HES1000 Spectrometer

Software User Guide

www.is-instruments.com

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Table of Contents

About this Manual

Who's this for?

This manual is intended for the operator of the HES1000 spectrometer (BlackFly version). It will allow the operator to understand how to get the most out of this new product.

What's in it?

This manual provides the operator with instructions on how to use the HES1000 software package included with your spectrometer.

A separate manual is available that describes how to unpack, install, calibrate and use the HES1000 spectrometer. This is included on the USB stick provided, along with the most recent version of this manual.

Introduction	Contains an overview of the HES spectrometer and the methodology of how to use it
Installation	Instructions on how to install the software
Start the GUI	How to get the software up and running
Operating your HES1000 software	Details of how the software is operated using the menus and button commands
Acquiring Data	Details on the process you should follow to acquire data
Data Display	Explains the various ways you can view your data, in both real time and historic saved files
Appendix A: Troubleshooting	Gives some suggestions on what to try if you have a problem
Appendix B: Calibration	Takes you through the process of recalibrating.
Appendix C: Apodisation	Explains some of the apodisation techniques available in the software
Appendix D: File Format	Shows you how your data file is made up

Warranty

All ISI's products come with a 1-year warranty covering parts, labour and shipping needed to repair manufacturing defects that occur during the warranty period. Shipping costs are limited to shipping to and from our customers during the warranty period. The warranty will be void if the system is handled inappropriately or if the housing has been opened.

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Changes are periodically made to the product and these will be incorporated into new additions of the manual.

1. Introduction

1.1. What's the product?

The HES1000 spectrometer is a Static Fourier Transform spectrometer providing high etendue measurements. Etendue is commonly referred to as throughput of a spectrometer. It is a measure of the ability of a spectrometer to capture and utilise individual photons from a particular area of a target or field of view. A more complete description of this can be found on our website – It's all about throughput.

Some of the key features are detailed below:

Model	HES1000	HES1000B	HES2000
Operating range	< 200 – 2400 cm^{-1}	< 230 – 1800 cm^{-1}	< 200 – 2300 cm^{-1}
Resolution*	~ 3 cm^{-1} per Fourier bin	~1.5 cm^{-1} per Fourier bin	<3 cm^{-1} per Fourier bin
Fibre coupled	SMA or FC/PC	SMA	SMA or FC/PC
Fibre aperture	<1 mm as standard	910 µm	≥1 mm as standard
Fibre NA	0.22	0.22	0.22

*Unlike most other systems, the HES spectrometers are linear in wavenumber space, meaning you won't lose resolution as you move from the starting wavelength. Unlike conventional spectrometers there is no slit present so no blurring is observed. (A minimum of 3 bins are required to resolve 2 lines)

1.2. System requirements

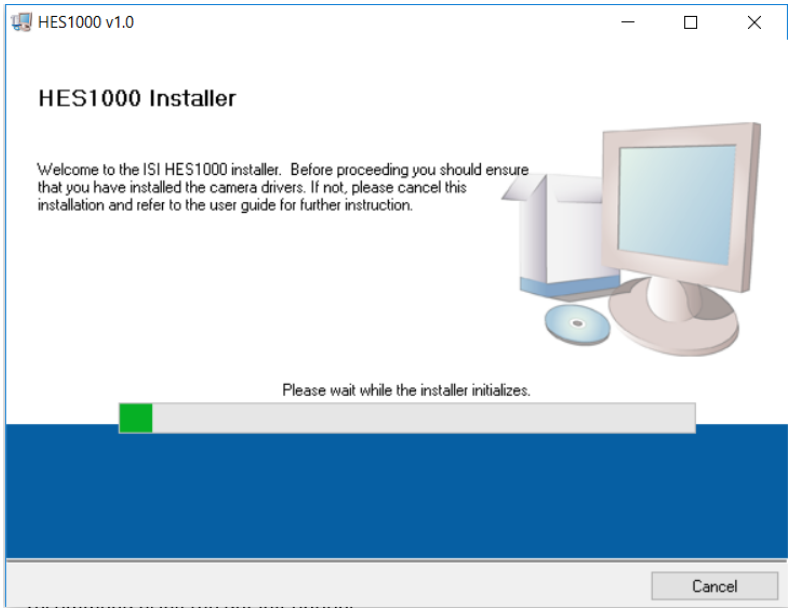
To run the system software, you will need a compatible device, running Windows 7 or later.

The compatible device will need a USB3.0 port and approximately 350 MB disk space. Performance requirements are minimal - a 2GHz single core processor and 1GB RAM will be sufficient.

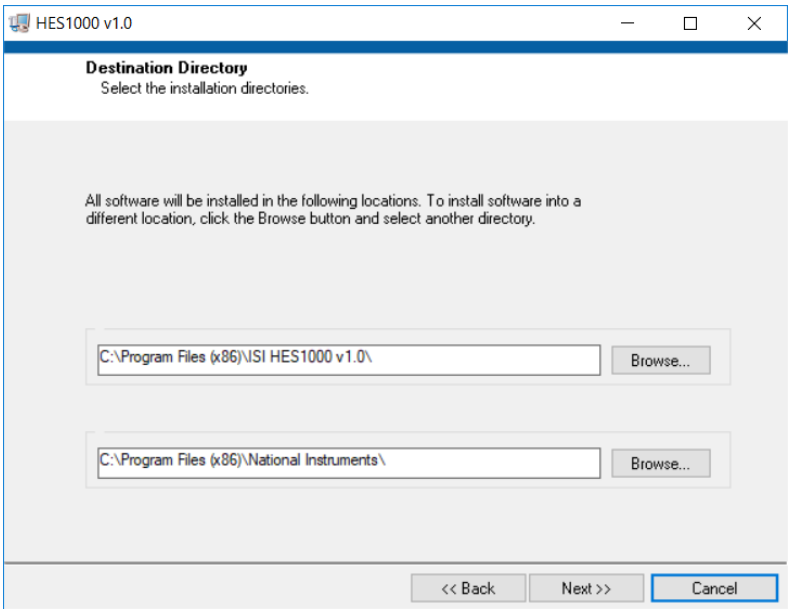
2. Installing Software

The software may be included as a USB stick or as a direct download from our website. You will need to run the 'setup.exe' file located in the 'HES1000 Installer\Volume' directory. This will start the installation routine. You may receive a 'This file is from an untrusted source. Do you want to run it?' message. Click '**Yes**' to continue.

You should then see the following screen:

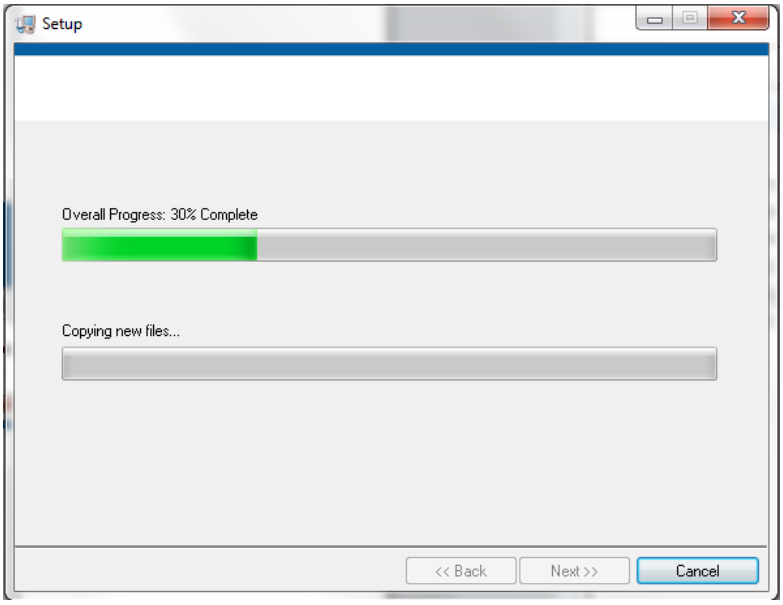


After the installer initializes you will be prompted for the installation location. We recommend using the default options.

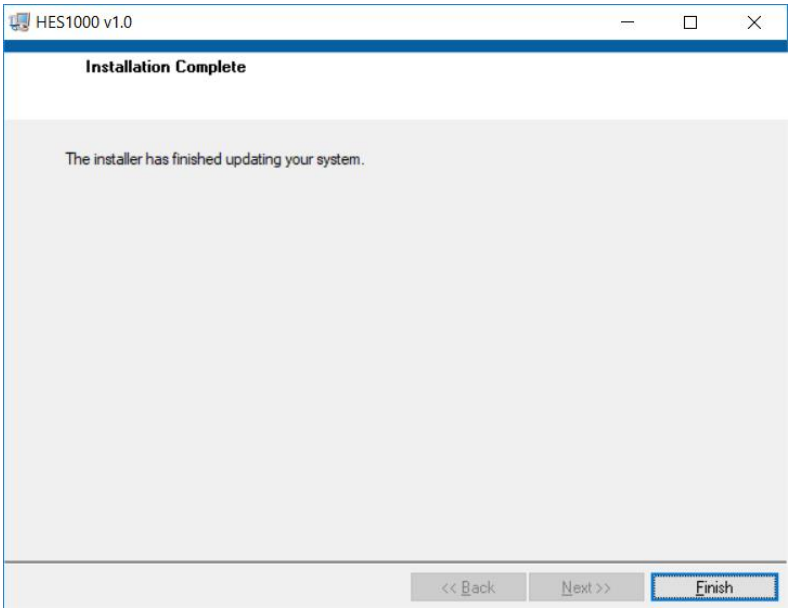


Click '**Next**' twice (you may need to select whether to disable Windows Fast startup – we have not experienced problems with this so uncheck it, but this may be platform specific).

