GUI Tools for an Enhanced User Experience

P.A. Kienzle

1National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

(Dated: October 31, 2002)

For instruments with many occasional users, it is important to have easy to use software. To support the frequent users it is important to be flexible. Using a scripting language to design a GUI and exposing it to the user allows us to do both. We present our work on a GUI for reflectometry data reduction and analysis written in Tcl/Tk and Octave, with underlying C code for the numerically intensive portions. As well as being easier to train new users, the new software allows existing users to do in minutes what used to take hours.

I. INTRODUCTION

Reflectivity data reduction and analysis at the NCNR has been a mix of various command line tools written in C and Fortran, often hidden behind scripts. Over the past year we have been reimplementing the functionality of these tools using a combination of Tcl/Tk1 and Octave2.

As we describe reflectometry data reduction and analysis there are a number of themes to keep in mind. Software should do the right thing most of the time. Software should allow you to do the wrong thing if necessary. Software should not be limited to just those features that are programmed in by hand. Users should be free to perform special calclations on their data without losing all the benefits of the GUI environment.

II. REFLECTOMETRY

A reflectometer consists of an incident beam, slits to control beam width and beam divergence, attenuators to control flux, the sample mount, and one or more detectors. Users can control the slits, the attenuators, the incident angle of the beam and the reflected angle to the detector. The slits are chosen such that the sample is fully illuminated throughout the entire range of angles. At very low angles the slits are fixed slightly open otherwise the beam intensity would go to zero.

After reducing the reflectometry data, the user is left with a reflectivity curve giving the proportion of reflected beam as a function of Q in reciprocal space. In practice, users want to be able to see both Q and angle theta throughout the reduction process.

There are four scans that are used to compute the final reflectivity, as determined by the incident and reflected angles. Keeping the reflected angle equal to the incident angle measures the specular reflection. Keeping the reflected angle slightly above or below the incident angle measures the off-specular reflection. Under the assumption of a perfectly flat sample, the off-specular reflection is considered to be background noise, and is to be subtracted from the specular reflection when producing the final reflectivity curve. The positive offset and a negative offset background scans are averaged before subtracting them from the specular scan. Keeping the incident and reflected angles at zero but gradually opening the slits measures the slit scan. This records the power of the incident beam which you need in order to normalize the final reflectivity curve.

There is also the rocking curve. Here the incident angle is fixed and the reflected angle is varied. If the peak does not occur when the reflected angle matches the incident angle, then the user knows that the sample is not mounted properly. The rocking curve will also give an indication of the validity of the assumption that the sample surface is perfectly flat. Using a set of detectors at different reflected angles rather than a single one, users can measure an entire rocking curve at a time. At present this is used to estimate the specular and background signals simultaneously so it makes more efficient use of the instrument. A topic of research is how to extract information about the surface of samples which are not uniform from the grid of rocking curves taken at various incident angles.

There are a variety of other measurements that are made, such as fixing slits and angles but varying temperature or field (or occasionally on NG7, the height of the sample). Our software can display these curves, but they do not enter into further reduction or analysis.

III. DATA SELECTION

Many raw data files are required to produce one reflectivity curve. Individual runs are used to cover different parts of the Q range due to things such as differing counting times, sampling densities or beam attenuation. With polarized beam, the data for each polarization state (A, B, C or D) is taken separately. In an extreme case (polarized data with positive and negative Q ranges each split into several runs) over 100 files may be required to produce a single reflectivity curve.

The attenuators are placed in the beam by hand, so each time an attenuator is changed, there will be another file created. Because the detector needs time to recover between events, we need attenuators whenever the rate of neutrons entering the detector is too high. This is mainly an issue for slit scans because then the detector is exposed directly to the beam.

The motor control program only allows motors to be
moved by fixed increments during a single run. At low angles the user has fixed slits, so low angle data must be in a separate run. Depending on what they are measuring, users will want to sample some parts of the reflectivity curve more densely than others. Each change in sampling density requires a new run.

The measurable reflectivity signal can change by seven orders of magnitude from below the critical angle where it is one, to high angles where it is indistinguishable from background. To get statistically significant counts throughout the entire range, different sections are measured for different times. Whenever the measurement time changes, a new run is needed.

One instrument has flippers to change the polarization state of the neutrons. A complete set of data consists of A,B,C,D files depending on which of the pair of flippers is activated. Sometimes reflectivity is measured through front and back surfaces, so each positive Q run will have a corresponding negative Q run.

For a variety of reasons the same Q range is often measured several times. Sometimes it is because the sample is dynamic. Users will reject the first few passes because the specular curve is still changing, but they will want to combine the remaining passes in the final reflectivity. Plus there are the usual problems that crop up during an experiment which cause some runs to be aborted or some ranges to be remeasured.

