LabSpec 5 (LS 5)
Notation

- Names of icons and menu items are denoted in **bold**.
- Names of windows are denoted in *italic*.
- Names of columns, rows or entries in a window are denoted in all **CAPITAL**.
Configuration Utility
Versatility

• We provide a wide range of Raman microscope/spectrometer instruments (analytical, research, processing, etc.), which require various configurations to meet the need of the applications specified by customers.

• While we can optimize the system to yield the best results in the target application, the service (maintaining existing systems, adding accessories, upgrading obsolete parts, etc.) could become a daunting task.

• The design goal of LabSpec 5 is to provide a platform that can adapt and control dynamically changing configurations without having to replace the software.

• The task is accomplished mainly through Config utility, where the specific configuration of the instrument is specified.
Accessing Config

- Double clicking **Config** icon opens the *Config Login* window, the operator can access the configuration of the LabSpec 5 in three levels.
  - **No password**: Clicking **OK** button with no password will prompt a message box that informs that changing configuration will be disabled. Clicking **OK** button of the message box opens the *Config* window in read-only format.
Config

- Each element comes with a list menu, from which the specific component and its configurations can be defined.
- Module option is where customized options are listed. When activated, corresponding icons or controls will become available in LabSpec 5 main window.
Overview
Main Window

File I/O

Experiment setup
Data acquisition

Axes and Cursors

Data Information

Data processing

Switch lasers

Neutral density filter

Confocal hole diameter

Spectrometer

Grating/Objective

Exposure time

Laser block/unblock

Slit width
Video Acquisition

Video
Continuously capture and display the video image. Both camera and lamp can be polarized.
Video

Menu options available for Video
Spectrum RTD (Real Time Display)

Spectrum RTD
Continuous capture and display the spectrum at the current spectrometer position

Spectrometer position
The spectral range is defined by the size of the CCD, laser wavelength and grating

RTD exposure time is set separately from the Data Acquisition exposure time
Spectrum

Menu options available for Spectrum
Spectrum Acquisition

Extended Range Acquisition
Setup the spectral range(s) for the Spectrum Acquisition

Spectrum Acquisition
Acquire a single spectrum

Exposure time and number of accumulation
When there are more than one spectrum in the memory, the operator can switch the display between them from here with the color coded radio buttons.
Map Acquisition

Interactive menu options to setup (lateral) map.
Map Acquisition

Mapping Properties
Setup the map and/or batch acquisition
Map Acquisition

Acquire a series of spectra as setup in **Mapping Properties** and **Extended Range Acquisition**.
Map

Max/min spectral intensity across the entire data set

Video image overlaid with the integrated intensity maps

Spectrum at the current cursor position in the Video or Map

Integrated intensity maps defined by three pairs of cursors (color coded)
Maintenance
Spectral Axis Calibration

- X-axis (spectral axis) of a Raman microscope is calculated using the full trigonometric relationship involving the included spectrometer angle.
- When the instrument is well aligned, there is a linear relationship between the spectrometer parameters and the spectral axis coordinates.
- The slope (KOEFF) and intercept (ZERO) of this linear relationship can be ‘tweaked’ to adapt to the daily fluctuation of the environment (e.g. temperature).
- The best practice is to keep record of changes made to these parameters.
- Please contact HORIBA Jobin Yvon if a significant drift in spectral axis is suspected or observed.
Spectral Axis Calibration

1. Place Si reference target on the sample stage
2. Change the X-axis unit to nm by selecting Options / Unit / nm
3. Set Spectrometer to Zero Order
4. Check zero position (laser line) using Spectral Real Time Display
5. If the laser line position is off zero, select Setup / Instrument Calibration and adjust the value for ZERO. Make sure to check zero position after every adjustments by repeating steps 3 and 4.
6. Change the X-axis unit back to 1/cm by selecting Options / Unit / 1/cm
7. Set Spectrometer to 520 cm⁻¹, where Si line should appear.
8. Check Si line position using Spectral Real Time Display
9. If the laser line position is off 520, select Setup / Instrument Calibration and adjust the value for KOEFF. Make sure to check line position after every adjustments by repeating steps 7 and 8.
Spectral Axis Calibration