You will then get the progress bar showing you how much remains

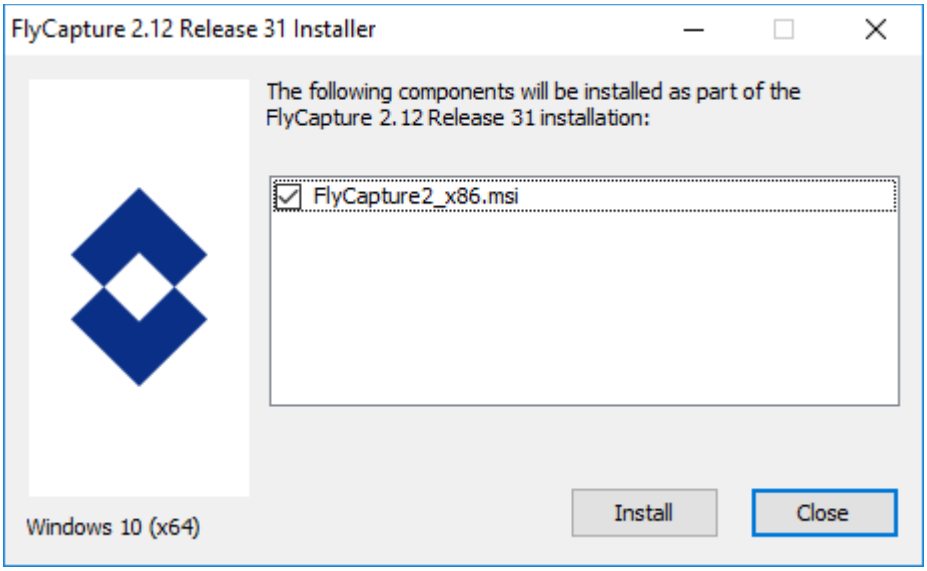


Followed by the 'Installation complete' display.

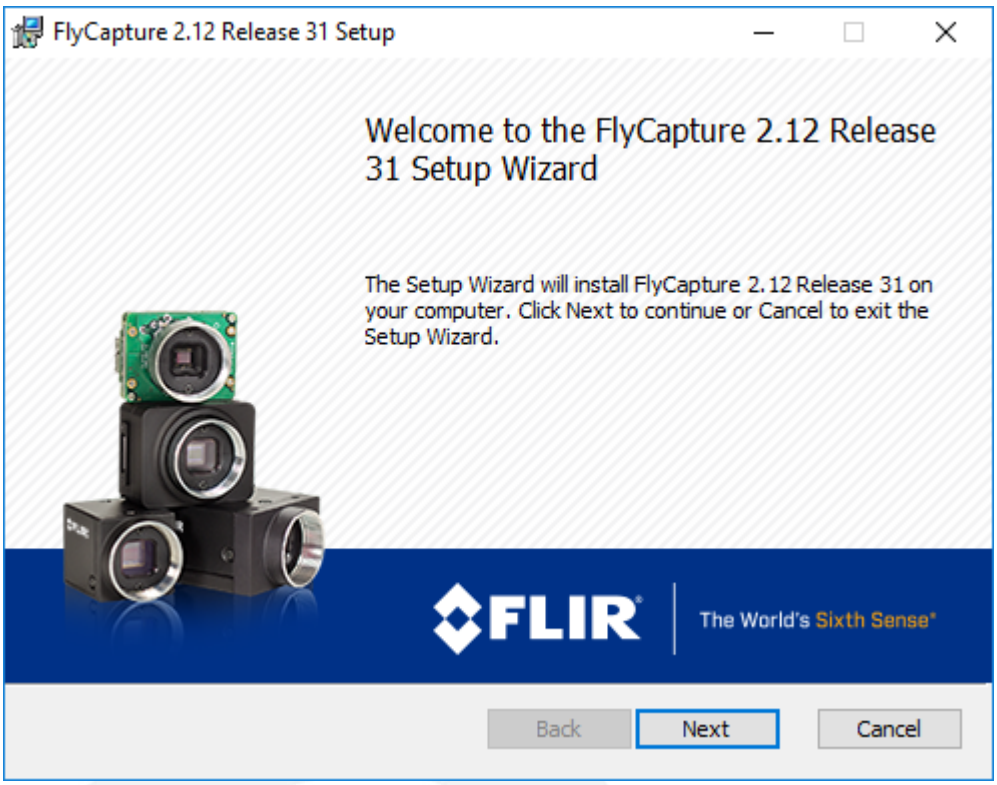


Click '**Finish'** to complete.

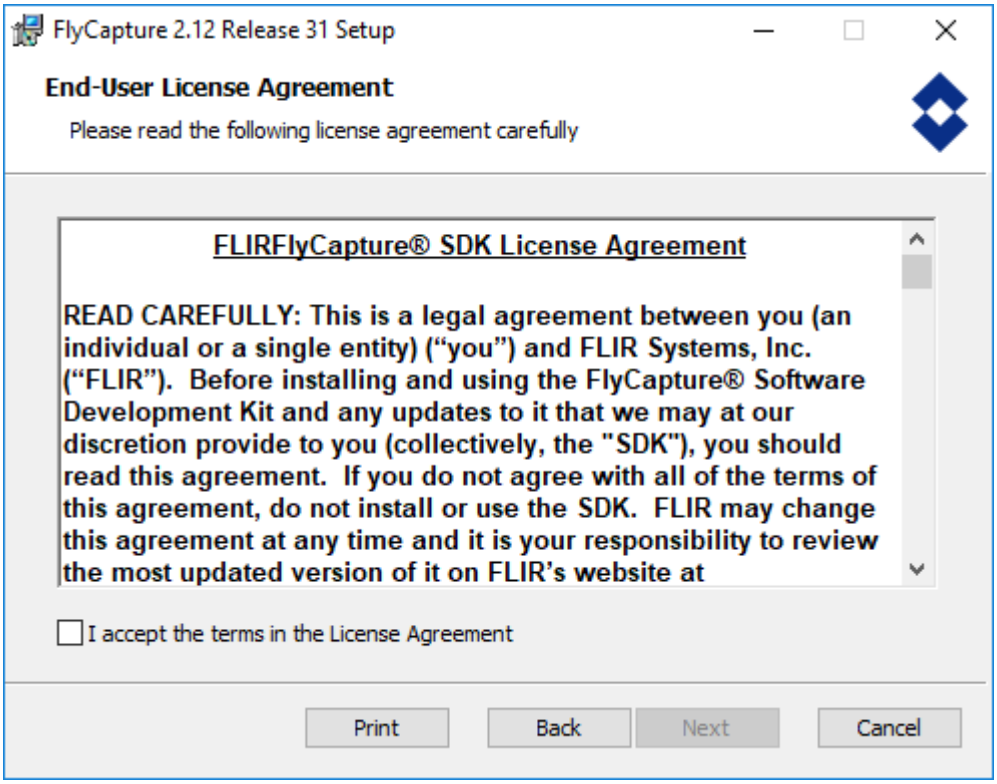
Next, another installer will launch to install the FLIR/PointGrey BlackFly USB drivers.



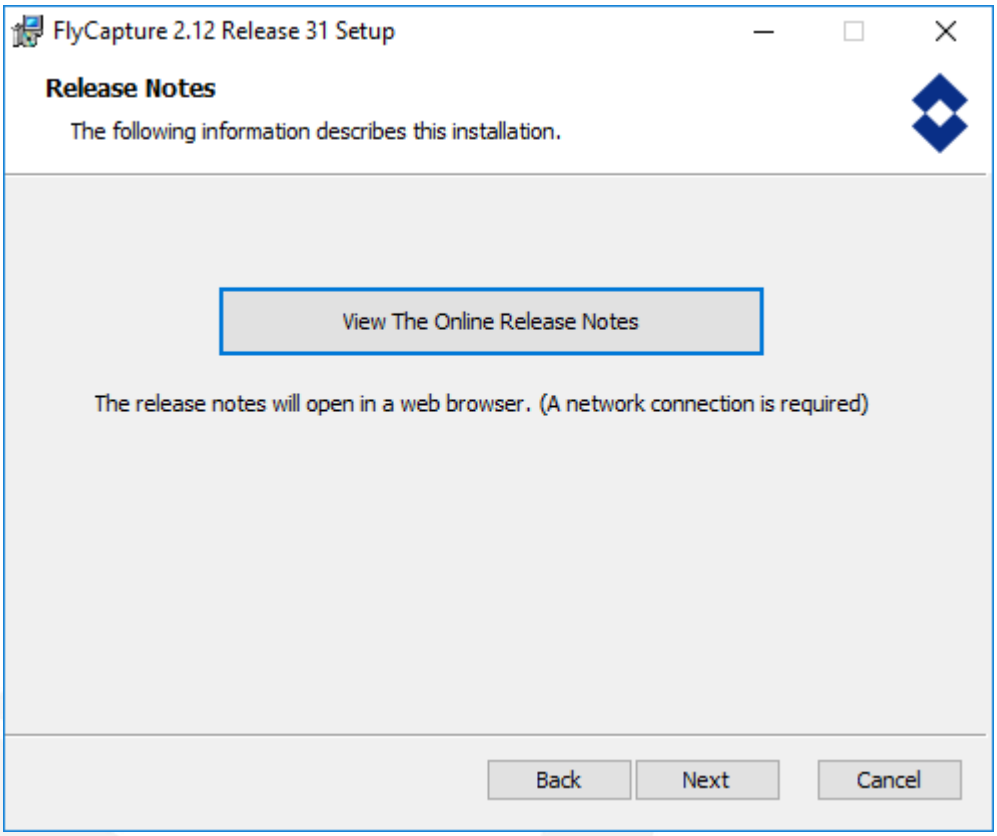
Click 'Install'



