E1)/RY	E1/RY = -72.87735554
1	8	5	0.	1	0	0	1	0.00000000	
2	10	3	53644.	-3	1	0	2	0.48884297	
3	5	3	53686.	-3	1	2	2	0.48921835	
4	3	3	53768.	-3	1	4	2	0.48997075	
5	6	4	110586.	-1	1	2	2	1.00773254	
6	7	2	138633.	3	1	0	3	1.26331362	
7	4	2	138674.	3	1	2	3	1.26369166	
8	2	2	138756.	3	1	4	3	1.26444154	
9	1	1	154402.	1	2	4	3	1.40701900	
10	9	6	191560.	1	0	0	3	1.74562274	

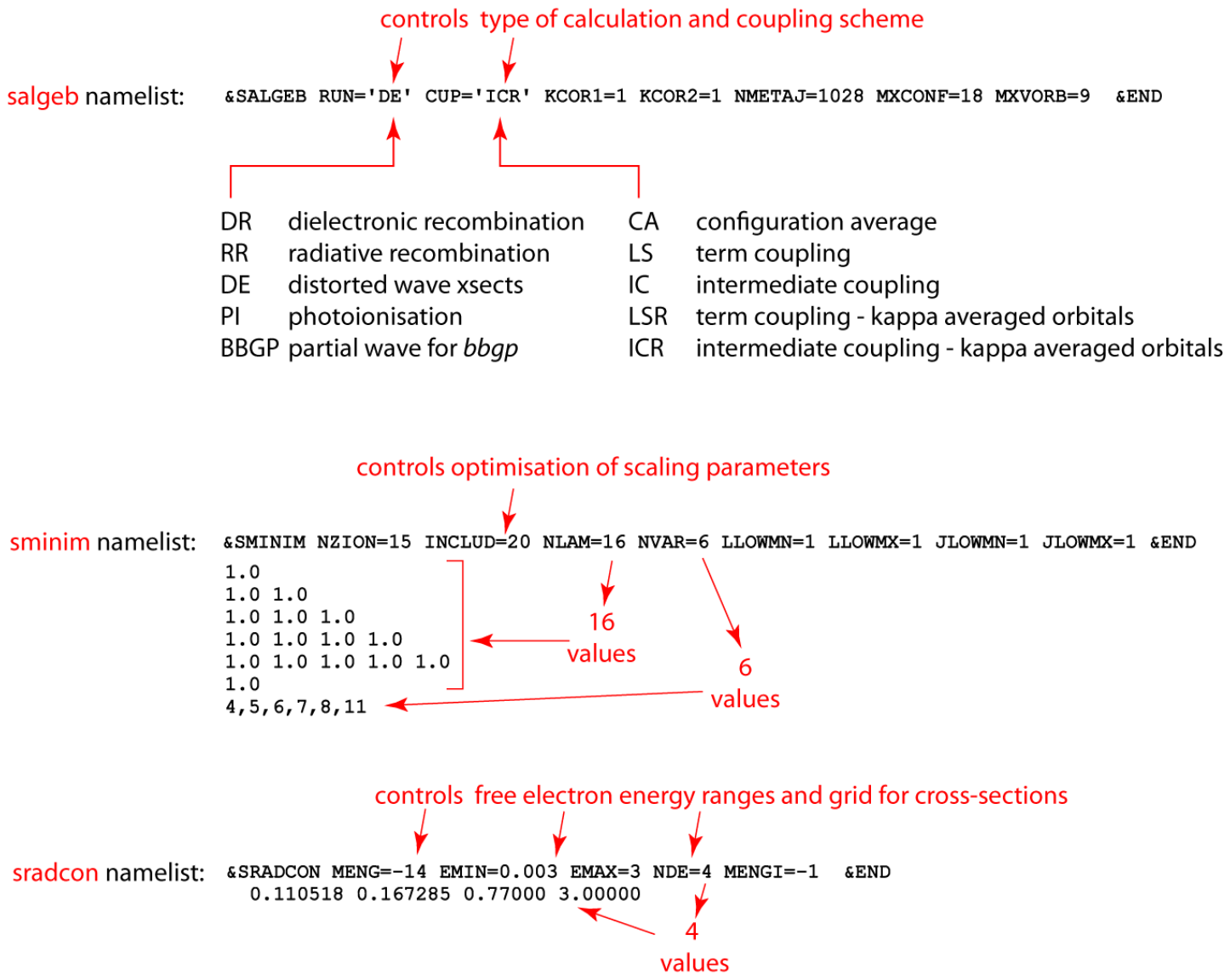
- absolute ground level energy
- algebraic level indexing
- algebraic term indexing
- level energies

3.2 Control of AUTOSTRUCTURE with namelist parameters

The AUTOSTRUCTURE code has been in continuing development for more than 30 years. It is now one of the most versatile codes of its kind in the world.

Much of its operation in recent years has been tuned to ADAS needs. It writes directly to ADAS formats such as *adf04*, *adf09*, *adf38*, *adf39* and *adf48*.

It can be used from the command line or via the interactive ADAS code ADAS701.



3.3 Using AUTOSTRUCTURE for dielectronic recombination

An original purpose of AUTOSTRUCTURE was the calculation of state selective dielectronic recombination coefficients.

The input data set is a driver of data format *adf27* of sub-category *dr* . It is designed to create dielectronic data tuned to bundle-n and bundle-nl population models.

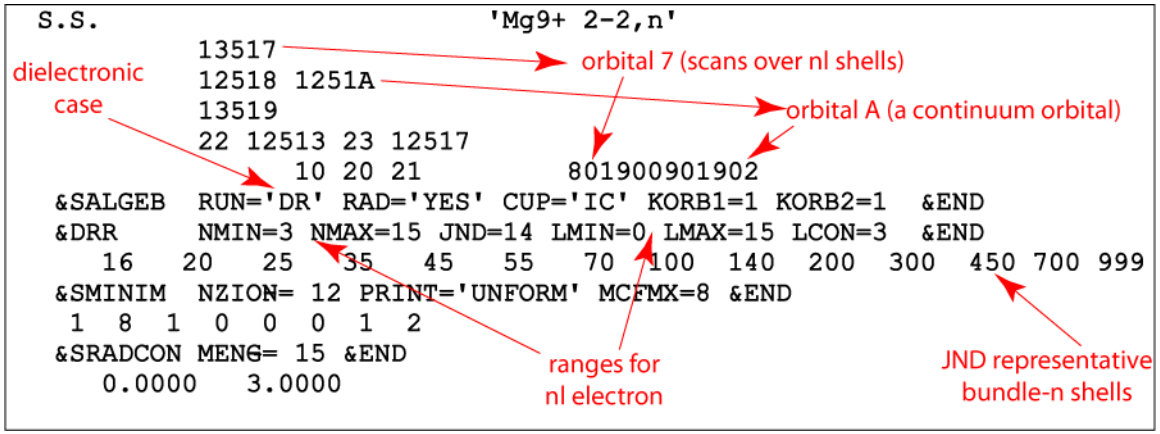
The dataset name:

/../adf27/dr/lilike/jc00#li/*mg9ic22-n.dat*

informs that it is a lithium-like Mg^{+9} which is recombining via 2-2 parent transitions capturing into higher n shells.

