Getting Started with Profit

A Tool for Visualizing High-Resolution Spectra

A Product of the *XMM-Newton* and *Suzaku* Guest Observer
Facilities and the
Laboratory for X–ray Astronomy
NASA/Goddard Space Flight Center

Contents

List of Figures

List of Tables

Chapter 1

Overview

Profit is a GUI (graphical user interface) tool for displaying and analyzing high- and moderate-resolution spectra. Although designed with high-resolution ($R > 300$) X-ray spectra in mind, *profit* will also work reasonably well with CCD resolution data ($R \sim 50$) and will work with spectra in other wavebands as well. *Profit* can read spectra in a number of formats, including simple ASCII text. It allows users to identify emission lines, to convert an identified line into velocity units using a user-selected wavelength, to store (and restore) individual spectra, to fit lines to gaussians, and other features. *Profit* is meant to handle the "exploratory" phase of analysis, although it has some powerful features. Combining the velocity function with the ability to store and plot multiple features, it is very easy to see if lines from a particular ion or isosequence are systematically red- or blue- shifted, asymmetrical, or broadened.

Profit's GUI is based on ROOT (`http://root.cern.ch`), a multifunctional library developed at CERN for high energy physics analysis. ROOT was chosen because it is well-supported and designed to handle histogram data smoothly. Although ROOT features and functions are used "behind the scenes" in *profit*, the user does not need to have any familiarity with ROOT to use *profit*, and in fact, ROOT users might find *profit* incomplete as we have removed many features in order to make a simple and robust tool. *Profit* runs natively on a variety of systems, including Linux, Mac OS X, and Solaris.

This manual describes *profit* version 1.0. We plan to continue developing *profit* to add functionality, and welcome suggestions from users as to what features would be most useful. Requests, bug reports, and questions can be submitted at the Feedback form on the *profit* web site, `http://heasarc.gsfc.nasa.gov/docs/software/profit/`; this can also be found at `http://heasarc.gsfc.nasa.gov/cgi-bin/Feedback`.

Chapter 2

Installation

Installing *profit* is straightforward, although it helps if you are familiar with unix "tarballs" and directory structure. Mac OS X users should be able to download the binary version which will expand either automatically or after double-clicking on the file.

Profit binary tarballs come in two types:

Complete: These include everything needed for *profit* to run, and can be downloaded, untarred, and run immediately. Each tarball is $\sim$ 80 MB. We recommend using the complete version if possible.

Update: These only update *profit* to the latest version. *Profit* requires a small binary and library of its own, and is compiled using a specific version of the ROOT (http://root.cern.ch) library and ATOMDB (http://asc.harvard.edu/atomdb/) database, which must also be installed (and is provided in the complete package). Our intent is to change the ROOT and ATOMDB versions infrequently, and therefore these will be left out of update releases to reduce unnecessarily large downloads.

2.1 Step-by-Step Installation

2.1.1 Download *Profit*

Download the most recent binary *profit* distribution for your operating system, or download the source distribution. If available for your operating system, we recommend the binary distribution as it is quicker and easier to install. Binary distributions are available which were built on

- Intel/Linux Fedora Core 1 (glibc version 2.3.2) with g++ 3.3.2.
- Mac/OS X Panther with g++ 3.3.
- Sun/Solaris 8.0 with Forte compilers v. 7.0.

The Linux binaries are likely to work only if the runtime libraries are compatible with the versions of glibc and the compiler described above. Linux users are therefore more likely than others to need to build from source. The Mac/OS X binaries are known to work fine on Tiger. The Solaris binaries should work on most versions of Solaris, but this has not been widely tested.

2.1.2 Unpack and Install (Binary)

To install a binary distribution, untar the distribution in a convenient directory:

```
unix% cd profit_dir
unix% tar zxf profit-version-ostype.tar.gz
unix% cd profit
```

At this point, *profit* is ready to run; see §2.2 for more details.

2.1.3 Unpack and Install (Source)

Source code builds are supported on all platforms, although *profit* requires a recent C++ compiler. We have tested the following compilers:

- g++ 3.2.3 or later.
- Sun Forte compilers 7.0 or higher.