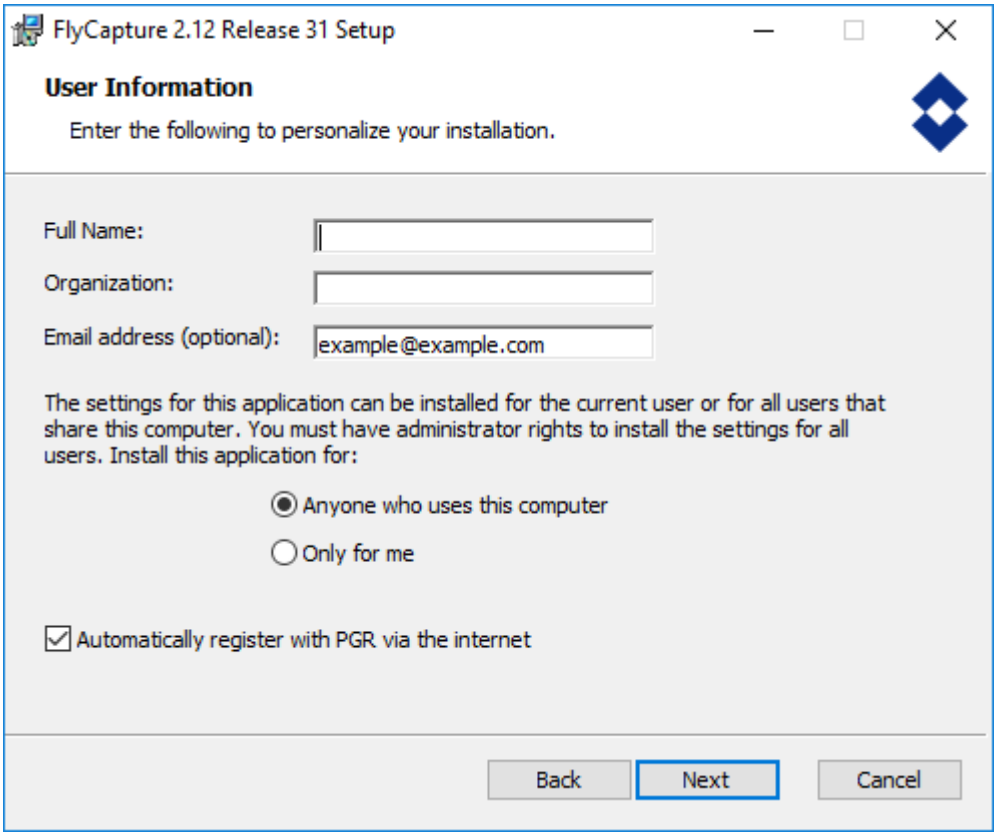
Click 'Next'



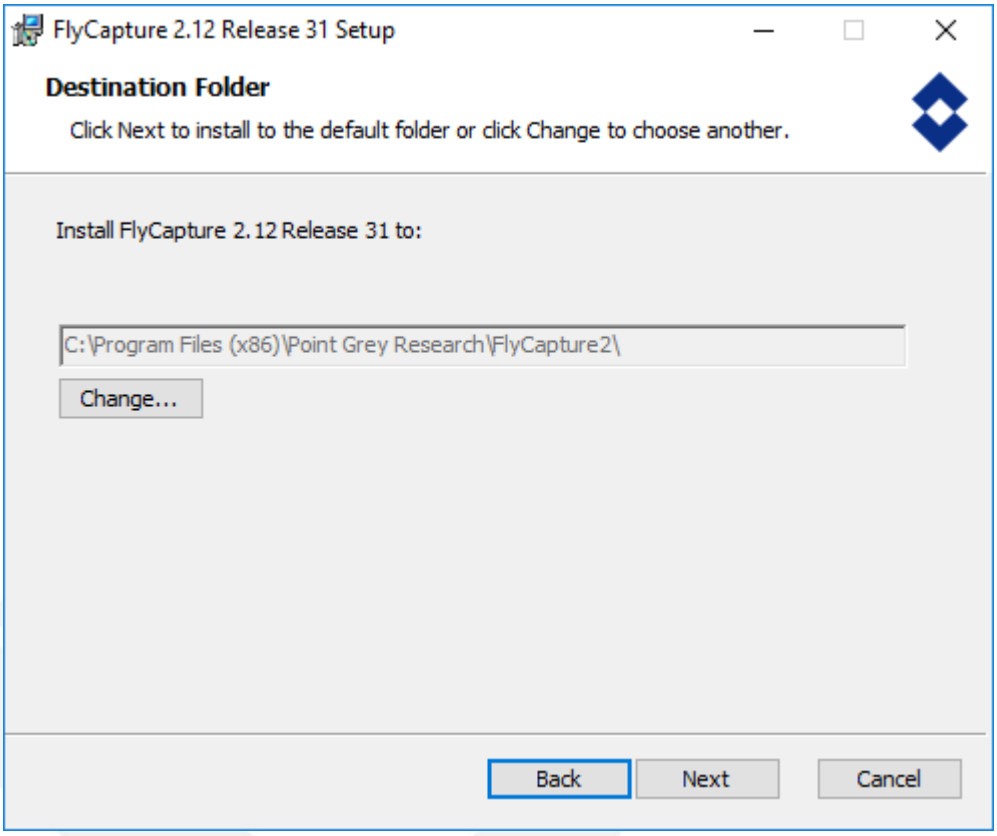
Agree to the terms to proceed.



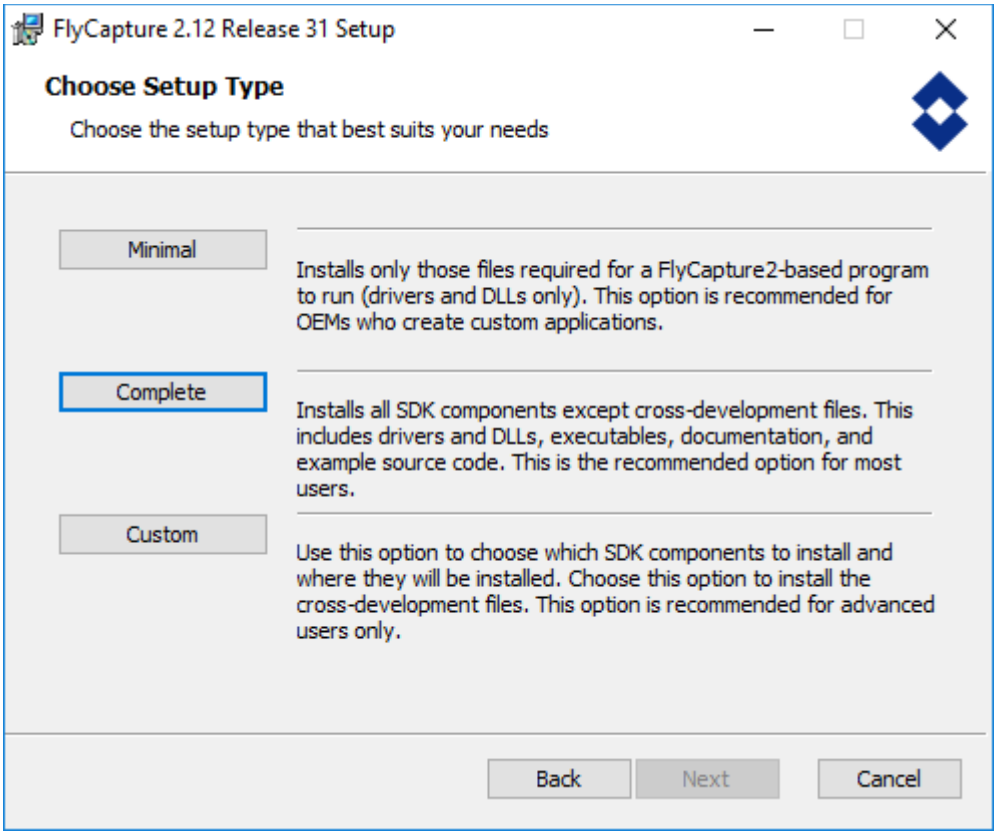
Click 'Next' when you are ready to proceed.



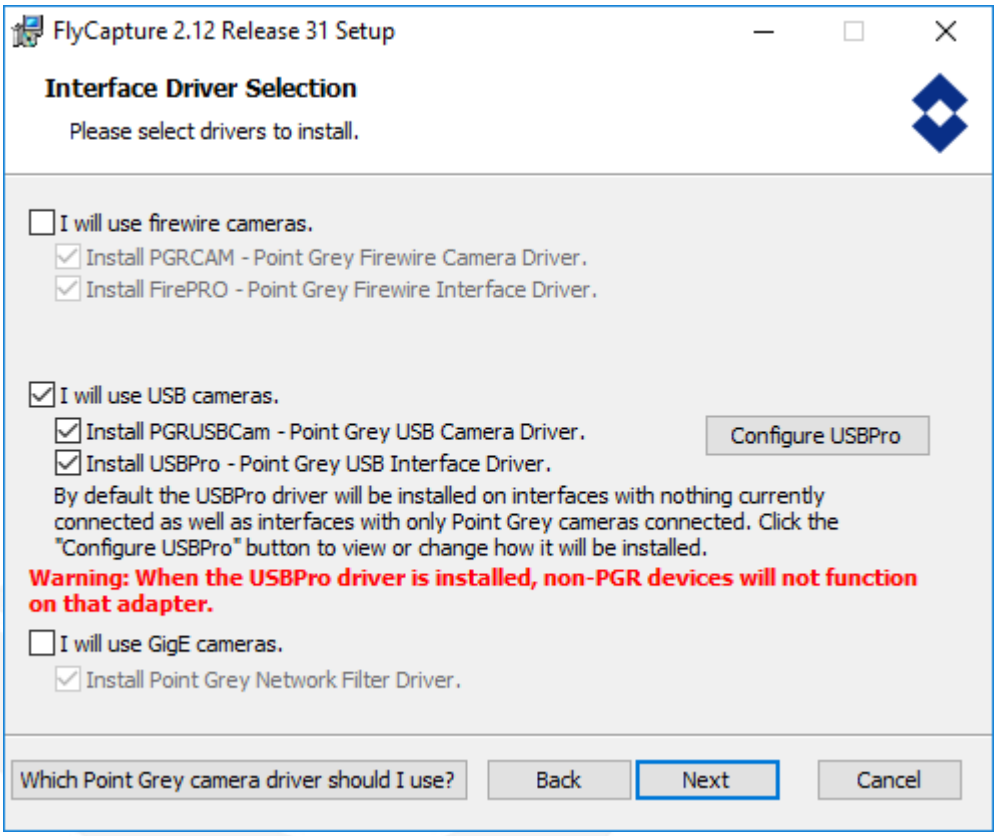
Registering is optional and at the discretion of the user. If you do not wish to register, untick the 'Automatically register…' option before clicking 'Next'.