The driver can be used interactively by the code ADAS701 or offline by ADAS7#1. It creates a number of datasets including the *olg* file and the *ols* and *oic* files of Auger rates in *ls* and *ic* coupling.

The code ADAS702 assembles energy level, transition probability and Auger data to obtain dielectronic coefficients of format *adf09*.

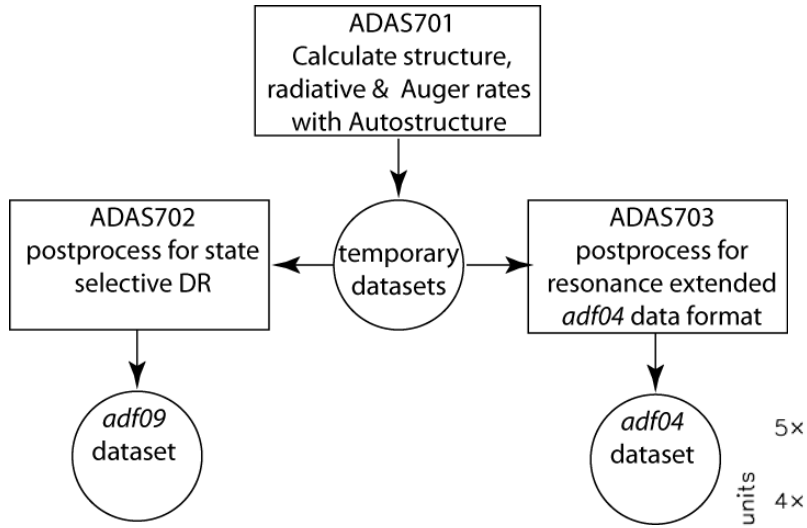


The ADAS project has a long history dating from ~1990 of dielectronic data preparation to the *adf09* format. Originally prepared in *ls* coupling, since 2000, it has been prepared also in *ic* coupling. Isoelectronic sequences up to Al-like have been completed spanning elements up to zinc. The drivers are archived similarly in format *adf27/dr*.

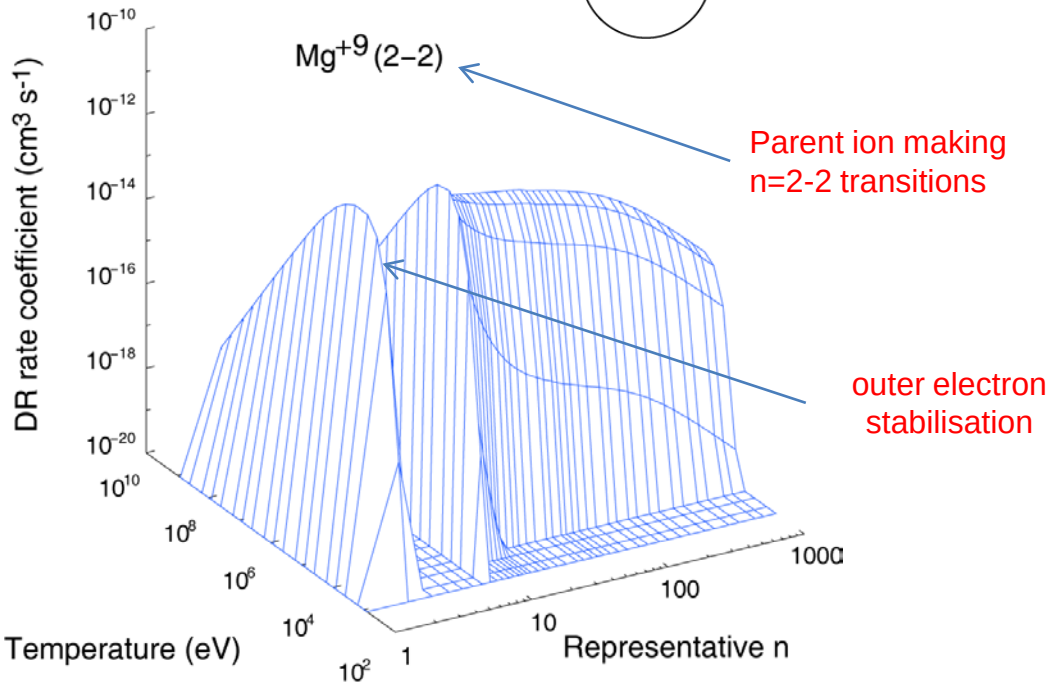
It is probably the largest repository of such data amounting to some 1.5 Gbytes.

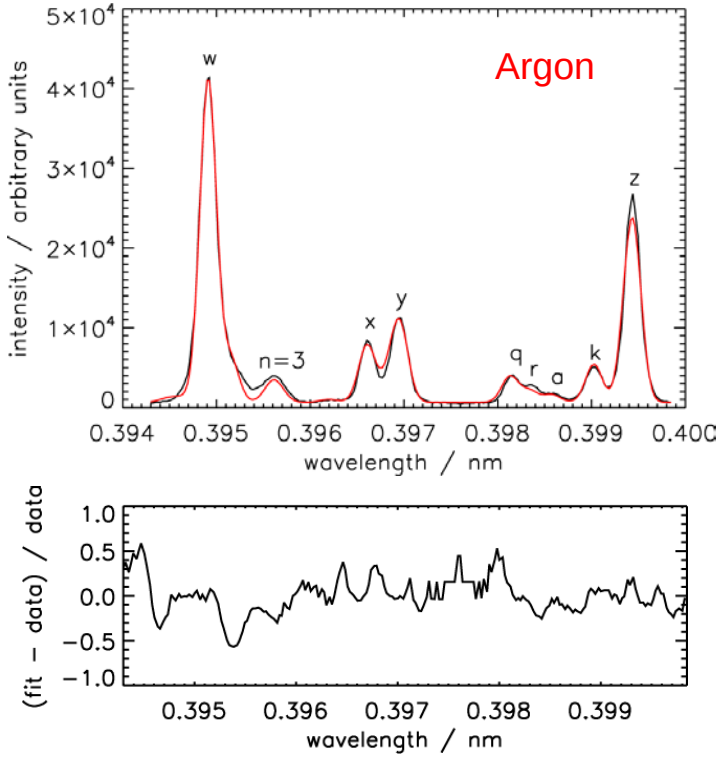
3.4 Postprocessing Auger data for ADAS applications

The adf09 database is one of the most important parts of ADAS. It is noted that correct modelling of dielectronic recombination in plasmas requires attention to capture to quantum shells as high as n~1000.