- To ensure the linearity over the full spectral range, the procedure in the previous page can be repeated with different spectrometer position.
- From the step 7, set the spectrometer to 600, 700, etc., and repeat the rest of the steps.
- Sharp and strong peaks from other samples of well known spectra can be used as well. (e.g. Aspirin, Chloroform)
Data Acquisition
Video Acquisition – Real Time

- Video
  - Continuously capture and display the video image

- Both light source (white lamp) and detector (camera) can be polarized

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Video

Menu options available for Video
Transmission Light
Pyroxine

Parallel polarization

Cross polarization

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Reflection Light

Parallel polarization

Cross polarization
Extended Video Acquisition

- Requires a motorized xy-stage.
- Select NGSExtendedVideo.dll in Config to activate, which adds an additional icon to the LS 5 tool bar.
- Selecting the icon opens the Extended Video window for setting up the extended video acquisition.
Extended Images

- Extending the field of view by patching multiple images together.
- This is **NOT** a real time image.
Move to the Cursor Position

- Requires a motorized xy-stage.
- Select NGSMouseTable.dll in Config to activate, which adds additional icons to the left tool bar of Video
- When the Target is selected, a bulls-eye appears on the video image, which defines the current center.
- Clicking on a new location in the image moves the bulls-eye and the stage moves automatically to center at the new position.
Spectrum Acquisition – Real Time

- **Acquisition / RTD**
  - There are two Real Time Display (RTD) modes
  - Selecting **Acquisition / RTD** menu opens RTD window
  - Image binning X and Image binning Y apply to **Detector Image RTD**.
    - Number of pixels specified here are added and read out as one pixel.
    - Increasing number of binning speeds up the read-out process.
  - Readout zone applies to both **Detector Image RTD** and **Spectrum RTD**.
    - There are three Readout zone modes: **Spectrum**, **Image** and **Full**
    - **Spectrum** and **Image** are defined in **Acquisition / Detector** and window
      the detector read-out regions
    - Usually, Readout zone is set to **Spectrum**
  - When selected, Accumulate image takes the number of accumulations (set in the bottom tool bar) into account.
  - (RTD) Exposure time can be modified here as well as in the bottom tool bar.
- **RTD** is triggered on by clicking Icons on the LS 5 tool bar.
Spectrum Acquisition - Options

- **Acquisition / Options**
  - Exposure time and Accumulation number can be set here as well as in the bottom tool bar
  - The name of the spectrum (or the data set) is set to **Data name** and a increasing integer suffix by default
  - Refresh time: Refresh the data measurement in progress at the set interval
  - Binning factor: Read out the set number of pixels as one. Increasing binning factor lowers the spectral resolution while increasing the signal.
  - Accumulation mode: Average, Sum, Detector
  - Spike filter: None, Multi (auto add), Multi, Single
  - Autofocus: Off, Before acquisition, Before each point
  - Scanning: Stage (point mapping mode), Scanner (line scanning mode).
  - Use detector : Active detector, Both
  - Signal mode : Signal, Signal-Dark
Extended Range Acquisition

- Selecting Acquisition / Extended Range menu or Extended Range icon opens Extended Range window.
- Select Auto-overlap and Combine Data options to use CREST (Continuous Rapid Extended Scanning Technology) to measure the spectrum.
- Spectrum acquisition is started by clicking Spectrum Acquisition.
Map Acquisition

• Setting up the surface map
  – Icons to define mapping properties appear on the left tool bar when the Video window is selected.
    • Each icon represents a map of a different shape.
    • Selecting an icon overlays the selected shape on top of the video image (pink dots).
    • The size of the map is adjusted by clicking and dragging with the mouse.
Map Acquisition

• Setting up the surface map
  – **Mapping properties** icon opens *Mapping properties* window
  • Array Size and Increment must be defined here.
Map Acquisition – Other Parameters

- **Mapping properties** window provide the place to set up parameters other than x and/or y scanning.
  - Depth profile is performed by employing the parameter Z
  - Other variables such as slit width and confocal hole diameters can be set to scan over a range at an increment.
  - Right clicking on the parameter list activates context menu. Select **Insert** to open **Device** window. Select variables to scan. (e.g. SLIT, HOLE)
Map Acquisition – Other Parameters

• Priorities of the variables
  – The order of the variables sets their priority during the mapping. The bottom parameter has higher priority, the top parameter has lower priority.
  – When set as below, the measurements will be made along x-axis at a constant y position before moving to a new y position to repeat the process.
  – To change the order of variables, right click on the variable name to activate the context menu. Use Remove, Up, Down menus to change the list and order of variables.
Map Acquisition – Options

• Increment
  – When the INCREMENT box is checked, the measurements are performed at the set increment.
  – When the INCREMENT box is not checked, measurements are performed at the increment calculated from FROM, TO and ARRAY SIZE.

