Interactive Spectral Analysis under X–Windows

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Abstract

Devices based on the WIMP (Window-Icon-Mouse-Pointer) paradigm have rapidly become very common tools in the astronomical community. Data analysis systems have to cope with this new reality, and need to exploit their capabilities, in order to be attractive to users.

In this paper, the design and the implementation of a system to perform interactive spectral analysis in an X-Windows environment are described. After a discussion of the basic requirements for efficiently analyse spectra, and particularly high-dispersion spectra covering a wide wavelength range, the features of the system are described.

In particular, the continuity with some of the former MIDAS spectral analysis commands (`SELECT/LINE` and `ANALYSE/SPECTRUM`) is stressed, and the evolution from VTU-based commands to tools exploiting WIMP capabilities is pointed out.

1 Introduction

Back in the late 70's and in the 80's, the astronomical community started building software environments to analyse their data. While fine pieces of such software (AIPS, MIDAS, IRAF, ST–SDAS) were being conceived and built, in the computer market devices based on the WIMP (Window-Icon-Mouse-Pointer) paradigm became rapidly available and popular. In the last couple of years, devices such as workstations and X-terminals have become increasingly inexpensive and therefore common also in the astronomical community.

The above-mentioned data analysis systems, on the other hand, concentrated on portability across different hardware platforms and, while striving for generality, lost some of the unique characteristics of WIMP devices. In other words: workstations have been treated just as multiple alphanumeric/graphic/image display devices, and few other windowing capabilities have been actually exploited.

Only lately, in order to be attractive to users, some of the best-known data analysis systems started using these new capabilities. A fine example is SAOimage, which has been built as a standalone package, but has been integrated into IRAF as the standard image-browsing tool. Also MIDAS is now importing packages based on windowing capabilities: graphic interfaces have been developed for XSPECTRA, distributed in the 91NOV version [5], and for the echelle reduction package [3].

In the following we will discuss background, concepts and implementation features of an interactive spectral analysis package which has been built under X–Windows and which uses a graphic user interface (GUI), designed to be easily integrated in any data analysis system. Integration with MIDAS has already been tested.

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1.1 OAT Background

There is a number of reasons which led us to the development of an interactive spectral analysis software under X-Windows. First of all, in Trieste there is plenty of expertise in spectral analysis. There is a wide community of users, both in the Observatory and in the University Department of Astronomy, which has been using spectral analysis packages for quite a long time. Such a community has declared preference for an interactive analysis paradigm, since it is felt that the scientist needs to maintain control at all times during the analysis phase.

This is why an interactive spectral analysis package to deal with photographic spectra, ELSPEC, has been designed back in 1977 and built on a PDP ([6, 7]); the system has evolved to VAX in 1982 [8] and distributed to the Italian astronomical community. The core of the package has been implemented in the VMS version of MIDAS as a couple of commands (`SELECT/LINE` and `ANALYSE/SPECTRUM`) in 1987 [4].

On the other hand, the Trieste Observatory (OAT) also has plenty of X-Windows expertise. OAT has planned and implemented the evolution of its computing facilities by installing since 1986 a non-homogeneous environment based on Unix workstations. The first version of the X-Windows driver for the Image Display Interface for MIDAS has been developed by OAT in 1988. Finally, during 1991, OAT has designed and built the user interface for the Galileo telescope under OSF/Motif ([1, 2]).

2 Concepts

When designing the system, a number of requirements were kept in mind. They are listed in the following:

- The software should use all possible attractive features of WIMP devices while keeping **simple**. This means that the GUI should allow to use pull-down menus, dialog boxes, interaction using the mouse, *etc.*, but by no means the user should feel lost by the number of options which he/she is allowed to choose from. In other words, there should always be an obvious path to the action the user wishes to perform (*e.g.* a default menu).

- All of the basic tools needed should be **visible** immediately. This is a corollary of the above statement. The main menu should contain all of the basic actions the user wishes to perform grouped under classes having obvious names.