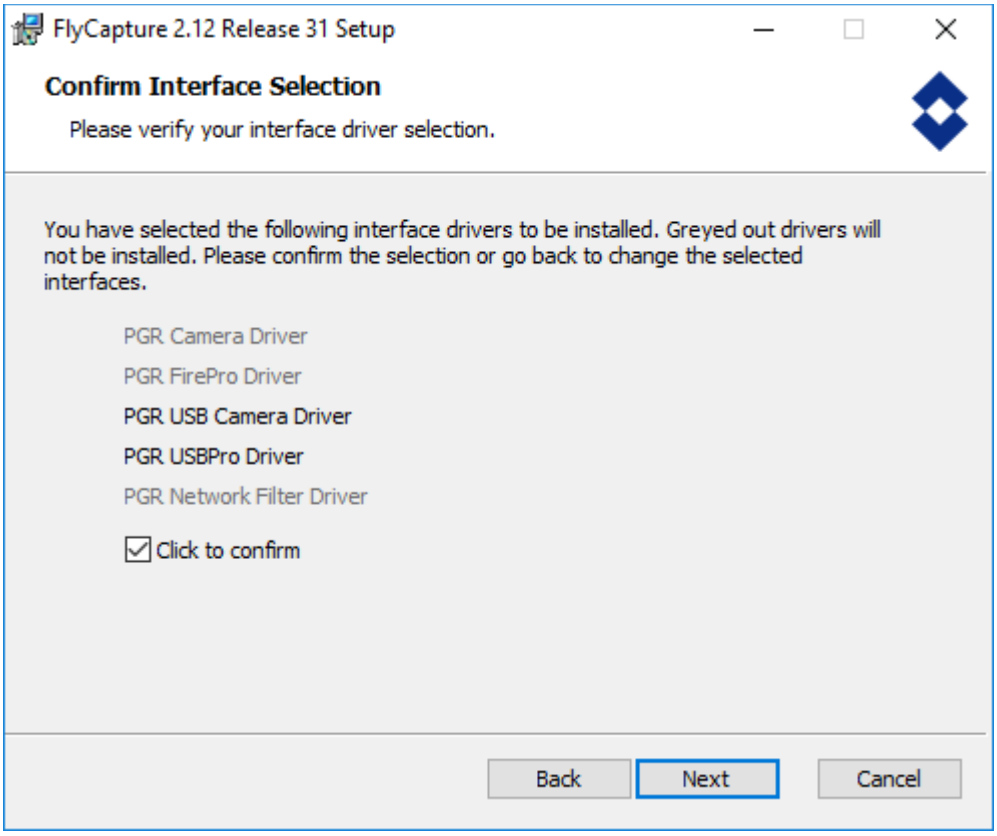
Select the installation location before clicking ‘Next’.



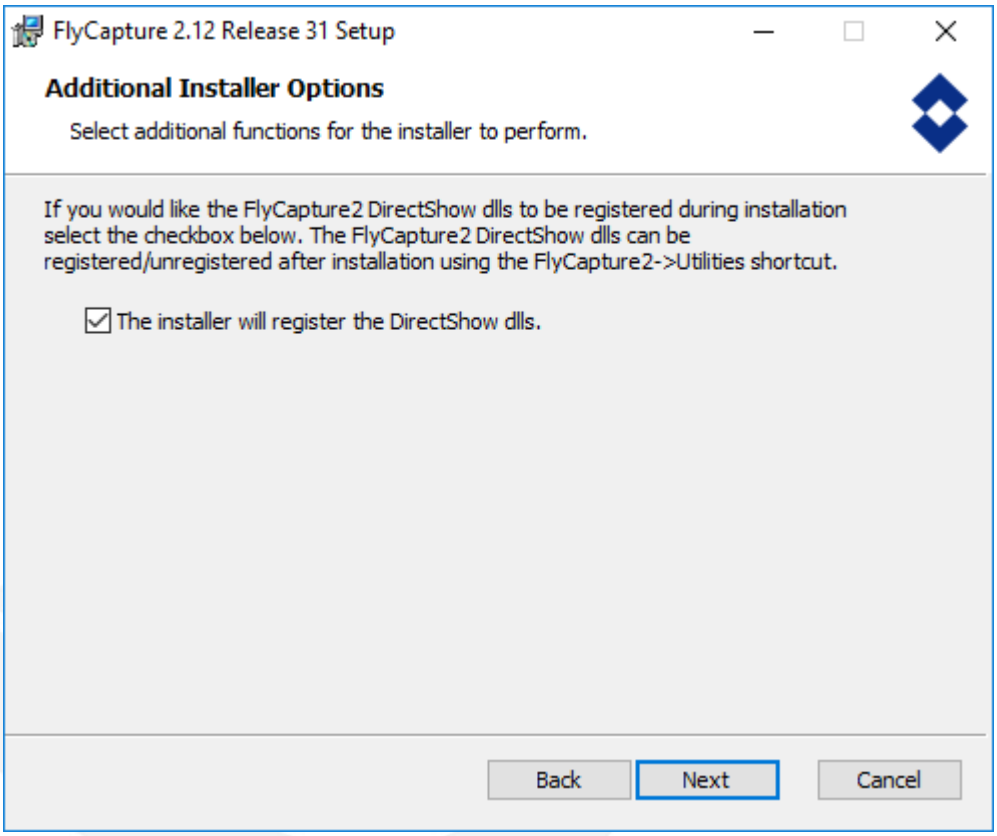
Select ‘Complete’ before proceeding.



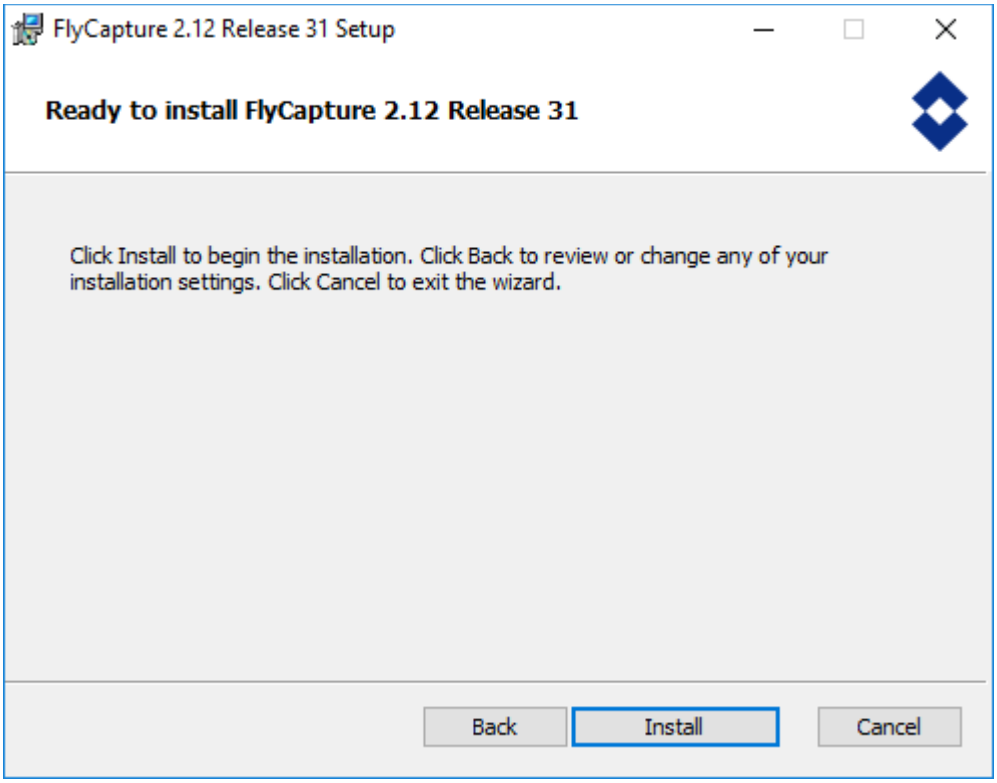
Select ‘I will use USB cameras’ before proceeding.



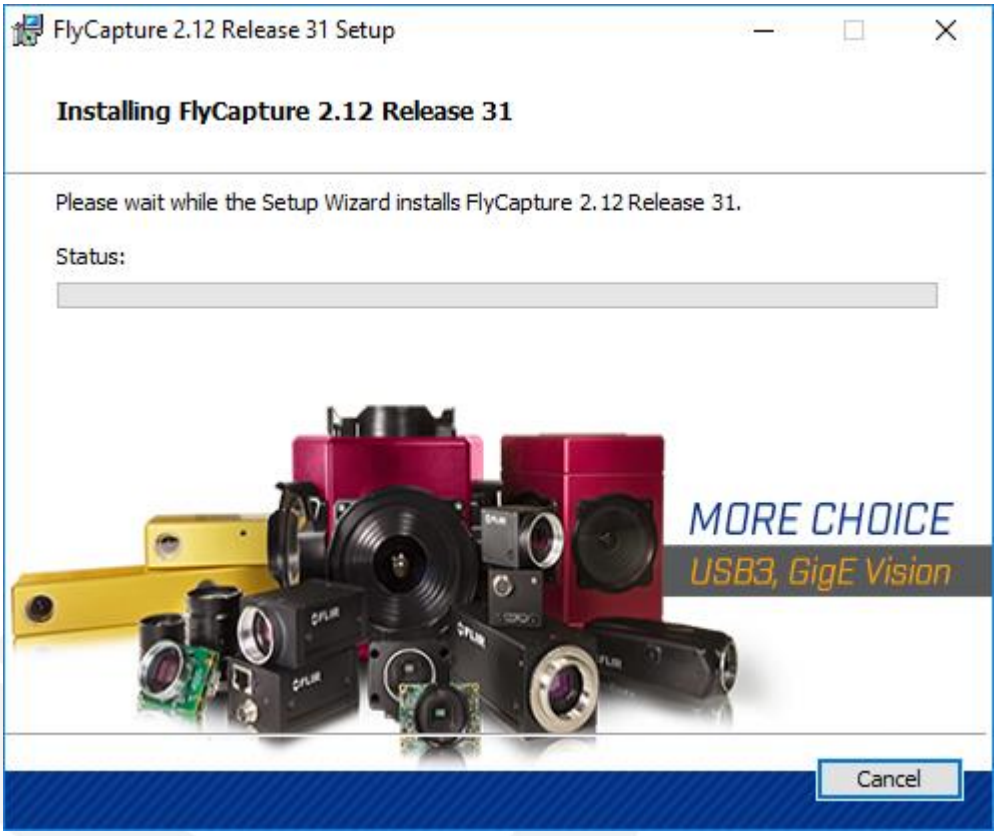
Click to confirm before proceeding.

