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Atomic and Molecular Databases in the Context of Virtual Observatories

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Abstract

Numerical and bibliographic Databases in Atomic and Molecular Physics are essential for both the modelling of various astrophysical media and the interpretation of astrophysical spectra provided by ground or space-based telescopes. We report here on our current project concerning the access to Atomic and Molecular Databases within the Virtual Observatories. This presentation aims at informing people about interoperability matters, in order to put together the efforts which have already started in this domain, to evaluate the needs and requirements of the targeted interrelation between atomic and molecular data bases and VO projects. Collaborations in this domain are welcome.

Keywords:

database, virtual observatory, interoperability

1. Introduction

Atomic and molecular databases are an example of distributed resources which are used in numerous astrophysical applications. However, specific problems raised by the access to these databases in the Virtual Observatories paradigm have not yet been addressed. It is important to make atomic and molecular data widely available in interrelating databases with VO projects ; this would allow in particular uniqueness of data used in astrophysical models and automatic access to these data from Web applications developed for spectrum analysis or modelling.

2. Virtual Observatories

The Virtual Observatory can be defined as "*an enabling and coordinating entity to foster the development of tools, protocols, and collaborations necessary to realize the full scientific potential of astronomical databases in the coming decade*". Since the first conference "Virtual Observatories of the Future", June 2000, various projects started in different countries : Astrogrid (UK) [1], AVO (Europe) [2], NVO (USA) [3], JVO (Japan) [4] and more. An International Virtual Observatory Alliance (IVOA, Fig. 1) [5] started in 2002, its aim is to facilitate international coordination through agreeing upon common standards for data and interfaces. The alliance consists of representatives from all funded international VO projects who meet on a regular basis to refine the roadmap and reach consensus on choices for "the common ground" issues.

Fig. 1 The IVOA consortium

There is a collaborative Web [6] site with forum of discussions and information on the different groups that define standards. The working groups are:

- Resource Registry: The Registry standard addresses the need for an astronomer to be able to locate, get details of, and make use of, any resource located anywhere in the IVOA space, ie in any Virtual Observatory.
- Data Modeling: addresses modeling of various items : Spectra, Quantity, Observations, Transforms, Interferometry, Simulations, etc...

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- Unified Content Descriptors (UCD) : formal vocabulary for astronomical databases
- Data Access Layer: The task of the DAL working group is to define and formulate VO standards for remote data access. Client data analysis software will use these services to access data via the VO framework; data providers will implement these services to publish data to the VO.
- VOTable: The VOTable format is a proposed XML (eXtensible Markup Langage) standard for representing tabular data in the context of the Virtual Observatory.
- VO Query Langage : This working group has developped the Astronomical Data Query Langage (ADQL), which is an XML language for constructing queries. The mechanism of passing a query to a node is also developped in the VOQL working group (SkyNode Interface).
- Grid and Web Services, Standards and Processes.

Other groups of interest, such as VO Architecture, VO Applications, GGF Astro-RG, Data Curation and Preservation, VOTheory are also established.

The **VOTheory group** is the group that will be active in working on the access of atomic and molecular databases within the VO. The aim of this group is to work out what should be added to the standards in order to meet the requirements of theory. The theme of atomic and molecular data has been officially introduced in the IVOA during the September 2004 Interop meeting in Pune (cf [6]). Even more recently the SpectralLinelists sub-group [7] has been created in the DAL working group, its purpose is to provide a simple access to spectral line lists.

3. Unified Content Descriptors (UCD)

The UCD was the first work that we undertook on standards for atomic and molecular data. Each UCD describes a concept, which is similar to classes in object oriented programming. The UCD concept vocabulary is restricted in order to avoid proliferation of terms and synomyms, and controlled in order to reduce ambiguity as far as possible. UCDs play a central role in ressource discovery and processing in the VO. Services may publish the UCDs that describe their ouputs. Looking at these UCDs human users or machine agents can find sources of information they are looking for. All information on UCDs can be found at [8].

Definition in Version 0.2 : A UCD is a string which contains textual tokens called ”words”, separated by semicolons (;). A word is composed of “atoms”, separated by periods (.). So the hierarchy is the following : atoms → words → composed words.

UCDs have been recently changed and updated, and we participated to the new definition of UCD for atomic and molecular physics. The first generation of atomic and molecular physics did not follow any logical classification and is not complete. We adressed all these points and provided a starting working sheet. We divided the field into 5 main topics: identification of elements, identification of levels, radiative transitions between bound states, photon-matter interaction, some specific UCDs for various quantities. From this classification, some UCDs have been proposed and will be discussed by the board working in the IVOA, here is an extract from the proposed list :
Identification of elements:*phys.at.element* : atomic element

- **phys.at.name**: name of the element [Actinium, Lead, ...]
- **phys.at.number**: atomic number [Z]
- **phys.at.symbol**: [He, H ...]
- **phys.at.ion**: ionisation stage [CII]
- **phys.at.isotopic**: [^{9}Be, ^{10}Be]
- **phys.at.weight**: atomic weight
- **phys.at.qn.I**: nuclear spin quantum number (see below for explanation of *phys.at.qn*)

Identification of levels *phys.at.level*: atomic level

- **phys.at.term**: atomic term
- **phys.at.configuration**: atomic configuration
- **phys.at.parity**: parity
- **phys.at.sweight**: statistical weight
- **phys.at.lande**: lande factor
- **phys.at.lifetime**: lifetime
- **phys.at.qn**: atomic quantum numbers
  - **.S**: electronic spin
  - **.L**: electronic L
  - **.J**: resulting from coupling of S and L
  - **.F**: resulting from coupling of J and I

4. Conclusion

Atomic and Molecular Databases are concerned with the Virtual Observatories because their data are used in tools for spectral analysis and in codes simulating astrophysical objects. Those applications will be made available for a large public through Web interfaces and will use VO standards. The first step towards standardisation is to insure the uniquiness and a full documentation on the quality of the atomic and molecular data that are used in the applications. This first step could be done by the various data centers, or could be carried out by a dedicated service for specific applications. It is clear that the involvement of data centers would be preferable. The next step is to work on the data model for atomic and molecular data and to work on scientific "use cases". We are currently involved in all these topics.

References

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[6] http://www.ivoa.net/twiki/bin/view/IVOA/WebHome
[7] http://www.ivoa.net/twiki/bin/view/IVOA/SpectralLineLists
[8] http://vizier.u-strasbg.fr/UCD/