To install, first untar the distribution in a convenient directory (note that XXX is the version number for this release of *profit*), and compile it as follows:

```
unix% tar zxf profit-<i>version</i>-src.tar.gz</td></tr>
unix% cd profit/profit/XXX</td></tr>
unix% ./configure
unix% make all >& make-log
unix% make install >& install-log
```

There is one known issue when building from source on Mac/OSX. The `make all >& make-log` step will most likely fail with errors about not being able to find libfreetype.dylib. If this occurs:

```
unix% cd /path/to/my/profit/extern/root/4.04.02f
unix% mkdir powerpc-apple-darwin7.9.0
unix% mkdir powerpc-apple-darwin7.9.0/lib
unix% cp -p root/freetype/src/freetype-2.1.9/objs/.libs/libfreetype.dylib powerpc-apple-darwin7
```

Then go back to the source instructions starting from the `./configure` command.

When building from source on Solaris there are numerous issues. We are working to resolve, or at least minimize and document these.

2.2 Running *Profit*

After either source or binary installation, the main *profit* executable file will be named `profit`, and will be located in the directory `profit/bin` inside the directory in which the tarball was unpacked.

2.2.1 Linux/Solaris

To invoke *profit* from a UNIX shell prompt, simply give the complete path to this executable:

```
unix% /path/to/my/profit/bin/profit
```

Optionally, users may add the path to the PATH environment variable, as shown here for csh/tcsh-type shells:

```
unix% setenv PATH $PATH\:/path/to/my/profit/bin
```

or as follows for sh/bash/ksh-type shells:

```
unix# PATH=\$PATH:/path/to/my/profit/bin
unix# export PATH
```

These commands may be included in the .cshrc file (if you use the tcsh shell) or .bashrc file (if you use the bash shell) to add *profit* to the path automatically when a new shell is started. Links to this file can be made and placed in any directory.

2.2.2 Mac OS X

Profit on the Mac requires X Windows; either the Apple X11 server or the XFree server must be installed. After ensuring that X Windows is running, simply open the "bin" directory and double-click on the `profit.command` icon. This has the side-effect of running the "Terminal" program, and will fail if X Windows is not running. The Terminal program can be exited after running Profit. This is a workaround that we hope to avoid in a future release.

If you have problems installing *Profit*, please inform the developers using the Feedback form on the *profit* web page, `http://heasarc.gsfc.nasa.gov:/docs/software/profit/`

Chapter 3

Using Profit

Profit's interface is designed to make most operations straightforward. Many features are accessed by either clicking a button or selecting a region. However, some features require short explanations. The main *profit* "view" is shown in Figure 3.1.

3.1 Reading Spectra

The Spectrum Information Window will always show the filename and other relevant information (source name, observation date, exposure time, etc) for the currently displayed plot. If multiple spectra have been loaded into *profit*, any of these can be brought forward into view by using the Spectrum menu, in the Menu Bar.

To load a new spectrum, use the "Open" command under the File menu. This will present a standard file dialog box, allowing any file to be selected. Currently, *profit* can read OGIP standard spectrum files (often called "pha" or "pi" files), as well as properly-formatted ascii text files. We discuss each type of file here.

3.1.1 OGIP Spectral Files: .pha and .pi

These file formats were defined by Arnaud, George, and Tennant (1992), and are used extensively by the X-ray spectral analysis packages XSPEC and Sherpa[1]. In its most basic form, this spectral format contains only the number of counts in each detector channel. The energies or wavelengths associated with each channel are not listed. As a result, *profit* requires a second file known as the "response" file (usually ending in .rmf or .rsp) to be designated. This file contains the energy bounds ("EBOUNDS") for each channel. In some cases, the spectral file internally lists the appropriate response file, and in this case, *profit* will automatically read the response file.

An extension to the OGIP standard defined the "Type II PHA" file, allowing one file to contain multiple spectra. This format is the default for *Chandra* HETG and LETG grating data. When *profit* reads a Type II PHA file, it simply lists each of the spectra (by number) in the **Spectrum** menu bar. The user is then responsible for loading the appropriate response. In *Chandra* Type II files, the number of spectra depends upon the grating and detector system used, as well as how the data were processed. Table 3.1 shows the default association for the three standard grating/detector combinations, but the user should be warned that non-standard data reduction can change these.

[1]For more details see `http://heasarc.gsfc.nasa.gov/docs/heasarc/ofwg/docs/summary/ogip_92_007_summary.html`.

