ADAS
Atomic Data and Analysis Structure

University of Strathclyde Glasgow

Uncertainty of medium-weight and heavy element line power coefficients

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Motivation

- **Focus in magnetic fusion and astrophysics is moving towards medium-weight and heavy elements**
  - This talk will focus on tokamak related aspects (see other talks for astrophysics overview)

- **Wall materials in tokamaks (e.g. Fe, Mo, W) often migrate into the plasma**
  - Conditions for 'burning' tokamak plasmas are highly dependent on ion power functions
  - $P_{\alpha} = P_{loss} = P_{trans} + \mathbf{P_{rad}} = P_{trans} + \mathbf{N_e^2(f_Z L_Z)}$

- **Future tokamak designs (i.e. DEMO) are exploring the concept of using seeded impurities (e.g. Ar, Kr, Xe) to dissipate the large exhaust heat loads through radiation**
  - Main modelling uncertainty in current DEMO design systems is from power functions
  - There must exist some uncertainty on the derived atomic data inputs

Moving to a new baseline in ADAS

- **Currently ADAS provides high precision GCR data for ions up to neon**
  - Above-baseline quality data available only for a selection of ions
  - Expand GCR data to medium-weight and heavy elements

- **The ADAS GCR data will form the new baseline in ADAS, replacing the current baseline (89) data**
  - Now using Autostructure with intermediate coupling (*ic*) level resolution
  - Possibility of R-matrix (resonances), DW (spin changing transitions) and PWB cross-section calculations are key to Autostructure's usage

- **In addition, we aim to provide a 'worst-case' uncertainty of the derived atomic coefficients**

What are the main sources of uncertainty associated with the derived atomic coefficients within ADAS? → Focus of talk

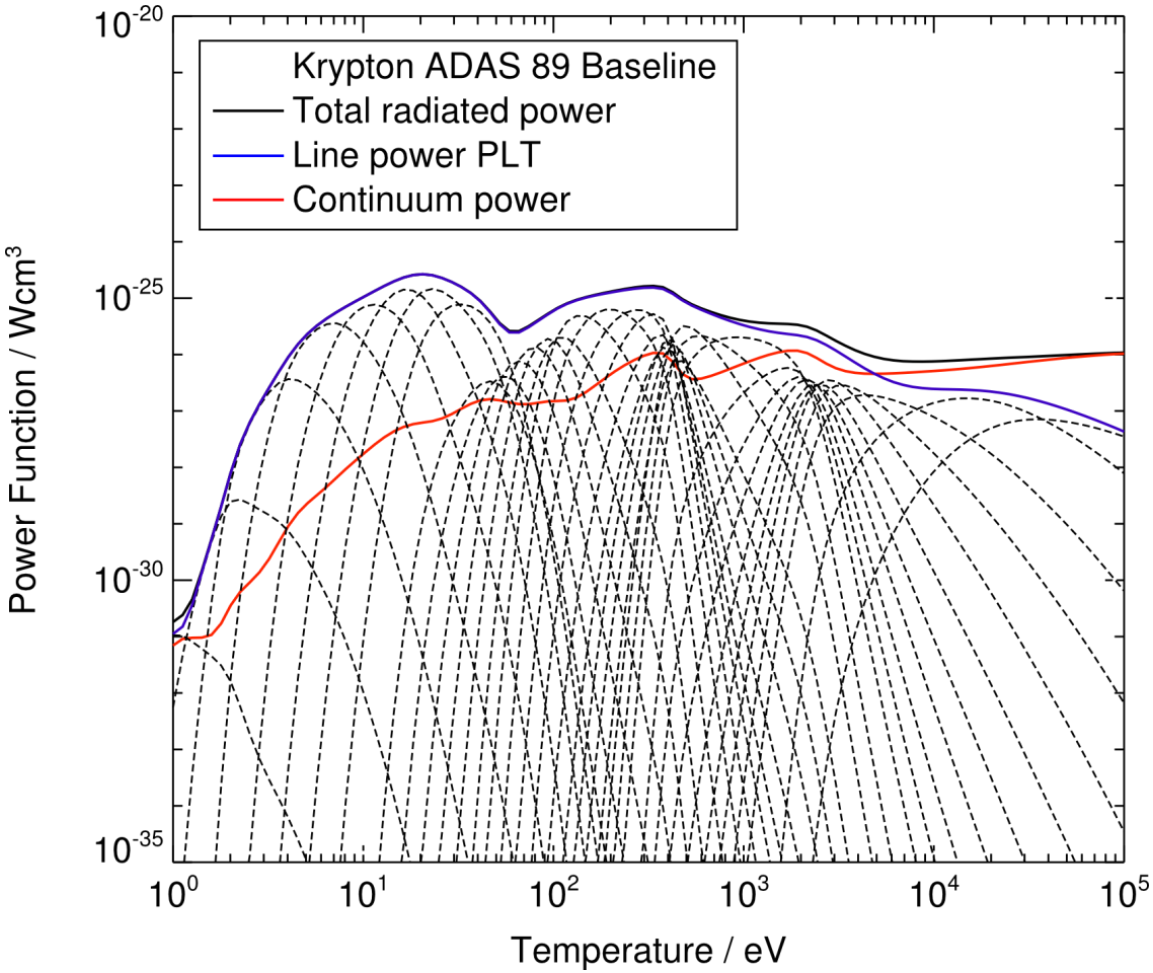
Power function overview

Ionisation balance uncertainties:

- Ionisation rates
- Recombination rates
- Focus of ***other*** talks

Line power P_{LT} uncertainties:

- Configuration selection
- Atomic structure and energy levels
- Collisional excitation cross-sections
- Focus of ***this*** talk