- The software should have the capability of handling spectra covering a **wide wavelength range**. As an example, analysis should be allowed on echelle spectra after orders have been merged (typically, in the order of 10^5 pixels).

- The software should have the capability of handling spectra containing **quality flags**. Spectral data gathered by instruments installed on space-bourne observatories such as IUE or HST include quality indicators. "Bad" pixels should be discarded.

- The software should have the capability of handling **non-uniformly-sampled** spectra. The above item points out for the need of handling spectra with missing values ("bad" pixels); furthermore, spectra gathered by instruments providing variable bin sizes (*e.g.* prism data) should be handled.

- The software should have the capability of analysing **photographic** spectra. In the era of CCDs, the use of photographic material may look quite obsolete; anyhow, it can still be useful to check archive data. As an example of the interest for such an activity, the Commission no.

29 of IAU has endorsed the creation of a working group which is to define an internationally-accepted policy for the creation and maintenance of spectral archives, including vaults of photographic material.

- The software should have the capability of analysing spectra with **fixed ITF**.
- The software should provide **continuity** with ELSPEC and with the `SELECT/LINE` and `ANALYSE/SPECTRUM` commands of MIDAS/VMS. In other words, the software should support the evolution of previous code using a VTU-based interaction paradigm into a set of tools exploiting WIMP capabilities.

3 Features

The design of the system has been completed, and currently most of the features have already been implemented. A first release of the package is expected in summer 1992.

The software has been developed on Unix (Apollo workstations under Domain OS and Hewlett–Packard workstations under HP/UX). The X–Windows interface used is OSF/Motif, and the X–Windows version of the AGL library is used for graphics. The main program has been written in Kernighan & Ritchie C, while the analysis routines are coded in Fortran 77, since they have been ported from previous packages. The C–to–Fortran interface has been kept to a minimum, since it may create some minor portability problem in different environments.

One of the main features of the package is the ability of reading the input file(s) in a variety of formats:

- **MIDAS BDF:** this format was supported in the MIDAS/VMS `SELECT/LINE` and `ANALYSE/SPECTRUM` commands, and still is.
- **MIDAS table:** two columns are required as a minimum. Their labels are `:WAVELENGTH` and `:FLUX` by default. Furthermore, the possibility of defining a third column (labeled `:QUALITY` by default) and a value for "good" data are supported. A fourth column, containing the bin size can be finally defined as an option.
- **ASCII table:** as in the previous case, two columns are required as a minimum, a quality column can be defined together with "good–data" values, and the binsize column is supported as an option.

The package has been tested up to now on HST data formatted as MIDAS tables, and on IUE/ULDA and IUE high resolution data formatted as ASCII tables. The package has been dimensioned in such a way that spectra up to 100000 pixels can be analysed.

4 The system

The current version of the package can either be run under the MIDAS environment, or standalone. The only required input is the name of the input file; the name of the output file can be defaulted. If the input file is a table, the location of the wavelength and flux columns are required; the location of the quality column and the "good–data" value, and the location of the binsize column are further optional inputs.

Once the input data file is read, possibly skipping values having "bad" quality flags, a graphic window is opened, where the original spectrum is plotted, and the GUI of the package (shown in Figure 1) is displayed. The main menu of the GUI contains a *display* item containing a number of display functions, an *analyse* item allowing the system to start line analysis, and the *select*,