To make sorting through the data easier, our software automatically categorizes each file according to what it is trying to measure. This is easy for reflectometry because that information is completely determined by the motor movements as recorded in the data file. The data range is displayed along with the run number. This makes it easy to see which runs compose the entire Q-range of the curve without having to select the files or read from the log book. Double-clicking the first file in the Q-range automatically selects all files of the same type which extend the Q-range. Data taken with different flippers or different slits or at different temperature or different field are skipped. Users can add or remove files individually, and with a little extra effort they can force otherwise incompatible files to be selected together. An ongoing theme is to provide convenience without sacrificing flexibility.

Even as a tool for sorting data files without performing any reduction, experienced users have found our software to be worthwhile. Being special purpose software it knows how to plot reflectometry data and automatically normalize for things like monitor count. What you can do with a double click would take several minutes to do with command line tools. The result is that data reduction which used to take hours can now be done in minutes.

Even better, our software encourages users to examine the data at each step of the reduction process. In one case a subtle problem with the instrument controller lead to a small discrepancy in one of the scans. Because the data is visible at every step of the way the discrepancy was easy to spot. With command line and batch files, there isn’t a strong inclination to view the data every step of the way, and the discrepancy wasn’t noticed.

For novice users the software is a boon. Yes they benefit as much from the data browsing capabilities as the experienced users, but they also benefit from the consistency checks which restrict the data that can be selected together. Furthermore certain questionable data points such as those in which the data rate exceeds the known recovery time for the detector are automatically tagged for exclusion. While it may not be obvious to the user why the points are being excluded, it should be enough of a clue that they will ask a more experienced user what is going on. Better that than to quietly accept questionable data. Users can override the exclusion easily enough in keeping with the theme of convenience and correctness without sacrificing flexibility.

IV. DATA REDUCTION

Once the files are selected the data reduction process is fairly straight forward. A set of specular, background and slit scans are selected. Specular runs are averaged and the average background is subtracted. The result is divided by the slit scan and by the incident medium transmission coefficient if the beam is attenuated by the sample environment. If the data was taken with fixed slits at low Q, users need to apply a footprint correction to account for the fact that some of the beam spills over the edges of the sample.

There are of course complications. For example, the slit scan is based on slit configuration rather than angle so specular and background data need to carry slit information along with them so they can be normalized later on. That means the data saved in intermediate files must also record the slits associated with each data point. This complicates saving and reloading data files. There are also the same sorts of complications which arise with data selection: the software tries to ensure that the scans selected for reduction are consistent, allowing the user to override if necessary.

Again the GUI interface allows a novice user to easily learn the necessary steps for data reduction. The software can keep track of the state of the data reduction and warn if for example the user tries to do a footprint correction before selecting the slit scan which will normalize the data [this is work in progress].

V. DATA ANALYSIS

After the data has been reduced to a reflectivity curve, the next step is to try to find a density profile which gives rise to that profile. If you can change a property of the sample such as the fronting medium you can solve the inverse problem directly. Without additional constraints however, finding the density profile is an ill-posed problem since many different profiles can give rise to the profile you observe. The software tries to ensure that the scans selected for reduction are consistent, allowing the user to override if necessary.

After the data has been reduced to a reflectivity curve, the next step is to try to find a density profile which gives rise to that profile. If you can change a property of the sample such as the fronting medium you can solve the inverse problem directly. Without additional constraints however, finding the density profile is an ill-posed problem since many different profiles can give rise to the profile you observe. The software tries to ensure that the scans selected for reduction are consistent, allowing the user to override if necessary.

For novice users the software is a boon. Yes they benefit as much from the data browsing capabilities as the experienced users, but they also benefit from the consistency checks which restrict the data that can be selected together. Furthermore certain questionable data points such as those in which the data rate exceeds the known recovery time for the detector are automatically tagged for exclusion. While it may not be obvious to the user why the points are being excluded, it should be enough of a clue that they will ask a more experienced user what is going on. Better that than to quietly accept questionable data. Users can override the exclusion easily enough in keeping with the theme of convenience and correctness without sacrificing flexibility.
same reflectivity curve. This situation is exacerbated by a search space with many, many local minima and an expensive cost function (about one second per function evaluation for a profile of moderate complexity on my slow machine).

Some fitting tools are model independent in that they try to find a density profile which generates the reflectivity curve without making any assumptions about the shape of the profile other than an initial guess. Other fitting tools are model dependent in that they assume the sample is made up of particular layers of particular depths with particular diffusion across the layer boundary. The user then codes constraints among the parameters the software finds the best fit.

An example of the latter program is mlayer. This is the first analysis program for which we have provided a GUI interface. Unlike other model-based interfaces, ours lets the user directly manipulate the density profile. As they drag interfaces, roughnesses and scattering length densities, users are treated to automatic updates of the theoretical density curve overlaid on the reflectivity data which they are trying to fit. Users can also enter specific known values into a table of layers.

VI. TOOLS

The GUI interface we have been working on over the past year has been developed primarily in Tcl/Tk. Tcl is an excellent scripting environment in this case because it is simple to learn but still powerful. Because it is a popular language, there are a number of tools available for it. Usually, if you need some kind of interface widget it is a matter of finding one that somebody else has written rather than writing a new one for yourself.

