
# GCR calculations for Magnesium, Argon, Iron and other elements

## *A different ADAS approach*

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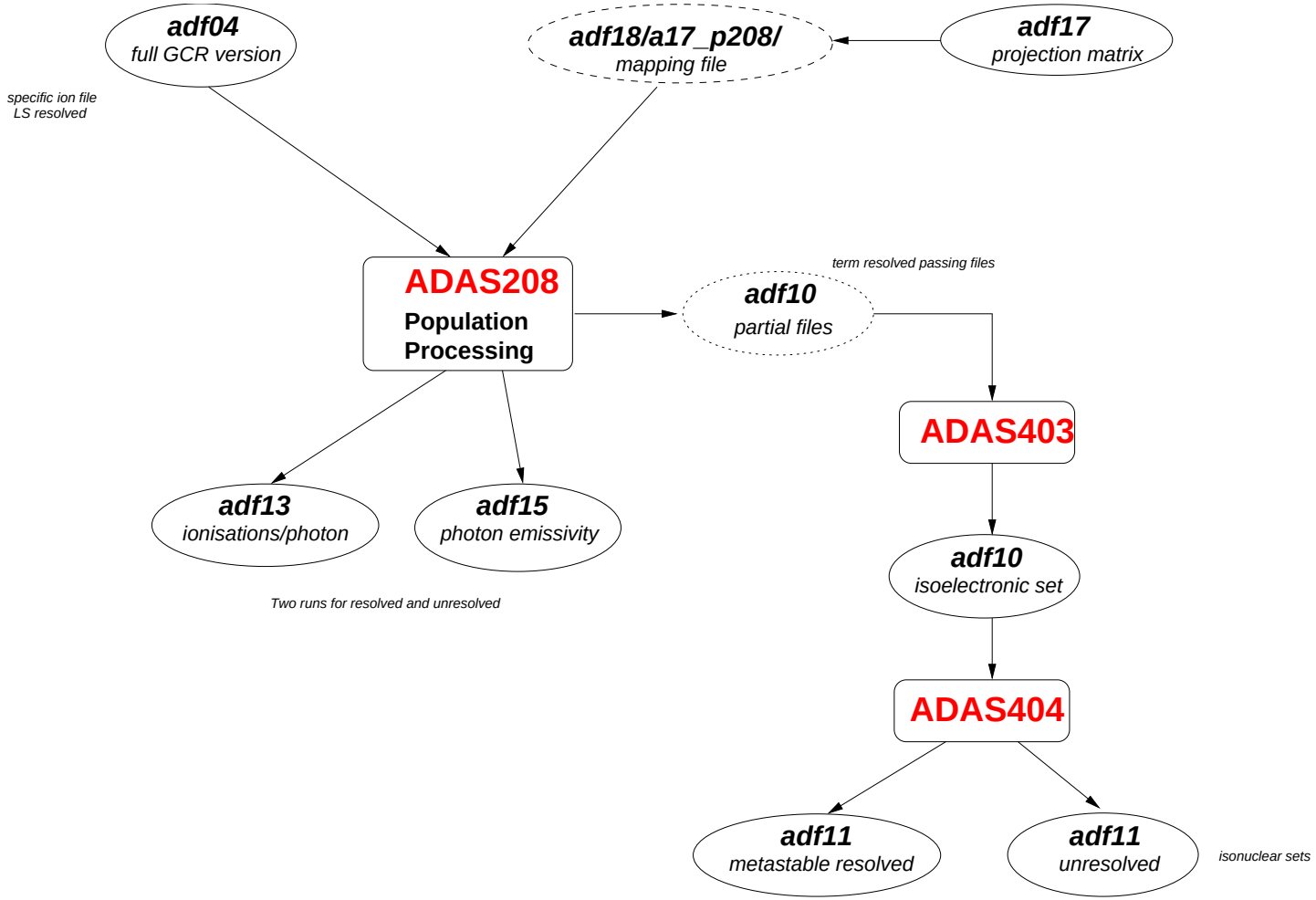
# Current GCR modelling

The current system could (kindly???) be described as baroque.




*A small part of the work-flow through generalised collisional-radiative (GCR) data production*

# Beyond the light elements

Current and future needs:

- To date the most sophisticated ADAS models have been applied to the light elements ($1 \leq Z \leq 10$) only.
- In both the astrophysics (Mg, Si, Fe) and fusion (Ar, Ni, W, Re ) domains modelling and interpreting the behaviour and emission of heavier elements is essential.