The ADAS703 processing path creates an enhanced adf04 dataset which includes resonance capture and Auger breakup transition data lines. So satellite line modelling is enabled. Results below are from ADAS605.





3.5 Current extensions of dielectronic calculations

- On progressing to systems with more electrons, the size of *adf09* datasets has increased markedly. It is unlikely that further large scale production in the standard *adf09* *ic* pattern will be produced.

- The complexity of heavy element ions has caused us to introduce a new hybrid approximation, combining an *ic* parent description with a configuration average intermediate state representation. This is much more economical in space requirements and ideally tuned to the bundling population models to be used for heavy species ions. This method will be introduced in ADAS and AUTOS releases in the near future.

- Dielectronic recombination at very low electron temperatures, typical of photo-ionised plasmas has been under extensive revision in recent years. The general assumption that dielectronic recombination gives way to radiative recombination at very low temperatures is not sustained, due to the common occurrence of 'at threshold' dielectronic resonances.

- Special measurements for W^{+20} obtained for ADAS-EU reveal extremely large resonance contributions which influence effective recombination markedly even up to electron-excited plasma temperatures.

- Theoretical examination of the problem, suggest that its origin lies in strong interaction of many configurations best described as an ergodic-like spreading of Auger rates amongst very many doubly excited states. Current calculations, near threshold begin to reproduce the experimental results. We anticipate these effects being introduced into the dielectronic data as we progress into the difficult heavy element ions.

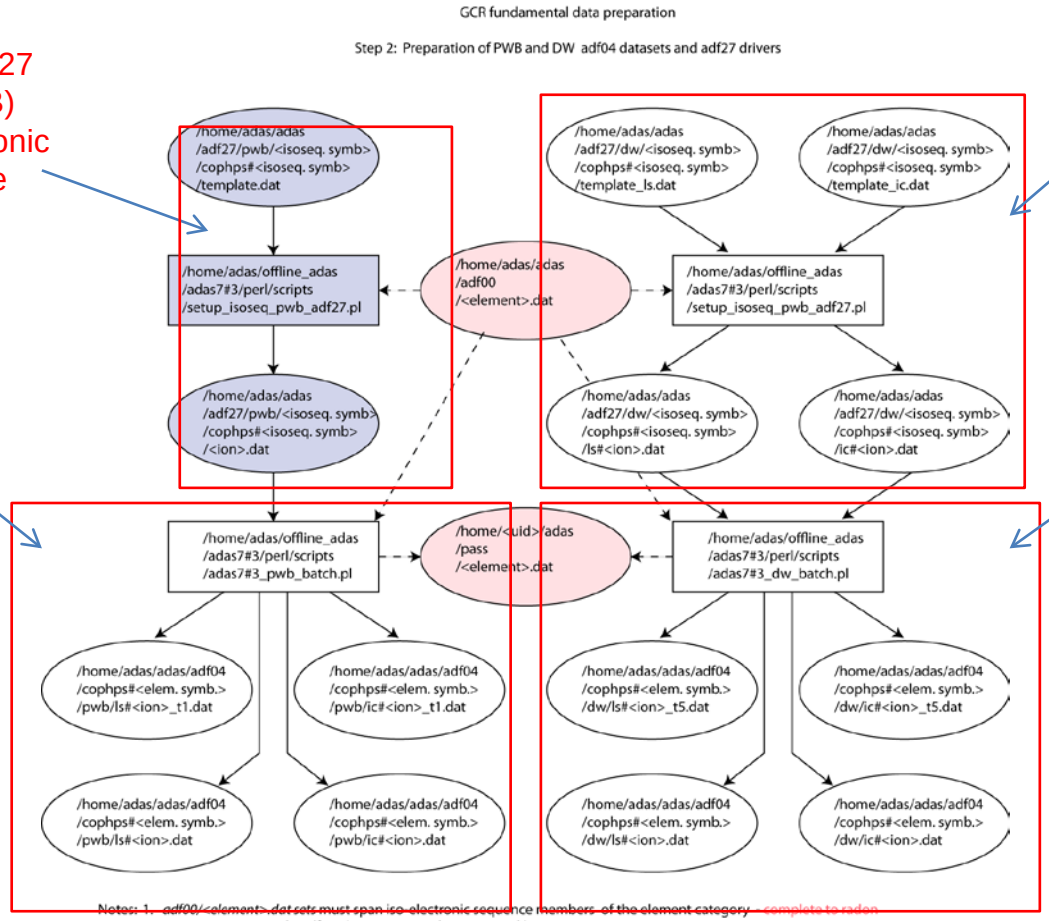
4.1 AUTOSTRUCTURE PWB and DW mass production

Set up drivers of format adf27 for plane wave born (PWB) calculations for an iso-electronic sequence from a template

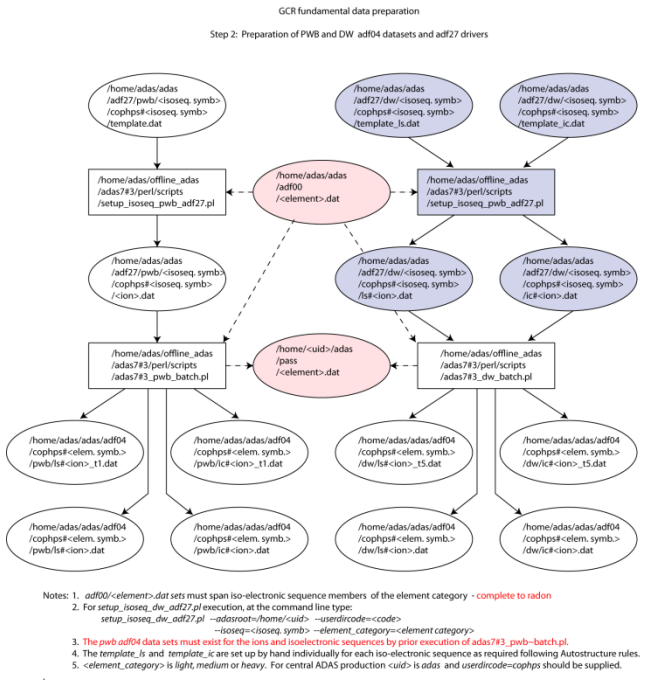
Execute distributed processer calculation of adf04 type 1 and type 3 *ls* and *ic* datasets in PWB approximation for the iso-electronic sequence

