HORIBA Scientific

Technical Note

Raman

SO-TN04

Raman Customization and Automation with LabSpec 6

HORIBA Scientific's LabSpec 6 software platform offers virtually every possible function for data acquisition, processing and display that a typical spectroscopist will require. This includes acquiring multidimensional spectral arrays, ranging from simple 1D time profiles, through to 3D XYZ confocal volumes, and beyond. However, despite these comprehensive capabilities we acknowledge that sometimes users want to do things in their own way.

LabSpec 6 includes three modules which make complete customization and automation of a user's Raman experiment a reality. The recordable Methods module allows routine multi-step tasks to be stored and recalled at will; visual basic scripting (VBS) allows complete customization and automation of almost every possible LabSpec function via user scripting; and finally the ActiveX module allows LabSpec 6's functionality to be called remotely from third party software.

Methods

The Methods module provides a simple and intuitive 'mouse click recording' facility for data acquisition and processing functions. This allows a user to very simply create a customized stack of operations (the Method) and subsequently run the operations sequentially with one click. At any time the method can be saved, re-opened, edited and run as desired by the user.

A typical example of using the Methods module is for automatic survey analysis of a new sample with multiple lasers and multiple gratings. A method can be created to acquire six spectra with high and low spectral resolution measurements using green, red, and infra-red lasers. When the method is run, the six spectra will be acquired automatically and presented on screen; the user can then evaluate results and judge the best combination for further analysis. The method could easily be extended to include batch processing of the data – perhaps to baseline and normalize each spectrum, for easier comparison. This just requires two additional operations within the Method.

Creating such a method is easy – see Figure 1. The Methods tab in LabSpec 6 has an intuitive interface – click the [Record] button to start recording mouse clicks. Any software button compatible with methods (which includes virtually all data acquisition and processing functions) displays a clear indicator with a mouse hover.

Click on the button, and that operation is added to the Method.

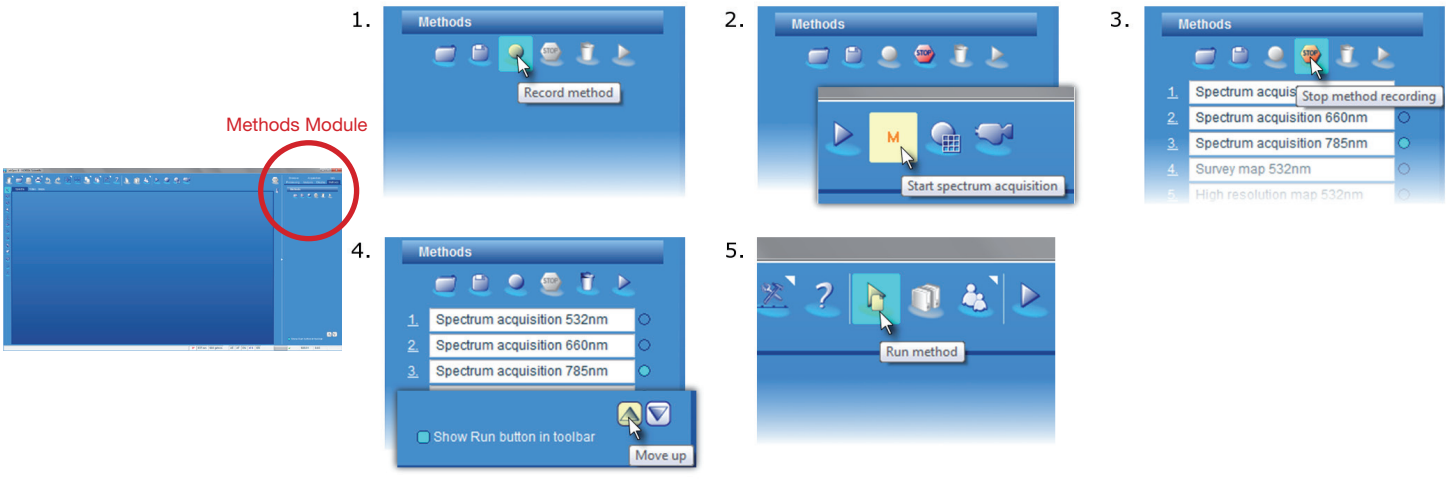

Figure 1: Creating and running a method, step-by-step.