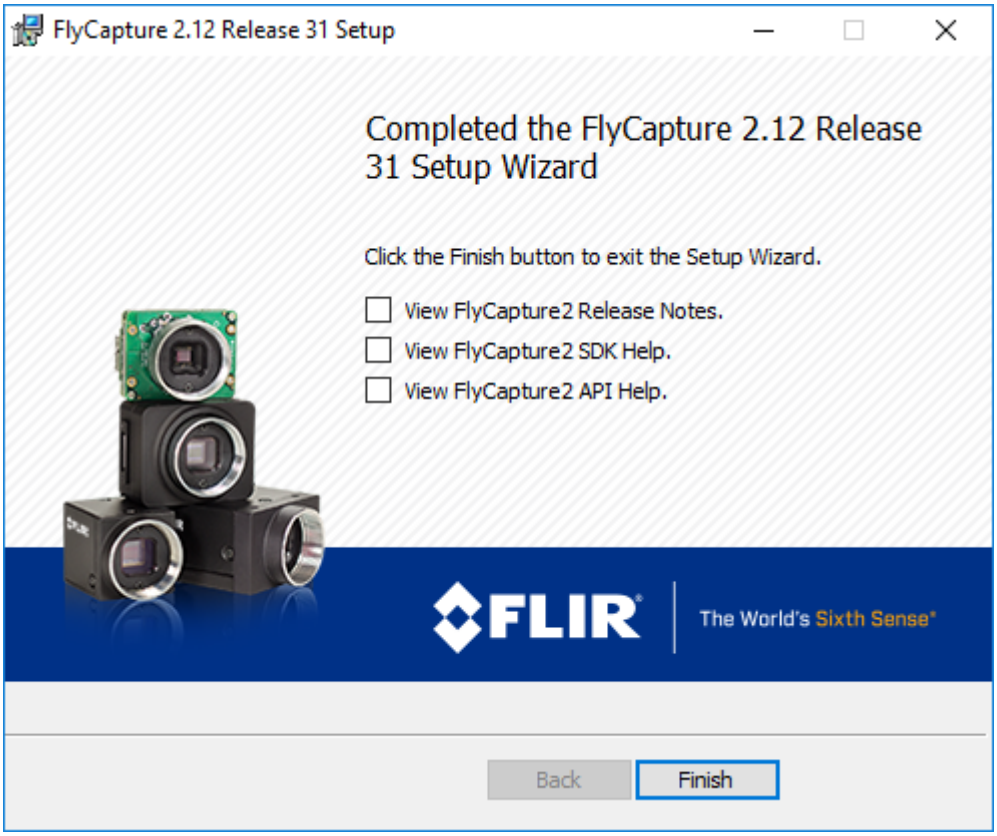


Click to register the dlls before proceeding.



Click 'Install' to begin.





If you wish to view the help files this is a good opportunity, otherwise click to finish.

Your software should now be ready to go, but we advise restarting your machine first to ensure the correct files are registered on your computer.

Shortcuts should be provided for you to run your software, but if this has not occurred due to local settings on your machine, then the HES1000.exe file can be found in the 'Program Files(x86)' directory.

The 'Operators Guide' provides full instructions on how to install your hardware.

3. Start the GUI

To start the HES1000 GUI click on the desktop icon or select 'Programs' via the START button in the Windows task bar and navigate to 'All Programs / ISI HES1000' (or under ISI HES1000 in Windows 10 from the Windows button).

This should open the main window GUI, as shown below in

.

Figure 1 Starting view of GUI

On first use a dialog box will appear asking for a 'Data Save Location'. This is the file path to the location where any files saved automatically. The software will create a directory with today's date to store the files. Note that when 'Save As' options are used, the files will be saved in a location of the user's choosing.

Afterwards a camera selection window will open (Figure 2).

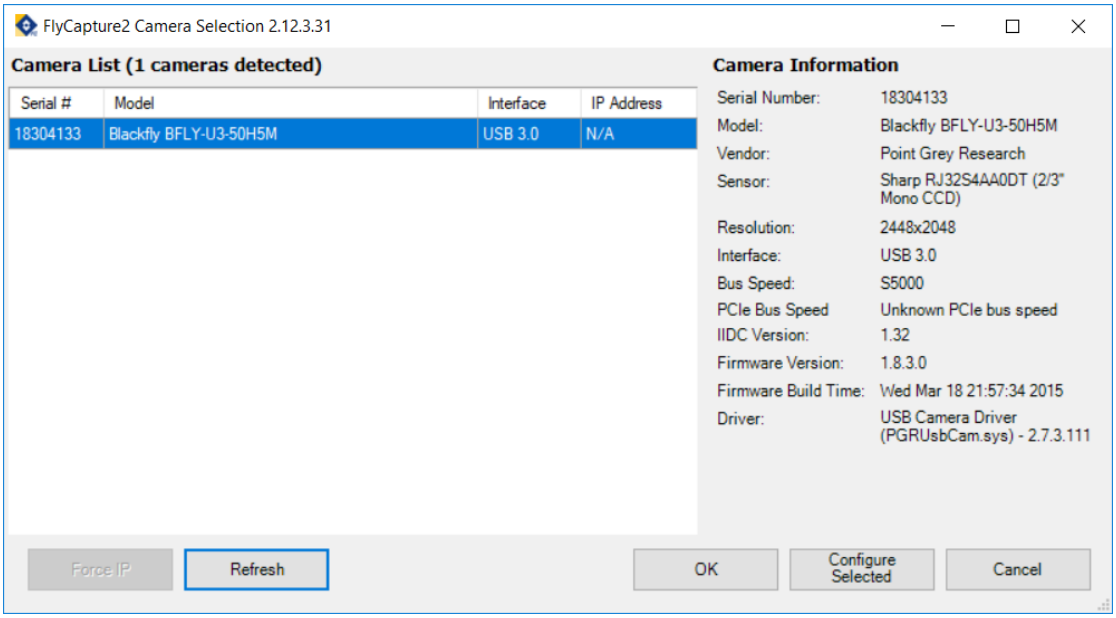


Figure 2 Camera Selection window

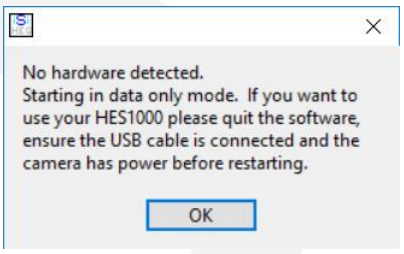
All the compatible cameras (FLIR/Point Grey) will be displayed in this window. Shown above is the correct model (Blackfly BFLY-U3050H5M). Ensure this is highlighted and click 'Configure Selected'. This will open another window that contains all the settings for the camera. This configuration window can also be opened from the main GUI to adjust the camera settings during operation. Details of how this can be used to configure your camera can be found in section 4.2. For now, it is best to go to the 'Custom Video Modes' tab and make the following changes:

- Pixel Format: Mono 16
- Image: Left – 0, Top – 975, Width – 2448, Height – 400

Click on 'Apply' and close the window. This returns you to the camera selection window (Figure 2). Click on 'OK' to proceed.

The software will then try to detect if your HES1000 is present. Please note that each installation contains calibration data for the HES1000 it was supplied with. Contact ISI if you wish to use more than one HES1000 on a single local machine.

If the software fails to detect a HES1000 a window appears saying "Error 3". You should click on 'continue' and then the following error message will appear:



If you are happy to proceed in 'Data Only' mode, then click 'OK' and begin investigating the files you have already saved. The HES1000 GUI provides this additional feature in that it can be used as a data viewing tool without needing the spectrometer to be present. It also allows basic data analysis techniques to be performed. The operation

of the software is identical to when a spectrometer is present, but with some functionality removed. Details of how to use this mode can be found in section 5.2.

If you were expecting the spectrometer to be detected then you should quit the software (section 7), check the USB connections, confirm the FlyCapture camera driver has been installed and restart the software. If the problem persists, please contact IS-Instruments Ltd.

With a HES1000 connected the GUI will appear slightly differently, with more controls enabled and some new ones appearing (Figure 3).