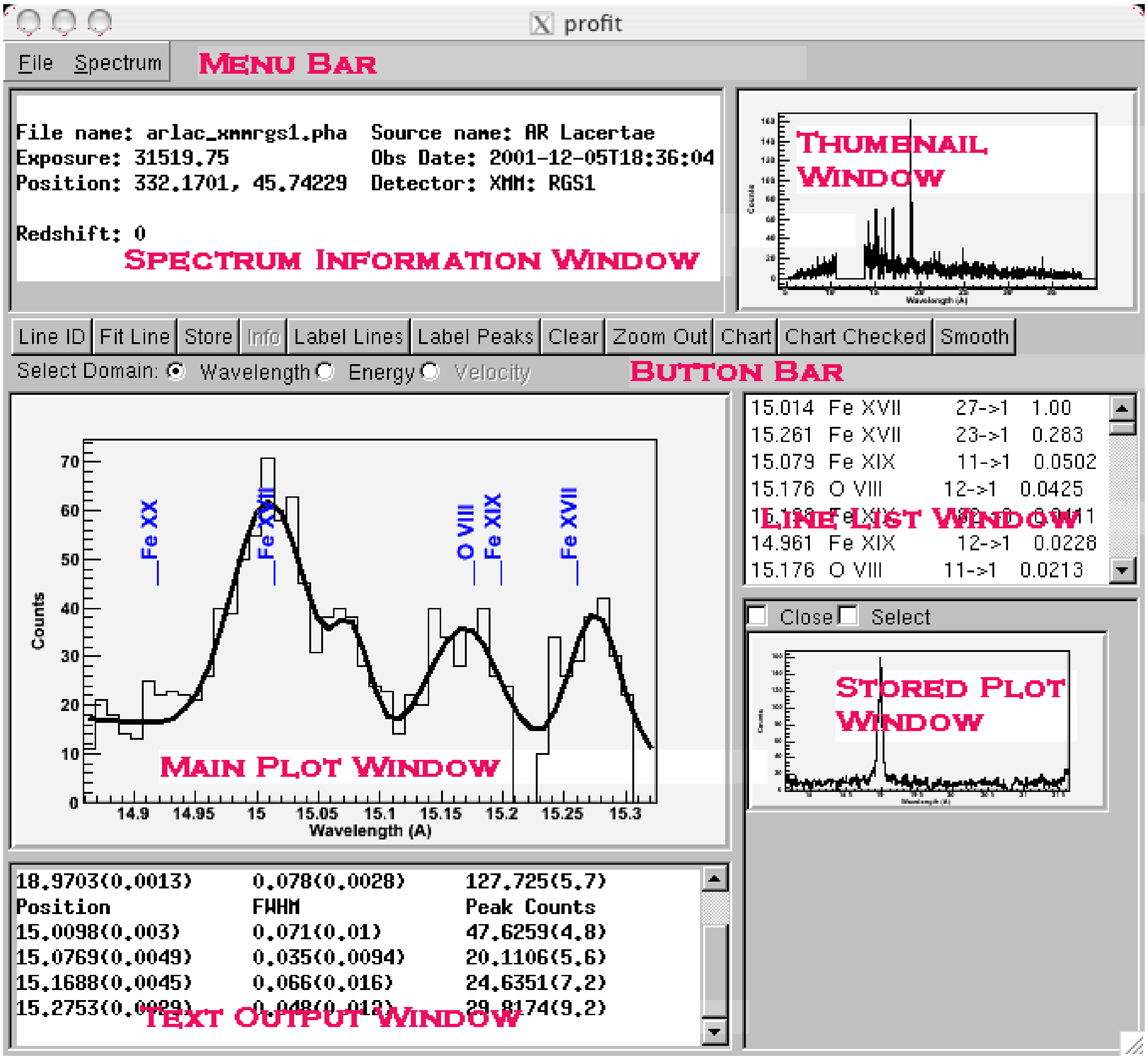

Figure 3.1: A sample *profit* session, showing an XMM RGS observation of AR Lac with the primary windows labelled in red.

We note that at the present time the *Chandra* archive does not include the response files; therefore, the user is expected to create specific response files for each dataset. As an alternative, generic grating response files can be downloaded from `http://asc.harvard.edu/caldb/prop_plan/grating/index.html`, although these may not be appropriate for grating observations done in non-standard modes.

3.1.2 Using ASCII text files

Profit can also read a simple text file which lists the energy and counts in a spectrum. In this case, some basic formatting is necessary for *profit* to understand the file. The first line of the file must be:

`FORMAT = profit`

and the second line should be

`TTYPE = E_MIN E_MAX COUNTS`

Table 3.1: *Chandra* grating Type II PHA datafiles and associated responses.