• Relative
  – When the RELATIVE box is checked, then the current position of the image is the (0,0,0) position of the map table.
  – When the RELATIVE box is not checked, then the (0,0,0) position of the image is the (0,0,0) position of the map table.
Map Acquisition – Options

• Extra Images
  – **Acquisition / Extra images**
  – When the autofocus is activated, extra images like the Reflection (on the autofocus detector) and the Z position (after each autofocusing) are available.
  – These are recorded
    • At the same time as the Raman mapping if you select MAP
    • Without recording any spectrum if you select IMAGE and click on IMAGE.
    • If you use IMAGE then you only obtain a topographic picture of the sample and the variation of reflectivity over the surface of the sample.
Data Treatment
Basic Data Treatment

- Baseline correction
- Spectral normalization and correction
- Smoothing
- Fourier transform
- Math
- Peak searching and fitting
- Profile from image

Math → Peak searching and fitting → Profile from image

Fourier transform → Spectral normalization and correction → Baseline Correction

Smoothing
Baseline Correction

Build the baseline by adding points at the cursor position

Remove the points defining the baseline

Build the baseline automatically and subtract from the current spectrum

Build the baseline automatically but NO subtraction

Copy the baseline

Paste the baseline to an other spectrum
Spectral Normalization and Correction

- **Normalize:** Normalizes all traces to same area value (100).
- **Zero:** Moves all traces to the minimum intensity level.
- **Get:** Takes the activated spectrum and put it in Corrector frame. This data object will be used as parameter.
- **Delete:** Removes the Corrector spectrum.
- **Subtract:** Subtracts the Corrector spectrum from all traces.
- **Multiply:** Multiplies the trace on the Corrector spectrum.
- **Correct:** Subtracts the Corrector spectrum from all traces. The intensity of the Corrector is multiplied to fit the intensity of the trace.
- **Thr:** Removes all trace with maximum intensity less than threshold value (in % to maximum data intensity).
Spectral Normalization and Correction

LIMITS: Check the box if you want that only a part of the trace is used for operation. This parameter is used for Normalize and Correct operation.

FROM and TO: Edit these fields to modify the limits of the selected region (linked to the red vertical cursors).
Smoothing

- Savitsky-Golay smoothing.
- First derivative
- Second derivative
- Median filter smoothing
Fourier Transform

- This is another smoothing tool
- When a spectrum is Fourier transformed, the low frequency data (spectral features) and high frequency data (noise) are separated.
- Therefore, eliminating high frequency region in the Fourier transform domain removes high frequency noise.
  - Fourier transform the spectrum
  - Cut off high frequency region
  - Reverse Fourier transform to spectrum
Fourier Transform

- LIMIT: Position of the cut off point in %. This parameter defines the smoothing factor.
  - 0: Fully smoothed,
  - 100: No smoothing.
- Click on the Go button to apply the value or drag the pointer to select the LIMIT visually.
- APOD: Type of the apodization function with apodization value reaching zero at a Limit point.
- FILTER: Select here the type of the filter function

None: No filter function
Traffic: Traffic function

None: No apodization function
Line: Linear function
Sqr: Parabolic function
Cos: Cosine function
**Math**

- **FUNC 1 and FUNC 2**: Basic math functions (+, -, *, /, ^), negating, power, log, exp, sin, cos, asin, acos, atan, abs, sqrt, step.
- **Go**: Perform the operation
- **x**: denotes the active object
- **y**: denotes other objects of the active window
- **a, b, c, d……..**: values of the axes for each data point (next slide)

Combine data objects into a single object
If we apply the formula ‘x+2*a’ to a **spectrum**, x is the intensity and a the Raman at each point.