Set up drivers of format adf27 for distorted wave (DW) calculations – *ls* and *ic* - for an isoelectronic sequence from templates

Execute distributed processer calculation of adf04 type 5 and type 3 *ls* and *ic* datasets in DW approximation for the iso-electronic sequence

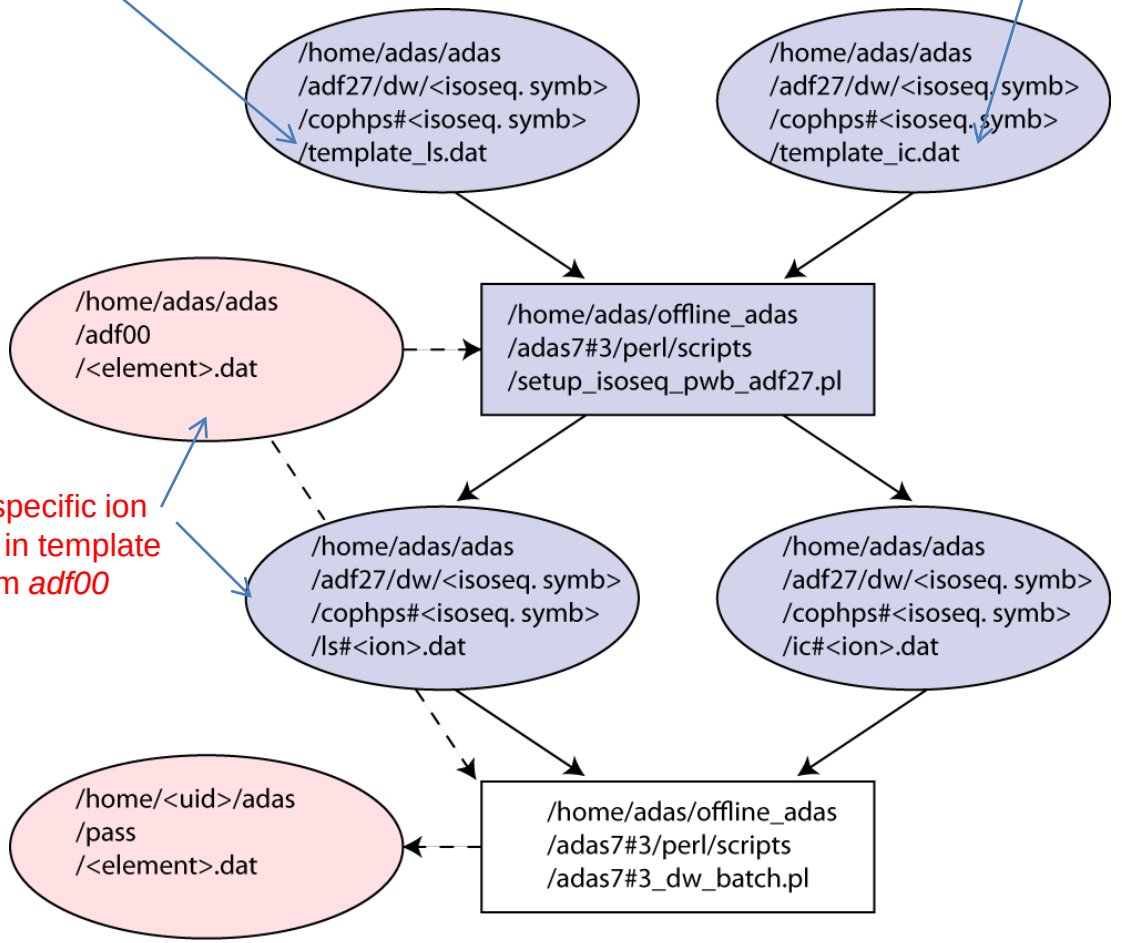


4.2 Creation of adf27 DW drivers from templates



ls template for an Autostructure *dw* calculation

ic template for an Autostructure *dw* calculation



fill in specific ion details in template from *adf00*

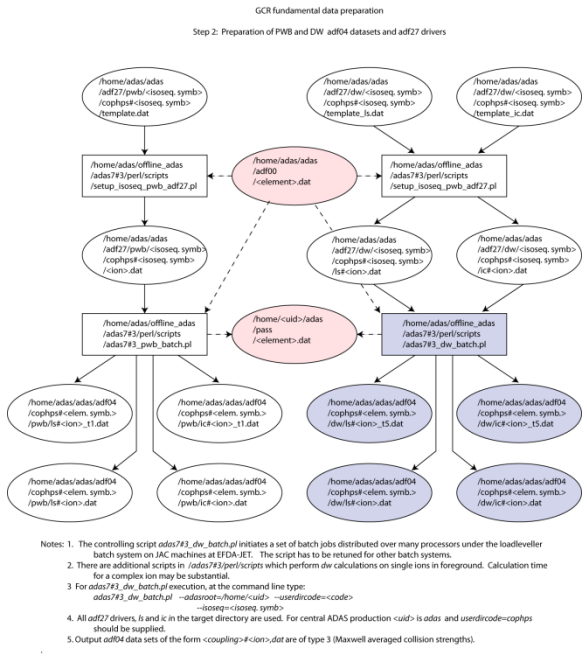
In mass generation of data it is advantageous to work with iso-electronic sequences.

The configuration sets and scaling parameters for a range of iso-electronic sequence members can be the same.

ADAS is highly organised for this, carrying out the preparation and runs in distributed processing and under the control of master scripts.

The first stage of *dw* production is isolated to the right.