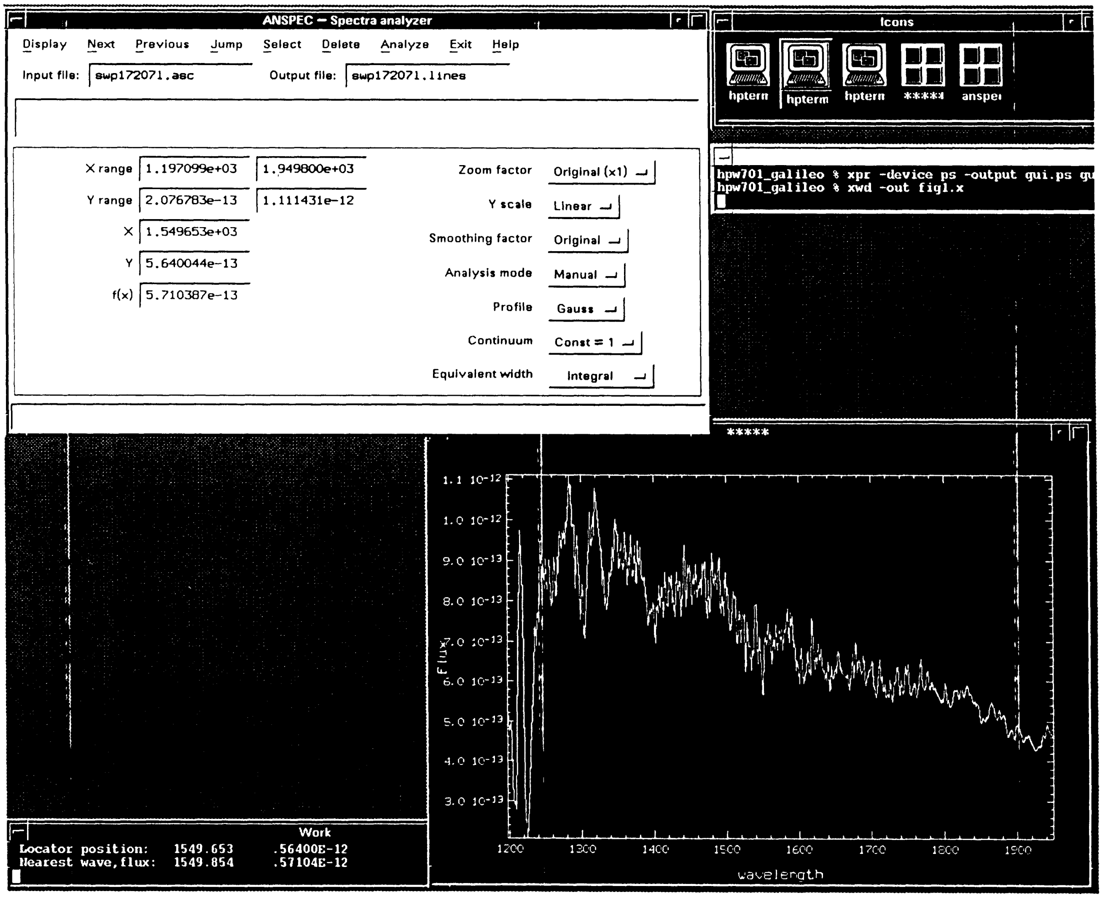

Figure 1: The initial setup of the spectral analysis package. Two windows are opened: a graphic one (AGL), where the original spectrum (an IUE low-resolution spectrum, SWP17207L, taken from the ULDA Italian National Host) is plotted, and the GUI of the package.

delete, *next*, *previous* and *jump* items allowing selection of lines chosen for further analysis and their display. A *help* item and the *exit* menu selection complete the main menu.

Display and analysis options can be chosen by using the buttons at the right-hand side of the GUI. Some read-only fields are furthermore available: at top, a help field where the user can find suggestions on the action which needs to be performed as a consequence of the option chosen; at the bottom, an error field where error and warning messages are displayed. At the left-hand side of the GUI the X and Y ranges of the displayed section of the spectrum are given, together with the X, Y and pixel value of the last graphic cursor action.