**Before operation**

<table>
<thead>
<tr>
<th>Raman shift</th>
<th>100</th>
<th>200</th>
<th>300</th>
<th>...</th>
<th>a</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intensity</td>
<td>200</td>
<td>250</td>
<td>500</td>
<td>...</td>
<td>x</td>
</tr>
</tbody>
</table>

**After operation**

| Intensity values | 20000 | 50000 | 150000 | ... |

If we apply the formula ‘x+b-a’ to a **image**, x is the intensity, a is the x distance and b is the y distance.

**Before operation**

<table>
<thead>
<tr>
<th></th>
<th>10</th>
<th>20</th>
<th>30</th>
<th>...</th>
<th>a</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>40</td>
<td>500</td>
<td>250</td>
<td>500</td>
<td></td>
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<tr>
<td></td>
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<td>50</td>
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<td></td>
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<td>0</td>
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<td></td>
<td>...</td>
<td></td>
<td></td>
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<td></td>
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</tbody>
</table>

**After operation**

<table>
<thead>
<tr>
<th></th>
<th>530</th>
<th>270</th>
<th>510</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>90</td>
<td>150</td>
<td>420</td>
</tr>
<tr>
<td></td>
<td>80</td>
<td>40</td>
<td>530</td>
</tr>
</tbody>
</table>
Operations using constants can be performed interactively using icons as well.

Add/subtract a constant

Multiply/divide by a constant
Peak Searching and Fitting

Search: search peaks automatically

Approx: approximate the peak position, height and width without fitting

Fit: start iteration

Init: initialize

Clear: clear all peaks and calculation results if there is any

Convert: convert the fitted spectrum with the calculation result

Peaks: open Peak window

Variables: open Variables window
Peak Searching and Fitting

Right clicking in the table activate the context menu, which allows add or remove peaks to fit.

Parameters of fitting functions can be adjusted for each peak from Variables window.

The entire peak fitting table can be copied and pasted using the Copy and Paste button.
Vertical or horizontal profile over an image can be obtained from Profile window.

You can apply to a profile the same operations as for a spectrum, then using the **Corr** button to put the corrected data back to the image where the profile was extracted.
Advanced Data Treatment

- Analyzing map image and profiles
- New spectral profile
Analyzing Images and Profiles

**Map:** Display integrated intensity of Raman images or profiles

**SpIm:** Contain all data of the image/profile

**Point:** Display the spectrum at the current cursor position
Analyzing with Cursors

Check USE box to generate the corresponding map.

Check BASE box to subtract baseline.

Check GREEN/BLUE box to generate the map of the corresponding ratio.

Check SPECTRUM box to see the spectrum of the selected data point(s).

Edit FROM and TO fields to adjust the limits of the spectral regions.

Click on the Correct button to modify data on the selected data point(s).
The initial method for analysing a mapped image or profile is to use three cursors (R, G and B) to define regions.

The image is generated by displaying the spectral intensity between these cursors.

The three cursors are simply selected from the three coloured cursor.

These three cursors appear when the window SpIm is activated.

If one or more of the cursors aren’t currently displayed on screen, they can be returned by clicking on the Cursor normalization icon on the toolbar.
Example

• Sample description
  – A raw pharmaceutical pellet. The map shows the distribution of 3 widespread fillers in pharmaceutical pellets: Cellulose, Starch and Magnesium stearate.

• Measurement
  – A large map is recorded onto the surface of the pellet.

• Acquisition conditions
  – Instrument: LabRam HR
  – Laser wavelength : 633 nm
  – Grating : 600 gr/mm
  – Confocal hole : 600 µm
  – Objective: ×50
  – Map size: 400 × 400 µm and 36 × 36 data points
  – Acquisition time: 10 s/point
The map displays the distribution of 3 components: Starch, Cellulose, and MgStearate.
To display the integrated intensity map, position pairs of Red, Green, and Blue cursors around selected Raman bands in *Point* or *SPlm* by selecting the corresponding color arrow on the left toolbar.
Sometimes, an intensity profile along a line can provide useful information such as diameter of agglomerations. Select a map (right tool bar) and click Profile icon (top tool bar). The intensity profile of the selected intensity map is displayed along the vertical or horizontal cursor line (red cross in Map window).
Modeling

- Supervised or unsupervised factors
- Normalize model
If the spectra of the pure components are available, they can be taken into the modeling program.