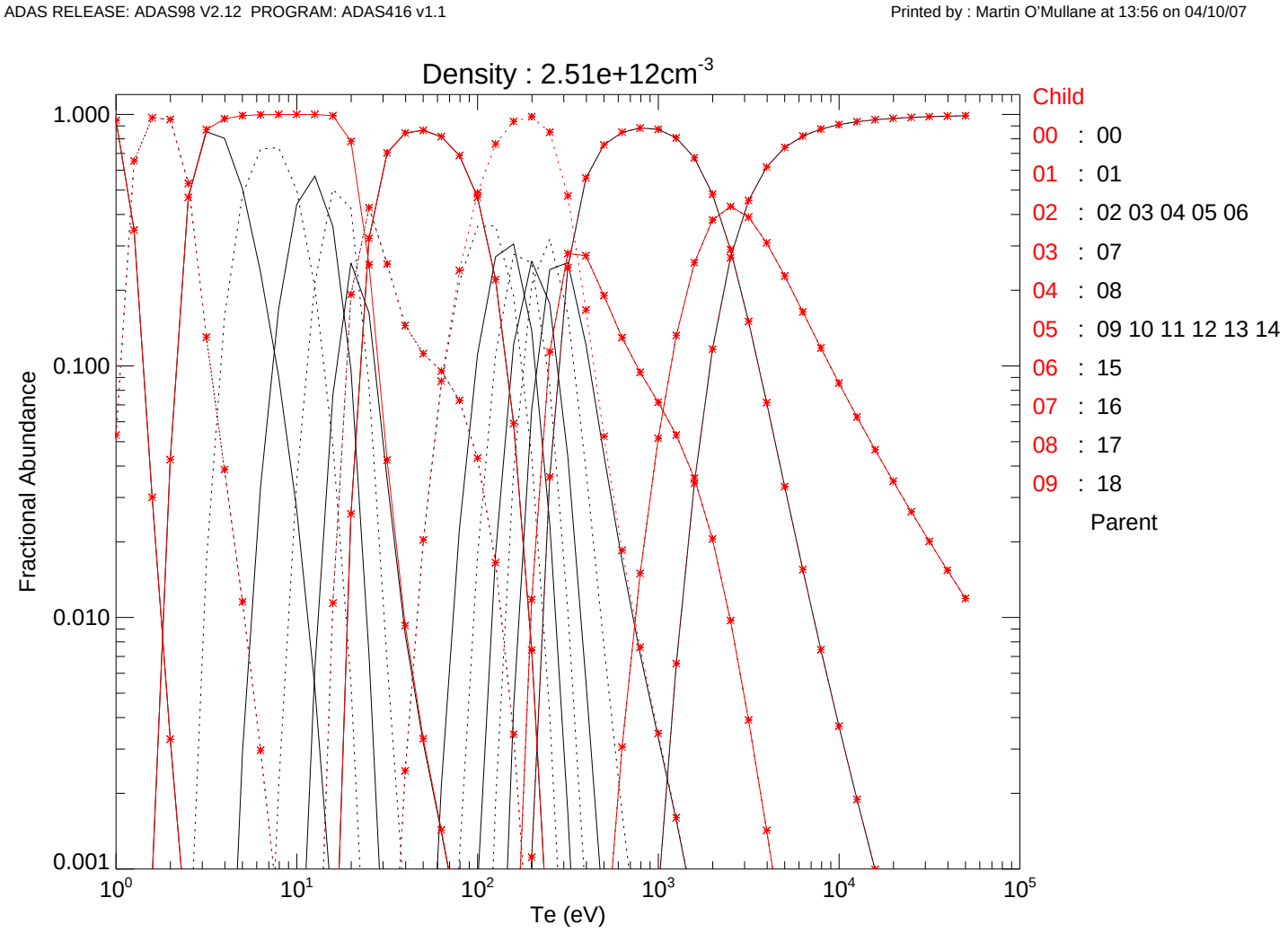
The future needs present a number of challenges.

- What degree of metastable resolution is appropriate.
- Is the ion stage model correct — LS or IC?
- Sources of data — structure, excitation, ionisation and recombination.
- Methods to sensibly ascribe data uncertainty.
- New archiving and naming schemes.

Automation is essential.

# Model and resolution

A universal metastable resolved picture (partition #00) is inappropriate for higher Z.




Partitioning and superstaging approaches will be used more widely.

# Does LS coupling remain a good model?

## For GCR modelling of higher Z elements:

- Detailed spectroscopy requires *J*-resolved data.
- LS breaks down as a good description due to increase in energy separation.
- However for (very) heavy elements a configuration average (CA) description may be more than sufficient.

## Current state of intermediate coupling data and codes:

- *adf04* is varied.
- *adf08* radiative recombination need simple adjustment in *adas211*.
- *adf09* DR data is archived in IC but is scarce for ions above the Na-like iso-electronic sequence.
- Projection data assumes *nS*, so either
  - must move to $J_p(nlJ)$.
  - or CA for high-n fill-in.
- The population codes (205/208/810) are independent of resolution.