4.1 Display

If the *display* item of the main menu is chosen, a pull-down menu is generated allowing a certain number of actions. *Hardcopy* allows to save the current AGL metafile on a permanent file which is then replayed on a hardcopy device. *Set Range* starts the graphic cursor on the AGL window: the user is allowed to choose interactively the bottom-left and upper-right corners of the area he/she wants to see. *Scroll Left* and *Scroll Right* shift the wavelength ranges of the displayed area by 20%. *Cursor Pick* starts the graphic cursor on the AGL window, and the user can read X, Y and

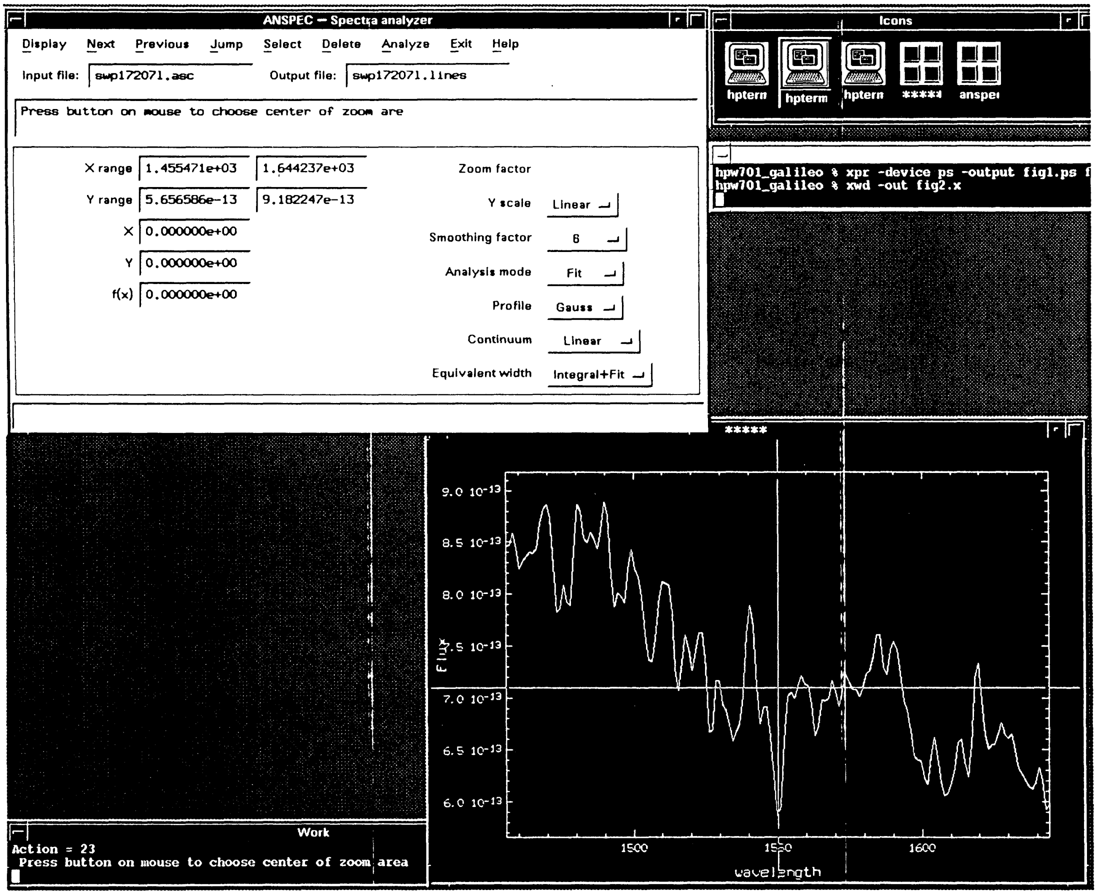

Figure 2: The spectrum originally displayed in Figure 1 has been smoothed by a factor of 6, and zoomed by a factor of 4 around the position defined by the graphic cursor.

spectrum value of the specific points chosen with the cursor by pressing a button on the mouse; the values are shown on the output fields at the left-hand side of the GUI.