HETG/ACIS		**LETG/ACIS**		**LETG/HRC**	
#	Response	#	Response	#	Response
1,6	3rd order HEG	1,6	3rd order LEG	1,2	All orders LEG
2,5	2nd order HEG	2,5	2nd order LEG		
3,4	1st order HEG	3,4	1st order LEG		
7,12	3rd order MEG				
8,11	2nd order MEG				
9,10	1st order MEG				

if the file has three columns of data, listing both the minimum and maximum energies of each bin. Alternatively, this line should read
`TTYPE = E_MIN COUNTS`
if the data lists only the central energy and counts in each spectrum. At the moment, *profit* assumes the errors are Poissonian; we expect to include a facility for including errors in a future release.

Some additional "keywords" can be included, which *profit* will read and put into the Spectrum Information Window. For example, the following lines added at the beginning of a text file:

```
EXPOSURE=3600
DATE-OBS=2005-04-01T02:21:38
INSTRUMENT=B21LAB
GRATING=BRAGG
OBJECT=Run10583
! Note: Neon and Iron plasma run with T = 0.7 keV, n = 1e13 cm-3
```

will make *profit* list the exposure as 3600 seconds, the observation date as listed, the detector to be B21LAB:BRAGG, and the source name to be Run10583. Finally, comments can be included in the file if they are prefaced with an exclamation mark (!).

3.2 Manipulating Spectra

After a spectrum is loaded into *profit*, a thumbnail of the entire spectrum is placed in the Thumbnail Window (using the default units, wavelength or energy, as selected in the File→Preferences menu item), and it is also put into the Main Plot Window. At any time, the Main Plot Window can be reset to the plot shown in the Thumbnail Window by double-clicking on the Thumbnail plot.

Profit's most fundamental ability is to zoom into and around particular spectral regions. This is done by clicking in the Main Plot Window, either on the plot itself or its x-axis, with the left mouse button, and dragging (*i.e.*, holding the mouse button down) to the right until you have selected the region of interest. If you overshoot, simply reselect on the new region; if you undershoot, the "Zoom Out" button (on the "Button Bar") allows you to expand the selected region slightly. In some cases, *profit* will ignore a request to zoom into a very small selection, since it is difficult to determine the difference between a small selection and a random click of the mouse. In this case, simply select a larger subspectrum and then zoom in further from there.

Profit can also slide spectra back and forth at a constant zoom. To do this, simply hold down the right mouse button on the Main Plot Window and simply slide the mouse left and right; the spectrum view will slide along with the mouse.

The X-axis coordinates used to display plots defaults to wavelength (Å) units, but can be easily changed to energy (keV) units temporarily by using the Energy radio button. Clicking the energy button will simply transform the spectrum displayed in the Main Plot Window into energy units, and vice versa for wavelengths. A more permanent change (which will affect future spectra loaded into *profit*) can be effected from the File→Preferences window. To convert to velocity units, a line must be selected to use as the 0 point; see §3.3.4.

3.3 Identifying Features and Fitting

3.3.1 Line ID Button

The "Line ID" button fills the Line List Window with a list (based on the atomic database in use) of the lines or features in the selected range shown in the Main Plot Window. The list includes the line position (either in energy (keV) or wavelength (Å) units, depending upon the current display), the ion emitting the line, the energy levels involved, and an estimate of the line strength relative to the strongest line in the list. Currently, two databases are available, either the ATOMDB (`http://asc.harvard.edu/atomdb`) collisional plasma database or the XSTAR (`http://heasarc.gsfc.nasa.gov/docs/software/xstar/xstar.html`) photoionized database. The line emissivities are calculated by considering a range of either temperatures or densities and using the peak intensity. As a result, these intensity estimates can be misleading and should only be used as a rough guide when identifying lines.

3.3.2 Info Button

After selecting a line in the Line List Window, the "Info" button will become usable. After clicking "Info" *profit* will extract and display more information about the line (such as its oscillator strength and the atomic level descriptions of the transition) in the Text Output Window.

3.3.3 Label Lines, Label Peaks, and Clear Buttons

The Label Lines button overplots every line present in the displayed spectrum on the Main Plot Window. The default limiting flux is 10^{18} ph cm^3/s, but this can be changed to whatever limit the user prefers in the File→Preferences window.

