Modernizing the ESRF beamline software architecture with generic Python modules

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Introduction

This article describes the new application software architecture on the ESRF beamlines. It will show its basic elements and comment on the level of their advancement.

The work has been mainly done in the BLISS group (Beamline Instrument Software Support) and by CSS (Certified Scientific Software) for the Spec Server. The list of contributors to this project include G. Berruyer, A. Gobbo, L. Claustre, T. Jouve, J. Klora, E. Papillon, N. Pascal, V. Rey, A. Sole, D. Spruce, and G. Swislow.

The global beamline control software structure

The beamline software architecture at the ESRF is built around the commercial data acquisition package SPEC. SPEC talks to our hardware mainly via the ESRF TACO device servers. The device servers can either be specific to one type of device or just represent the hardware channel to talk to a device (i.e., a serial line). For a small number of device types (i.e., stepper motors) which represent however the majority of hardware items used on the beamlines (i.e., we have about 3000 motors on our beamline) the code to talk to these devices has been added to SPECs internal codebase. For the rest of devices the access is done via SPECs macro language. The end user does normally not see a difference between these methods.

The data display routines in SPEC are not sufficient for our beamlines. We have therefore decided to add external data visualization tools (i.e., for CCD cameras). The communication between the different programs is done using shared memory with specific header informations.

GUI user interface are put on top of SPEC. In the past we were using a program which mixed the standard user input from the keyboard with the input from the GUIs. SPEC sent information back to this program via a
dedicated pipe. Multiple GUIs can be used at the same time. The information sent has been distributed to the GUIs in some type of event.

Two types of such GUIs have been used at the ESRF. There is a general SPEC GUI written in Motif which had a built in editor for graphical panels. The relatively simple panels were used to gather information to start SPEC macros. No programming had to be done in the GUI. There exists also a GUI written in Tcl/Tk dedicated to Protein crystallography experiments. This GUI contains much more dedicated logic but will also in the end send commands to SPEC to carry out the experiments. It will however do many things in addition (i.e. add information to a central data base).

The new building blocks

The modernization of the control system keeps the general structure described in the last paragraph. Individual components are replaced with modules and applications written in Python. We can therefore distinguish the following areas:

- The external program which mixes keyboard input and the GUI communication to SPEC has been replaced by a new server mode in SPEC. When started in server mode, SPEC listens to requests from clients and sends events to them. We have a Python client library which provides access to SPEC with an object oriented interface.

- A plotting framework (PyDVT) has been created. The framework defines classes in the following areas:
  - visualization (like 2D images or contour plots)
  - data sources (like input from a file or from SPECs shared memory)
  - user selections (like cuts)
  - filters (like fitting routines or color selectors)

  It makes it then possible to define the data flow between them.

- Applications for visualization have been created from this framework. They work either standalone with data from files or integrated in the online data visualization with data from SPEC shared memory. Examples of these applications are given later.

- A new configuration editor has been created. This editor can be freely configured. It integrates the functionality of SPECs config editor and our own in-house configuration tools.

- A general GUI framework application has been started in Python. The application allows to load Python classes and integrate them into the running system. There is an built in editor to create simpler panels interactively without any programming.

Why Python

Our choice for Python was relatively simple to make. We wanted a scripting language which can be easily used by the scientists on the beamline. Python can be extended with modules in Python or other languages (i.e. C). The language is very compact, easy to read, and offers an enormous amount of built-in functionality. It is largely platform independent. You can read more on www.python.org.

Unluckily the choice of the toolkit for Python was less obvious. We started using the most widely used toolkit Tk (coming from Tcl/Tk). We did have to program many standard widgets for our projects and the final programs didn’t have the "look and feel" we wanted. We decided therefore to try Qt with Python bindings (www.trolltech.com) and are very happy with the functionality. Python/Qt is however not very widely used. We tried therefore to be as independent of the graphical toolkit as possible in the basic classes.
The Spec Server

SPEC when started in server mode accepts connections on a socket. Multiple clients can connect and send messages. Clients can execute commands, talk to motor or counter objects in the server, read variables (i.e. global variables or motor parameters) from the server, and be automatically informed about changes of these variables. Events can be sent from SPEC to the clients.

The SPEC server does execute one macro at a time. It will queue macro executions if the macro unit is currently occupied. This restriction is the easiest way to avoid uncontrolled mixing of experimental procedures. There are three points why this restriction is not very important for practical purposes.

1. Not many incoming requests will lead to the execution of a macro. For example, it is possible to ask the value of a global variable while a scan macro is executing.

2. The event nature of the communication leads to a reduction in the client server traffic. The client is automatically informed when something interesting for him changes (i.e. a motor stops).

3. The level of commands. The client tells the server for example to start a movement but will then be free to do other things. A graphical user interface can start a movement on a motor, start later another movement of another motors and all that while the server is counting on a detector.

The SPEC server and client can be started and stopped independently and will reconnect automatically. There currently exists a Python client library and other SPEC versions can be used as clients too. It is for example possible to configure a motor in a client SPEC version to refer to a motor in a SPEC server. One client can talk to multiple servers.

The development of the SPEC server mode has been accompanied by a new method of writing pseudo motors and counters. Only these pseudo motors will be fully functional in server mode. The new method consists of calling predefined macro code from SPECs built in C code.

