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New data in ADAS in support of GCR

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ADAS development

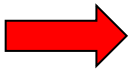
Needs:

- Reconstructing the emission and interpreting the behaviour of elements heavier than Ne is essential in both fusion and astrophysics: developments in the fusion context (e.g. ITER) and new analysis in the lower temperature solar chromosphere and transition region (e.g. need of Si^{1+}) required the extension of the range of species up to Argon and beyond.

- Extension of *Generalised Collisional-Radiative* (GCR) *model* to medium-heavy elements.

Requirements:

- Increasing the baseline.
- Automation and precision.
- Appropriate resolution.



Extension:

- **Infrastructure and mass data production.**
- **GCR derived data production.**

Infrastructure and mass data production

(1) *Ionisation potentials - adf00*

- basic data – ionisation potentials, ground configurations and quantum numbers from NIST (H - Kr)

- *ls* and *ic* ionisation, excitation, metastable specification quantum numbers from NIST (H – Fe): <*elem*>_ls.dat , <*elem*>_ic.dat (e.g. ar_ls.dat, ar_ic.dat)

- access - the *adf00* reading routines have been revised: **xxdata_00.for**, **read_adf00.pro**

- automatic creation and update – perl scripts: /adas1#1/scripts/

Infrastructure and mass data production

Example of ic adf00 for argon

ar_ic.dat

number of metastables for each ionisation stage

configurations

ionisation potentials and excitation energies

quantum number specifications

```
argon            -18  4  6  6  5  6  5  4  1  4  5  6  5  6  5  4  1  2  1 /wf=   0.00000/
 0     1.57596112d+01  1s2  2s2  2p6  3s2  3p6                    ( 1)0(  0.0)
    1  0.00000000d+00  1s2  2s2  2p6  3s2  3p6                    ( 1)0(  0.0)
    2  1.15483539d+01  1s2  2s2  2p6  3s2  3p5  3d0  4s1          ( 3)1(  2.0)
    3  1.16236925d+01  1s2  2s2  2p6  3s2  3p5  3d0  4s1          ( 3)1(  1.0)
    4  1.17231605d+01  1s2  2s2  2p6  3s2  3p5  3d0  4s1          ( 3)1(  0.0)
 ...............................................................
 2     4.07350066d+01  1s2  2s2  2p6  3s2  3p4                    ( 3)1(  2.0)
    1  0.00000000d+00  1s2  2s2  2p6  3s2  3p4                    ( 3)1(  2.0)
    2  1.37891500d-01  1s2  2s2  2p6  3s2  3p4                    ( 3)1(  1.0)
    3  1.94683699d-01  1s2  2s2  2p6  3s2  3p4                    ( 3)1(  0.0)
    4  1.73701854d+00  1s2  2s2  2p6  3s2  3p4                    ( 1)2(  2.0)
    5  4.12442097d+00  1s2  2s2  2p6  3s2  3p4                    ( 1)0(  0.0)
 ...............................................................
17     4.42622267d+03  1s1                                       ( 2)0(  0.5)
    1  0.00000000d+00  1s1                                       ( 2)0(  0.5)
c-----------------------------------------------------------------------------------------------
c
c  New updated adf00 ic format dataset with current NIST values.
c  Replaces earlier dataset of same name.
c
c  Sources:    /home/adas/adas/adf04/nist#18/     ic form
c              /home/adas/adas/adf00/             base form
c  Code:       make_nist_ls_adf00.pl
c  Producer:   Hugh P. Summers
c  Date:       07-Sep-2012
c
c  Expected metastables are not satisfied by NIST adf04 datasets for ionisation stages:
c           Ion charge      Deficit
c               2              1
c
c-----------------------------------------------------------------------------------------------
```

Infrastructure and mass data production

(2) *Energy levels and rate coefficients - adf04*

- *ls* and *ic adf04* without cross sections: /nist#<*nuclear charge*>/

- AUTOSTRUCTURE PWB *ls* and *ic* – type 1 and 3 *adf04* (up to Kr-like H - Zn):
  /cophps#<*isoelectronic sequence*>/pwb/ls#<*ion*>.dat
  /cophps#<*isoelectronic sequence*>/pwb/ic#<*ion*>.dat

- AUTOSTRUCTURE DW *ls* and *ic* – type 5 and 3 *adf04* (up to Kr-like H - Zn):
  /cophps#<*isoelectronic sequence*>/dw/ls#<*ion*>.dat
  /cophps#<*isoelectronic sequence*>/dw/ic#<*ion*>.dat

