

Is there life after SPEC ?





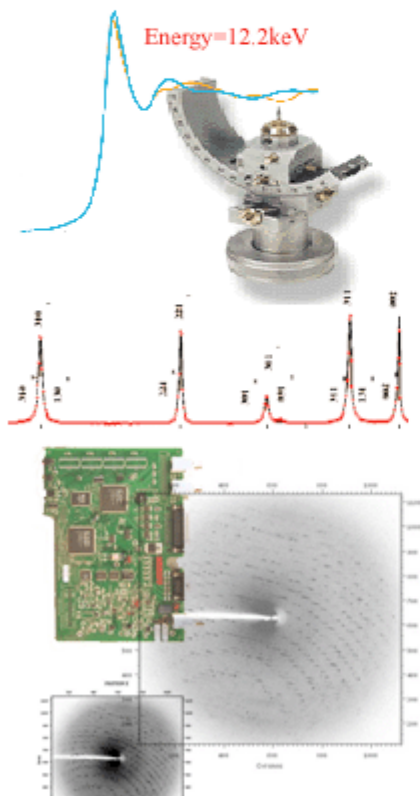
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... Meeting the software needs of scientists since 1985 ...

Welcome



Certified Scientific Software's **spec** X-Ray Diffraction and Data Acquisition software provides scientists with reliable instrument control at more than [550 X-ray and neutron diffractometers at over 200 locations worldwide](#).

Developed in 1986 for X-ray diffraction, **spec**'s portability, flexibility and power have made it a valuable data acquisition tool in a wide range of experiments. **spec** is available on UNIX/Linux platforms and supports numerous hardware configurations.

spec's [features and functionality](#) reflect years of input from a broad user base. Unlike typical home-grown or public-domain software, **spec** is well-documented and backed by committed

What is SPEC ?

spec

```

Current Positions (user, dial)
Motor 0
  m0
100.0000
100.0000

147.SPEC> ascan m0 1 100 10 1
Total 11 points, 11 seconds

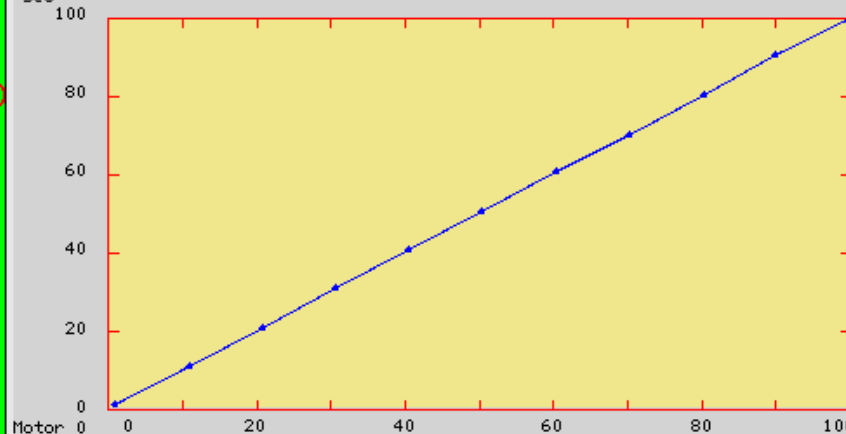
Scan 2  Fri May 28 00:15:54 2010
ascan  m0 1 100 10 1

#  Motor 0  Seconds  Seconds
0  1.0000    1         1
1  10.9000   1         1
2  20.8000   1         1
3  30.7000   1         1
4  40.6000   1         1
5  50.5000   1         1
6  60.4000   1         1
7  70.3000   1         1
8  80.2000   1         1
9  90.1000   1         1
10 100.0000  1         1

148.SPEC> 
```

spec 1

: Peak at 100 is 100. COM at 69.908.
FWHM is 50 at 50.



Motor 0	Scan 2 sec
0	0
10	10
20	20
30	30
40	40
50	50
60	60
70	70
80	80
90	90
100	100

What is SPEC ?

- A sequencer from CSS used mainly at synchrotrons with :
 - Reciprocal space calculator for diffractometer geometries
 - Support for lots of hardware drivers
 - Support for 0D, 1D and 2D detectors
 - A basic scan plotting package
 - Supports simple calculations on data
 - A macro language
 - A server mode
- Well known to synchrotron scientists
- Used on hundreds of beamlines for thousands of experiments

Why replace SPEC ?

