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A Survey of Software for the Manipulation and Visualisation of 3-D Sub-mm Spectral Line Datasets

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Abstract. 3-dimensional spectral line datasets are the end products of observations from single-dish telescopes and interferometers using widely differing instrument technologies over a broad wavelength range. Consequently, a range of software packages exist for the data reduction, analysis and visualisation of such 3-D data sets. These packages vary greatly in scope, generality, age, maturity and the availability of support and further development effort. Here we survey a range of relevant software packages emphasising packages suitable for the handling of submillimetre data sets generated by sub-mm focal plane arrays such as HARP/ACSIS on the JCMT. The conclusions are broadly relevant to future software development and re-use for a wide variety of astronomical instruments and wavelength regimes.

1. Introduction

This survey has been motivated by the imminent arrival of a 350 GHz 16-element focal plane array receiver (HARP) and its digital autocorrelation spectrometer (ACSIS) at the JCMT (Dent 2000). In combination, these will generate large ($\sim$ several GByte) data cubes in standard FITS and/or NDF formats. We needed to identify manipulation/visualisation software with a short learning curve which we could recommend to users with little or no experience in using traditional astronomical data reduction packages. Thus this survey excludes the traditional interferometer oriented packages such as AIPS and MIRIAD/GILDAS – the pros and cons of these should be familiar to users with a background in interferometry. Commercial packages with support for astronomical data import/export (e.g. IDL) are not considered here. Traditional spectral-line specific tools with some useful but limited map making capabilities, such as SPECX, CLASS and COMB are also not discussed here.

2. Some Typical User Requirements

- Strong, on-going development and support with open licensing (e.g. GPL).
- Reliable and robust handling of astronomical file formats (e.g. FITS).
- Ability to efficiently handle large data files (e.g. $>$ 4GB).
- Complete handling of astronomical co-ordinates, projections and units.
- Ease of use e.g. for graduate student on first observing run at the JCMT.

- Intuitive user interface, powerful scripting capabilities.
- Radio astronomy friendly - knows about dual sideband receivers, $T_{\rm sys}$ as a measure of expected noise, standard rest frames etc.
- Bad pixel (region) masking.
- Smoothing and decimation of spectral cubes.
- The mosaicking of spectral cubes.
- Spectral baseline fitting and removal across cubes.
- Mathematical operations on entire cubes (and regions).
- Truncation of spectral cubes.
- Display arbitrary 2D slices of 3D cubes (pixel and contour representations).
- Calculation of statistics over cubes (sub-cubes and regions).
- Calculation and display of 2D integrated intensity maps from 3D cubes.
- Calculation and display of higher-order moments e.g. velocity fields.
- Any 3D rendering capability is a plus.

3. Complete DR and Visualisation Packages

3.1. AIPS++

AIPS++ (McMullin et al. 2004) is a large, general purpose software package for the manipulation and visualisation of astronomical data. It was developed by a consortium of observatories, and saw its first public release in 1999. The consortium was disbanded in 2003 and software effort and support reorganised amongst the member institutions. Support of the central code base remains the responsibility of NRAO and the source code is freely available under the GNU Public License.

On a technical level, AIPS++ consists of a scripting language, glish, which acts as a software "glue" between pre-compiled C++ clients. The GUI is provided via the use of glish bindings to Tk widgets and PGPLOT primitives. The software is organised around the concept of distinct tools which can be created and destroyed via the glish command line or AIPS++ GUI. A wide range of tools exist for handling single dish and interferometric data, as well as general purpose tools for image analysis, astrometry etc. In addition, there are tools to perform telescope specific calibration and visualisation tasks.

2D and 3D image manipulation and visualisation is handled via the `image` tool. FITS data cubes can be read in and converted to the AIPS++ table-based image format. AIPS++ images can be viewed via the image viewer tool, which enables 2D slice (rasters and contours) and 1-D spectral profile display. Image tool functions include masking, mosaicking, image moment calculation, smoothing and decimation, region selection and statistics finding. Glish scripting provides the flexibility to combine operations to perform powerful, user defined 3D image manipulations.