Configuration selection

- **The main complexity in a structure calculation is usually the *correct* selection of configurations**
  - limited by the size of the calculation
  - ideally capturing as much of the radiated power as possible
- **For the low levels of the ion, we require a set of optimal configurations for each ion**
  - define the configurations in terms of promotion rules for each driving configuration
  - pick rule sets that produce highest ΔP_{LT} / ΔN_{Levels}
- **Optimisation method built on previous Ph.D. work by Adam Foster**
  - now using Autostructure
  - combining (and further optimising) configuration sets from metastable driving configurations

Promotion rules for configuration sets

A set of rules defining the promotion of electrons from a driving configuration can be used to generate a configuration set

– **Rule sets are stored in ADF54 data sets, e.g. adas/adf54/promotion_rules_zn_small.dat**

index	config						
160	1s2	2s2	2p6	3s2	3p6	3d1	4s1
161	1s2	2s2	2p6	3s2	3p6	3d1	
162	1s2	2s2	2p6	3s2	3p6	3d0	4s1
163	1s2	2s2	2p6	3s2	3p6		
164	1s2	2s2	2p6	3s2	3p5		
165	1s2	2s2	2p6	3s2	3p4		
166	1s2	2s2	2p6	3s2	3p3		
167	1s2	2s2	2p6	3s2	3p2		
168	1s2	2s2	2p6	3s2	3p1		
169	1s2	2s2	2p6	3s2			

index	160	161	162	163	164	165	166	167	168	169
n_el	20	19	19	18	17	16	15	14	13	12
no_v_shl	1	1	1	1	1	1	1	1	1	1
max_dn_v1	3	3	3	1	2	2	2	2	2	2
min_dn_v1	0	0	0	1	0	0	0	0	0	0
max_dl_v1	2	2	2	2	2	2	2	2	2	2
min_dl_v1	0	0	0	-1	-1	-1	-1	-1	-1	0
max_dn_v2	0	0	0	0	0	0	0	0	0	0
min_dn_v2	0	0	0	0	0	0	0	0	0	0
max_dl_v2	0	0	0	0	0	0	0	0	0	0
min_dl_v2	0	0	0	0	0	0	0	0	0	0
prom_cl	1	1	1	1	1	1	1	1	1	1
max_n_cl	3	3	3	3	3	3	3	3	3	2
min_n_cl	3	3	3	3	3	3	3	3	3	2
max_l_cl	1	1	1	0	0	0	0	0	0	1
min_l_cl	1	1	1	0	0	0	0	0	0	1
max_dn_cl	1	1	1	2	1	1	1	1	1	2
min_dn_cl	0	0	0	0	0	0	0	0	0	0
max_dl_cl	2	2	2	2	2	2	2	2	1	2
min_dl_cl	1	0	0	0	1	1	1	1	0	0
fill_n_v1	0	0	0	1	1	1	1	1	1	1
fill_par	0	0	0	0	0	0	0	0	0	0
for_tr_sel	3	3	3	3	3	3	3	3	3	3
last_4f	0	0	0	0	0	0	0	0	0	0
grd_cmplx	0	0	0	0	0	0	0	0	0	0

Iso-nuclear seq.

Rule set size

Driving configurations

Number of electrons

Valence shell promotions

Closed shell promotions

Extra options

Promotion rules and optimisation

1. Define list of promotion rule changes, e.g.

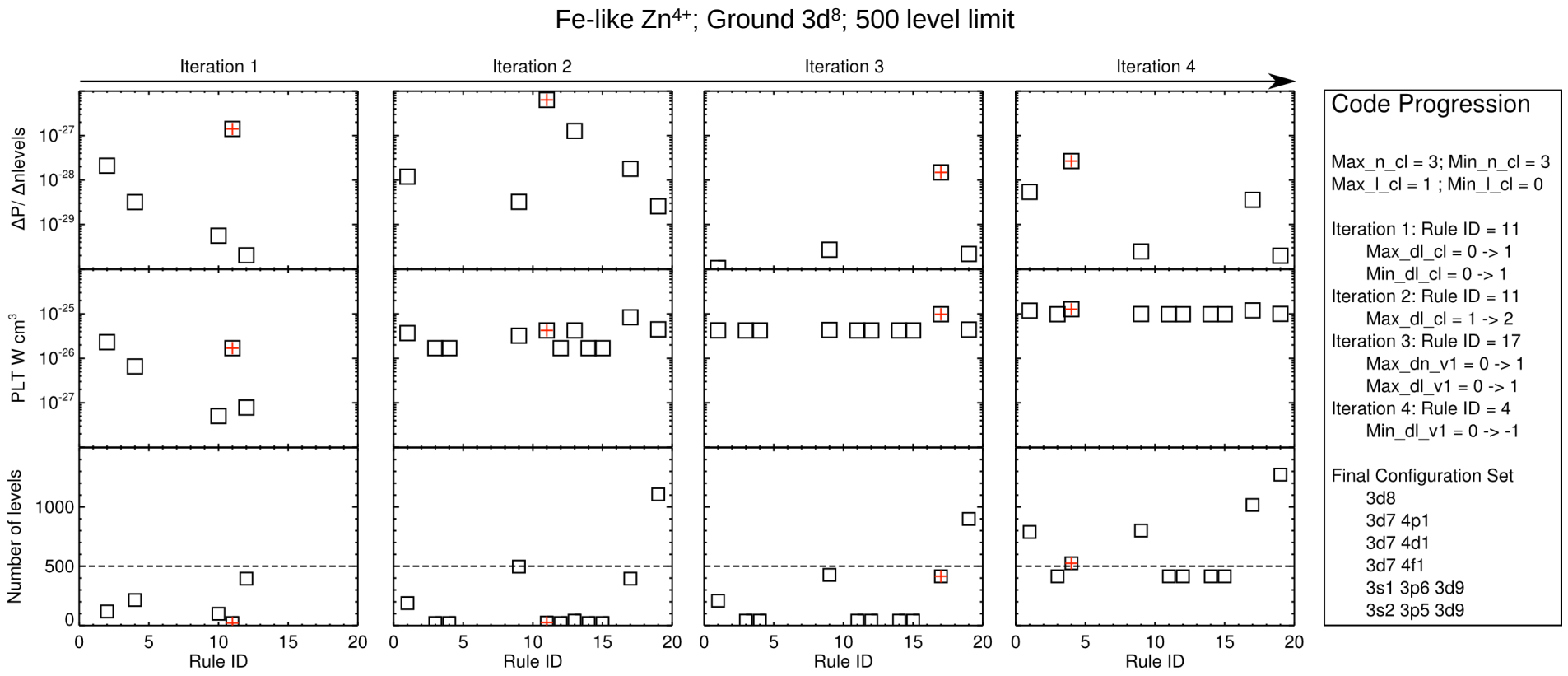
ID	Description	ID	Description
1	$\Delta n_{v1}^{max}+1$	8	$\Delta l_{v2}^{min}-1$
2	$\Delta n_{v1}^{min}-1$	9	$\Delta n_{cl}^{max}+1$
3	$\Delta l_{v1}^{max}+1$	10	$\Delta n_{cl}^{min}-1$
4	$\Delta l_{v1}^{min}-1$	11	$\Delta l_{cl}^{max}+1$
5	$\Delta n_{v2}^{max}+1$	12	$\Delta l_{cl}^{min}-1$
6	$\Delta n_{v2}^{min}-1$	13	Ground complex
7	$\Delta l_{v2}^{max}+1$	14-19	Extra options