- Despite the fact that SPEC has been used to do all experiments at the ESRF since 20 years it has some drawbacks :
 - the SPEC macro language is too limited in term of data structures, flow control and programming language features
 - SPEC doesn't offer multitasking abilities
 - SPEC has no centralized configuration
 - SPEC has no symbolic debugger
 - SPEC is not (easily) extensible
- The EDF data format used to store acquired data doesn't fit our needs anymore
- Online data visualization tools (while data acquisition is going on) need to be improved

SPEC++ Evaluation

- All SPEC++ potential solutions will be evaluated by interfacing them to the following TANGO devices
 - SimMotor, SimCcd, SimMca, SimCounterTimer, SimSampleController, SerialLine, Gpib
- The following scans have to be executed :
 - 0d : counter timer
 - 1d : one variable (motor, temperature, time...) + one or several counters/detector (0d, 1d and 2d)
 - 2d : two variables (motor, temperature, time...) + one or several counters/detectors (0d, 1d and 2d)

SPEC++ at the ESRF

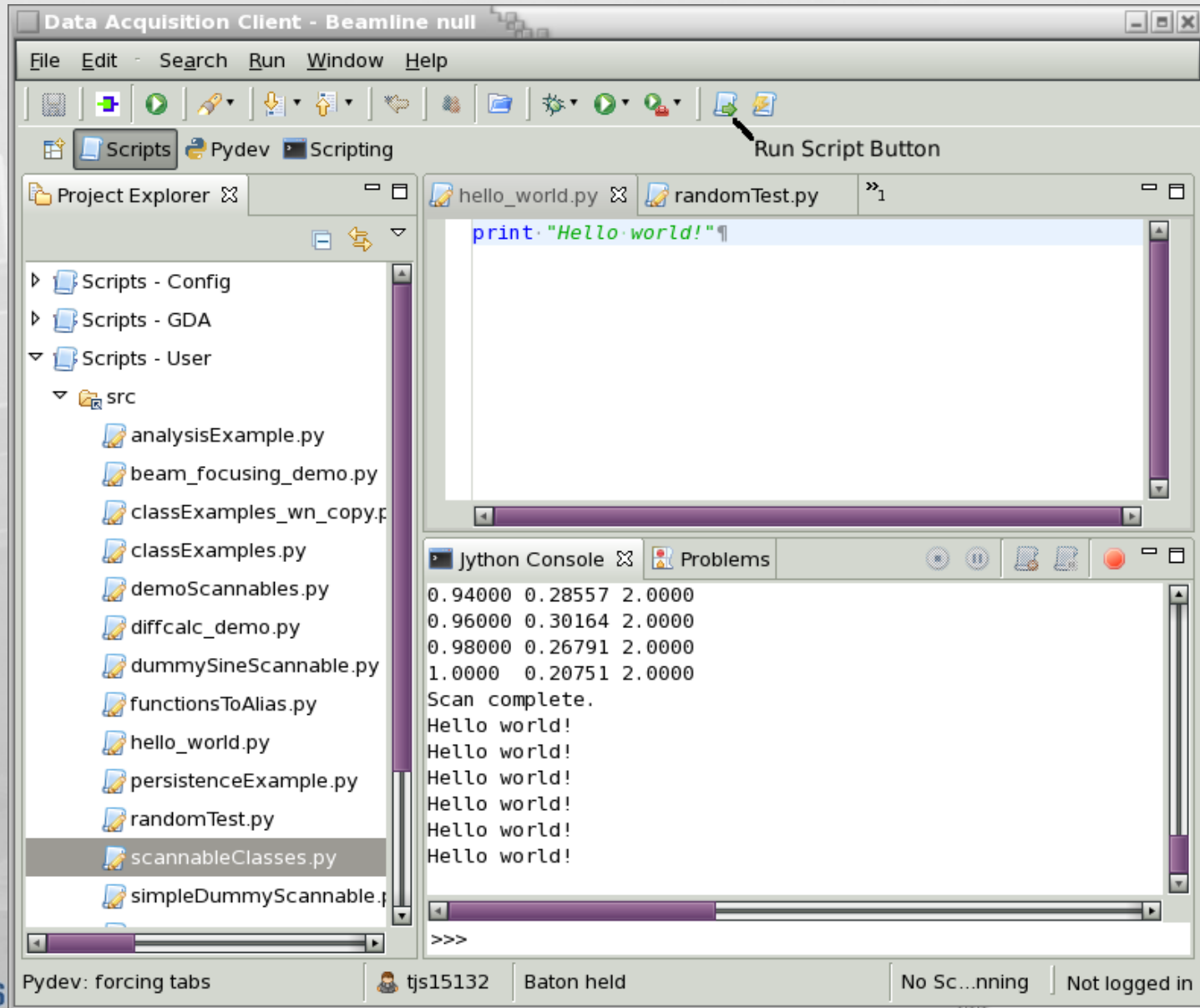
- Requirements + Specifications
 - We have produced a document as part of ESRFUP-WP10
 - ESRF will organise a workshop in 2010
- Evaluating
 - Sardana : an integrated solution from ALBA
 - Khoros : an proposal based on the KIS principle
 - GDA : an integrated solution from DIAMOND
- NO Decision yet