4.3 Production of adf04 type 5 and type 3 datasets from adf27 driver

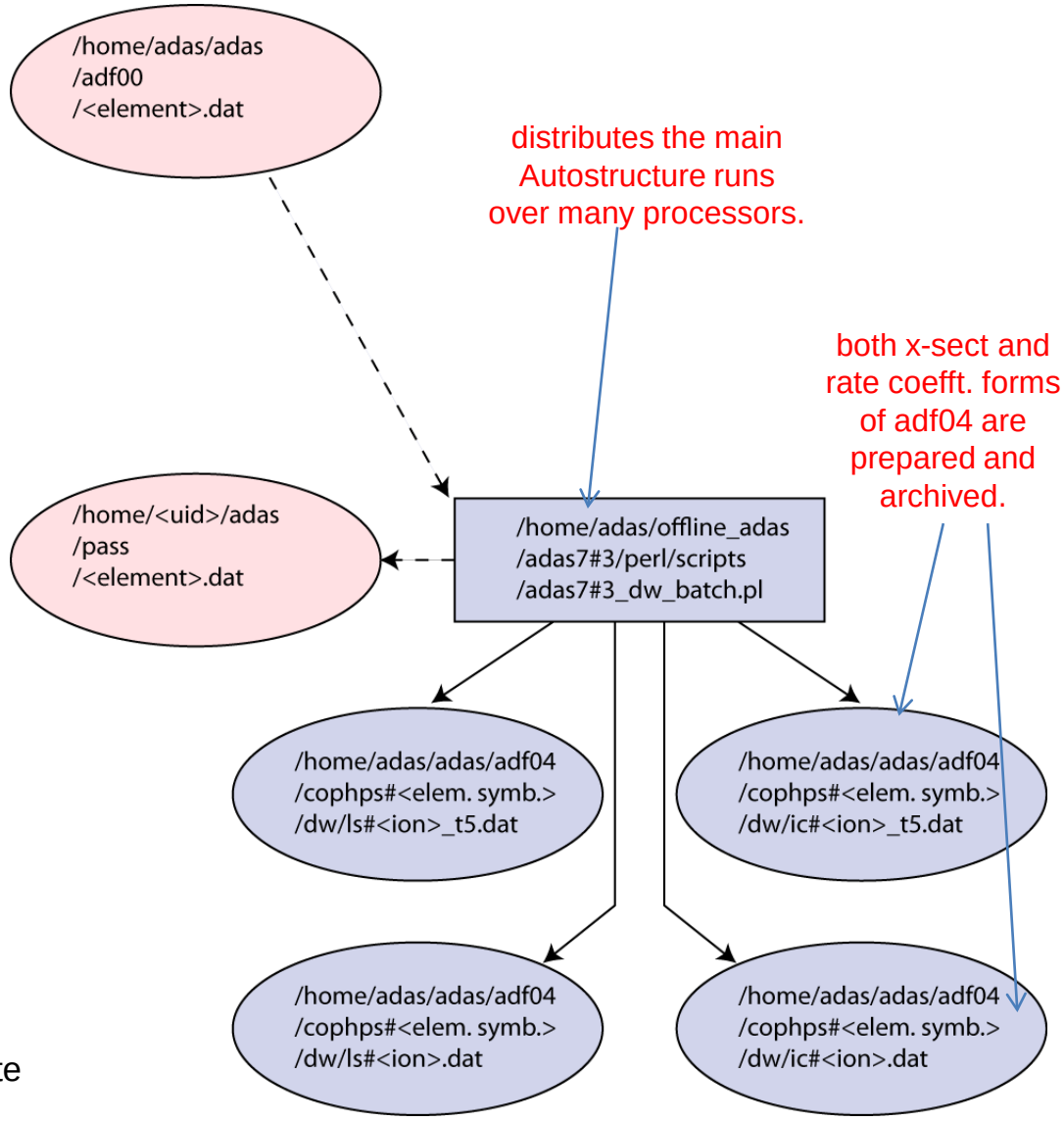


The organisation of the actual *dw* calculations is shown on the right.

The completion is the set of *adf04* datasets for the members of the iso-electronic sequence.

A sequence such as phosphorus-like for the light element set up to zinc takes ~1 week distributed over ~40 processors at the JET Facility.

ADAS archives *pwb* and *dw* calculations of both *ls* and *ic* resolutions and of both cross-section (type 1 or 5) and rate coefficient (type 3) *adf04* format.



4.4 Neutral and near neutral ion level adjustments

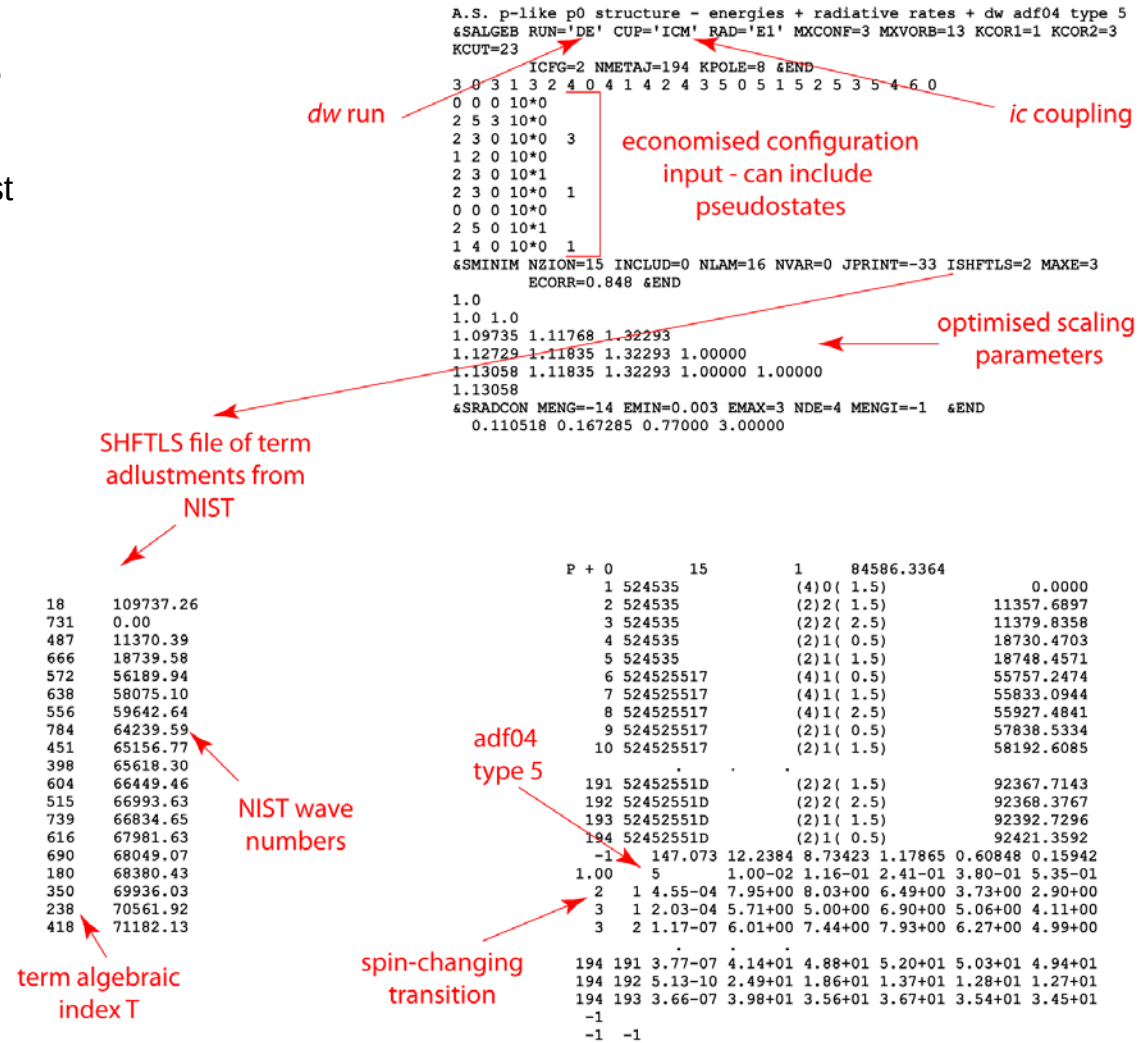
The neutral and near-neutral atoms are the most difficult systems to calculate, since the electron-electron Coulomb potential is not dominated by the Coulomb interaction with the nucleus.