If not, LabSpec 5 allows you to create a model automatically by using a factor analysis algorithm.

*In terms of normalization of the reference spectra:*

If the original spectra had not been recorded in the same conditions you wouldn’t lose any information by normalizing because the relative intensities were already unreliable.

But, if the spectra have been recorded in the same conditions, the relative intensities are representative of the relative Raman scattering power of each components. In this latter case, you lose information by normalizing.
Example

• Sample description
  – AsO$_4^{3-}$ can substitute for SO$_4^{2-}$ in sulfate minerals. Raman spectrometry proved very useful for investigating the formation of SO$_4^{2-}$ - AsO$_4^{3-}$ intermediate phases.
  – The sample comes from a former industrial site in France comprising mainly sulfate minerals similar to gypsum (CaSO$_4$.2H2O) and thenardite (Na$_2$SO$_4$) and with a high As content (8 to 18% w/w).

• Acquisition conditions
  – Instrument: LabRam HR
  – Laser wavelength : 633 nm
  – Map size: 51 × 70 µm
  – Step size: 1µm
  – Acquisition time: 10 s/point
Two phases are observed. The characteristic peak of each phase is displayed between Red and Green cursors:
To extract two pure spectra constituting the sample, click **Modeling** icon to open **Model** window. Set **FACTORS** to 2 and click **Create**.
Two phases are extracted by the Modeling procedure. The characteristic peak of each pure phase is displayed in Red and Green.
MODE: Overlay

To change the display mode of score images, right click in the image to activate window context menu and select Format and scale. Select TILE from MODE.

MODE: Tile
Open the corresponding video image, right click in the image to activate the window context menu, and select **Imposition**. Check OVERLAY IMAGES box. Select an intensity map or a score map to overlay.
It is also possible to use the band fitting results to create a map of peak position (p), amplitude (a), band width (w) and the area (a) of the peak.

Check MAP box of the parameter to map and click **Apply**.
Example

• Sample description
  – 1 mm square silicon structure.

• Measurements
  – A line measurement is recorded at mid-height of the square from one edge to the other.
  – A spectrum is recorded at every 15 µm.
  – The Silicon peak position in a non-stressed Si crystal is 520.7 cm⁻¹.
  – If a tensile or a compressive stress is occurring in the structure (due to a defect, a coating, a boundary, etc.), then the position of the peak shifts to lower (tensile) or higher (compressive) wavenumbers.

• Acquisition conditions
  – Instrument: LabRam HR
  – Laser wavelength: 532 nm
  – Grating: 1800 gr/mm
  – Confocal hole diameter: 200 µm
  – Step size (x-axis only): 15 µm
  – Extended video image: the picture is recorded over a very large surface area.
SpIm displays all the spectra recorded along the line. **Point** shows the spectrum at the cursor position selected either in Video or Map. The line of analysis is superimposed on the video image. **Map** displays up to three parameters that are selected in SpIm.

Red cursors are position in SpIm to map the intensity of the silicon peak along the line. The intensity drops at the edge of the silicon square.
To display $SpIm$ in 2D, right click in $SpIm$ window to activate the window context menu and select **Format and scale**. Select 2D from DIMENSION.

To display the line of measurement on the sample image, select **Video** and right click in the image to activate the window context menu. Select **Imposition**. Check SHOW DATA PPOINTS box.
The profile is displayed in 2D in SpIm such that the color scale corresponds to the Raman intensity. The curve shape of the 2D map illustrates the shift of the Silicon position along the line of analysis that is displayed on the video image.
When the profile is displayed in 1D, peak fitting can be applied to the image in order to map the peak positions. Select **Add peak**. Click at the peak position. This adds a peak to be fitted.
Click **Approx** and then **Fit**. When finished, click **Peak**. From **Peak** window, check MAP box for **P** and click **OK**.