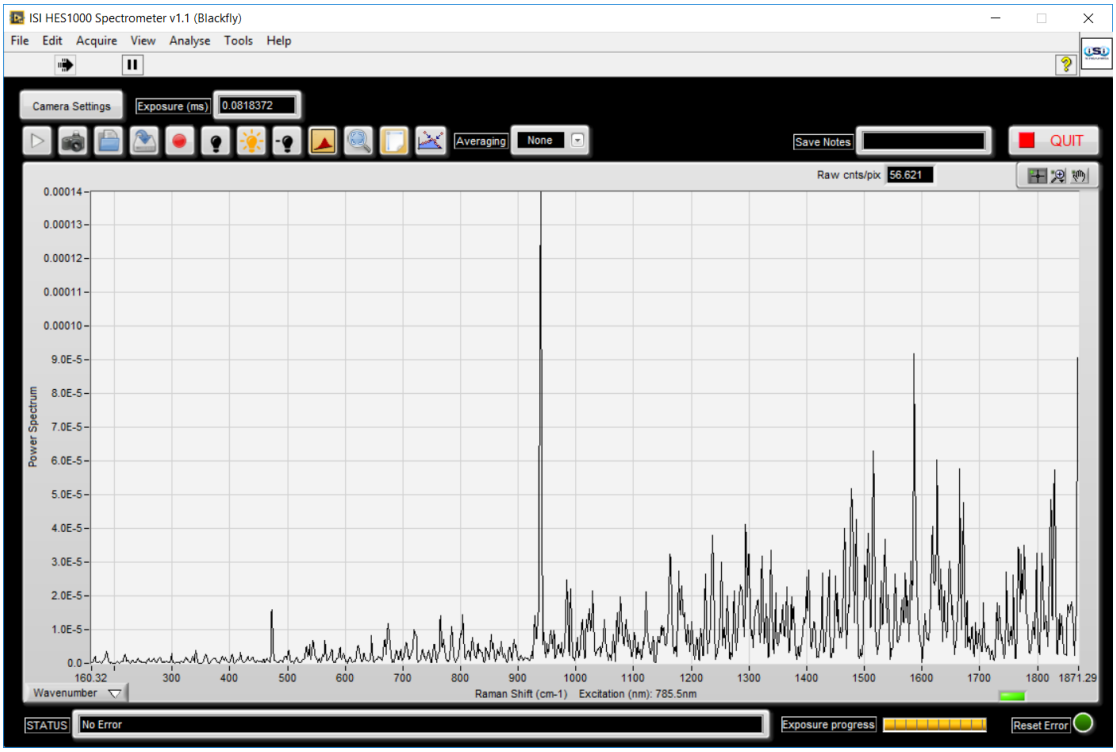


Figure 3 The GUI with a HES1000 connected

In this mode, the software will allow you to fully drive your HES1000 and provide the same functionality as the data only mode.

4. Operating your HES1000 software

With the GUI up and running your HES1000 will be just about ready for use.

4.1. Main Window Commands

The main window is your interface to your spectrometer. The various commands that you can use can be accessed via the menu bar, or by using some of the shortcut buttons provided. Some of these will only be available under certain conditions and may be disabled or completely disappear. Some of the commands are only available by clicking on the buttons, such as the 'Autoscaling' and 'Zoom Pop' commands. The various commands on each menu will be described below.

4.1.1. 'File' Menu

Command	Button	Description
Open Spectrum		Opens a previously saved spectrum
Open Image file	-	Opens a previously saved image file
Open Dark Image	-	Opens a previously saved dark image file
Overlay Spectrum	-	Opens a previously saved file and overlays it on the current display
Store Reference Spectrum		Stores the last acquired spectrum to a temporary storage location
Subtract Reference Spectrum	-	Subtracts the stored reference spectrum from the current display
Overlay Reference Spectrum	-	Overlays the stored reference spectrum on the current display
Delete Last Spectrum	-	Removes the last overlaid spectrum from the current display
Save		Saves last acquired intensity spectrum (.spec), power spectrum (.pspec) and raw image (.hes) image automatically to the selected data directory
Save As…	-	Saves the last acquired spectra & image (as above) to a user selected name and location
Save Dark Image		Saves the last acquired image as a dark image for future use & stores as dark frame
Record		Continuously saves the spectra (only) to the selected data directory
Data Location		Allows the user to adjust the location in which the data are automatically saved

File info	-	Displays the file header information for the last opened data file
Quit	QUIT	Shuts down the HES and closes the software

4.1.2. 'Edit' Menu

Command	Button	Description
Undo	-	Standard Windows operation
Redo	-	Standard Windows operation
Cut	-	Standard Windows operation
Copy	-	Standard Windows operation
Paste	-	Standard Windows operation

4.1.3. 'Acquire' Menu

Command	Button	Description
Start		Start to continually acquire spectra
Stop		Stop acquiring spectra
Snapshot		Acquires a single spectrum
Camera Settings	Camera Settings	See section 4.2
Save image	-	Continually save the raw image also if 'Record' is in use (advanced use only). Select to toggle on/off.
Dark Frame	-	Allows use of dark frames that are a common tool used to remove unwanted background/contaminants
Dark Frame > Store		Store a dark frame for background removal
Dark Frame > Apply		Subtract the dark spectrum from the current display
Apodise > [*options*]		Apply selected apodisation – see Appendix C

4.1.4. 'View Menu

Command	Button	Description

X-Axis	-	Allows you to set the x-axis
X-Axis>Wavelength	Wavelength	Set the spectra to be displayed in wavelength (nm). Click on arrow to switch to Wavenumber.
X-Axis>Wavenumber	Wavenumber	Set the spectra to be displayed in wavenumber (cm^{-1}). Click on arrow to switch to Wavelength.
Y-Axis	-	Allows user to set the y-axis
Y-Axis>Power Spectrum	-	Displays the power spectrum (default)
Y-Axis>Intensity Spectrum	-	Displays the intensity spectrum
Autoscale		Autoscales the spectrum display area (default is 'ON')
Zoom Pop		Stops the acquisition and 'pops' a window out to allow you to zoom in to the spectrum. See section 6.1.1.
Display	-	Allows you to view the data in different states of analysis
Display>Spectrum	-	The default mode. This displays the output spectrum
Display>Raw Image	-	Displays the output of the camera, an interferogram.
Display>FFT	-	Displays the output of a 2D FFT on the interferogram

4.1.5. 'Analyse' Menu

Command	Button	Description
Averaging	-	Allows you to apply averaging to the data in real time
Averaging>None		No averaging is applied
Averaging>Add		Add a set number of acquisitions together to produce a single spectrum
Averaging>Running Mean		Applies a running mean to consecutive spectra (also known as a rolling mean or moving average)
Averaging>Block Mean		Applies a block mean to the data (a set number of acquisitions are used to create a single result before starting a new block).
Averaging>Median		Applies a Median filter to the interferograms. Helps to remove transient events.
Averaging>Size	-	Allows you to set the number of acquisitions to be used in the ADD/MEAN
Median Filtering	-	Median filter the spectra in real time
Median Filtering>None	-	Remove Median spectral filtering
Median Filtering> Interferogram	-	Apply median filtering to an interferogram
Median Filtering> Spectrum	-	Apply median filtering to the spectra
Median Filtering>Rank	-	The amount of median filtering. A low rank is a small amount of filtering (0=none)

4.1.6. 'Tools' Menu

Command	Button	Description
Peaks	-	Allows you to automatically locate and label the peaks in your spectra
Peaks>Locate	-	A submenu for configuring the peak detection algorithm
Peaks>Locate>Threshold		Only peaks with heights above this level will be detected and labelled
Peaks>Locate>Width		The FWHM of the peaks to be detected
Peaks>Display		Displays the location or height of the peaks detected in your spectra
Peaks>Display>Location	-	Display the location of the peaks in wavelength/wavenumber
Peaks>Display>Height	-	Display the height of the peaks
Calibrate	-	Allows you to adjust the calibration of your HES1000 (advanced use only)
Calibrate>Adjust Coeffs	-	Prompts you to enter the new coefficients
Calibrate>View current	-	Only peaks with heights above this level will be detected and labelled

4.1.7. 'Help' Menu

Command	Button	Description
Instrument Setup	-	Displays the spectrometer's setup characteristics in a dialog box
About	-	Displays details about the software

4.2. Camera Settings

For the Blackfly camera, the manufacturer's configuration tool (Figure 4) had to be incorporated into the control software due to limitations in compatibility.

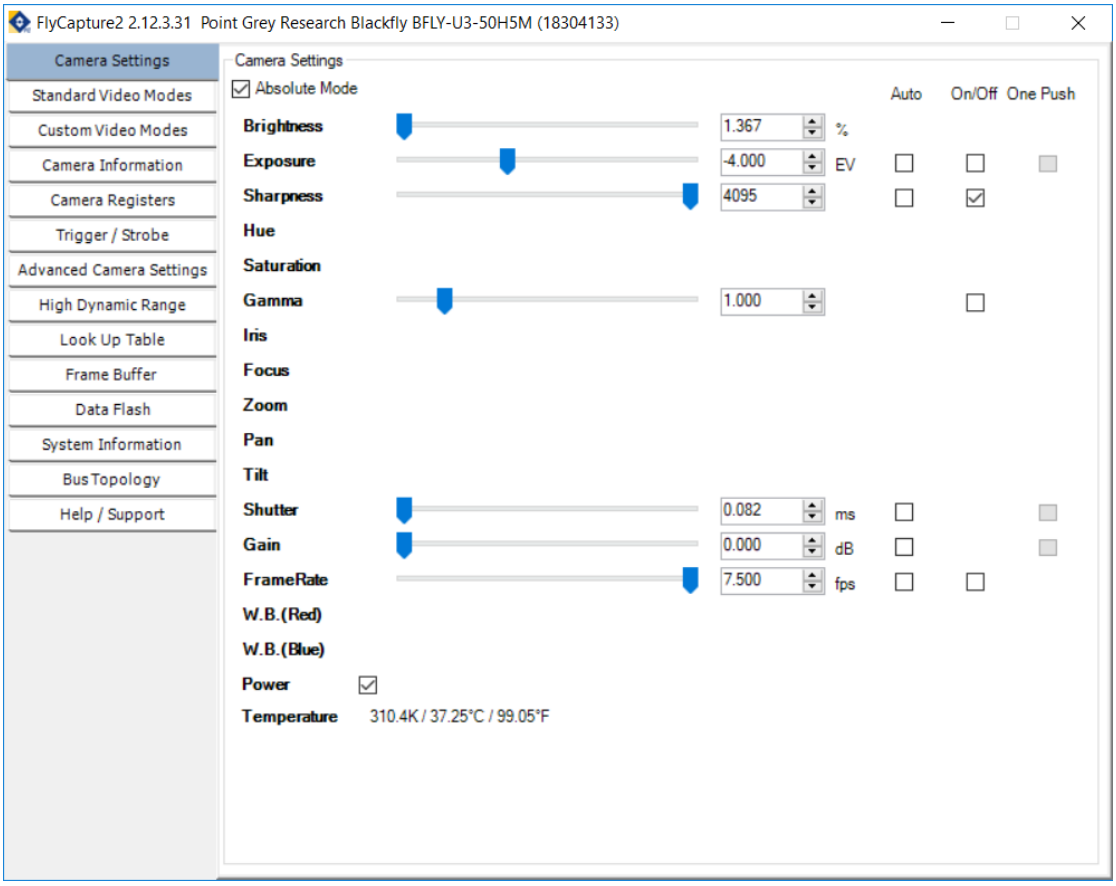


Figure 4 Manufacturer's camera configuration tool

This control window provides many features that are either unnecessary or detrimental to the operation of the camera inside the HES spectrometer. These controls have been turned off programmatically. These are Brightness and Exposure. If you accidentally switch them back on, they will be turned off automatically.