Much more extensive configuration interaction must be included and optimisation of potential scaling parameters. In spite of this, level energies are insufficiently precise for spectroscopy and must be adjusted.

The National Institute of Standards and Technology (NIST) is the primary atomic energy level source. ADAS uses periodic automatic scanning of NIST to assemble *ls* and *ic* *adf04* data sets of energy levels without collisonal data archived element directories as:

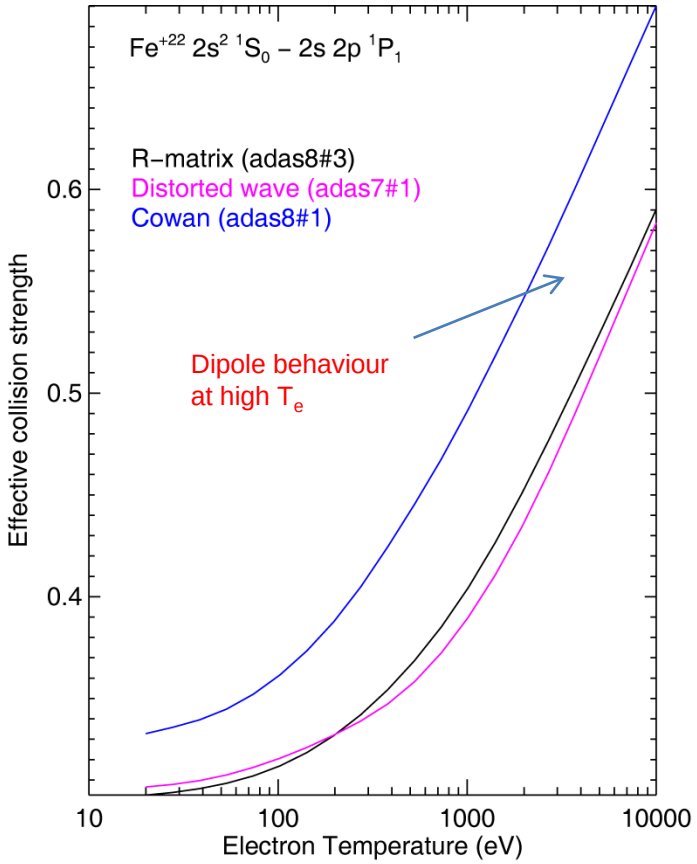
/.../adas/adf04/nist#<at. numb.>/

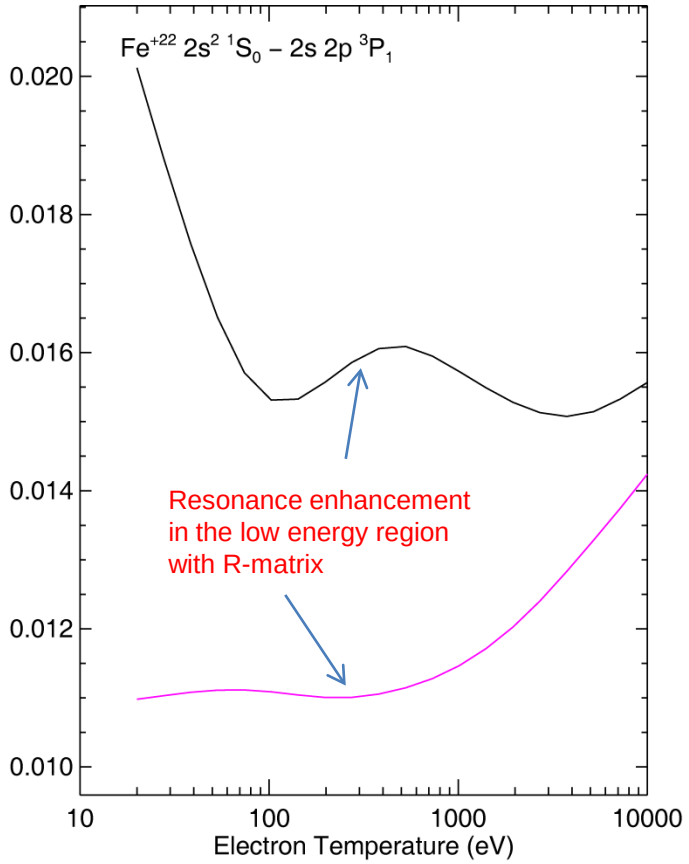
ADAS uses these data for Autostructure adjustment. ADAS also has special codes for matching and merging *adf04* datasets: /adas705/g5mrg4.for.



4.5 Cross-section illustrations and comparisons

There is no valid Born cross-section for this spin change transition although residual weak spin breakdown does give a non-zero cross-section





5.1 The R-matrix method and electron impact cross-sections

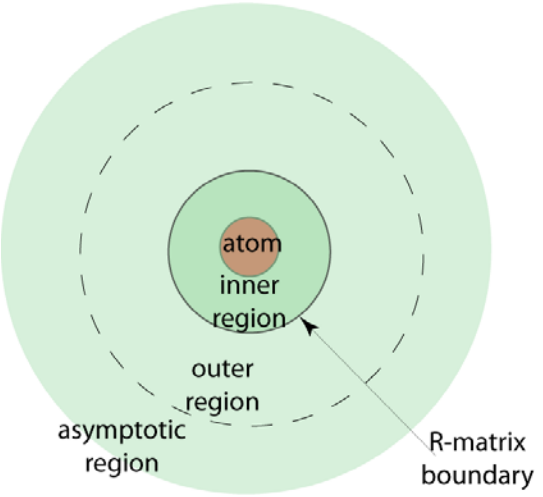
The R-matrix method is the most versatile, high precision method available for calculation of electron impact excitation cross-sections.