2. Start from a driving configuration (usually the ground) and cycle through each rule change

3. On each iteration, calculate the CA P_{LT} for one T_e and N_e and store 'figure of merit' ratio – ΔP_{LT} / ΔN_{Levels}
4. Rule change with highest ratio is set as reference scenario, and step 2 is repeated

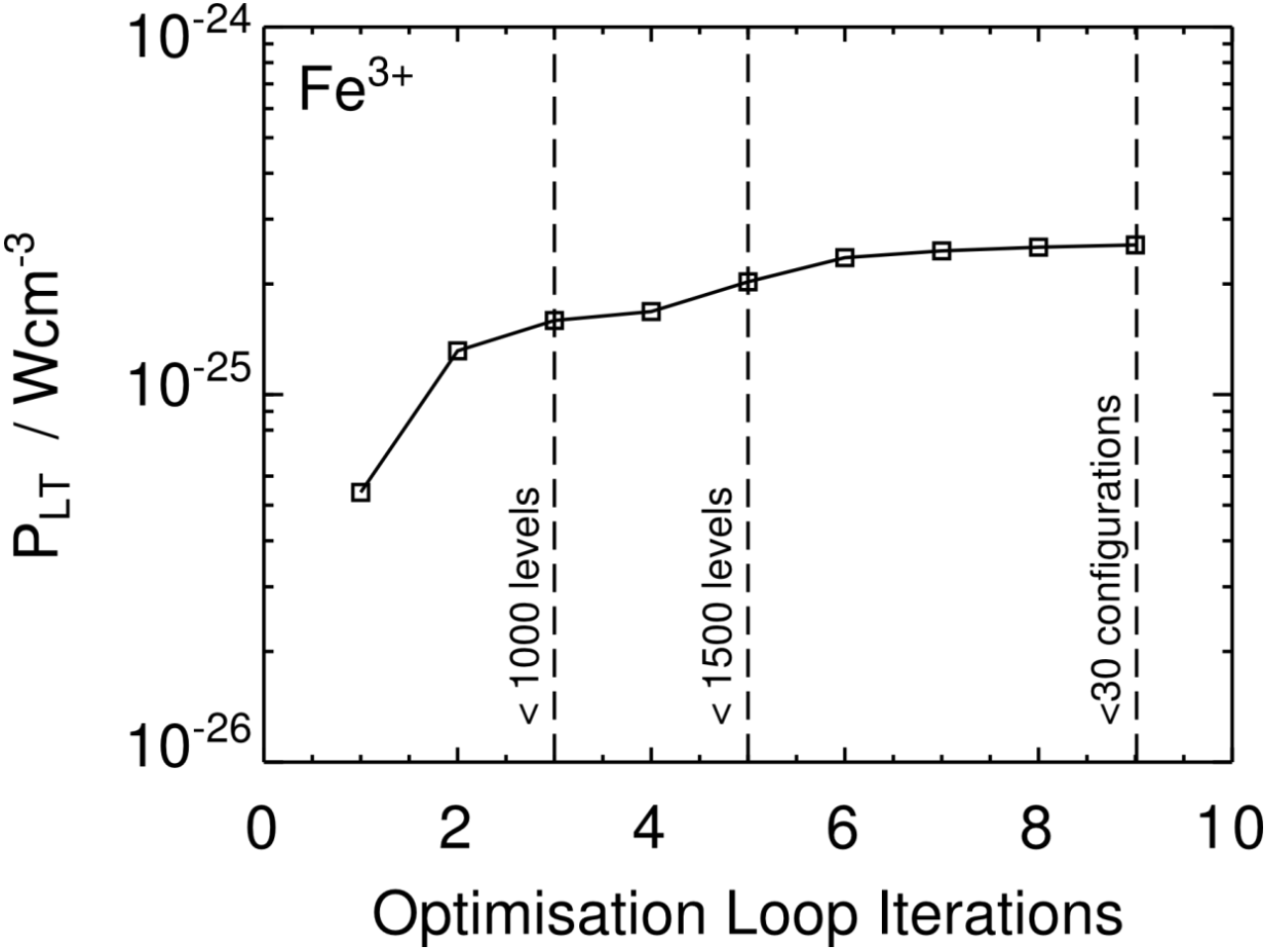
5. Loop continues until the number of configurations/levels is greater than pre-defined limits