A new window appears with the plot of the peak positions along the line. It gives an accurate idea of the strain in the silicon structure:
Spectral Profile

- Create a Raman map out of spectra that were recorded separately.
  - Open the files that are to be made into a map
  - Select the first spectrum of the new spectral profile.
  - Input a name and click New. New SpIm window with the given name is created automatically showing the selected spectrum. Corresponding Map window is also created.
  - Add other spectra one by one by selecting and clicking **Add** or **Insert** button.
  - **Add** – adds the selected spectrum to the end of the spectral file.
  - **Insert** – inserts the selected spectrum to the position selected in the Map window
Graphic Tool Panel

- Window Context Menu
- Activated by clicking right mouse button with the mouse positioned in a window.
- Graphic Tool Panel is sensitive to the characteristics of the window it is linked to. Therefore, the specific elements listed change depending on the window the menu has been called for.
- Each Graphic Tool Panel is composed of two sections, separated by a line. Elements in the top section are common to all windows. Elements in the bottom section are window specific.
Graphic Tool Panels

Window displaying individual spectra.
**Spectrum Model**

Window displaying individual video images.
**Video**

Window displaying maps.
**Map Score**
Graphic Tool Panels

Window displaying a collection of spectra in 1D. 
*SpIm*

Window displaying a collection of spectra in 2D. 
*SpIm*

Window displaying a collection of spectra in 3D. 
*SpIm*
Common Elements

Format and scale
Format the window setting. Often used options are
– Mode: Select display modes out of Single or various Multi modes.
– Rel: Allow multiple spectra/images be displayed with independent scale for easy comparison.

Shortcut icons on the right tool bar
Toggle between single and selected multi display modes
Common Elements

**Image colors**
Select and format color palette for the window
Common Elements

Fast settings
Activate the interactive formatting from the data window itself.
Elements that can be changed are underlined.
Shortcut icon on the right tool bar

Rescale
Rescale both X and Y axes to show the full data range.
Shortcut icon on the top tool bar

Swap x axis
Reverse x-axis direction
Window Specific Elements

Axes
Format axes and grids.

Legend
- SINGLE: Legend is displayed when Single display mode in Formatting and scale is selected.
- MULTI: Legend is displayed when one of Multi display mode in Formatting and scale is selected.
Window Specific Elements

Spectrum
Select to display spectrum as a set of Lines, Points or Bars.
Format line style, color and thickness.

Cursor
Select pointer types:
- Line: single vertical line
- Cross: vertical and horizontal lines
- Level: vertical and horizontal lines with the horizontal line position locked to the intensity
- Double: two vertical lines
- Peak: three vertical lines with positions of two outer lines locked to the approximated FWHM.
Window Specific Elements

**Scale bar**
Format color and font of scale bar.

**Image**
Select to display image with or without interpolated rendering, and change the default image color.

**Imposition**
Overlay elements of *Maps* or *Score* windows on top of *Video* image. Check boxes of desired elements and then select the *Map* or *Score* window to overlay.
Window Specific Elements

**Spectra**
Format 1D rendering of SpIm window

**Image 3D**
Format 3D rendering of SpIm window
Visual Basic Script (VBS)
A scripting language to automate LabSpec
What is VBS?

- What is VBS?
  - In order to simplify complex or repetitive tasks, LabSpec 5 can be automated, using VBS, a well known Scripting Language.
  - Visual Basic Script is an interpreted, scripting language.
  - It allows very fast implementation, high level programming.
  - It does not requires an external development environment.

- What can be automated?
  - Motor movements
  - Data Acquisition
  - Data Treatment
  - 2D Map or 1D Profile Generation
  - Instrument calibration
  - File import/Export
  - Video
What is Different about VBS?

- There are basically two kinds of programming languages:
  - Compiled languages (C, C++, Pascal, Delphi, etc.)
    - They are low level programming languages that require a program called compiler to convert source code to the machine language.
    - Advantages: Very powerful, flexible and fast to execute.
    - Disadvantages: Hard to code, require a compiler, not intuitive.
  - Interpreted languages (VBS, JavaScript, Python, PHP, ASP, etc.)
    - They are high level programming languages that do NOT require a compiler.
    - A program called interpreter converts at execution time the commands to the machine language.
    - Advantages: Very fast to implement, easy to code, very intuitive
    - Disadvantages: Much more limited and slower than compiled languages, no visual interface.
How Does it Work?