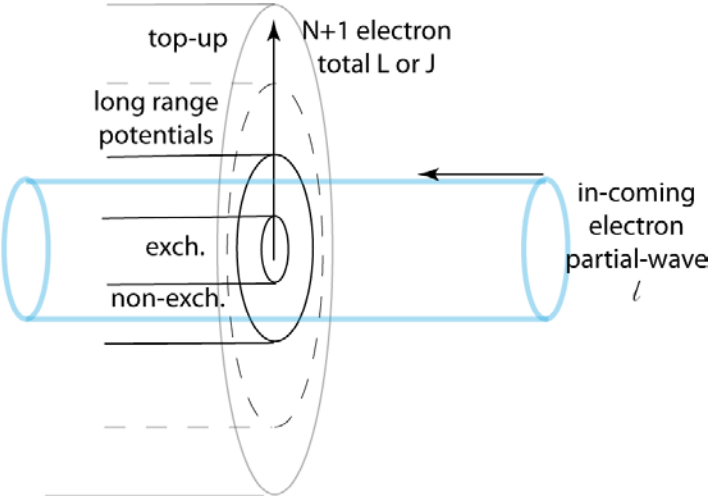
It treats resonant structure in the N+1-electron system correctly at root, but is a complex method which is demanding on computer resources.

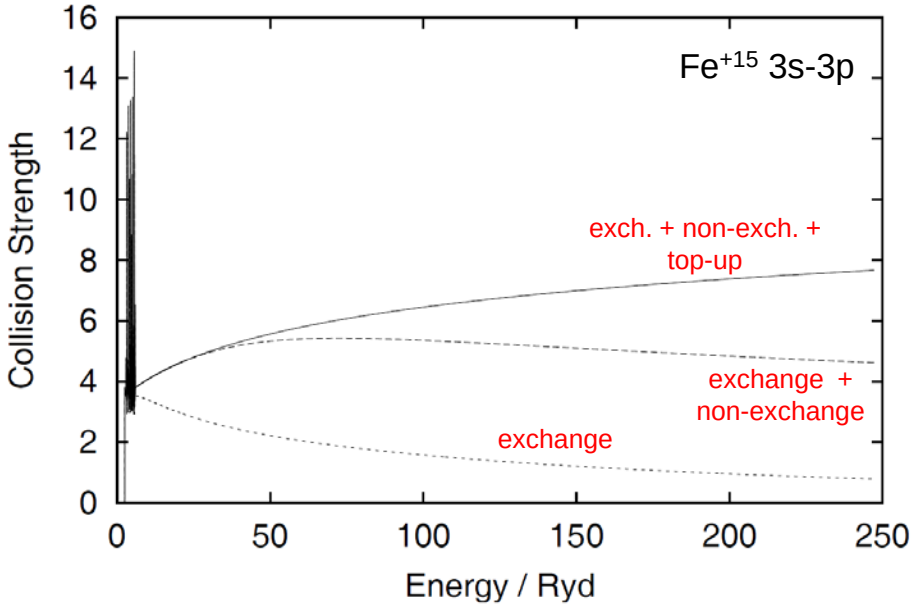
The variants are able to handle light systems in *ls* coupling, semi-relativistic systems in Breit-Pauli *ic* coupling and fully relativistic systems in the Dirac formalism.

With inclusion of pseudo-states, it can address neutral and near-neutral systems – including ionising collisions.

Most current development and production using R-matrix methods are coordinated between Strathclyde University, Auburn University and Queen's University of Belfast and are closely linked to the ADAS Project.







5.2 Using the R-matrix method with ADAS: Fe^{+15}

autos

```
A.S.
&SALGEB RAD='ALL' CUP='LS' MXVORB=3 MXCONF=3 KORB1=1
KORB2=3 KUTSO=0 BORN='INF' &END
3 0 3 1 3 2
1 0 0
0 1 0
0 0 1
&SMINIM NZION=26 RADOUT='YES' &END
```

stg1

```
S.S.
&STG1A &END
&STG1B MAXLA=2 MAXLT=12 MAXC=20 MAXE=100 &END
```

no. of continuum basis orbitals

maximum energy

stg2

```
S.S.
&STG2A &END
&STG2B MAXORB=6 NELC=11 NAST=3 INAST=0
MINLT=0 MAXLT=12 MINST=1 MAXST=3 &END
1 0 2 0 2 1 3 0 3 1 3 2
3
2 2 6 0 0 0 0 0 0 0
2 2 6 1 1 1 1 1 1 1
2 2 6 1 0 0 0 0 0 0
2 2 6 0 1 0 0 0 0 0
2 2 6 0 0 1 0 0 0 0
2 0 0
2 1 1
2 2 0
1
2 2 6 0 0 0 0 0 0 0
2 2 6 2 2 2 2 2 2 2
2 2 6 1 0 0 0 0 0 0 2
```

min. & max. LT and ST (N+1-electron system)

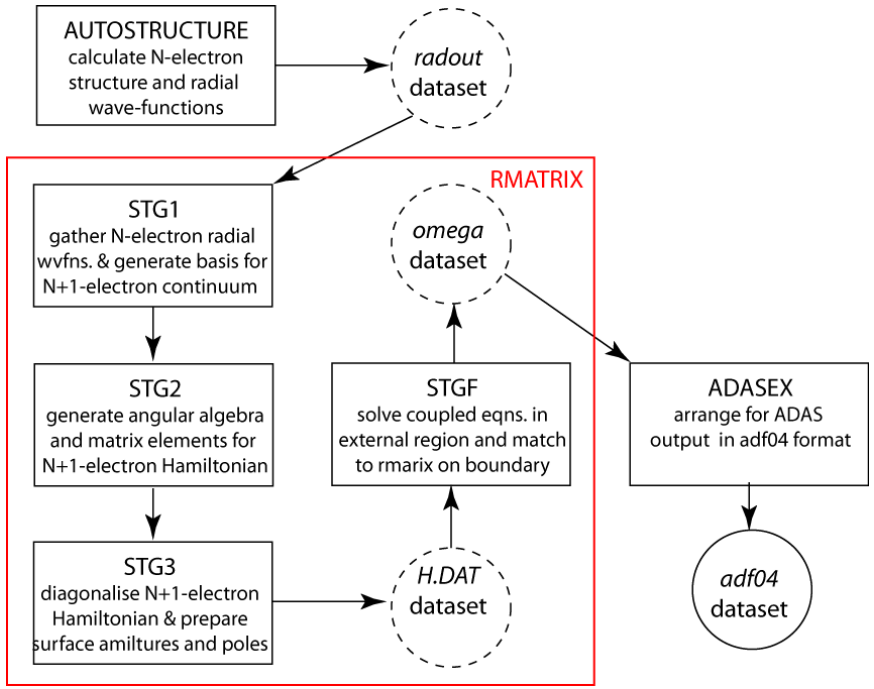
atom configs. (N-electron system)