- access - the *adf04* reading routine **xxdata_04.for** has been revised to cope with the NIST *adf04*s

- automatic creation and update – perl scripts: /adas7#3/scripts/

- semi-automatic NIST merge (in progress): cophps#<*iso.seq.*>/pwb_nist/ls#<*ion*>.dat
  cophps#<*iso.seq.*>/dw_nist/ls#<*ion*>.dat

Infrastructure and mass data production

Example of NIST adf04 for krypton (Kr^{28+})

ic#kr28.dat

energy levels

configurations

```
Kr+28        36        29    26036000.00
    1  521522543            ( 3)1(  2.0)           0.00
    2  521522543            ( 3)1(  0.0)      160700.00
    3  521522543            ( 3)1(  1.0)      423820.00
    4  521522543            ( 1)2(  2.0)      524890.00
    5  521512553            ( 3)1(  2.0)     1674650.00
    6  521512553            ( 3)1(  1.0)     1864320.00
    7  521512553            ( 3)1(  0.0)     2133800.00
    8  521512553            ( 1)1(  1.0)     2377700.00
    9  521522533519         (  ) (  3.0)    20142200.00
   10  521522533519         (  ) (  1.0)    20162300.00
   11  521512543517         (  ) (  2.0)    21161800.00
   12  521512543519         (  ) (  3.0)    21570000.00
   13  521522533510         (  ) (  3.0)    22281100.00
   -1
   -1   -1
c-------------------------------------------------------------------------------
c
c  adf04 format dataset with NIST energy levels.
c
c  Source   = http://physics.nist.gov  -> /home/hps/nist_energy_level_tables/
c  Code     = process_nist_to_adf04.pl
c  Producer = Hugh P. Summers
c  Date     = 07-Sep-2012
c
c-------------------------------------------------------------------------------
```

The empty fields are due to the change of coupling in NIST (e.g. *jj* instead of *ic* or *ls*)

Infrastructure and mass data production

(3) *Ionisation rates - adf07*

- basic data – *adf23* CADW: /cadw/ca<*year*>_<*element symbol*>.dat
  adf07 CADW : /cadw#<*nuclear charge*>/ca<*year*>_<*ion*>.dat

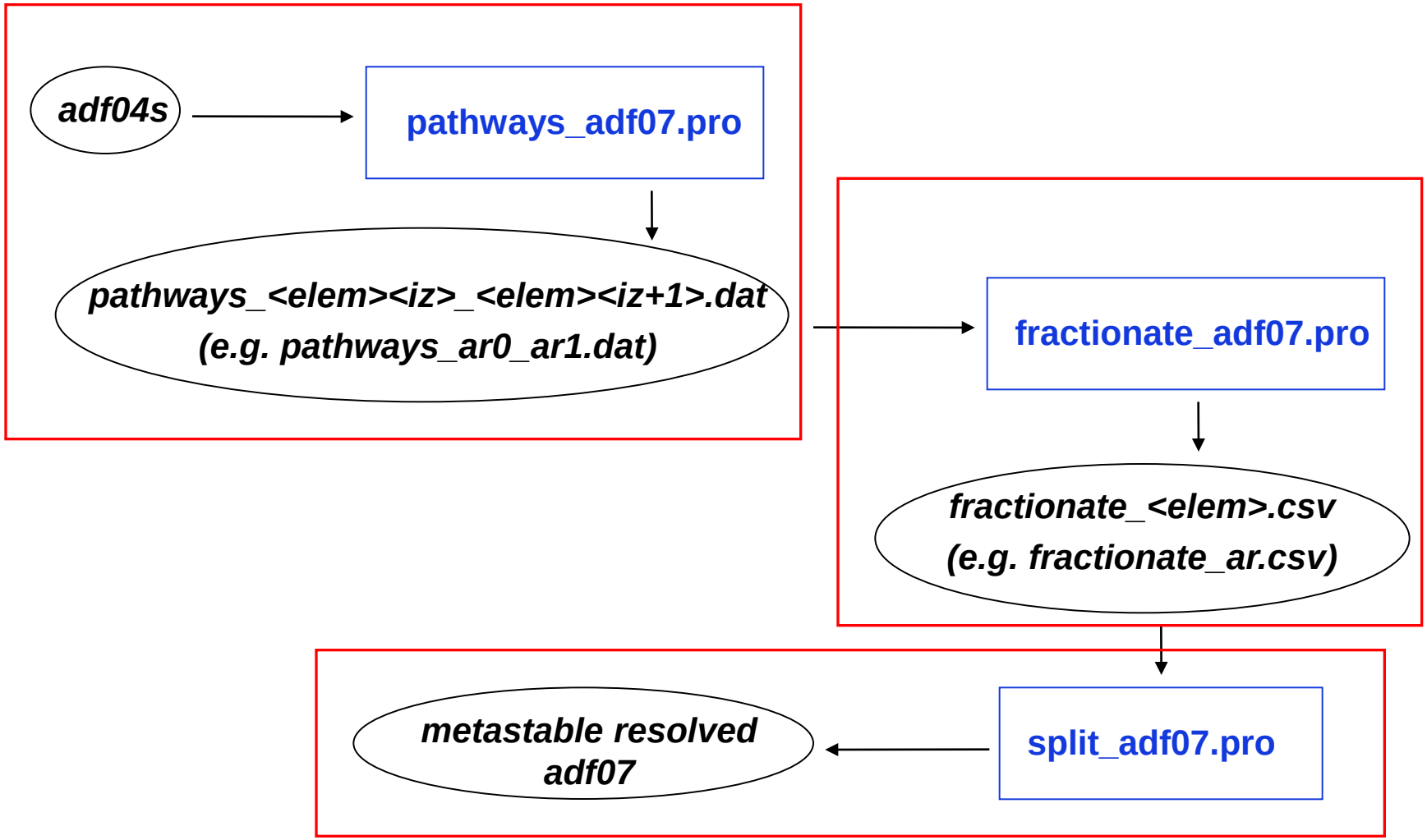
- metastable resolved (H – Fe):
  /cop<*producer*>_cadw/ls#<*element symbol*>.dat