An Integrated Solution

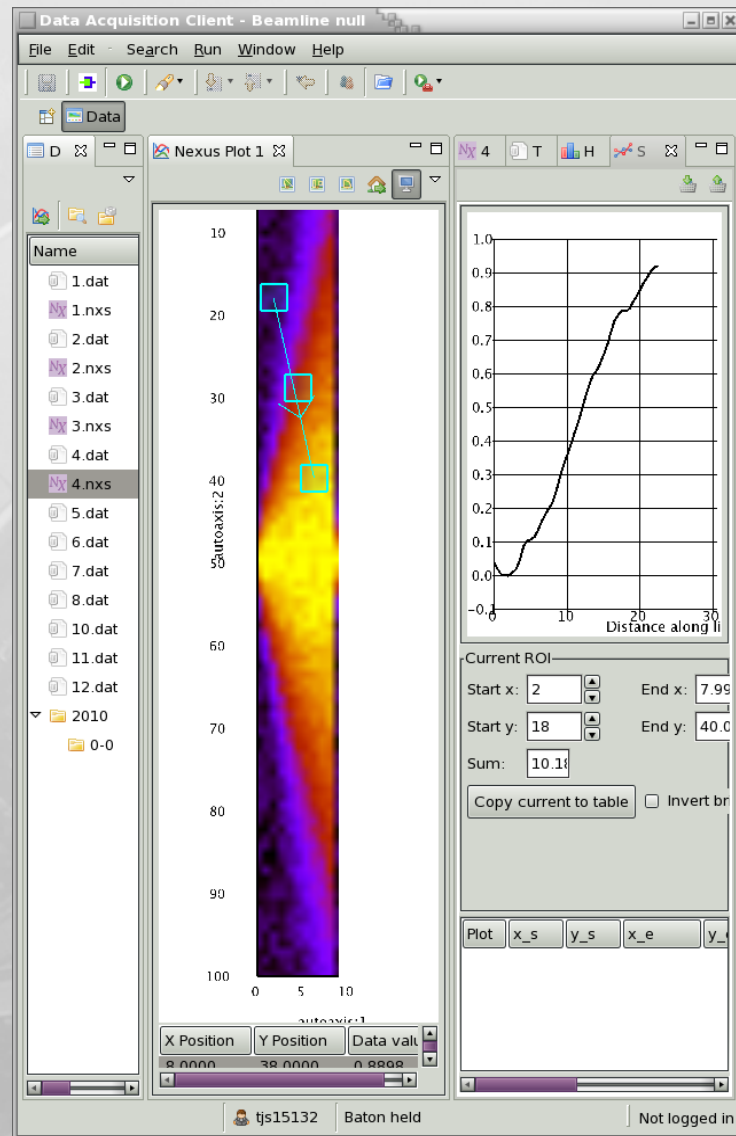
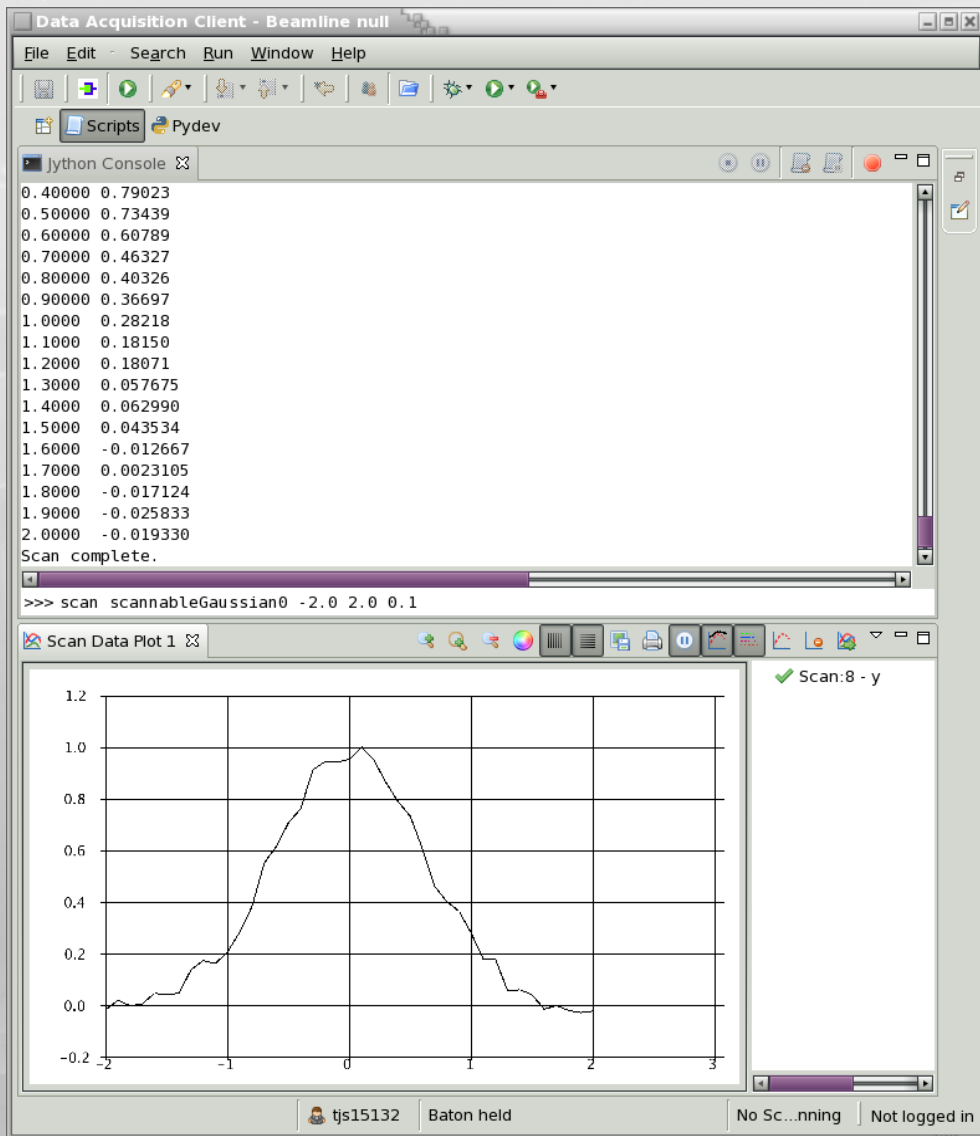
- We do not only need a Sequencer to replace SPEC but also :
 - Hardware control not part of the Sequencer
 - A Configuration Manager and Editor
 - A Data Manager for managing the data + metadata
 - An Experiment database for archiving experiments database
 - Online Data Analysis to steer the experiment
 - A link to the Offline Data Analysis tools
 - All of this in a well documented Integrated Environment
 - Under Open Source Licence free for the user to take home

