CASSIS: A TOOL TO VISUALIZE AND ANALYSE INSTRUMENTAL AND SYNTHETIC SPECTRA.

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Abstract. The advent of high spectral resolution and wide band instruments has left us with an almost overwhelming amount of rich spectra. The analysis of such datasets would be tedious and time consuming, without adequate tools. At IRAP, we have been developing a software, CASSIS, designed to help the astronomer with these tasks. We presented the tool during the SF2A meeting, and the link between databases and interoperability.

Keywords: ISM: molecules, Line: identification, Molecular data, Radiative transfer

1 Introduction

With the wealth of high-resolution, wide-band astronomical spectra that can be and have now been obtained with new generation receivers on ground-based telescopes and with space-based observatories, the need for an efficient and user-friendly software for line analysis has become crucial. Moreover, in order to better understand the physics, dynamics, and chemistry of the observed astronomical objects, it is necessary to develop theoretical models that can be compared with the observations. The goal of the CASSIS software is to provide a set of tools to make such a comparison easier in order to find the best set of parameters that reproduce the observations. Since 2005, we have developed, at the Institut de Recherche en Astrophysique et Planétologie, the CASSIS line analysis package (Centre d'Analyse Scientifique de Spectres Instrumentaux et Synthétiques*) to speed-up the analysis of high spectral resolution spectra (and particularly broad spectral surveys) from ground or space-based telescopes. CASSIS is one "Service d'Observation" of the OVGSO (Observatoire Virtuel du Grand Sud-Ouest) of the OMP (Observatoire Midi-Pyrénées). This package brings together the astronomical data from the telescopes, the telescopes parameters (main bean efficiencies, beam size in order to deal with the beam dilution), the atomic and molecular spectroscopic databases (JPL[†], CDMS[‡], NIST[§]) as well as collisional databases (BASECOL[¶] and LAMDA[‖]) in order to constrain the chemistry and physics of the source, such as the column density (and consequently its abundance), the kinetic or excitation temperature, the molecular hydrogen density, the line width, the line multiplicity.

2 CASSIS design and implementation

2.1 Spectra queries

CASSIS uses the SSA protocol (Single Spectral Access) to access the IVOA (International Virtual Observatory Alliance) services in order to retrieve any spectra (Hubble, Corot, Splatalogue, ISO, etc; the complete list can be found at the http://registry.euro-vo.org webpage) via our SSA module. Also CASSIS uses SAMP (Simple Application Messaging Protocol) that enables astronomy software tools to interoperate and communicate.

CASSIS can visualise any fits spectra, as well as spectra obtained with the CLASS/GILDAS software, widely used in the millimetre community.

2.2 Molecular databases queries

Line identification and radiative transfer modelling require repeated queries to molecular and atomic databases such as CDMS, JPL, and NIST. CASSIS also provide a database where the ortho/para separation has been performed on some species (H_2D^+, H_2O, H_2CO, NH_3, c-C_3H_2, H_2S and isotopologues) as well as the A/E separation on CH_3OH, CH_3CCH, $HCOOCH_3$. Both CDMS and JPL databases have been used to perform the separation, and the related partition functions are also computed and provided. Regular updates are performed to provide the most recent modifications of the official databases. The whole database is provided during the software installation. CASSIS can also deal with your own private catalog. It is also able to retrieve some useful information for the modelling or identification from databases (CDMS, JPL, BASECOL) through the VAMDC (Virtual Atomic and Molecular Data Centre) TAP protocol (Table Access Protocol) based on IVOA format. TAP provides virtual data and allows to plug in the query language VSS2 and the data model VAMDC-XSAMS (the latter being an output format).