The Label Peaks button first attempts to identify peaks in the observed spectrum, and then uses a simple algorithm that uses the location and estimated strength of the possible matching emission lines to label these features. It can fail if there are too many features (more than 50-100) present in a spectrum, in which case a message to this effect will be printed in the Text Output Window.

The Clear button will erase all labels from the plot.

3.3.4 Velocity Coordinates

Profit can calculate the velocity shift for a spectrum if told what atomic line to use for v=0. To switch into velocity space, generate a list of potential lines using the Line ID button, and then select a likely line from the Line List Window by clicking on it. At this point, the line should highlight, and the Info button and the Velocity radio buttons will also activate. Clicking on the Velocity button in the second line of the "Button Bar" will put the plot into velocity (km/s) coordinates with 0 km/s centered on the selected atomic line.

By default, switching to velocity plotting forces the spectral range to be -3000 to +3000 km/s. However, these values (-3000, +3000) can be changed to the users' specification in the File→Preferences window. In addition, if desired, the "forcing" effect itself can be eliminated, and the entire displayed spectrum simply transformed as it is with the energy and wavelength buttons.

3.4 Line fitting

One of *Profit*'s most powerful abilities is that it can "fit" a spectrum, automatically identifying and fitting features. We caution users that line fitting is a complex problem, which *profit* has only begun to address. Currently, *profit* attempts to fit the spectrum shown in the Main Plot Window using a straight line for the continuum and a series of Gaussians for line emission. The algorithm can be confused by a spectrum with many lines, a curved continuum, or simply a small number of counts in each bin. These problems are intrinsic to non-linear fitting and should not be considered "bugs" *per se*. However, the code works well when there are only a small number of well-separated lines with 20 or more counts and a flat continuum.

Due to the difficult nature of non-linear fitting and the many different combinations of machines and operating systems that can run *profit*, it is possible that *profit* will take a very long time to complete a fit, or even crash, if asked to fit a large region with many features, or one that cannot be easily fit with the simple *profit* model of a continuum plus Gaussians.

3.5 Other *profit* Features

3.5.1 Chart button

Clicking the Chart button creates an entirely new plot, consisting of the data and labels found in the Main Plot Window but "chopped" into (by default) 5 separate plots. This is entirely a convenience tool, allowing a dense spectrum with many identified features to be separated into smaller subplots for examination. This new plot can only be printed to a file; it is not "live," and cannot be manipulated with the mouse.

3.5.2 Storing and Restoring Plots

Profit can store plots in the main window into the Stored Plot Window. These plots can be brought back to the main window by double-clicking on them, or deleted by clicking the Close button above each plot (only one stored plot is shown in Figure 3.1). To create a single plot showing multiple stored plots, simply click the Select button for each desired plot and then click the Chart Checked button in the "Button Bar".

Stored plots can be restored at any time to the Main Plot Window by double-clicking on them.

3.5.3 Smooth button

Clicking on the Smooth button will do a simple smoothing based on the smoothing algorithm 353QH (Friedman, Proceedings of the 1974 CERN School of Computing, Norway, 11-24 August, 1974). This is similar but not identical to a tophat smoothing algorithm. We expect to improve upon this method in a future release.

Chapter 4

Planned Features and Known Issues

4.1 Known Bugs

Problem: A small spectral region is selected but fails to expand.

Workaround: Begin with a larger region and then refine your search from there. This is a ROOT issue.

Problem (OS X only): Double-clicking on profit.command fails to start *profit*.

Workaround: Check to make sure X11 is available and running before double-clicking profit.command. Also, do not install *profit* into a directory tree that has a space (ie, ' ') in the name. This will confuse the profit.command script.

Problem: The X and Y axis labels on "Chart" plots are too small to be read.

Workaround: None yet available.

Problem: After changing the redshift, the stored plots are changed as well

Workaround: At the moment, *profit* can only have one redshift per session, which is applied to all spectra immediately. If you need to have multiple redshifts for different objects, please use multiple *profit* sessions.

Problem: Pressing the "Clear" button does not remove the fit line.

Workaround: We are working improve the interface to allow either the fit line or the labels to be removed individually. At the moment, to remove a fit line simply double-click on the thumbnail and reselect the specific region.

Problem: Pressing "Smooth" repeatedly changes the line and continuum flux.

Workaround: We will be implementing a flux-conserving smooth; at the moment, please use "Smooth" as a visualization tool only.

Problem: At times, my stored plots lose their fit lines or show a different fit line than they should.