The three upper buttons at the right-hand side of the GUI allow for further display actions by activating pull-down menus: *Y scale* allows the toggling between *linear* and *log*; *Smoothing factor* gives the user the choice of the number of iterations a smoothing-by-threes algorithm will go through to make the displayed data more pleasant to look at. The *Zoom factor* button starts the graphic cursor on the AGL window and allows the user to zoom by a specified factor around a chosen central point.

These display features have been proven to be particularly useful to scientists dealing with long spectra.

In Figure 2, the spectrum (a low-resolution IUE spectrum extracted from the Italian national host site of the ULDA archive, at OAT) has been smoothed by a factor of 6, and zoomed by a factor of 4 around the position defined by the graphic cursor. Wavelength and flux ranges of the displayed data and the values of the pixels related to the last interactive action are displayed on the left-hand side of the GUI.

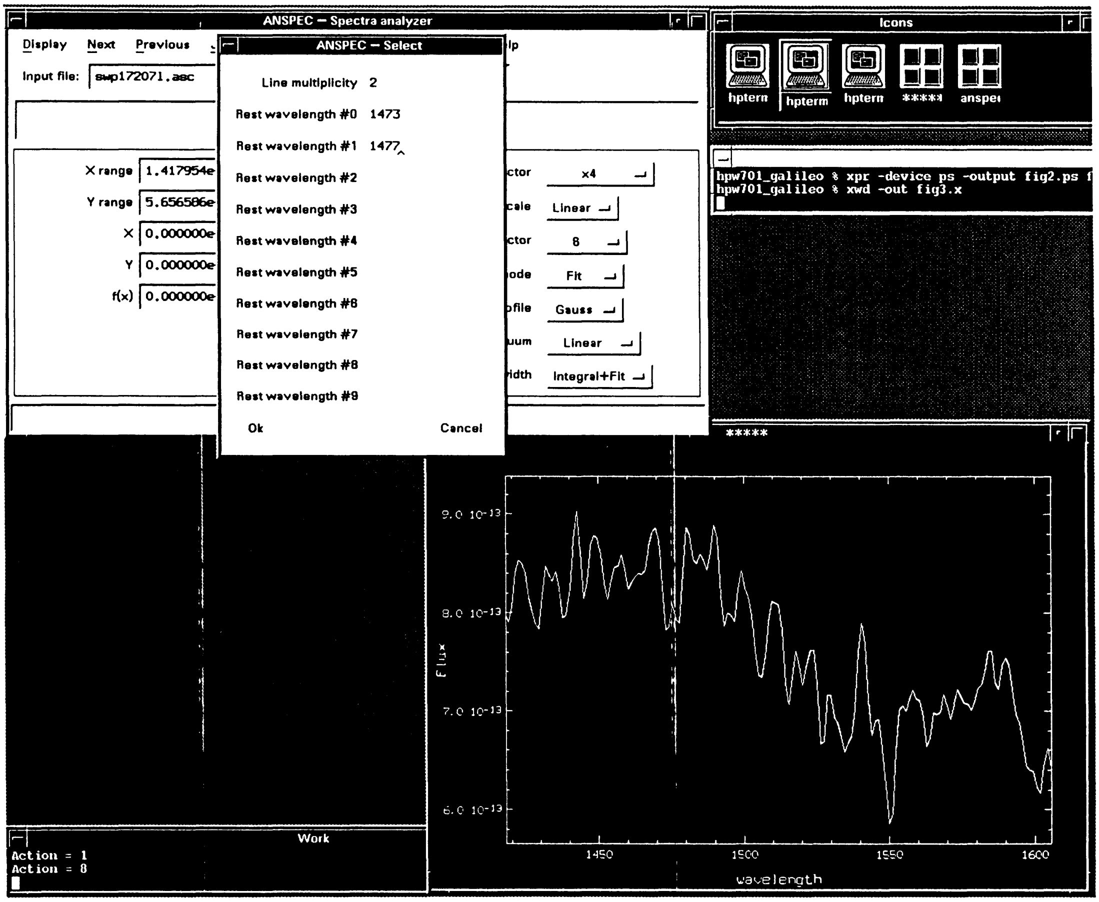

Figure 3: Running the *select* option in the main menu. The user is prompted for line multiplicity and for rest wavelength(s) in the case radial velocity analysis is desired.