Optimisation example

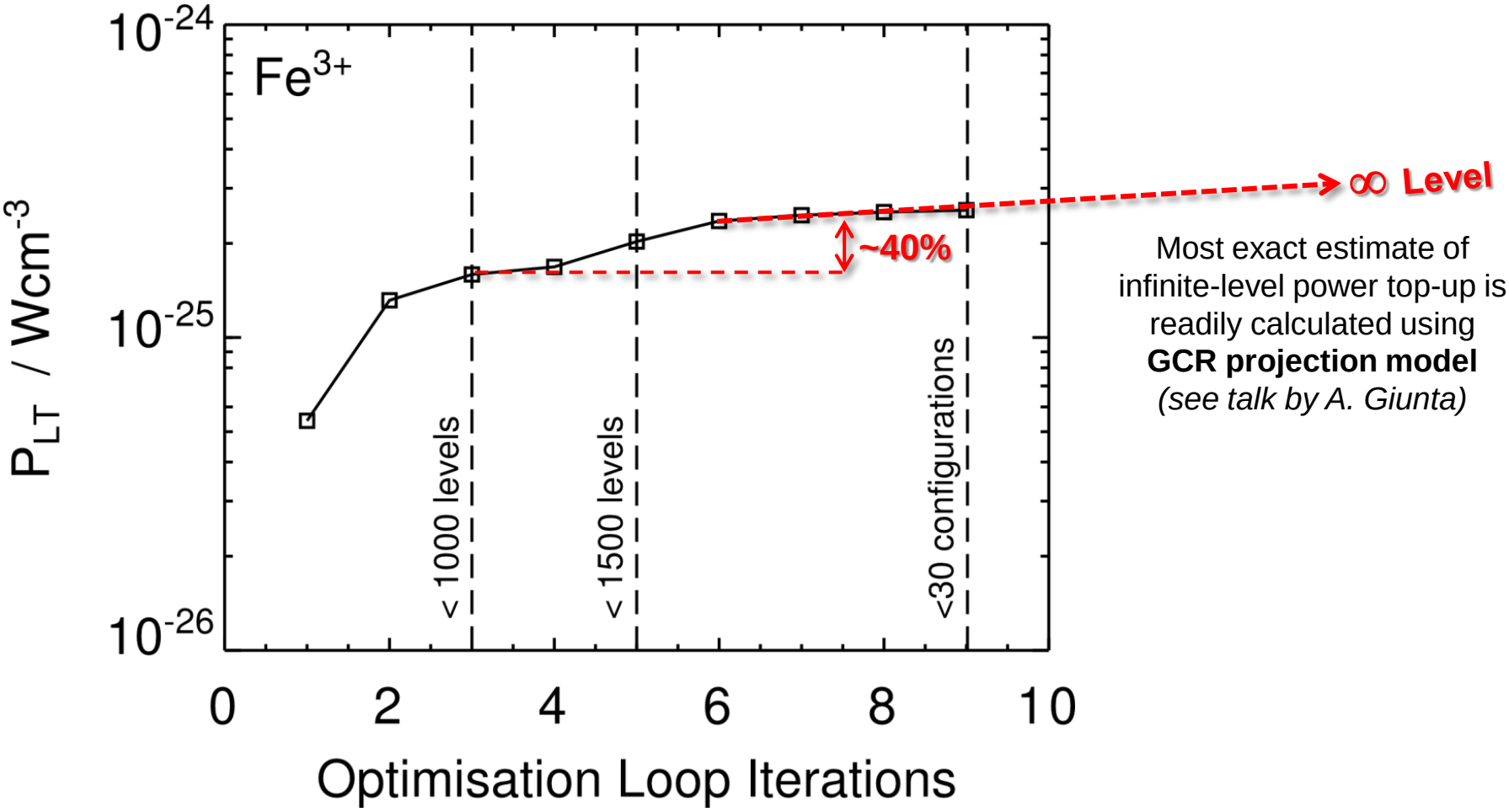


Note: Different rule changes used for first iteration to force dipole transitions

Optimisation example



Optimisation example



Most exact estimate of infinite-level power top-up is readily calculated using **GCR projection model** *(see talk by A. Giunta)*

Multiple driving configurations

We now have a set of configurations for *each* driving configuration

– But an ion may have a number of driving configurations (i.e. metastables)
– The final configuration set should be based on ***all*** driving configurations

Further optimisation required using GCR model with ion-impact collisional excitations *(see talk by M Bluteau)* to determine relative populations of metastable configurations

Further optimisation steps:

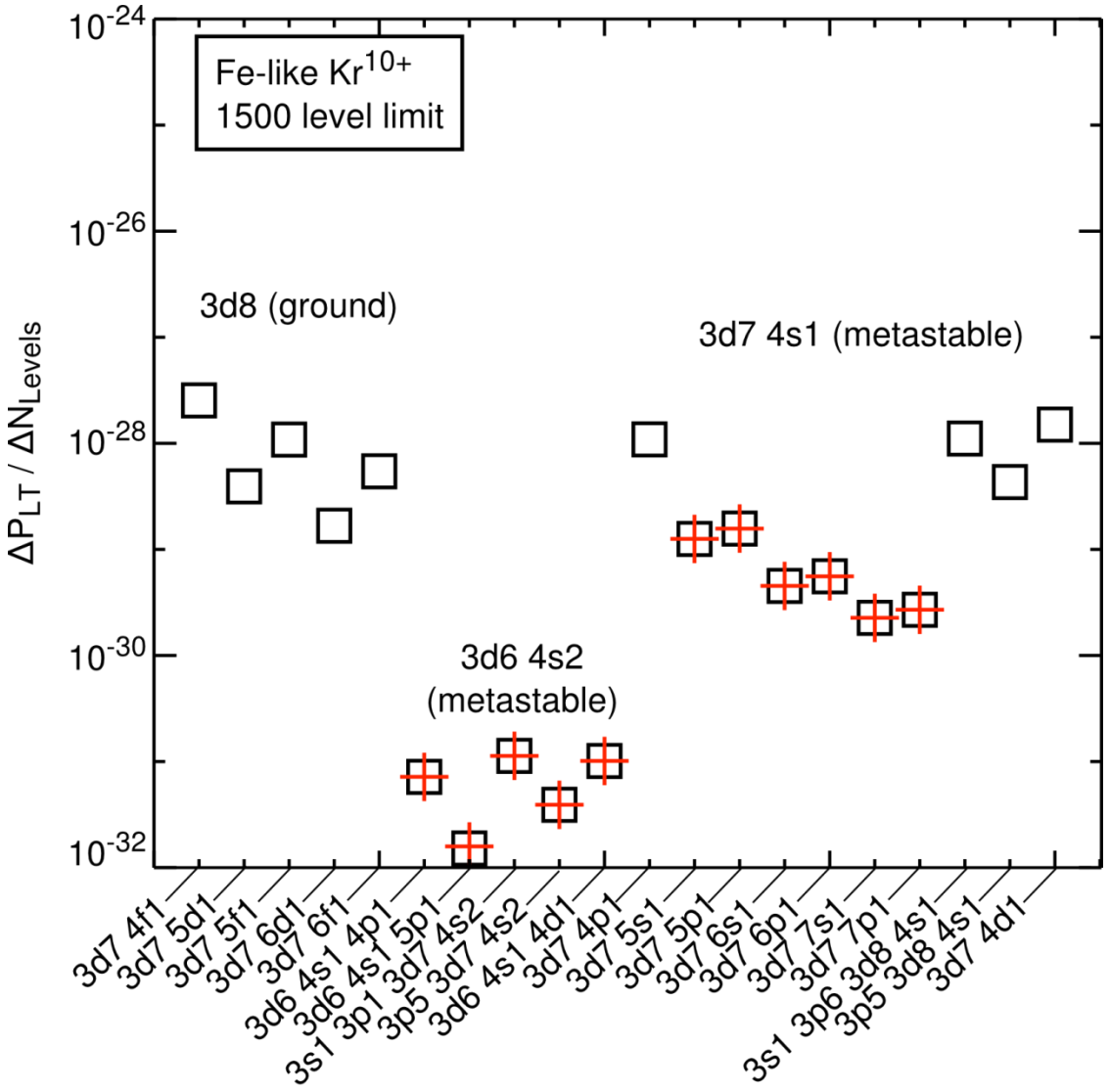
1. Combine configurations from each driving configuration (removing any duplicates)