Overall, the reception of AIPS++ by the astronomical community has been somewhat mixed and widespread adoption slow. It has developed a reputation for being non-user friendly, probably due mostly to the poor integration of the GUI and command line interaction and the lack of conceptual integration between tools. Features such as full support for the draft spectral FITS WCS standards, rotations between pixel and sky frame axes and support for handling spectra from dual-sideband receivers have not yet been implemented. AIPS++

and glish have arguably found more success as a lower level toolkit for the development of facility-specific data reduction software such as the parallel real-time data reduction system for the ACSIS spectrometer, which is built around glish messaging and AIPS++ libraries. Plans for future development of the AIPS++ code base will be more targeted towards application for particular instruments, such as ALMA. The glish scripting language has the disadvantage of a small user community and low manpower availability for core language support and development. Thus, much work is being done to decouple the AIPS++ C++ libraries from glish, so that they can be used with other, powerful, wide user scripting languages, most notably Python. Unfortunately, this focus on core software infrastructure and ALMA-specific goals by the AIPS++ development team means there is less effort for more "user-centric" feature requests and bug fixes. Also, it is hard to recommend AIPS++ to users with the knowledge that the UI (scripting language and GUI) will change rapidly over the next few years.

3.2. Starlink

The Starlink (Draper et al. 2005) Software Collection consists of an array of tools targeted towards astronomical applications at a wide range of wavelengths. Much of the software is mature and has a wide user base, particularly from the UK astronomical community. Recent work includes moving the code base into CVS, simplifying build procedures using autoconf, ensuring MacOS X compatibility and migration to the GPL license.

One strength of Starlink is its hierarchical data format NDF (N-dimensional Data Format). NDF can support data of arbitrary dimension and can contain variance and data quality arrays in additional to image data. AST data objects describing WCS (World Co-ordinate System) information provide sophisticated astrometry handling. AST also handles spectral co-ordinate axes, such as the one-to-many mappings which arise in dual-sideband heterodyne systems. Starlink includes a `convert` application to handle conversion to and from NDF and other formats such as FITS. `convert` allows one to easily specify the required FITS header convention e.g. classic AIPS, WCS paper III compliant etc. Direct manipulation of 3D NDF data cubes is mostly achieved through the Starlink `kappa` package. It consists of 180 general purpose command-line programs for manipulation, image processing and visualisation of NDF data. While `kappa` includes no GUI frontend other than a PGPLOT display window, its commands are mostly reasonably self-explanatory and well suited to use with scripts (e.g. UNIX shell, Perl etc.).

Starlink offers the `datacube` package to handle higher level, 3D spectral data specific visualisations. `datacube` is a collection of scripts, run from the command line, which use lower-level Starlink applications, such as `kappa`, to achieve visualisation tasks. `datacube` allows slice-by-slice steps through 3D cubes, interactive plotting of spectra at given sky positions, as well as the generation of velocity and line-peak maps following interactive Gaussian fitting to spectra within a cube. 3D data cubes from contiguous areas of the sky can be mosaicked together into larger datacubes using `makemos`, part of the Starlink `ccdpack` package. `makemos` can handle 3D NDF data easily and allows the user fine control over what happens to any regions of overlap between component subcubes.

To summarise, applications provided as part of the Starlink collection can meet most of the typical user requirements described above. However, using Starlink software does involve some user-friendliness related disadvantages. Firstly, the required functionality comes from a variety of different software packages, with separate documentation. Secondly, the user interaction with most of the relevant software is almost exclusively via the command line. This second disadvantage is shared by most "traditional" astronomical data reduction packages (AIPS, MIRIAD etc.), and at least maintains flexibility at the expense of a steeper initial learning curve.