4.2 Line selection

Spectral features to be analysed at a later stage can be interactively selected by choosing the *Select* option in the main menu. The user is prompted for line multiplicity and for rest wavelength(s) in the case radial velocity analysis is desired (Figure 3). Then, using the graphic cursor on the AGL window, a wavelength range containing the relevant spectral feature is chosen. Selected lines are marked with a horizontal bar at the upper end of the AGL window (Figure 4).

Once a number of ranges have been selected, they can be displayed choosing the *Jump* (Figure 5), *Next*, or *Previous* options. When a range is displayed, analysis can start on the spectral features included in such a range.

4.3 Analysis

No effort has been made for the time being in upgrading the spectral analysis algorithms: as a matter of fact, in this version of the software they are the same as in the former `ANALYSE/SPECTRUM` MIDAS command.

Before the user selects the *Analyse* option on the main menu, he/she needs to choose between the analysis modes allowed, choose among the various analytical models for the line(s) (Gaussian, Lorenzian, Moffat, Voigt), choose how to define the continuum (constant, linear, spline), and choose

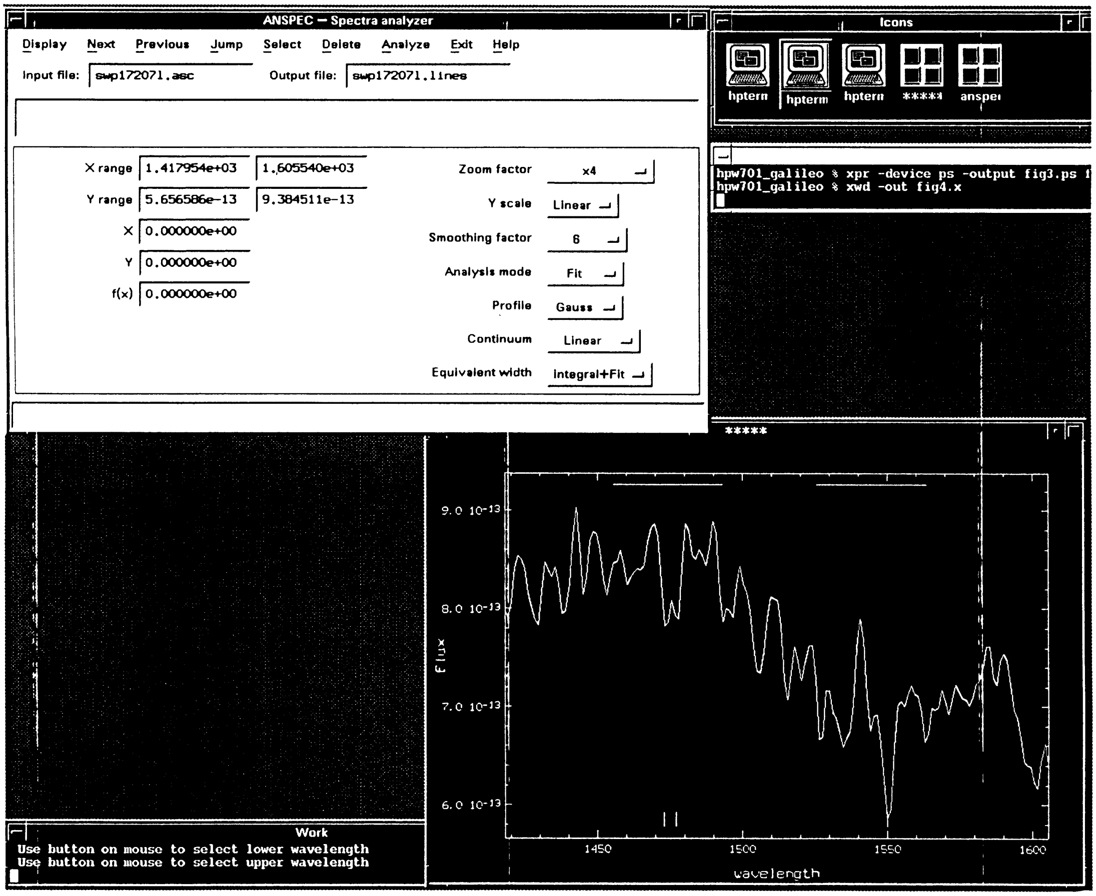

Figure 4: Running the *select* option in the main menu. The selected lines are marked with a horizontal bar at the upper end of the AGL window.

if the equivalent width of the line is to be computed as the integral of the line above/under the continuum, or as it results from the fitting procedure. Defaults are obviously available.

Two basic analysis modes are allowed: *manual* and *fit*. The system requires that the initial guesses of the local continuum, and the central wavelength, central depth and FWHM for every component are interactively defined. Up to 10 line components can be specified: this is not a limit of the analysis algorithm, but rather a reasonable limitation set by the difficulty of graphically interacting with the data.

Once the line(s) parameters have been initialized, a fit to a given analytical model previously chosen from a menu of shapes is performed using a modified Fraser-Suzuki method.

At the end of the analysis, the results can be either validated or rejected; in the latter case, the analysis step can be re-run. In both cases, another selected line can be displayed via the *Jump*, *Next*, or *Previous* options in the main menu, and analysed.

4.4 Handling the results

At the end, a table is stored in memory containing all of the selected lines and, for the analysed lines, all parameters of interest computed in a statistically correct way. Parameters included are: central depth of the line, wavelength of the peak, left HWHM and right HWHM (for each, the initial