2. Distinguish between the metastable and promoted configurations

3. Systematically remove each promoted configuration in turn

4. Remove configurations with lowest values of $\Delta P_{LT}/\Delta N_{Levels}$ until limits satisfied

Multiple driving configurations

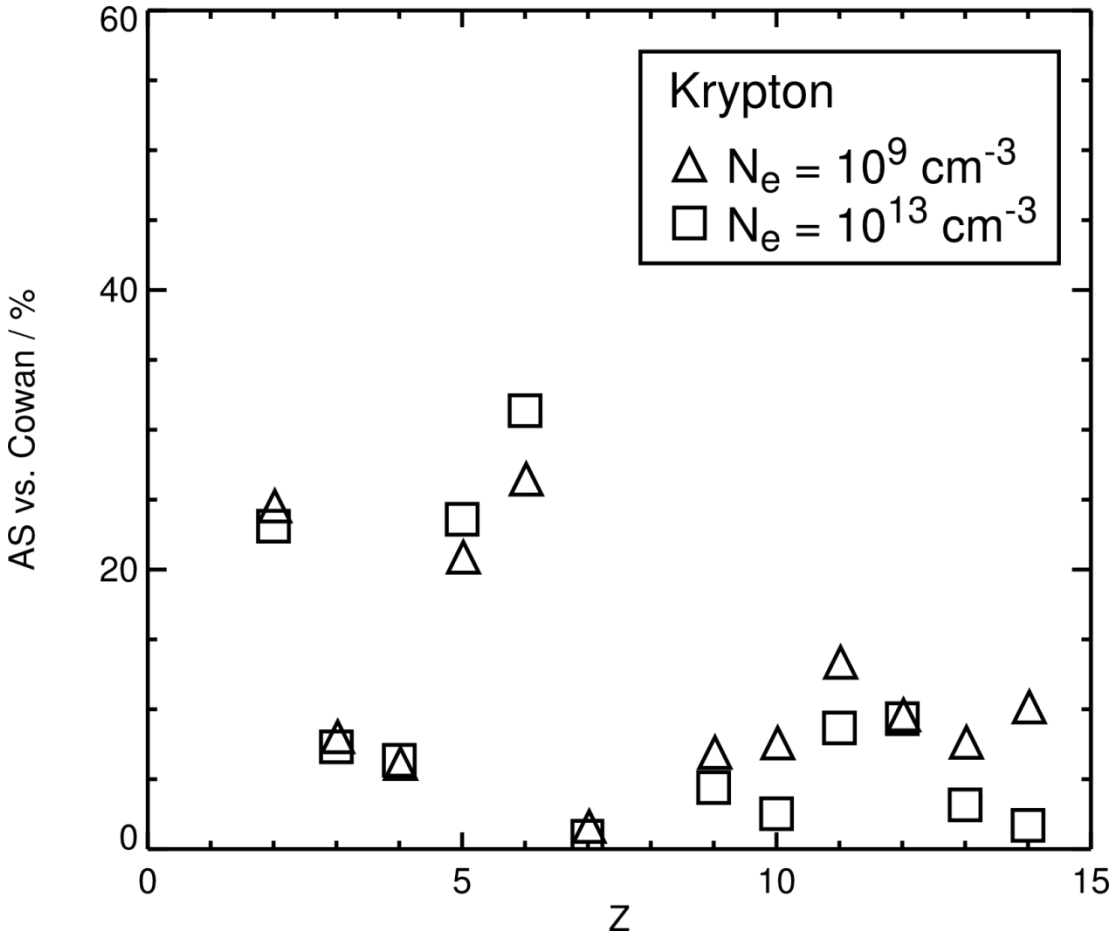


Case study: Krypton

- **Perform analysis P_{LT} uncertainty analysis for Kr iso-nuclear sequence**
  - ions in the range 1<Z<15
- **Atomic structure uncertainty**
  - compare Autostructure vs. Cowan using PWB *ic* resolution
- **Collisional excitation cross-section uncertainty**
  - compare DW vs. PWB using Autostructure in *ic* resolution
- **Compare P_{LT} with previous (89) ADAS baseline**

Uncertainties from atomic structure

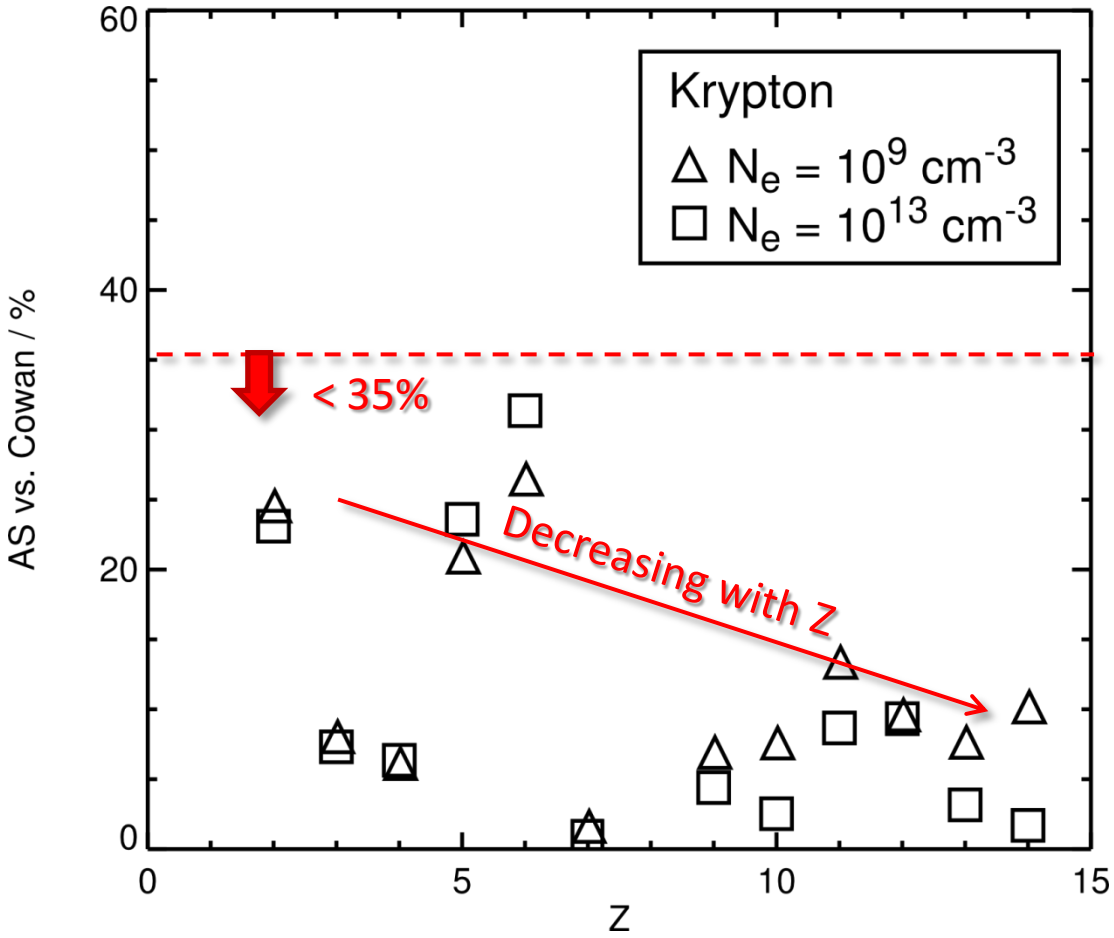
Compare Autostructure vs. Cowan (*ic* PWB) PLT at ionisation potential



- **Near neutral ions are a problem case, where further optimisation of Autostructure scaling parameters is required** – currently in development