Sharpness, Gamma and Gain can provide useful enhancement of the data for signal to noise improvements but can introduce unwanted errors. FrameRate control has also been switched off as this can limit the measurement lengths available.

These features have been left enabled but can be adjusted by the user. Sharpness will be on and set to its maximum by default, Gamma, Gain and FrameRate will be switched off by default.

A full description of this and the camera selection tool can be found under FlyCapture SDK Help, which should be found in the START menu under 'Point Grey FlyCapture2 SDK>Documentation'. The main controls that should be used will be described below. Any other controls may affect the performance of the system and will not be documented. If the system becomes unstable, quit the software, unplug the camera from the PC, wait ~ 6s, replug the camera into the PC and restart the software. This should reset the camera to its default settings.

4.2.1. Camera Settings

The camera settings tab is the one which will be used most commonly. Full explanations of each control can be found in the SDK help, but the key controls here are:

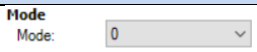
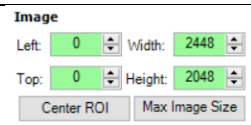
Shutter: Length of the measurement in milliseconds

Please note that adjustments on this tab take effect immediately, so care should be taken to avoid overexposure or prolonged unwanted measurements.

The system does, however, suffer some measurement lag. Usually, two images are acquired with the old settings, prior to the changes being made. For example, when the shutter is changed from 1 ms to 100 ms, 2 x 1ms images will be acquired and displayed, prior to the 100 ms images being available.

4.2.2. Custom Video Modes

This tab should be used initially to set up the camera, but not adjusted routinely. The key controls are described below:

Command	Button	Description
Mode		Enables the binning modes of the camera. Use of this feature is not recommended so Mode 0 should be selected.
Pixel Format		Allows the user to select the ADC bit depth of the camera. Due to compatibility limitations only Mono 8 & Mono 16 are recommended. Mono 16 will provide the best sensitivity.
Image		Allows the user to select a region of interest. The camera will only acquire data in the selected area, which can help reduce the influence of read noise as the data are only captured in a narrow letterbox on the detector. At manufacture the settings were: Left = 0 Width = 2448 Top = 975 Height = 400 User adjustment away from these values may limit performance or improve it.

The other controls should not be adjusted.

Adjustments to these controls only take effect once the 'Apply' button is clicked.

4.2.3. Updates

Whilst updates may become available for this camera driver, it is advised not to update without first contacting ISI, as the updated driver may be incompatible with your HES software.

4.3. Other controls

Whilst most of the controls have been covered in the previous section, a few have not been discussed as they do not have menu-based commands.

Text (e.g. experiment details) can be entered here that will be included in any data file that is saved.

If your software gets stuck, which can happen from time to time with USB devices, clicking on this can sometimes clear the problem. See Appendix A for help with troubleshooting.

There are also some indicators that provide useful information.

This will display the file path of either the last saved file or of the last opened file, depending on what you are doing at the time.

This will provide information on what is happening with your system at the moment.

	This gives you an indication of how many photons are being detected. In 2D mode it is the mean number of counts seen over the pixels of the camera (1600 x 1200 for IDS UI3250). .
	This indicates if the camera is possibly being over exposed. If so it will turn red and you should reduce either the exposure time or the amount of incident light immediately. Therefore, you should always start with a very low exposure (e.g. 1 ms) and slowly increase
	Shows the current exposure time
	Progress bar for current exposure

5. Acquiring Data

In order to acquire data successfully you should follow the guidelines detailed in the Operators Guide for the setup of your hardware before starting the software.

5.1. The Process

To acquire data the following sequence should be followed:

- Prepare hardware setup
- Ensure the HES1000 is powered
- Start the software
- Set Exposure to a small value (e.g. 1 ms) to ensure no overexposure
- Start the acquisition
- If the light levels are ok gradually increase exposure time to desired level
- Stop acquisition
- Adjust other settings to suit (e.g. averaging, filtering, save notes, etc.)
- Start acquisition

It is often beneficial to take a 'Dark Frame' to improve signal to noise. To do this ensure no light can enter the system (also remove fibre). Use a long exposure, e.g. 10 s, in the mode you wish to operate. When it has finished click on the 'Store Dark' button and then continue with your acquisitions. You can apply the dark frame subtraction by clicking on the 'Subtract Dark' button. The software automatically calculates the dark ratio to remove based on exposure time. **It is imperative that the image size (set by AOI) is the same for both Dark images and measurement.**

Once you have finished your data collection you can view the files in this package, but you may wish to shut down the system first and use it in 'Data Only' mode (section 5.2). The correct procedure to safely shut down your system is simply to make sure you click on the 'QUIT' button and wait for the software to stop switching off the power or removing the USB cable.

5.2. 'Data Only' mode

As described earlier your software can be used as a file viewer for previously saved data. If your software is operating in this mode, then the main window will appear as shown in

with the acquisition-based controls being disabled.

To view a data file either use one of the 'File>Open…' menu commands or click on the open file button (section 4.1.1). Navigate to the desired .spec, .pspec or .hes file and select it. You will have the ability to perform some basic analysis on this file and adjust the viewing options. See Appendix D for information on the file formats.

6. Data Display

Once the data have been acquired there are several options for displaying it. There are three types of data display, each with their own way of navigating and adjusting the display. These are accessed via the View>Display menu.

6.1. Spectrum

This is the default mode that the software will always start in. It displays the spectrum that has been calculated from the raw image collected by the HES1000 camera. An example of a spectrum is shown in Figure 5. It should be noted that by default the data is apodised to improve the quality of the spectrum gathered.

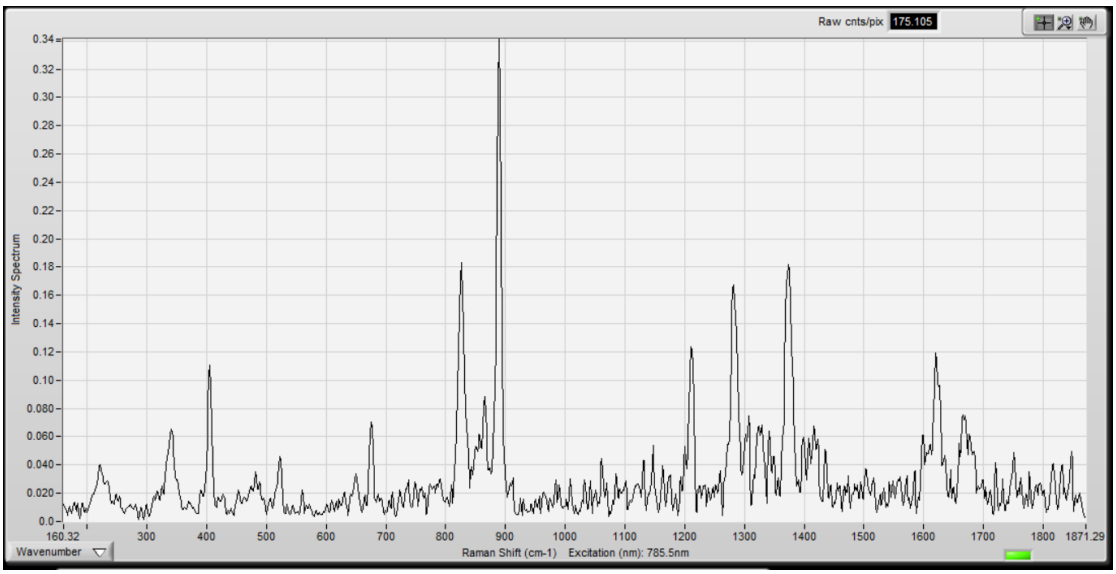


Figure 5 A paracetamol transmission Raman intensity spectrum taken by a HES1000 (1mm aperture 30s exposure without dark image subtracted).

In this display the Y-axis is a relative intensity or contrast. These values can be used to estimate the number of photons at a particular wavelength by multiplying by the number of pixels: 5 MPix for the full frame but reduced if ROI is used. This can be set as either the power spectrum, typical of Fourier Transform Spectrometers, or the intensity spectrum, typical of traditional dispersive spectrometers, by using the menu command (section 4.1.4). The system defaults to power spectral display.

The x-axis can be adjusted between wavelength (nm) and wavenumber (cm^{-1}) using either the menu command or button (section 4.1.4). The x-axis will then display the spectrum in the desired units.

By default, the display will have the 'Autoscale' option selected. This is designed to best display the data without the need for adjusting scales by hand, but sometimes it may not produce the best display. If this is the case, then switch it off by clicking on the button and begin manual adjustment. This can be done in several ways.

The first is to click on the start and/or end values on the scales and manually edit the values as required. The most efficient way is often to use the navigation tools at the bottom left of the display . These are described below.

	Not used
	Clicking on this provides several useful navigation options that allow you to zoom in/out in different manners. These are a window zoom, an x- and y-axis zoom, a zoom in and a zoom out. A reset option is also provided.
	Clicking on this allows you to move the data around inside the display by clicking and holding in the display area and moving the mouse around.

Another useful tool when viewing the data in this mode is the peak detection (section 4.1.6). This allows you to label the peaks in your data. Clicking on the peak detection button will label the peaks using the default settings. This may not be suitable for your data and the threshold and width may need adjusting. Typically adjusting the threshold level to be just above the noise level will provide the best results. The type of label can also be adjusted between location in the chosen x-axis and height (y-axis). An example of this is shown below in Figure 6.