Figure 5: Running the *jump* option in the main menu.

guess, the computed value, and the standard deviation are given); effective wavelength, FWHM, equivalent width, integral equivalent width, peak radial velocity and effective radial velocity (for each, the computed value and the standard deviation are given); the overall standard deviation of the fit, number of fit iterations to reach convergence, and the error code; finally, all inputs to the analysis (window range, rest wavelengths, rejected areas, analysis modes, *etc.*).

This table stored in memory is output to a file at the end of the program. The format, in this version of the software, can either be an ASCII table, which can be ingested by spreadsheets and database systems, or a MIDAS table.

5 Future Developments

As was previously stated, the initial version (1.0) will be available during the summer 1992, after a complete debugging phase and consistency checks have been performed. Version 1.0 will contain the features which have been described, and possibly some minor enhancements.

A number of upgrades will be included in new releases of the software:

- Automatic line selection (which was already available in the MIDAS/VMS `SELECT/LINES` command) will be added. The feature will be based, as before, on non-linear filtering and a thresholding mechanism.

- Full support for input files in FITS format (standard files, files with IMAGE extension, table files, and 3–D binary table files) will be guaranteed; other formats for input files will be supported if deemed to be necessary.
- A multi-file option will be supported, to allow users to easily being able of analysing a small number of lines over a large number of spectra.
- Additional software modules allowing support for analysis of photographic spectra will be added. Such modules include handling of files ingested by a microdensitometric system, wavelength and density–exposure–wavelength calibrations. This activity has anyhow a lower priority.
- Additional software modules allowing the interactive definition of the continuum on a large scale will be added.
- A number of different line analysis paradigms will be tested and, if the case, included in the package. In particular, auto-initialization of the line(s) analysis step may be interesting, when the initialization of the fit is simple and does not need to be performed interactively (*e.g.* line multiplicity = 1). Moreover, computation of left and right edge radial velocities will also be included.

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Part II
IR and UV Spectra