2.3 Radiative transfer modelling

In order to constrain the chemical and physical properties of an astronomical source, you can use the radiative transfer modelling provided by the CASSIS software. All the details on the theory can be found on the CASSIS website (Formalism for the CASSIS software[**], author: C. Vastel). Any prediction of spectra can be done from many telescopes provided by the software, using the spectroscopic databases (frequencies, energy levels, statistical weights, Einstein coefficients). Presently a LTE model as well as the RADEX (van der Tak et al. 2007) code are available. These models need some information about the source (size of the source, column density, excitation or kinetic temperature, H_2 molecular density, velocity in the local standard of rest, values of the continuum) which is provided as templates that can be exported or imported into the CASSIS database. The telescopes informations are provided as ASCII files (will soon be xml files) so that any telescope can be very easily added or modified. The software can obviously deal with emission and/or absorption features, depending on the excitation temperature and the value of the continuum. This allows, among a number of tools, to compute synthetic models to be compared with the observations via χ^2 minimization with regular grids of models or using the Markov Chain Monte Carlo algorithm. An example of the main CASSIS user interface is shown in Figure 1. The best fit LTE modelling of the CH species is presented in red, and compared with the Herschel/HIFI observations. The spectroscopic parameters are given when the user clicks on each transition, and the resulting opacity from the LTE modelling are also given.

Currently CASSIS harbours a rotational diagram tool. The observed integrated lines can be fitted (Levenberg-Marquardt or Amoeba fitter) and stored into a file which is called by the rotational diagram tool; the latter then yields the estimated column density and excitation temperature of the studied species (both with error bars) as well as the probability of occurrence (P-value) for a χ^2 value depending on the number of degrees of freedom. A set of results can be obtained varying the source size, but no automated best-fitting tool is available yet. One can also apply the opacity correction module if some of the points might not be optically thin. A change in the temperature for lines of different excitation might indicate that the source has different temperature components or that the lines considered are not optically thin and cannot be easily used to obtain a meaningful excitation temperature. As Goldsmith and Langer (1999) nicely said, this method requires quite a large number of transitions spread over a range of upper state energies. If you plan on performing a population diagram analysis on 2 points only, CASSIS will evidently not be able to provide the errors on the column density and excitation temperature nor the χ^2 and probability values. Note that CASSIS can perform the rotational diagram analysis assuming optically thin lines for multiplet transitions ($\sim$ same frequency, $\sim$ same upper energy), but not on blended transitions ($\sim$ same frequency, different upper energy). Also, the opacity correction cannot be performed on any of these transitions for the moment. After using the Rotational Diagram module, you might want to use the column density and excitation temperature values in the Line Analysis module in order to compare the synthetic spectrum with your observations. An example of the rotational

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[**]http://cassis.irap.omp.eu/docs/RadiativeTransfer.pdf

diagram module is shown in Figure 2 on 11 transitions in the Herschel/HIFI frequency range. The blue fit corresponds to a linear fit, giving the excitation temperature and total column density for CO. The red fit corresponds to a linear fit taking into account the opacity effect, more important for low energy levels. It results in a lower excitation temperature and a higher column density.

3   Perspectives

In addition to these features, we propose to provide a tool to interface the results of a number of publicly available codes and the visualization/analysis part of CASSIS. For a given code, the tool would allow the user to define the parameter space to be investigated (range and step for each parameter needed by the code) and where to store the results ; it would then run the code on a dedicated server for all sets of parameter values. Finally, CASSIS would perform the χ^2 minimization as it currently does for LTE and RADEX, and plot the result corresponding to the best set of parameters. The originality of the project presented here resides in the added value for the astronomers. Indeed, presently an astronomer has to define and code in his preferred environment all the steps needed to compare the results of a given model with an astronomical spectrum. He/she has to : (i) identify the lines of a desired species in a generally crowded spectrum (due to the current sensitivity of the instruments) ; (ii) install the available codes and define the grids on which the computation will be done, and (iii) define the minimization algorithm to find the physical parameters that best reproduce his/her data. What we propose to provide with this project is a common environment that will allow the user to easily define the grids on which the computation will be performed, but also a common minimization module for all models. This will allow to perform a comparison of the results of different models, using the same input assumptions. The link to VAMDC (Virtual Atomic and Molecular Database Center) and observational spectral databases via the Virtual Observatory (VO) protocols VAMDC-TAP and SSAP is already implemented in CASSIS, and we will make this VO access functionality also available for databases of physical parameters of astrophysical sources when they will become available. It is useful to check the most up to date spectroscopic data provided through VAMDC, as well as how to deal with the quantum numbers, that can be quite complex to identify from a non-expert in spectroscopy astronomer. Some models (RATRAN, LIME for example) can need large computer resources for large grids of models, therefore the Synthetic Spectra Builder will be developed to run in batch mode on any existing dedicated computing cluster. This will be made available through the STOP (Spectral TOols Platform, 2015, PI: S. Bottinelli) project funded for ∼15 months.