Uncertainties from atomic structure

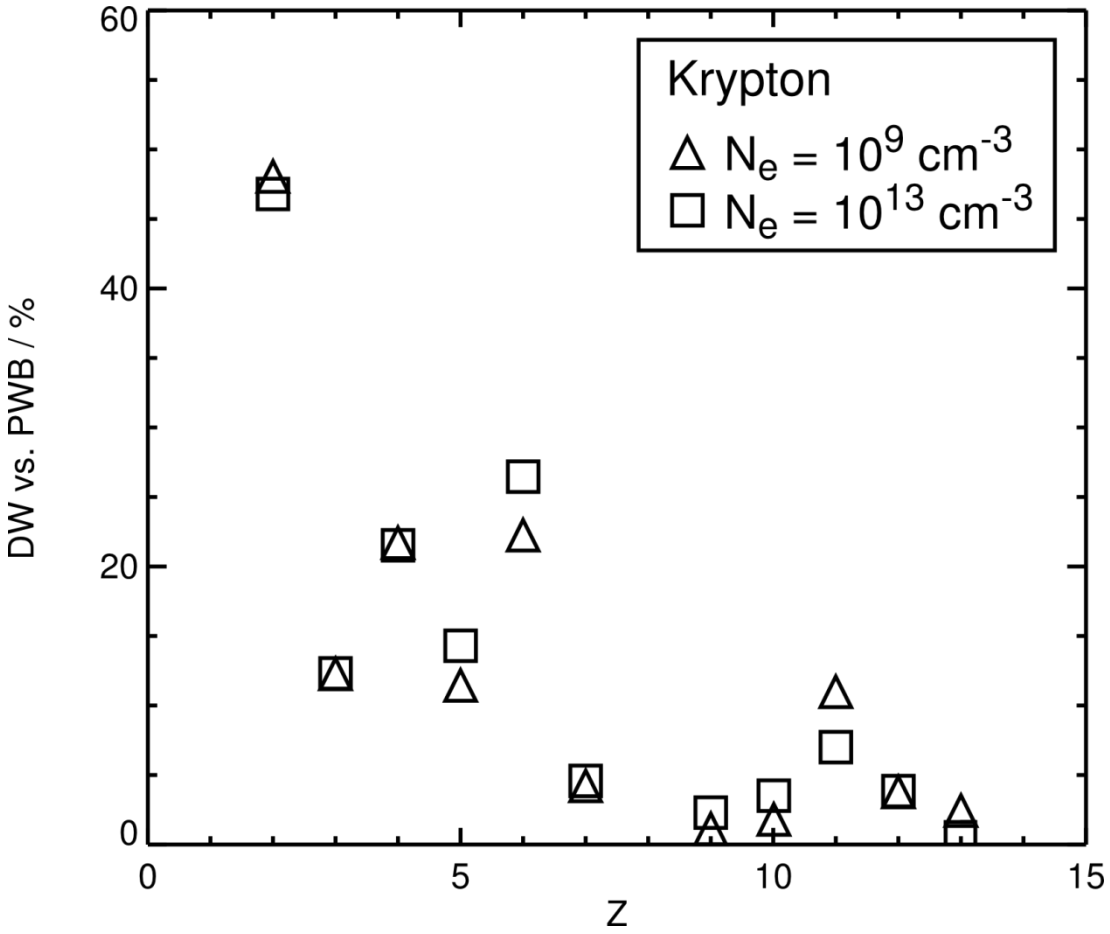
Comparison of Autostructure vs. Cowan (*ic* PWB) PLT at ionisation potential



- **Near neutral ions are a problem case, and therefore further optimisation of Autostructure scaling parameters is required** – currently in ADAS development

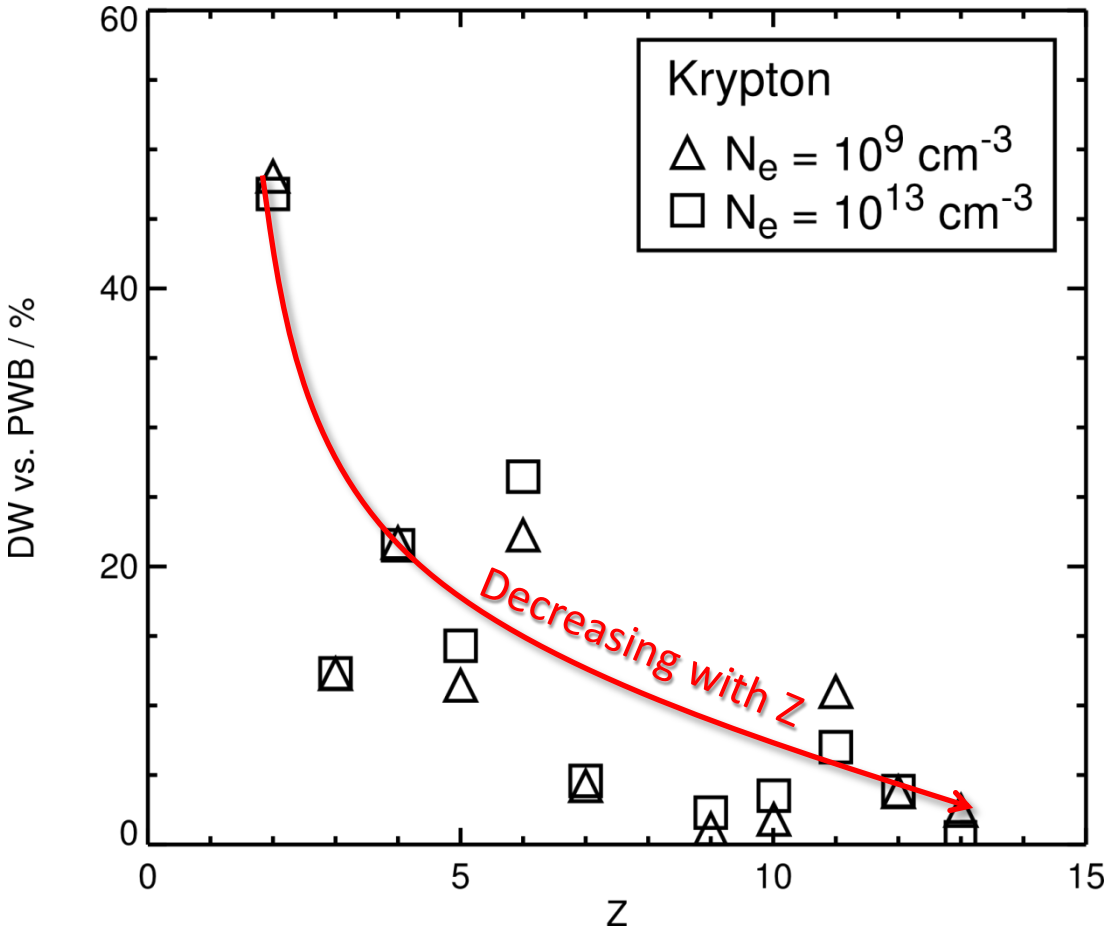
Uncertainties from collisional excitation cross-sections

