PP/E001254/1 — Applicants' responses to referees' comments.

Overview

The referees' reports show very strong support for the proposal, and all have given a high rating to its international standing and the importance of supporting it at the present time. Referees O2, O3 and O4, in particular, state the crucial role that the research has in an international context. Referee O1, however, does have some criticisms, which may be the result of inadequate explanations in the proposal, so we seek here to clarify these issues.

There are two main issues. Firstly, practicality, the referee appears to be thinking of serial computation — which would **indeed** take **a few decades to complete** — parallel computing reduces this by an order of magnitude. Secondly, relevance, the referee **seems to have misunderstood the nature of the project** — **we are not proposing** the usual **piecemeal** computation of data for a specific transition for a specific ion for a specific diagnostic — instead, we are concerned with the totality of data, **produced in a consistent, well tested, semi-automated manner**. **This approach was understood and** especially appreciated by Referee O2. Finally, there is **a further** misunderstanding that we are proposing to establish a new atomic database — we are not — rather we *are proposing to provide the complete set of atomic data we will produce to the astrophysics community through a dedicated server (SADA), on the lines of OPEN-ADAS.*

Detailed response to Referee O1's comments.

(1) The calculation of R-matrix collision data for all K- and L-shell ions up to Zn is not as massive an undertaking as it might have seemed a few years ago. **From our own experience, we are confident** that the advance of computer power, especially parallel **processors**, coupled with the development of robust parallel computer codes **and automated scripts** means that **reliable** parallel R-matrix calculations (200 levels) can be carried-out relatively easily. The large amount of atomic data generated requires equally good analysis tools. We have developed such management and analysis tools and have been piloting them on the F-like sequence, following our initial work on Fe (Whiteford et al, 2006, A&A 446, 361). The bespoke **year-long** calculations which were once associated with, say, a 29-state calculation on He a decade ago are now associated with M-shell ions, e.g., low-charge Fe.

We can and must think on a bigger scale **HELEN: SUGGEST DELETING THE BIT ABOUT THE USA - ONE COULD ARGUE IF THE FOLK IN THE USA ARE DOING THESE CALCULATIONS¡ WHY ARE WE BOTHERING?**. *GIULIO: I would write: For a large number of astrophysically-important ions, no collisional data are available. In recent years, other researchers have started to produce large-scale calculations, but using a distorted wave approach (HULLAC, FAC). It is now well established that R-matrix calculations are far more accurate.* The time is ripe **for the UK to lead the way in this effort**. **This part of the work has the highest priority in our research plan** and **will comprise** the initial main effort of the PDRA **DELETE - whatever their background** with the shell boundaries the priority sequences **SORRY, NOT QUITE SURE WHAT THIS MEANS - COULD IT BE PHRASED MORE CLEARLY?. DELETE NEXT SENTENCE. The PDRA will work systematically through the iso-electronic sequences**. Our piloting of the F-like sequence **enables us to have confidence** that this objective is achievable

within the **given** time frame. However, PDRA funding is critical. At the end of the day, we ask to be judged on our **previous?** record of deliverables.

NEXT PARAGRAPH REWORDED (2) Regarding relevance, three co-PIs (Mason, Young, Del Zanna) are heavily involved in using R-matrix atomic collision data for **s**olar diagnostics. Clearly, with approx 250 ions it was not possible to provide a critical evaluation of the current state of play of each one. We referenced our own work in this respect to demonstrate our experience and capability here. Indeed, for some ions, accurate calculations are already available, however the quality of available data is not uniform. It is our strong view (in this proposal) that it is time to step back from the piecemeal reactive nature of one-off calculations and to provide a comprehensive coverage from R-matrix for all ions of astrophysical interest in each iso-electronic sequence. Clearly, there will be existant bespoke calculations for certain ions and transitions, and it is our intention to publish comparisons with these atomic data. It is intended that benchmark calculations will be carried out for certain key ions or transitions.

Although one might expect that the identification of UV and X-ray spectral lines is well-known, this is not in our experience the case. For example, we note that something like 1/3 of emission lines seen by the SUMER spectrometer on SOHO remain unidentified. Many of these are likely due to n=3 transitions of abundant elements for which there are no atomic data available, or transitions of minor ions for which nobody has calculated data for in the past. The need in this sense is not specific in terms of a particular diagnostics or set of lines, but is general in that we want good data for *all* transitions to better understand the complete spectra of the Sun and other astrophysical objects.

GIULIO/PETER - MENTION FUTURE SOLAR PROJECTS? SOLARB? AS MENTIONED BY REF 04??

Finally, we do not agree that benchmarking collision data against laboratory and astrophysical spectra is not really possible. There are many line ratios that are insensitive to the plasma conditions and whose values depend on collision rates that can be compared with observation. *There is ample literature on the subject. Such method, or the approach of Del Zanna, Berrington & Mason (2004, A&, 422, 731) which looks at observed and theoretical emissivities for groups of lines at once, have demonstrated the ability to critically distinguish between sets of collisional data, and point out inaccuracies in the atomic calculations.* We can also look at the low- and high-density limits of density diagnostics which depend on collision rates. Examples of these are given in Young, Landi & Thomas (1998, A&A, 329, 291) and Storey, Mason & Young (2000, A&AS, 141, 285).

GIULIO: I am myself a bit confused now about what Nigel/Helen wrote. I would write: (3) Regarding databases. We are proposing to make the complete set of atomic data that we will either calculate ab-initio or process (e.g. observed wavelengths) available to the astrophysical community via a dedicated server, SADA, in a similar way as OPEN-ADAS, which is being set-up tailored to fusion research. The provision of this complete set, which includes the original collision strengths, and not just the rates, is needed by the community (e.g. to study non-equilibrium plasmas), as noted by Referee O2. SADA will ensure a wide international distribution of the atomic data we propose to calculate and benchmark. Being involved with ADAS and CHIANTI, we will obviously make the data available also through these atomic packages. We are not proposing to develop a general database of atomic data.

(3) Regarding databases. Perhaps two issues **have been** confused. There is the specific dissemination of the atomic data which we generate, from all objectives, and the access to and the tailoring to astrophysics of OPEN_ADAS. We are not

proposing to establish a new independent database. **We are proposing to make available through OPEN_ADAS the original collision data, not simply the collison data integrated over a Maxwellian velocity distribution. The relevance and importance of this type of atomic database was noted by Referee 02. OPEN_ADAS is being set-up and tailored to fusion at IAEA. We seek to take the opportunity to enable the astrophysics community to access our atomic data through ADAS and CHIANTI. This will ensure a much wider international distribution network.**

In summary, we believe that we have **fully** addressed the concerns raised by this Referee (O1), which are not shared by the other referees. Indeed, Referee O2's comment on the strengths of the proposal provides an eloquent exposition of the relevance.

Brief responses to the other referees' comments:

Referee O2: IP meet twice a year. We try to ensure that the PDRA and one of the PI's attend so as to maintain our collaborations.
Referee O3: Worldwide atomic activity maybe small in numbers but the atomic data are *used* by a huge solar and astrophysics community.
Referee O4: We cannot see from the report which requested resources are being recommended justified at a 'reduced level', especially given the uniformly 'high' ratings.

SHOULD WE COMMENT AT ALL ON THE CONTRIB OF PETE TO THE DIELECTRONIC WORK? I THINK IT IS MENTIONED BY REF 2