4   Conclusions

CASSIS is used in the community to deal with large spectral surveys (Herschel/HIFI, IRAM/30m), but also to prepare proposals for single-dish or interferometric astronomical facilities (IRAM NOEMA, IRAM 30m, ALMA, JCMT, SMA, CSO, HIFI etc...). It has been offered as a HIPE plug-in from version 5.0 of HIPE[††]. HIPE (Herschel Interactive Processing Environment) is a software package to interactively process Herschel data, including finding the data products, interactive analysis, plotting of data, and data manipulation. Using any CASSIS model inside HIPE creates a new HIPE variable. It is possible to overlay any CASSIS model with others CASSIS models or to display it in a new HIPE view. The software is constantly evolving, with the telescopes developments as well as new functionalities from astronomers feedback requests.

References

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van der Tak, F. F. S.; Black, J. H.; Schoier, F. L.; Jansen, D. J.; van Dishoeck, E. F., 2007, A&A 468, 627

[††]http://herschel.esac.esa.int/HIPE_download.shtml

Fig. 1. A screenshot of the main CASSIS window, showing an observed spectrum in black overlaid with a synthetic spectrum in pink. The blue lines indicate the position of the transitions of the species of interest, here CH. A click on these lines display spectroscopic information. Clicking on any modelled line also gives the excitation temperature, Tex, used to produce the model, as well as the opacity, which depends on the assumed column density.
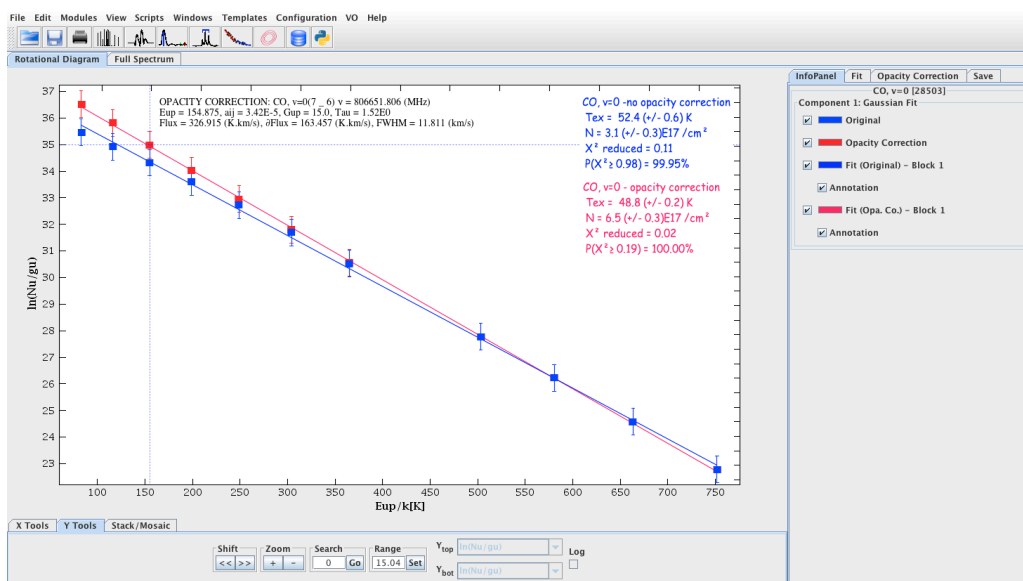

Fig. 2. A screenshot of the CASSIS window, showing the rotational diagram analysis without opacity correction (blue) and with opacity correction (red). Clicking on any line also gives the spectroscopic parameters as well as the line flux.