atomic terms (multi, L, π)

reson. configs. (N+1-electron system)

stg3

```
S.S.
&STG3A &END
&STG3B INAST=0 NAST=0 &END
```



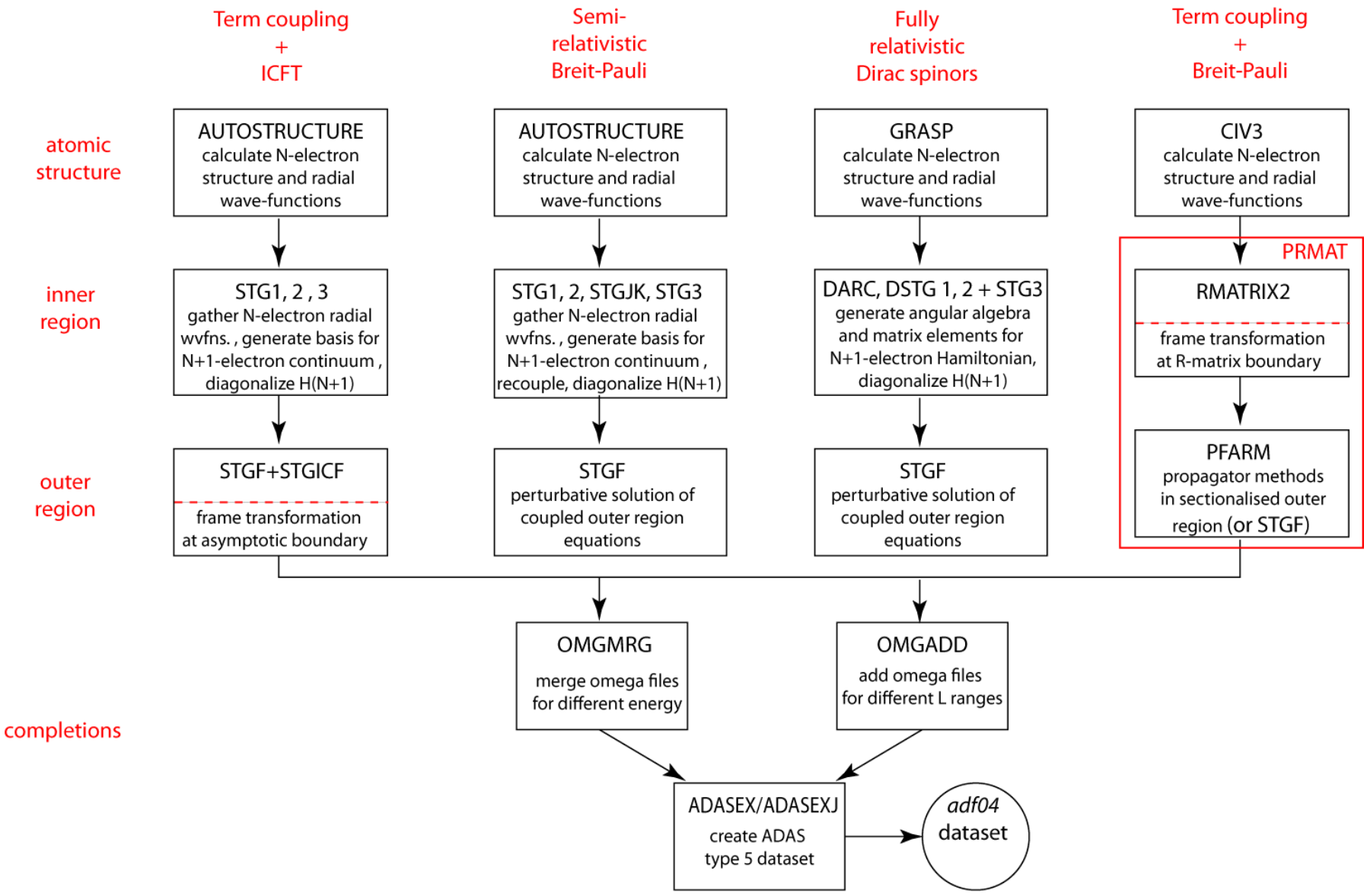
stgf

largest l for coll. strengths

```
&STGF IMESH=1 IQDT=2 PERT='YES' LRGLAM=12 IPRINT=-1
ELAS='NO'
IPRKM=4 IBIGE=0 &END
&MESH1 MXE=9000 E0=0.01 EINCR=0.00001 &END
```

energy grid, number, start and increment

5.3 The current family of R-matrix method implementations



5.4 Participation in R-matrix calculations

The preparations and infrastructure required for R-matrix calculations for the new species and ions of current interest for fusion are substantially beyond the usual needs of ADAS codes. Most calculations require parallel computing capabilities and often the power of massively parallel supercomputers.

It has usually been most fruitful and likely of success, to work closely with the Strathclyde/Auburn/ADAS teams in a first development, so that insight and experience can be communicated efficiently and work coordinated. Thereafter, trained researchers can progress satisfactorily back in their home laboratories.

Further information on the R-matrix codes is available http://amdpp.phys.strath.ac.uk/tamoc/. The recent user manual for the current parallel R-matrix codes, prepared by Ballance and Griffin, is added as an appendix to the lecture notes for module 7.

The ADAS implementation is to be found in the directory */home/adas/offline_adas/adas8#3/* . A *Makefile* downloads the current code versions and creates and complies the codes. A user password is required to access the download site. A PERL script for execution of a basic R-matrix run is available as *adas8#3.pl* . These require adjustment for specific local conditions and computer resources.

6.1 Conclusions

- The ADAS team and its coworkers have built up a very large capability for the calculation of the atomic structure of arbitrary atoms and ions and of electron impact collisional cross-sections with them.

- The ADAS fundamental data formats, including *adf04*, *adf07*, *adf08*, *adf09* provide one of the largest resources of such data in the world.

- ADAS can bring to bear three major atomic structure codes and four major cross-section calculation codes. These collectively provide very wide species coverage at baseline precision through to highest precision, leading-edge calculations for specific high-priority ions.

- ADAS-EU sub-contracting collaborations have been of major importance in refining treatments of special cases, such as neutral atoms and in clarifying behaviour in the most complex systems. The going ADAS research program is extending these collaborative linkages and enabling greater penetration of special studies into the collisional domain.

- Fundamental data production by ADAS and its coworkers is tuned to exploitation in the various collisional-radiative models of ADAS and to the production of the derived data required for application.

- ADAS can at some level address all elements and their ions occurring in the present fusion plasma environments and in the expected ITER environments.