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Ultranet: High speed data acquisition software for time-resolved spectroscopy

Contact greg.greetham@stfc.ac.uk

G. M. Greetham, D. A. Robinson, M. Towrie and M. Pollard
Central Laser Facility, STFC, Rutherford Appleton Laboratory, HSIC, Didcot, Oxfordshire, OX11 0QX, UK

M. Kogimtzis
Technology Department, STFC, Daresbury Laboratory, DSIC, Warrington, Cheshire WA4 4AD, UK

Introduction

Major facility developments require significant parallel software developments. Ultranet is a new program written in LabVIEW 8.6 (National Instruments) to control instrumentation, data acquisition (DAQ) and data processing in the facility development Ultra[1].

Ultra aims to increase the range of experiments available to the user community, in terms of more laser wavelength and spectroscopy technique combinations. Scaling of the facility requires attention to how new equipment is brought together, so that the laboratory remains accessible to user groups and experimental parameters are reproducible. DAQ in the Ultra laboratory is a computing challenge as the high repetition rate laser is combined with wide detector arrays. Processing the data real-time rather than taking a simple time average has significant advantages which improve sensitivity of the instrument.

Device control

The Ultra facility makes spectroscopic measurements over a range of conditions such as varying laser wavelengths and time delays[1]. Controls for various scanning devices are shown within tabs on the graphical user interface (GUI), labeled "Delay line", "TOPAS", "Rotator" and "Stanford", in fig. 1. Most of the devices discussed here are provided with LabVIEW drivers to enable fast setup of communication.

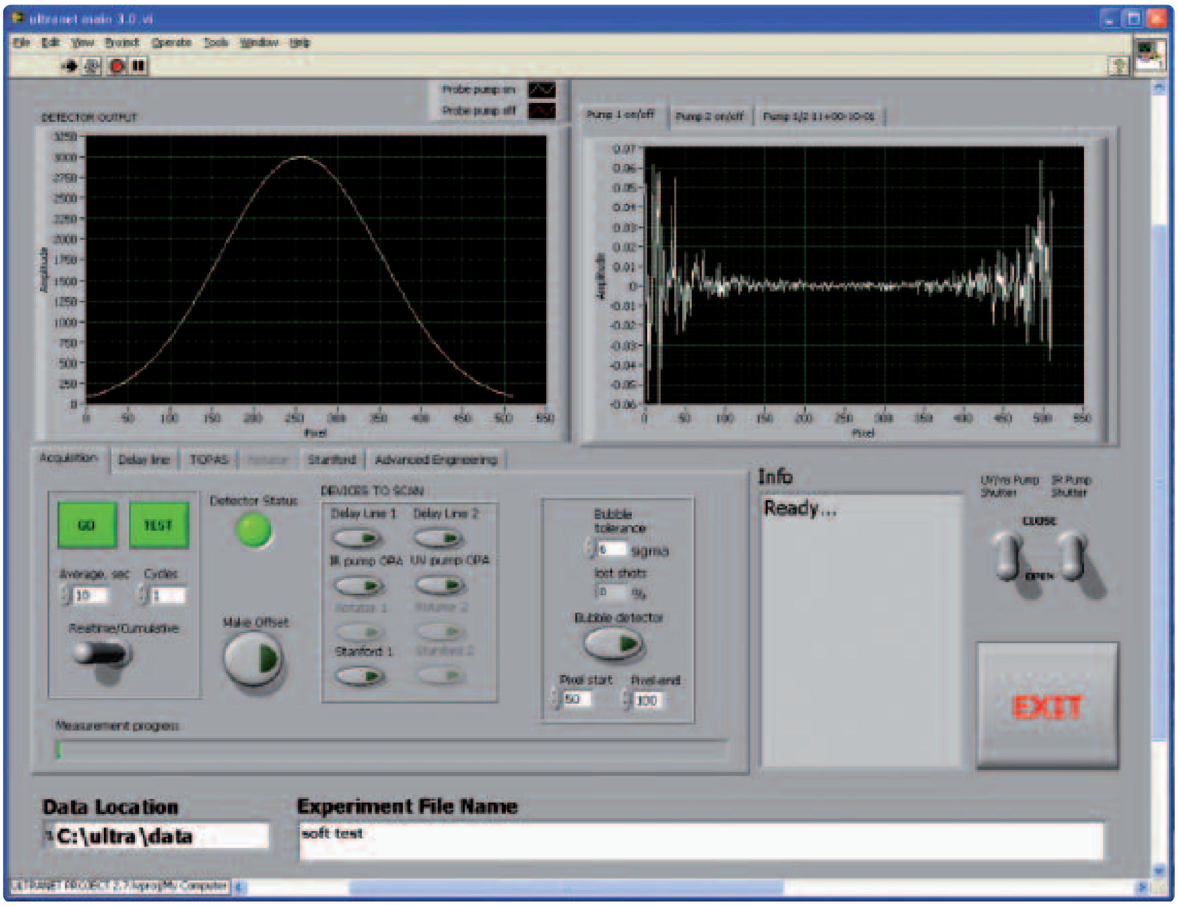

Figure 1. Front panel of Ultranet program. Results displayed in graph windows, with a refresh rate of 4 times per second. Device controls laid out in tabs on front panel.