Compare P_{LT} from DW vs. PWB calculations using Autostructure with *ic* resolution



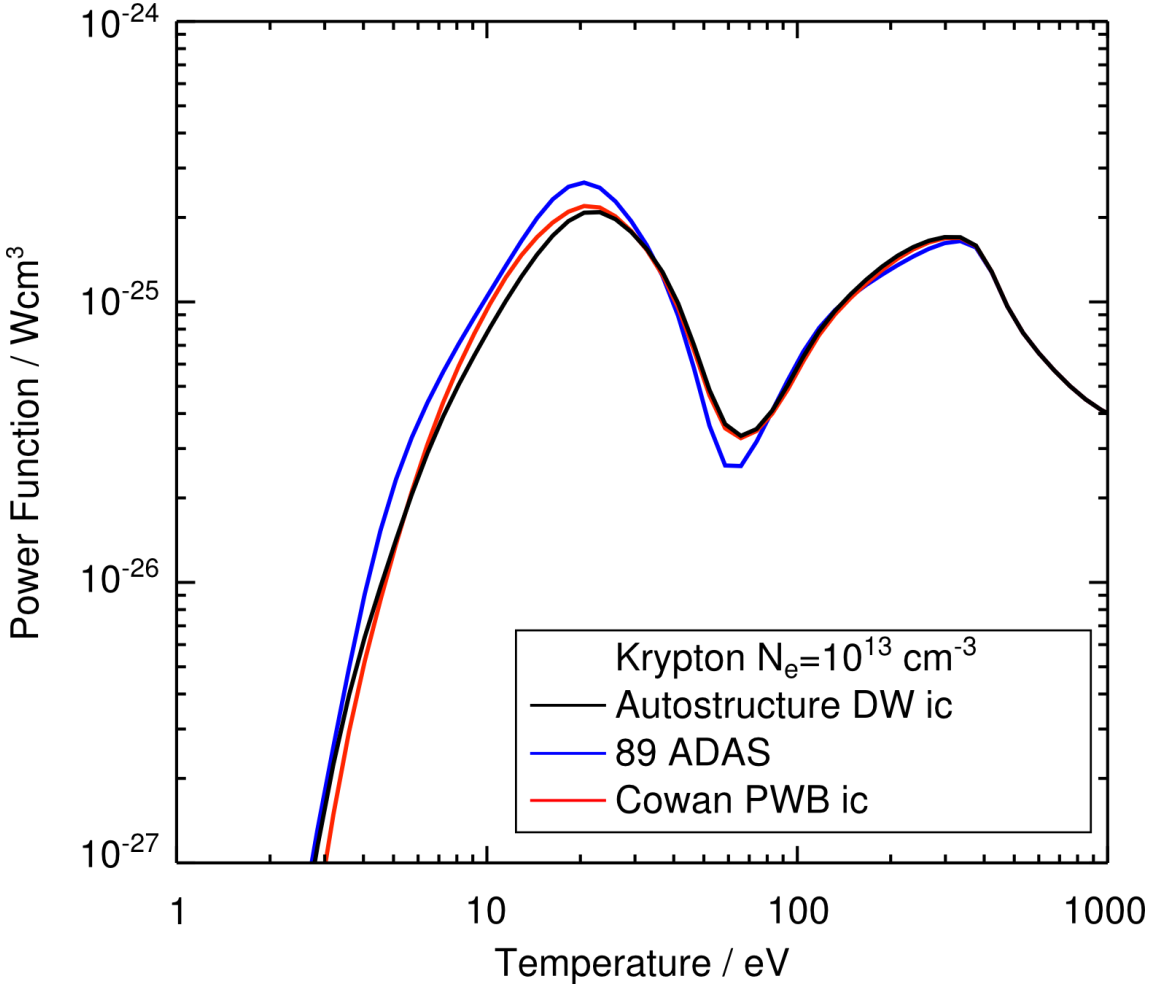
Uncertainties from collisional excitation cross-sections

Compare P_{LT} from DW vs. PWB calculations using Autostructure with *ic* resolution



Kr power function

Only uncertainties from P_{LT} included for 1 < Z < 15



Note: results require further testing and analysis – for visualisation purpose only

Summary & Discussion

- **ADAS baseline moving to Autostructure, DW and *ic* resolution for medium-weight and heavy elements**

- **Configuration sets optimised to power using promotion rules**
  - **secondary optimisation step for multiple driving configurations**

- **Uncertainty on P_{LT} from atomic structure and collisional excitation cross-sections typically below 30%**
  - **decreases with ion charge**

Discussion

➢ **How are uncertainties propagated and stored in ADAS?**