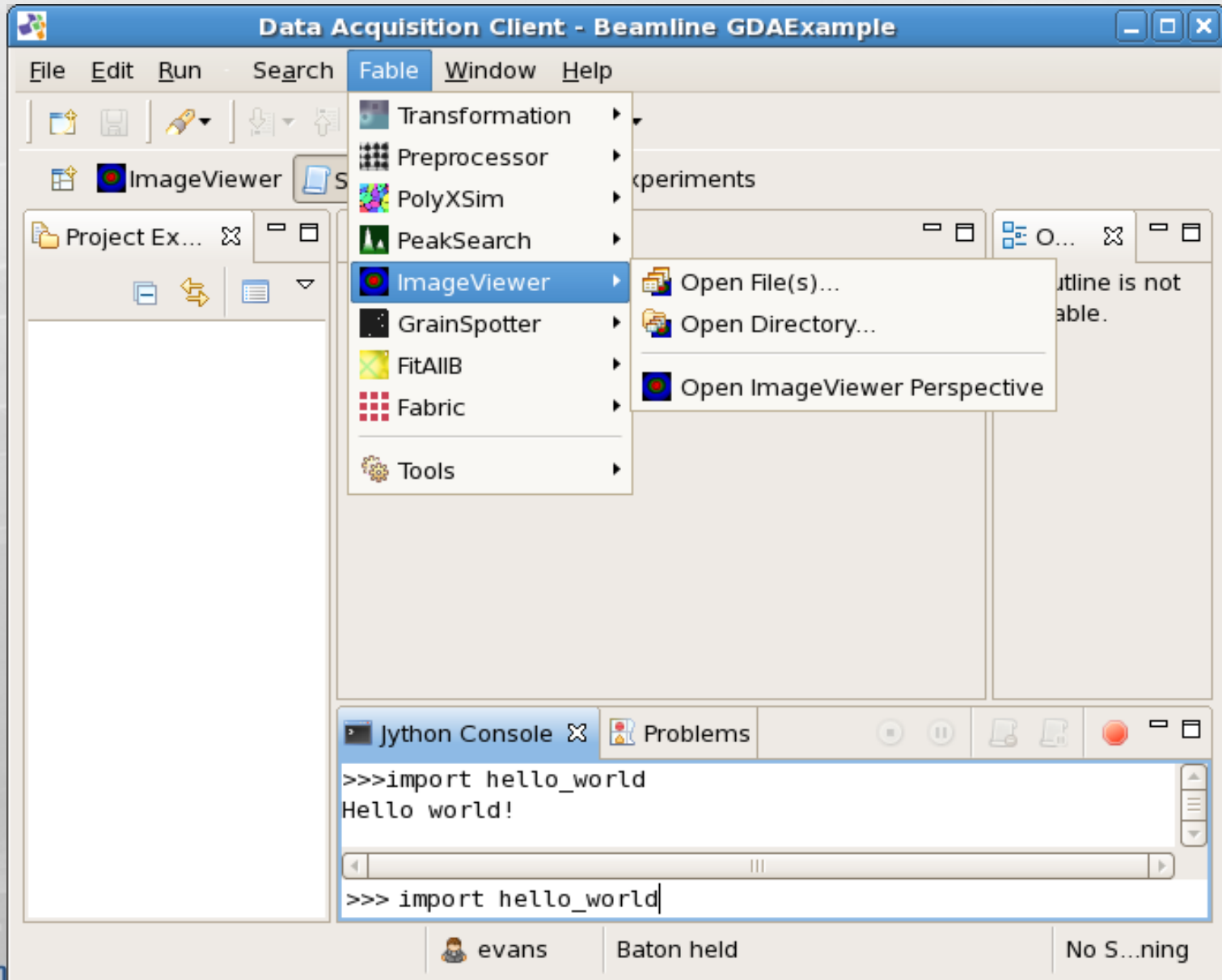
Why GDA ?