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Operations in the Method can be reorganised, to adjust their position in the final operation sequence; and of course they can be deleted, and new operations inserted if needed.

Other uses of the Methods module include automated sequential survey and detailed mapping of a sample (with large and small step size respectively), and acquisition of data to compare results with different hardware settings (such as laser wavelength, confocal depth resolution, spectral resolution etc). In multi-user environments, Methods is an ideal way for 'expert' users to create complex data acquisition and processing routines which can be used at the touch of the button by less experienced operators.

Visual Basic Scripting (VBS)

Visual Basic Scripting (VBS) is an active scripting language, designed as a lightweight programming tool within the Microsoft® environment. Within LabSpec 6 it can be used to create customized scripts which access nearly all functions available to a standard user within the interface – in combination with the standard VBS commands and functions it offers a real programming capability directly within LabSpec 6. In essence, VBS provides automation to a level beyond the Methods module, described above – it does however require a degree of background knowledge and understanding in VBS, so is not suitable for all users.
The library of LabSpec 6 objects for VBS include functions to set parameters/values within the interface (i.e., to set up measurement conditions), and acquire, process and display data. In addition, the native VBS functions such as logical decisions, looping, waiting etc, allow scripts to be generated which can encompass complete experiment protocols, with feedback of results and adjustment of parameters through the experimental process.
One potential drawback of VBS is speed – scripts are traditionally slow to run. In LabSpec 6 this does not present a problem. The script is used to set up processes, but the actual process is then carried out using LabSpec 6's native, high end compiled software modules. Thus, even time dependent functions such as detector read out, motor movement, and ultra-fast mapping can all be reliably controlled with VBS.

To open up access to VBS for less experienced users, and to speed up scripting for experienced programmers, LabSpec 6 includes a library of script "building blocks". These are pre-written functions which can be called and inserted into a user script very quickly using LabSpec's fully integrated script editor. This module acts as an ideal tutor in scripting for beginners, since they have at immediate disposal fully functioning script examples to start working with. For more experienced programmers, these "building blocks" will ensure ultra-fast programming. Users can even create new "building blocks" from their own code, allowing them to build up a library of their own code for future use.

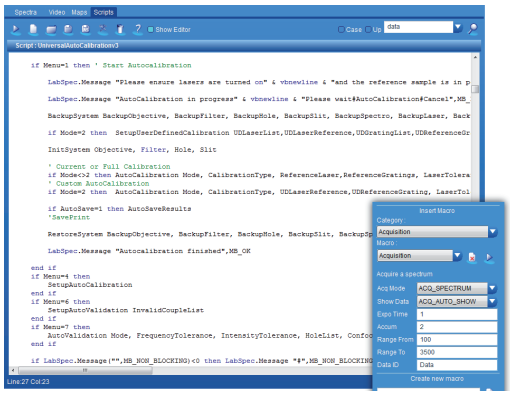

Figure 2: LabSpec 6's embedded VBS script editor and (inset) set up window for a code "building block".

ActiveX Remote Control

ActiveX offers a framework for re-using software components in a manner which is independent of the original programming-language. Relating to LabSpec 6, it allows the core functionality of LabSpec 6 to be integrated into third party software, including its hardware control, data acquisition and data processing capabilities.
Uses of ActiveX can vary, from basic examples such as allowing native LabSpec 6 data files to be directly imported by third party software, through to more complex scenarios such as lab automation projects. In the latter case, HORIBA Scientific's Raman instrument may be just one of a number of instruments being used. In such cases it is typical for the end-user (or external contractor) to write an all-encompassing automation software, which will control all necessary robot handling, data acquisition, decision making and feedback. LabSpec 6's ActiveX components allow the HORIBA Raman system to be fully controlled via the automation software – the programmer needs no in-depth knowledge of LabSpec 6 or its programming language. Knowledge in ActiveX, coupled with full documentation on specific LabSpec 6 ActiveX components, allows fast and complete programming that can exploit the full capabilities of LabSpec 6 and HORIBA's cutting edge Raman systems.

Summary

LabSpec 6 is a powerful spectroscopic software suite, for data acquisition, processing and display. Its approach to customization and automation allows it to be easily molded to specific requirements…whether by simple automation of standard spectroscopic routines via Methods, or near unlimited programming capability using visual basic scripting and ActiveX. It is a software which can easily adapt to the varying needs of analysts and researchers alike, whatever their demands.

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