- access: **read_adf07.pro**

- semi-automatic – perl scripts: /idl/adaslib/proc_adf/

Infrastructure and mass data production

Metastable fractionation scheme



Infrastructure and mass data production

(4) *Dielectronic recombination - adf09*

- AUTOSTRUCTURE *ls* up to Al-like:
  /<*producer*>93/<*ion*><*coupling*><*core transitions*>.dat

- AUTOSTRUCTURE *ls* and *ic* up to Al-like:
  /<*producer*>00/<*ion*><*coupling*><*core transitions*>.dat

- AUTOSTRUCTURE *lsh* and *ich* (hybrid), K - Co extending:
  /<*isoelectronic sequence*>like/<*ion*><*coupling*><*core transitions*>.dat

- access - **xxdata_09.for** under revision (HPS)

- semi-automatic creation continuing (NRB)

GCR derived data completion

- All the production and updates listed are sufficient to allow GCR to arbitrary complex system in a semi-automatic manner.

- The whole system, already implemented at *ls* resolution, is designed to allow *ic* GCR. This becomes more appropriate moving to medium and heavy species and more highly ionised ions.

Low levels / Parent+Valence	$C_{ij}^{(ls)}$	$C_{ij}^{(ic)}$
ls-ca	$ls\text{-}ca \rightarrow C_{ij}^{(ls)}$	$ls\text{-}ca \rightarrow C_{ij}^{(ic)}$
ls-bn	$ls\text{-}bn \rightarrow C_{ij}^{(ls)}$ *	$ls\text{-}bn \rightarrow C_{ij}^{(ic)}$ ◇
ls-bnl	$ls\text{-}bnl \rightarrow C_{ij}^{(ls)}$	$ls\text{-}bnl \rightarrow C_{ij}^{(ic)}$
ic-ca	$ic\text{-}ca \rightarrow C_{ij}^{(ls)}$	$ic\text{-}ca \rightarrow C_{ij}^{(ic)}$
ic-bn	$ic\text{-}bn \rightarrow C_{ij}^{(ls)}$	$ic\text{-}bn \rightarrow C_{ij}^{(ic)}$ ◇
ic-bnl	$ic\text{-}bnl \rightarrow C_{ij}^{(ls)}$	$ic\text{-}bnl \rightarrow C_{ij}^{(ic)}$ ◇

* the model exists

◊ the model almost exists

- All the material described above is already in the ADAS database or ready to be included, raising the quality of the baseline and increasing the size of the database by at least a factor 2.