The plotting framework

PyDVT is a framework for visualization tools. It defines different objects and the data flow through them. The data flows from the "source" to the graphical "view" window. On its way it passes through "filters". There are special selection classes to select which data to take from the source and also selection classes which refer to the graphical selection done by the user with the mouse.

view The views can be 2D display, contour plots, normal 1D plots, radial plots, 3D plot, data tables, or mesh plots. The underlying graphics kit is PLPLOT to which we added user interaction. Online display of fast 2D detectors requires a level of performance we could not get in this way. We therefore used a specifically written library in C and a pixmap widget for the 2D display.

source For the moment the data can come from either files or SPEC shared memory. The source also includes a trigger mechanism when the data has been updated. The user of the tool kit does not have to be concerned with the update of the plot in this way.

filters It is relatively easy to insert filters into the data-flow. There are filter fit-routines which take input from the data source and result in the fitted curve (which can then be displayed in a view possibly together with the raw data)

The toolkit is independent of the GUI toolkit. We currently use bindings for Qt and Tk.

Visualization Applications

General graphical applications have been created with the Python toolkit. Examples of these applications are:

PyMCA PyMCA is an application to work with spectra from multi channel analyzers. It can read the spectra from SPEC files or SPEC shared memory and display them. One can calibrate the spectra in user units (normally energy). Peak search and fitting are integrated.
PyDis PyDis takes two dimensional data from files or SPEC shared memory and displays it in different ways. The application can be extended with plug-ins. A poster presented at the workshop shows an example of PyDis extended for data analysis.

NewPlot Displays online or offline SPEC data from scans. Allows fitting of the data and all the common view operations.

The applications are finished but still need some validating before we can use them on our beamlines on a large scale.

A Configuration Editor

A common problem on our beamlines is the complexity of the configuration of its components. To add a device to the system we often have to add information in many different places. We decided therefore to create a configuration editor which could be easily adapted to input all the necessary information. It will replace the SPEC configuration editor and ESRF specific tools for configuration at our beamlines. It is also planned to use the editor in the NICOS control program of the Munich FRM II beamlines.

It consists of two parts:

1. A description editor which creates files which defines all the possible items to configure. It allows to create "properties" (i.e. the motor parameter "velocity", or the unit). Every property has a type and a default value. One can then define the properties of the objects in the system (i.e. that all motor objects have a "velocity" property).

2. A configuration editor which will use the information from the description editor to create the above objects and configure their properties. The editor allows to create groups (i.e. diffractometer or monochromator), enable and disable parts of the configuration, and generally assists the user during the configuration.

The program is in the final development phase. We still need to provide output filters to save the final configuration in the standard ("old") file formats (i.e. SPEC config file).
The general GUI framework

The general GUI framework is an attempt to integrate different standard graphical components with beamline specific parts. Starting from an empty application the individual elements are loaded interactively. This configuration is then saved. The general concept is born out of the experience from our generic SPEC GUI and specific GUI applications (i.e. ProDC for the protein crystallography beamlines). Both approaches had their advantages and disadvantages. While the specific interface pleased which its rich functionality we have to invest a lot of time to maintain it. We want to combine complicated graphical standard components with beamline specific panels. The framework consists therefore of two parts:

1. A wizard to load in Python classes into the application. These classes need to be Qt or Tk Widgets (both at the same time don’t work well at the moment). There is an optional mechanism to communicate with other classes with an “eventhandler” (classes can send and receive events).

A special type of classes is the placer type class. These “placers” once loaded into the applications accept other classes inside their window in a predefined way (a up/down placer might accept two windows it will place either in the upper or lower half of its window).

The wizard will therefore go through the following steps:

- ask a filename and make the user select a Python class
- ask the user where to put it on the screen (either in its own window or inside another one)
- ask additional parameters and create and instance

2. An integrated editor for simple panels with simple graphical elements like input widgets, buttons, frames, labels, and so on. These panels will display information from SPEC and send commands to SPEC.

This project is in its final stage but needs some more work.

FAQ

Why not build a scripting language on top of standard graphical components? We need to provide fast (sometimes in hours) a 90% solution. Our highest priority is to make an experiment possible however inconvenient. We will later try to automate certain steps and only later add a graphical interface for convenience.

Why not build a system where Python talks directly to the device servers? Apart from the obvious reason that SPEC had been more or less our only option when we started, there is a very import basic philosophy behind this decision - “Configure - don’t program”. SPEC allows us to hide all the different server implementations behind a standard layer. It allows us to adapt the system to the different experimental stations. Writing a specific application for an experimental station is relatively simple - but it is extremely difficult to maintain these type of programs. This approach becomes also inefficient with the large number of experimental stations as at the ESRF.

Conclusion

Python has been proven an excellent tool. It allows to quickly develop complex programs and helps to collaborate in the our group. On the down side we see that the installation of the finished software takes more effort and regret the absence of a powerful standard GUI toolkit. Our overall opinion stays however very positive.

The new concept is finished but some building blocks still need some more work. News about our progress will be available on [http://www.esrf.fr/computing/bliss/bliss.html](http://www.esrf.fr/computing/bliss/bliss.html).