A single motion controller (XPS, Newport) is used to control two translation and two rotation stages via Ethernet. Two micron-precision translation stages are used to control timing of two laser pulses arriving at the samples (hence "Delay lines") and two rotation stages can be used to control their polarization when fitted with polarization rotating optics. The delays and polarizations can be adjusted within the respective tabs and during an experimental acquisition they can follow a user defined scan automatically.

The wavelength of the lasers is controlled by optical parametric amplifiers (OPAs) (TOPAS, Light Conversion). Several OPAs can be computer controlled via a single RS-232 serial communication. Similar to the delay lines, these devices can be operated remotely to set the laser wavelengths and scan automatically.

Data acquisition and processing

Due to the intensive DAQ and processing requirements in the experiment, this part of the program is multithreaded by LabVIEW into the following categories; a) DAQ, b) data sorting, c) data processing, d) data archiving. A quad core computer allows each of these to be processed by an allocated processor. As the Windows operating system (OS) may occasionally interfere in the speed of DAQ and processing, the program must be set to high priority in the OS and large (20 MB) data buffers must be set to ensure no data is lost between processing threads to avoid loss of data.

(a) Acquiring and processing data in real-time has significant advantages in improving signal to noise levels, see below. Detector array systems (Quantum Detectors) with 16 bit, 512 element, <20 kHz data acquisition systems developed by STFC's Technology Department allow single shot measurements of the sample probe spectra. When acquiring at 10 kHz, the detectors send > 10 MB/s of data via UDP data transfer to the DAQ computer. UDP has an advantage over TCP data transfer in that is does not provide any data delivery handshaking, and thus provides a faster data throughput. This means the speed of the data transfer is maximized in UDP, although large receiving buffers must be set on the DAQ computer (~ 20 MB) to ensure no data is lost.

(b) Sorting of the data is done to ensure the data flow is coherent, i.e. each reference spectrum corresponds to the correct probe spectrum and each pump on measurement is compared with the correct pump off neighbor.

(c) By recording simultaneous reference spectra with the spectra of the laser passing through the sample allows one to normalize the shot-to-shot laser intensity and spectral fluctuations [2]. These fluctuations are a major source of noise in these measurements, as high as 5 % RMS shot-to-shot. The use of referencing can reduce these variations to <1 %. Secondly, the Ultra system uses a pump modulation technique, whereby probe spectra are collected at 10 kHz, with the photo-induced reaction being modulated by chopping the pump laser at 5 kHz [2]. The difference between the pump on and pump off spectra show the small changes in the sample due to the photo-induced reaction in question. Real-time pump modulation is a form of frequency filtering, i.e. the experiment and its respective background are taken within 100 µs of each other, so there is little change in conditions due to laboratory noise (e.g. vibrations and electrical noise <1 kHz). Adding a second pump, increases complexity, but the technique is still applicable, by chopping the second pump at 2.5 kHz. Absorption changes induced by the pump(s) are calculated in the equations below.

1 pump:

$$\Delta A_N = \log[1 + I_R/I_P[((I_{probe}/I_{ref})_{pump\ on} - (I_{probe}/I_{ref})_{pump\ off})] + \Delta A_{N-1}\,(N-1))/N$$

2 pump:

$$\Delta A_N = \log[1 + I_R/I_P[((I_{probe}/I_{ref})_{pump1\ on\ pump2\ on} + (I_{probe}/I_{ref})_{pump1\ off\ pump2\ off} - (I_{probe}/I_{ref})_{pump1\ on\ pump2\ off} - (I_{probe}/I_{ref})_{pump1\ off\ pump2\ on})] + \Delta A_{N-1}\,(N-1))/N$$

I_R and I_P are the final averages of the pump off spectra on the reference and probe side respectively, and N is the total number of acquisitions. Additional discrimination (labeled "Bubble Detector" on the GUI) can be applied to remove large fluctuations in the signal caused by unusually large variations such as those associated with gas bubbles in the sample flow stream, on a shot by shot basis.

(d) Typically, the real-time calculated difference spectra are averaged over several seconds to obtain a single high signal to noise data set. However, it is also desirable to archive every single shot of the data. This archiving is of potential benefit in developing new data processing (noise filtering) techniques for the future and diagnosing any noise sources on the data through Fourier transform methods.

Summary

Ultranet is a new program for acquiring pump-probe spectra in the Ultra laboratory. The LabVIEW based system allows simple GUI device control and graphical spectra output displays, while simultaneously applying high speed multi-threaded DAQ and data processing techniques within the Windows OS.

References

1. Application of ULTRA to 2D-IR, G. M. Greetham, I. P. Clark, M. Towrie, M. W. George, A. W. Parker, P. S. Codd, R. C. Farrow, P. Matousek, Z. J. Xin, CLF Annual Report, (2008-2009).
2. M. Towrie, D. C. Grills, J. Dyer, J. A. Weinstein, P. Matousek,http://apps.isiknowledge.com/DaisyOneClickSearch.do?product=WOS&search_mode=DaisyOneClickSearch&db_id=&SID=V29M2GjaNN8FJ8MEhII&name=Matousek P&ut=000184358300002&pos=5 R. Barton, P. D. Bailey, N. Subramaniam, W. M. Kwok, C. S. Ma, D. Phillips, A. W. Parker and M. W. George, *Applied Spectroscopy*, **57**, 367, (2003).