- GDA is an integrated Data Acquisition Solution from DIAMOND
- It is based on :
 - Eclipse/RCP + Jython sequencer + Object Server + Nexus + Data Visualisation + Online Data Analysis
 - It is a working solution (already used on almost 20 beamlines)
 - It is Open Source, free and well documented
- Advantages :
 - A Big collaboration at a higher level than TANGO and EPICS
 - Opens the door to solving higher level problems e.g. data analysis
- Disadvantages :
 - I am alone to think GDA is a good solution !



The screenshot shows the 'Data Acquisition Client - Beamline null' application window. The interface includes a menu bar (File, Edit, Search, Run, Window, Help), a toolbar with various icons, and a 'Run Script Button' (a green play icon) which is highlighted with an arrow. Below the toolbar is a 'Scripts' tab with a 'Pydev' sub-tab. The 'Project Explorer' on the left shows a tree structure with folders for 'Scripts - Config', 'Scripts - GDA', and 'Scripts - User', and a sub-folder 'src' containing several Python files, including 'hello_world.py' and 'randomTest.py'. The main editor area shows the content of 'hello_world.py', which contains the code `print("Hello world!")`. Below the editor is a 'Jython Console' window showing the output of the script: a table of numerical data followed by the text 'Scan complete.' and five instances of 'Hello world!'. The status bar at the bottom indicates 'Pydev: forcing tabs', the user 'tjs15132', 'Baton held', 'No Sc...nning', and 'Not logged in'.





Data Acquisition Client - Beamline GDAExample

File Edit Run Search **Fable** Window Help

- Transformation
- Preprocessor
- PolyXSim
- PeakSearch
- ImageViewer**
 - Open File(s)...
 - Open Directory...
 - Open ImageViewer Perspective
- GrainSpotter
- FitAIB
- Fabric
- Tools

Jython Console Problems

```
>>>import hello_world
Hello world!
>>> import hello_world|
```

evans Baton held No S...ning

The IDEAL solution ?

- A MODULAR Solution
- Modules :
 - Hardware Control
 - Sequencer
 - Data Manager
 - Data Visualisation
 - Experiment Database
 - Online Data Analysis
 - Command Line Interface
 - Unified Graphical Interface
- Agree to collaborate on at least ONE module

Session programme

- Sardana+Tau – Tiago Couthino
- Khoros – Matias Guijarro
- Soleil CLI – Alain Buteau / Majid Ounsy
- View from DESY – Thorsten Krachts
- Heated Discussion
- Agreement ;-)