Workaround: We are trying to eliminate this bug. If you can find a way to cause this problem consistently, please let us know.

4.2 Planned Features

1. Use effective area file to present spectra in physical units.
2. Return total counts or flux instead of peak counts in line fits.
3. Allow variable abundances, rather than only Anders & Grevesse values.
4. Allow user-selected label colors, sizes, fonts.
5. Store results of fits to a latex file.
6. Allow plots to be output as QDP files.
7. Make the XSTAR database work more like the ATOMDB database, so that atomic data are available.
8. Allow a wider range of axis units, such as nm or inverse cm.
9. Include undo feature.
10. Improve fitting to allow more options.

Chapter 5

Frequently Asked Questions

5.1 General Questions

Q1: I've found a bug! How can I find out if you know about it already?

A1: We will attempt to list all known bugs (and workarounds) on the "Known Bugs" page of the *profit* website, `http://heasarc.gsfc.nasa.gov/docs/software/profit`. If you do not see your particular issue there, or are not certain it is the same problem as one listed, please let us know via the Feedback form. We will attempt to recreate the bug and advise you of what can be done.

Q2: I need a new feature! Whom should I tell?

A2: Again, please let us know via the Feedback form. Please remember that *profit* is not (yet) anyone's main priority, so clear explanations of your new feature request, especially including examples of how it should work and even how it might be implemented will be most appreciated. At the same time, most of *profit*'s new features are due to user requests, so please do not be shy!

Q3: I want to read in a text file for a spectrum, rather than a FITS file. Is this possible?

A3: Yes! Please see the explanation in §3.1.

Q4: Who is responsible for *profit*?

A4: Randall Smith and James Peachey are the responsible parties, with encouragement and assistance from a large cast of others.

Q5: Why do we have to submit requests through a "Feedback Form?" Why not give a direct email address?

A5: Two reasons: spam and archiving. The Feedback form method reduces spam significantly, and all emails sent there are archived for later reference.

5.2 Fitting

Q1: I tried to fit but got an error message "Fit did not converge" even though it's a simple spectral region.

A1: Basically, it wasn't simple enough. Please see the explanation in §3.4. The fitting algorithm currently used works especially poorly on low-count data or regions where the continuum is curved. Also, to avoid degeneracies, the maximum line width is 100 eV.

Q2: I tried to fit but got an error message saying there were too many peaks? Why can't *profit* fit more than 20 peaks at a time?

A2: This is an attempt to avoid *profit* crashing. Currently, on some machines, fitting large numbers of lines leads to core dumps. We have found that limiting the lines to be fit to 20 or less significantly reduces this possibility.

Q3: I tried to fit but *profit* crashed!

A3: As noted in A2 above and in §3.4, we are trying to address this problem but given the many different machines and operating systems that can run *profit* the issue is complex. To avoid this, we recommend that you don't try to fit large regions until we can address the issue definitivity. However, please let us know via the Feedback form on the *profit* website if you find a file and spectral region where you can force a core dump consistently; we are searching for examples to test fixes against.

Q4: I'd like to do fits that include the detector response (.rmf) and effective area files (.arf).

A4: May we recommend using either XSPEC (`http://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/`) or Sherpa (`http://asc.harvard.edu/sherpa/`), both packages that do this and far more. We are in close contact with the developers of both packages, and may include more features like this in the future. At the moment, however, *profit* should be used an exploratory tool.

5.3 Other Questions

Q1: Why did you choose ROOT and not package XYZ?

A1: ROOT has the features we need and is actively supported by the high-energy physics community. Although different in many ways, both astronomers and high-energy physicists both use histograms and spectra as one of their primary data classes, unlike, for example, computer scientists or GUI designers who include histograms in their libraries only for completeness. Finally, we were familiar with ROOT and could rapidly develop *profit* with it. However, we are not wedded to ROOT if a superior package is available.

Q2: What other atomic databases will you include?

A2: Plans are fluid on this. If you happen to know of an atomic database you would like to add, please let us know via the Feedback form.

Q3: How is *profit* different from XSPEC/Sherpa/ISIS?

A3: *Profit* is meant to be a GUI-based tool for exploring a spectrum, discovering what emission lines are present and if they show signs of doppler shift or broadening. XSPEC, Sherpa, and ISIS are primarily meant for fitting models to spectra. *Profit* is meant to complement, not replace, those tools.

Q4: How is the name pronounced? Pro'-fit or Prah'-fit?

A4: We accept either.