4. 3-D Visualisation Software

As opposed to general purpose FITS viewers which can display 2D slices of 3D data (e.g. fv, GAIA, and DS9), the following packages offer more sophisticated 3D visualisation capabilities.

4.1. Karma

Karma (Gooch 1996) is a package specifically targeted for the visualisation of 3D astronomical data sets. It consists of a suite of visualisation tools as well as a programmers library and API distributed under the GPL and LGPL licenses. While Karma is mostly the work of single developer, the project is mature and continues to be actively supported. Karma has two main tools useful for visualisation, namely `kviz` and `xray`. `kviz` enables 2D slice viewing in raster and contour mode, spectral profile display, image annotation, higher order image moment generation and display, renzogram display and image statistics calculation. `xray` is a tool which enable powerful 3D volume rendering of datacubes. User interaction with Karma is via a fast graphical user interface.

4.2. OpenDX

OpenDX (`http://www.opendx.org`) is the open source version of IBM's Visualisation Data Explorer. It is aimed at the 3D visualisation of scientific data from a wide range of sources. Users include mechanical and electrical engineers, medical imaging professionals as well as astronomers. OpenDX is available for Unix platforms (inc. Mac OS X and Windows (under Cygwin). Visualisations are specified in OpenDX by preparing a "Visual Program" in a GUI-based Visual Program editor. These visual programs specify the interconnections of data-driven visualisation tools. These tools handle primitive visualisation operations such as file import, statistics calculation, surface rendering and colour table setup. There is great flexibility in combining these elements to perform a wide variety of visualisations.

For the visualisation of 3D astronomical datacubes Starlink provides a variety of Visual Programs for common datacube visualisation, such as displaying sequences of 2D slices of 3D cubes and displaying 3D isosurfaces. Starlink also provides software to convert NDF datacubes into the native OpenDX .dx file format. OpenDX is a well featured and flexible program for 3D visualisation suitable for astronomers with more specialised visualisation needs. The majority of observers will probably continue to look to conceptually simpler, astronomy-specific software packages for the most of their needs for datacube visualisation.

5. Useful Scripting Language Extensions

PDL (`http://pdl.perl.org`) is a Perl module, written in C, which gives Perl the ability to manipulate large N-dimensional data sets efficiently. The astronomer-oriented development team provide support for I/O in FITS and NDF formats.

Python has become a popular scripting language for scientific applications. Python modules exist for array manipulation (such as `numeric` and `numarray`) and the PyFITS module enables FITS I/O (Rottler 2005).

6. Some Concluding Observations

- No single software package meets all of the user requirements in Sec. 2.
- It is clear that a modern GUI which is well integrated with scripting capabilities requires considerable design and implementation effort.
- FITS has the advantage of file format simplicity but it is arguably too easy to develop multiple keywords/conventions. Publication of the FITS Spectral WCS standard is a helpful step here.
- The hierarchical NDF format is more sophisticated than FITS but has a steeper learning curve poor and end-user adoption outside of the UK.
- Much can be learned by comparing user requirements for 3D software across the whole electromagnetic spectrum. Such comparisons will encourage software reuse and prevent a fragmentation of software effort.
- Continuing support and development of a software package is an essential requirement for its adoption.
- The control that open-source licenses such as GPL give the user community over the software is highly derirable.
- The JCMT will recommend Starlink software and Karma to users for routine handling of ACSIS data. Some support for AIPS++ users will exist in the form of cookbooks. Support is expected for users wanting to import ACSIS data into older packages such as AIPS, CLASS and SPECX.
- Future developments include the Euro3D (`http://www.aip.de/Euro3D/`) project which aims "to provide standard software for the visualisation and analysis of datacubes" which aims for a first public software release is scheduled for December 2004. The developers stated aim is to produce tools which are "independent of data source", so hopefully the software will be useful at sub-mm/radio as well as optical/IR wavelengths.

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