

ROUND TABLE DISCUSSION OF THE SESSION: “INTERFACE TO LABORATORY DATABASES, AND THEORETICAL MODELS”

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Introduction: It is an important moment for the access of atomic and molecular line databases in the VO. Good news is that we have both a data model and an access protocol. They basically work, both for the laboratory databases community, and for the observational astronomy community, even in “exotic” energy ranges such as X-rays. These are potential issues, which the presentations in this session have highlighted: the modelling of the underlying atomic and molecular physics is complex (and it has not been attempted in the data model yet), proper line identification is a complex issue, existing databases suffer of incompleteness in some energy ranges, of data quality and uncertainties issues.

The main questions to be answered are:

- can the current data model support the basic needs of line databases (which would allow us to propose it to try and have it promoted to proposed recommendation at the next IVOA Inter-Op meeting)?
- in which direction do we primarily need to expand the model?

Piskunov: There are three aspects in the astronomical usage of line databases. In increasing level of complexity, these steps are:

1. identify features and perform crude estimations of plasma diagnostic observables
2. perform radiative transfer calculations to predict lines shapes, etc.
3. perform complex simulations of astrophysical systems

The answer to the first question depends on the level of complexity we wish to ensure. In all cases, we need to describe the information to allow systems to combine lines from different sources. Although I need to study the model in more details, I have the feeling that some important fields are still missing (line broadening, for instance?)

Müller: For atomic data, there is still room for improvement, but at least Step#1 above can be achieved in most cases. For molecular data, we are not even at Step#1 in many cases.

Piskunov: In the study of stellar spectra, the comparison of spectra highly dominated by molecules (depending on the environment) is an important issue for line identification.

Roueff: Identification is not straightforward. We see sometimes species in astronomical observations that we do not see in laboratory. We will never have information on them in the database structure. This is even more extreme for molecular lines.

Piskunov: For molecular data, there are several groups working on molecules in stars. One important source of information is the Heidelberg database. In stars, *e.g.*, water has half a million transitions. We do not use all of them for synthesis. It is unrealistically ambitious to have all this incredible wealth of information covered by the same standard.

Müller: Water is a good example of how a molecule can produce many problems. Only recently it has been treated. Other cases are simpler.

Guainazzi: If I may try to summarise the outcome of the discussion into a sort of general recommendation for the IVOA, I would say: go ahead with the model in its current status, but maintain the process open, and involve as much as possible the community. We need to maintain the process open to new developments, which we may expect in the field of laboratory or theoretical data.

Kerber: We should encourage the community to talk and contribute. Inputs are needed, but this won't happen alone. Everyone should participate, and encouraged to do so.

Genova: DCA has some budget to discuss standards. We may think at some point in the future to use it for a specific discussion on these topics. In the meanwhile, the participants should register to the DAL forum, read and post contributions. It is a good occasion to encourage people to register into the IVOA DM and DAL fora.

Soubiran: For theoretical spectra, three questions are the most urgent to address:

- which kind of models have not been implemented in the VO yet, and would be most critical for spectroscopic analysis?
- should VO provide grids of theoretical spectra (fixed nodes, not flexible) or codes to generate them with user-provided parameters (computational effort, redundancy)?
- automated methods to derive physical parameters rely on modelled templates. Such methods will become usual tools in the VO, whereas the validation of the models is usually not documented. How can this uncertainty be taken into account ?

Cerviño: Documentation and validation is main issue not only for VO, but for the scientific community in general. People should make their models available and take the responsibility to ensure the validity. It is the responsibility of the people who provide the service. Probably some tutorials are needed to use the models properly.

Richards: People in the radio domain are frightened to put their data in the VO, as users could use them without the proper knowledge. The way to proceed is to try and see. If there are problems, one needs to improve the documentation. For computation, authentication could be needed to put some kind of access restrictions.

Allen: Could photoionization codes such as `Cloudy` be included in VO? It is developed by a small group, which may not be very motivated.

Guainazzi: Active astronomers in the VO should try to promote science cases, that could encourage the publication of important codes into the VO. `Cloudy` could be a good test case.

Cerviño: `Cloudy` code is being re-written in C++, so it can be easily (and will be) adapted to the VO. More than science cases, we need tutorials to encourage people to use the tools.

Palacios: Many computational resources are now available. We should think to make them work in the VO. Both approaches (grid and computational) should coexist.

Skoda: There are some steps to be taken before a code can be made VO compatible. They may discourage some code developers. In the intermediate stage, would it be possible to create cgi-scripts that translate VO queries?

Piskunov: Tools capabilities and problems should be published in refereed journals. This is the only way to have a proper scientific assessment. The tools should be flexible, not computational expensive, and robust. And the application should complain, if you do something stupid.

Genova: VO cannot be the police for tools. Users should be guided in their choice, and they should know what the applications do. Perhaps IVOA should bless or not applications but we cannot forbid people registering applications if they wish.

Allen: I agree with that. VO does not remove the need for astronomers to think of what they are doing. They should discriminate. You still need to be an astronomer to do science using the VO.

Genova: One needs to realise that it is not easy to publish applications capabilities on a refereed journal. There have been some actions at the level of the Astronomy & Astrophysics editorial board to try and ease this process. However, generally a supporting science case is required for a paper to be accepted, and this is not always easy.

Piskunov: Nonetheless, this is the only safe way. VALD has 5 or 6 papers published on refereed journals.