- You said VBS is slow, but I want fast measurements!
  - LabSpec automation allows VBS (easy to code, but slow) to call LabSpec C++ (hard to code, but very fast) functions!
  - This way, you can have both an easy to code scripting language and very fast functions for acquisition and treatment.

<table>
<thead>
<tr>
<th>VBS Script</th>
<th>LabSpec 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Move Spectro to 520.7 cm⁻¹</td>
<td>Fast, C++ engin</td>
</tr>
<tr>
<td>Start Acquisition</td>
<td></td>
</tr>
<tr>
<td>Do Peak Fitting</td>
<td></td>
</tr>
<tr>
<td>Save data to file</td>
<td></td>
</tr>
</tbody>
</table>
What do I Need?

- LabSpec 5 has an integrated script editor, with auto-completion and syntax colouring.
- It includes Full pdf documentation.
- A ‘Getting Started’ tutorial to get familiar with VBS and LabSpec programming is also available.
Where Can I Use?

• Examples in Data Acquisition
  – Spectra with different lasers
  – Spectra with different gratings
  – From low power to high power (D2, D1, D0.6, …)
  – Depth profiles with different confocal hole diameters

• Examples in Data Processing
  – Sequences
    • filter + baseline + peak fitting
    • peak fitting + plasma position correction
  – Create new functions
    • create special data smoothing functions
Where Can I Use (cont’d) ?

• Examples in Data Display
  – Create a profile from single spectra
    • 1 D profile with access to axis definition + possibility to have non-equidistant data
    • 2 D profiles (re-create maps from single spectra)

• Examples in Data Export
  – Export in specific format for other software
Visual Basic Script (VBS)  
One Practical Example in Detail
Step 1

• Objective: Automate a Linkam heating/cooling stage
  – This example will show you how easy and how fast VBS prototyping can be, even with a relatively complex project.

• Requirements:
  – Manage a temperature ramp (From $T_1$, to $T_2$, Step, Speed, Holding time and Experiment name)
  – Take a video snapshot before each spectrum (save image to file)
  – Do a Raman Acquisition (save spectrum to file)
  – Create a profile Intensity vs. Temperature (save profile to file)
Step 2

1. Create a function to manage the temperature ramp
   • Temperature ramps are defined by 6 parameters. Let’s write a function that can handle these parameters.

   **Function** DoTemperatureTest (ExperimentName, StartTemperature, StopTemperature, Speed, HoldingTime, TemperatureStep)

   **End Function**

2. Setup the Linkam stage with the correct speed and holding time
   • LabSpec specific functions are identified by “LabSpec.” prefix. These functions are fully documented, specific parameters are explained and a short example is provided.

   ‘Set Heating/Cooling Speed
   LabSpec.ManageTemperature CONSTANT_SPEED, Speed, 0, Speed, 0, HoldingTime
ManageTemperature

• Overview
  – Description: Manage Linkam stage parameters
  – Keywords: Cooling, heating, speed
  – Type: AutoVBSAct

• Syntax
  – `long ManageTemperature (long Mode, double HeatingSpeed, double HeetingTime, double CoolingSpeed, double CoolingTime, double HoldingTime)`

• Parameters
  – `Mode`: Heating and Cooling mode
    • CONSTANT_SPEED: Use constant speed (°C/min) during heating/cooling
    • CONSTANT_TIME: Use constant time (sec) for heating/cooling
    • FREE_TEMPERATURE: Free the cooling stage (other parameters are ignored)
Step 3

3. For each point, heat or cool the Linkam stage
   – The Linkam stage can be used as any other motor (spectro, hole, slit, etc.)
   – The unique command to drive all motors is “LabSpec.MoveMotor”
   – MotorName is “Temperature” and MotorPosition (°C) for point i can be calculated by: Temp (i) = StartTemperature + i × TemperatureStep

‘Calculate the number of spectra
NbSpectra = (StopTemperature – StartTemperature) / TemperatureStep + 1

‘Heat/Cool to the first/next step
For i = 0 To NbSpectra – 1
   LabSpec.MoveMotor “Temperature”, StartTemperature + I * TemperatureStep, “”, MOTOR_VALUE
Next
MoveMotor