# Example of Lithium

The number of ADAS datasets can be large for even the simplest systems:

```
adf04/adas#3/cpb02_ls#li0.dat
adf04/adas#3/cpb02_ls#li1.dat
adf04/adas#3/cpb02_ls#li2.dat
adf04/adas#3/cpb02_n#li2.dat
adf04/copmm#3/ls#li0.dat
adf04/copmm#3/ls#li1.dat
adf04/copmm#3/ls#li2.dat
adf04/copmm#3/ls#li3.dat
adf04/lilike/lilike_cpb02#li0.dat
adf04/helike/helike_cpb02#li1.dat
adf04/hlike/hlike_cpb02#li2.dat

adf07/szd02#li/szd02#li_li2.dat
adf07/szd02#li/szd02#li_li1.dat
adf07/szd02#li/szd02#li_li0.dat

adf08/rrc98#h/rrc98#h_li2.dat
adf08/rrc98##/rrc98##_li3.dat
adf08/rrc98#he/rrc98#he_li1.dat

adf10/acd96/pj#acd96_h11.dat
adf10/acd96/pj#acd96_he11.dat
adf10/acd96/pj#acd96_he12.dat
adf10/acd96/pj#acd96_li11.dat
adf10/acd96/pj#acd96_li21.dat
adf10/met96/pj#met96_h##.dat
adf10/met96/pj#met96_he##.dat
adf10/met96/pj#met96_li##.dat
adf10/plt96/pj#plt96_h##.dat
adf10/plt96/pj#plt96_he##.dat
adf10/plt96/pj#plt96_li##.dat
adf10/prb96/pj#prb96_h10.dat
adf10/prb96/pj#prb96_he10.dat
adf10/prb96/pj#prb96_li10.dat
adf10/prb96/pj#prb96_li20.dat
adf10/qcd96/pj#qcd96_he12.dat
adf10/qcd96/pj#qcd96_he21.dat
adf10/scd96/pj#scd96_h11.dat
adf10/scd96/pj#scd96_he11.dat
adf10/scd96/pj#scd96_he12.dat
adf10/scd96/pj#scd96_li11.dat
adf10/scd96/pj#scd96_li21.dat
adf10/xcd96/pj#xcd96_li12.dat
adf10/xcd96/pj#xcd96_li21.dat

adf11/acd96/acd96_li.dat
adf11/scd96/scd96_li.dat
adf11/prb96/prb96_li.dat
adf11/plt96/plt96_li.dat
adf11/acd96r/acd96r_li.dat
adf11/scd96r/scd96r_li.dat
adf11/prb96r/prb96r_li.dat
adf11/plt96r/plt96r_li.dat
adf11/qcd96r/qcd96r_li.dat
adf11/xcd96r/xcd96r_li.dat
adf11/acd89/acd89_li.dat
adf11/scd89/scd89_li.dat
adf11/ccd89/ccd89_li.dat
adf11/prb89/prb89_li.dat
adf11/plt89/plt89_li.dat
adf11/prc89/prc89_li.dat
adf11/pls89/pls89_li.dat

adf13/sxb96#li/sxb96#li_pjr#li0.dat
adf13/sxb96#li/sxb96#li_pjr#li1.dat
adf13/sxb96#li/sxb96#li_pju#li1.dat
adf13/sxb96#li/sxb96#li_pju#li0.dat
adf13/sxb96#li/sxb96#li_pjr#li2.dat
adf13/sxb96#li/sxb96#li_pju#li2.dat

adf15/pec96#li/pec96#li_pjr#li0.dat
adf15/pec96#li/pec96#li_pjr#li1.dat
adf15/pec96#li/pec96#li_pju#li1.dat
adf15/pec96#li/pec96#li_pju#li0.dat
adf15/pec96#li/pec96#li_pjr#li2.dat
adf15/pec96#li/pec96#li_pju#li2.dat

adf17/cbnm96#li/cbnm96#li_li0ls.dat
adf17/cbnm96#he/cbnm96#he_li1ls.dat
adf17/cbnm96#h/cbnm96#h_li2ls.dat
adf18/a09_a04/drm96#he/drm96#he_li1.dat

adf18/a09_a04/drm96#li/drm96#li_li0.dat
adf18/a17_p208/exp96#h/exp96#h_li2ls.dat
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adf18/a17_p208/exp96#he/exp96#he_li1ls.dat
adf18/a17_p208/exp96#li/exp96#li_li0ls.dat
adf18/a09_p204/drm96#h/drm96#h_li2n.dat
adf18/a09_p204/drm96#he/drm96#he_li1n.dat
adf18/a09_p204/drm96#li/drm96#li_li0n.dat

adf25/bns96#h/bns96#h_li2.dat
adf25/bns96#he/bns96#he_li1.dat
adf25/bns96#li/bns96#li_li0.dat
```

How can the numbers be reduced?

# Streamlining data production

The heavy species project has introduced automated methods out of necessity. These can be exploited to extend the GCR-quality data production.

- Generate a baseline *adf04* set with heavy species tools.
  — automated configuration selection and data production available
- We still have to assemble the highest quality *adf04* for stages of diagnostic or ionisation balance importance, by any means possible/available.
- Neutral and near-neutrals will always require special attention.
- S-line data is an ancillary output of the offline *adas8#4* codes.
- DR from (new) BBGP code — either archived as *adf09* or from a sub-routine call.
- Projection data generation under discussion — similar approach to *adas316*.
- Need to alter population codes to output *adf11* rather than *adf10* datasets.
- Use partitioning codes *adas416* to produce iso-nuclear *adf11* data.

Naming conventions may need to be changed:

- The current year system (89, 92, 96) is not flexible enough.
- Should we use multiple years — 07, 08, 09 etc.
- Or sub-years — 07a, 07b, 08c etc.?