One big piece missing from Tcl/Tk for scientific programming is that it does not deal well with vectors and matrices. There are some pure Tcl implementations of matrix operations but they are too slow. The BLT package provides vectors and some vector operations, but many operations are not available. Instead we use the Octave numerical environment as a compute engine. Again it is a simple language to learn, and again it is similar enough to Matlab that large number of tools are available for it. Usually, if you need to solve some kind of numerical problem it is a matter of finding a solution that someone else has written.

While not a full featured publication quality graph layout application, the graph widget we use (BLT) provides enough control to make an excellent data browser. Being tightly bound to the rest of our GUI allows us to implement certain conventions which we could not easily do with a separate graphing application such as switching from log to linear by clicking on the axis or displaying the point under the cursor as both Q and angle coordinates which are very useful in our application.

Because we are using a scripting language, we can open up a console which allows us to enter commands directly in that language, including commands for manipulating data that is shown on the screen. For example, certain specialized processing of the counts may be required to correct for an instrument error. These procedures only need to be applied to a few files (e.g., 3 months worth the runs) so it isn’t reasonable to expect support for the specialized processing to go into the general reflectivity reduction software. Instead they should be able to modify the affected files by hand (e.g., using a correction script) and continue processing the data using the usual gui interface.

Once the experiment is running smoothly, data is taken very regularly. In that case it should not be necessary to select all the data by hand for reduction, but instead be able to write a script which reduces all the data, showing a few key steps along the way so that the user can be sure that the data is reasonable. If it is not, the user should be able to take corrective action using the usual user interface then continue with the script. The script should also allow the user to perform steps that cannot be automated, such as selecting the linear part of the fitted slit region used to fit the footprint correction. In this way, processing data sets can be reduced from minutes to seconds. Even more importantly, instrument responsibles can set up automated procedures for their users to follow for particular kinds of experiments. If all goes well, they should then be able to process their data with little hassle or detailed knowledge of the usual sequence of steps required.

Providing a scriptable interface is a medium term goal for the project. We have not yet formalized the underlying data manipulation in a way that makes this convenient. An issue with all GUI programming, no matter what the language is that it is by nature anathema to modular programming. Because the user is free to wander backward and forward through the process, it is difficult to implement the procedural aspects of the interface. For example, footprint correction requires that the user fit a curve to the flat portion of the onset of the background subtracted, slit scan divided data. However, changing the background runs may change the position of the flat portion of the onset, so the footprint that the user specified is no longer applicable. So somehow selecting new background data has to signal that the footprint correction used elsewhere in the program is now invalid and should be ignored. This two way flow of information is very disruptive.

In my experience Tcl/Tk facilitates hiding the interconnections better than most. Individual widgets can take a variable name as a parameter rather than the current variable value. They then put a trace on the variable so that the widget is notified when the value is read, written or deleted. Using techniques like this, we should be able to make the GUI independent of the scripting language, so that new gui elements can be added without updating the existing gui elements or the scripting interface.

Again, because it is a scripting environment it is rel-
atively easy to support extensions to the environment. As the project has grown from supporting one data format (NG-1) to four (NG-1, NG-7, X-RAY, NG-7 with position sensitive detector), it has become necessary to modularize the file loading process. Adding support for a new file type now consists of writing two functions, one to quickly load the header so that the file can be categorized, the data range displayed, and constraints applied to the selection process, and another to load the data and do initial conversions to Q vs intensity. There is also some code to associate file extensions with the file categorization function which needs to be changed in several places, so further refactoring is necessary. Also, as different instruments have different capabilities and limitations, some aspects of the reduction process will need to change elsewhere in the program.

VII. CONCLUSIONS

While not yet complete, our data reduction and analysis tools lead to a marked increase in productivity. So much so that even long time users with dozens of specialized scripts for data reduction are happy to convert to using them. Through careful design we have managed to provide convenience and flexibility in the same package.

While a concern throughout the development, modern PC’s are able to handle the performance penalty of running scripted applications. The user interface is adequate even on a relatively old pentium II, 300Mz computer. In the case of mlayers, the GUI is bound by the cost of generating the reflectivity curve for the layers so I would not anticipate a significantly enhanced user experience if the whole interface were translated into C.

Tcl/Tk plus Octave has proven itself to be a fine platform for rapid development of scientific applications. Interface ideas can be tested quickly and the more promising ones can be developed more fully without too much overhead. This allowed us to experiment with a number of different interfaces in less time than we would take to produce a single interface in C.

1. Tcl Developer Xchange http://www.tcl.tk
2. Octave home page, http://www.octave.org
3. J. F. Ankner and C. F. Majkrzak, Subsurface profile refinement for neutron specular reflectivity Neutron Optical Devices and Appl. 1738, 260 (1992).
4. N. F. Berk and C. F. Majkrzak, Using Parametric B Splines to Fit Specular Reflectivities Phys. Rev. B 51, 11296 (1995).
5. C. F. Majkrzak and N. F. Berk, Exact Determination of the Phase in Neutron Reflectometry by Variation of the Surrounding Media Phys. Rev. B 58, 15416 (1998).