• Overview
  – Description: Moving a specific motor
  – Keywords: Script, step value, string index
  – TypeL AutoVBSAct

• Syntax
  – `long MoveMotor (LPCTSTR MotorName, double PositionValue, LPCTSTR PositionName, long Mode)`

• Parameters
  – `MotorName`: Motor name (see Motor Name List)
  – `PositionValue`: Value to reach
  – `PositionName`: Position name (only for named position motors such as microscope)
Step 4

4. Capture a video snapshot
   - Waiting for the video to be ready may take some time, for example to move the beam splitters in ARAMIS.
   - The video image is being saved to a native “*.ngv” file here, but it can also be saved as a TIFF or JPEG image

```
'Take Video Image
LabSpec.Video START_VIDEO 'Start the live video

Do 'Wait till video is ready
  VideoID = LabSpec.Video (GET_VIDEO_ID)
Loop Until VideoID > 0

'Save the live video image
LabSepc.Save VideoID, Path & ExpermentName & "\Video_" & i+1 & "_" & CurrentTemperature & "deg.ngv", "ngv"

LabSpec.Video STOP_VIDEO 'Stop the live video image
```
Video

- **Overview**
  - Description: Display video image
  - Keywords: Camera
  - Type: AutoVBSAct

- **Syntax**
  - `long Video (long Mode)`

- **Parameters**
  - `Mode`: Start/Stop video
    - `START_VIDEO`: 0, Start video
    - `STOP_VIDEO`: 1, Stop video
Step 5

5. Spectrum Acquisition
   – Raman Acquisition is totally similar to the video acquisition

   ‘Take Spectrum

   ‘Start acquisition
   LabSpec.Acq Mode, IntegrationTime, AccumulationNum, AcqFrom, AcqTo

   ‘Wait till spectrum is ready
   Do
     SpectrumID = LabSpec.GetAcqID()
   Loop Until SpectrumID > 0

   ‘Save the spectrum
   LabSpec.Save SpectrumID, Path & ExperimentName & “\Spectrum_” & CurrentTemperature & “deg.ngs”, “ngs”
Acq

• Overview
  – Description: Start an acquisition
  – Keywords: VBS ActiveX, VB, integration time, Accumulation
  – Type: AutoVBSAct

• Syntax
  – `long Acq(long Mode, double IntegrationTime, long AccumulationNum, double From, double To)`

• Parameters
  – `Mode`: Acquisition modes
    • ACQ_SPECTRUM: 0, Start a spectrum acquisition
    • ACQ_IMAGE: 1, Start a CCD image acquisition
    • ACQ_LABSPEC_PARAM: 2, Start spectrum acquisition with LabSpec interface parameters
    • ACQ_SPECTRAL_IMAGE: 3, Start spectral image acquisition with LabSpec interface parameters
    • ACQ_AUTO_SHOW: 10, Add to any other acquisition mode to automatically show acquired data
  – `IntegrationTime`: Spectrum integration time (sec). Ignored if ACQ_LABSPEC_PARAM mode is selected.
Step 6

6. Add each spectrum to a profile

‘If the profile does not exist and the current spectrum is the first spectrum of the profile, the profile is created.
If i = 0 then ProfileID = LabSpec.Profile (0, 0, SpectrumID, CurrentTemperature, “Degree”, “Temperature”)

‘If the profile exists, the current spectrum is added the profile, and the profile is updated.
If i > 0 then ProfileID = LabSpec.Profile (1, ProfileID, SpectrumID, CurrentTemperature, “”, “”)
Profile

• Overview
  – Description: Create spectral image from spectra
  – Keywords
  – Type: AutoVBSAct

• Syntax
  – `Profile (long Mode, long profileID, long SpectrumID, double Value, LPCTSTR Unit, LPCTSTR Label)`

• Parameters
  – `Mode`: Profile modes
    • `CREATE_PROFILE`: 0, Create a profile with one spectrum (ProfileID is ignored)
    • `ADD_TO_PROFILE`: 1, Add a spectrum to the profile
    • `ProfileID`: ID of a previously created profile. Relevant only for `ADD_TO_PROFILE` mode
  – `SpectrumID`: ID of a spectrum to add to the profile
  – `Value`: Extra dimension value for the current spectrum
Results