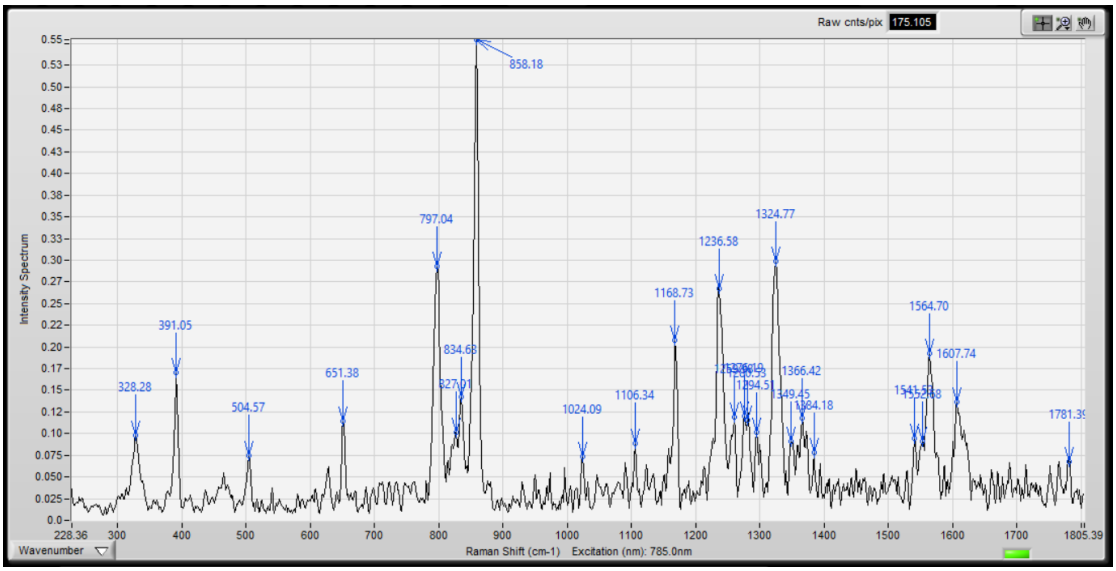


Figure 6 The paracetamol spectrum with some of the peaks labelled

The final display tool is the Zoom Pop.

6.1.1. Zoom Pop

This is a feature designed by us following discussions with some users about what they wanted to see in their software. The 'Zoom Pop' will stop the acquisition if it is in progress and will open a new display, as shown below in Figure 7. The spectrum is still displayed but in a slightly smaller window. On the right, a small window appears that will display sections of the spectrum in more detail.

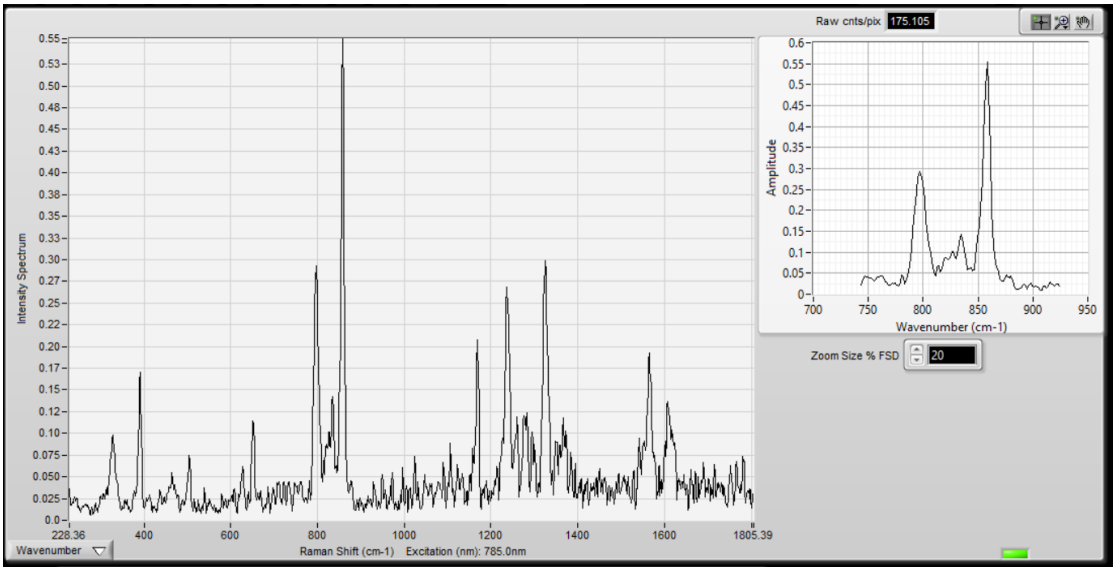


Figure 7 The Zoom Pop display

The size of this zoomed area can be adjusted using the provided control and the location is controlled by moving the mouse pointer across the spectrum in the larger window. This display autoscales to the data. To return to the standard mode simply click on the button once more.

6.2. Raw Image

This mode displays the raw data collected by the camera and is not designed for everyday use. These data are an interferogram. However, all cameras have intrinsic noise and one of the main contributors is read noise, potentially reducing the SNR. This can be optimised by using the AOI, which can be set in the 'Acquire' menu. This allows the user to specify the region in which the data are being collected and not process extraneous data, potentially adding extra noise. An example of an apodised interferogram is provided in Figure 8.

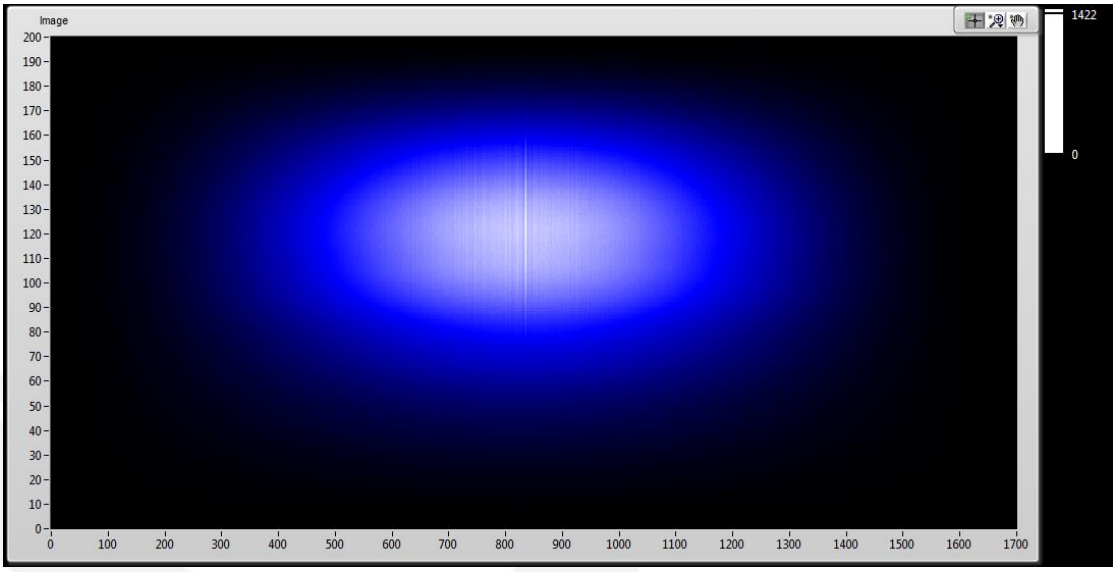


Figure 8 Interferogram (produced by HES2000)

As with the spectrum navigation, the axis values can be manually adjusted by clicking on the values and editing. Similarly, the navigation tools at the bottom left of the display can be used in the same manner. The only main difference is the inclusion of an intensity scale on the right of the display. This provides the colour ramp for the data and can be adjusted in the same manner as the x- and y-axes. However, it is set by default to autoscale so if you wish to adjust the values you will first have to switch off the autoscaling on this colour ramp. This is done by right-clicking on the colour ramp and unchecking the 'Autoscale' option. You can now manually edit the top and bottom values.

6.3. FFT

This option displays the results of a 2D Fast Fourier Transform (FFT) on the interferogram in pixel space. Figure 9 shows an example of this display.

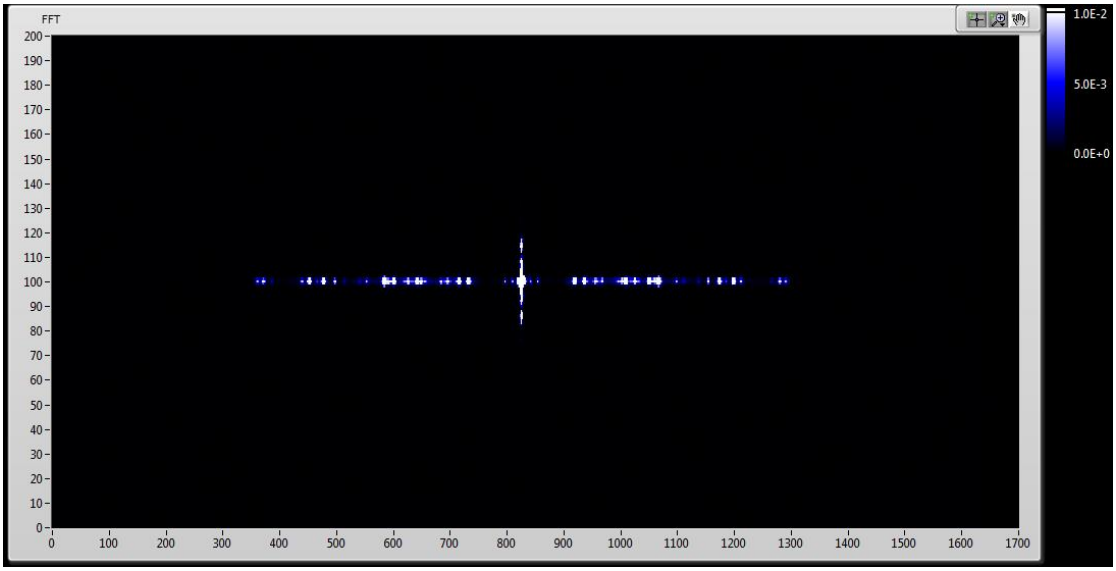


Figure 9 FFT of the above 2D interferogram

This display is navigated in the same manner as the raw image, but the colour ramp is not autoscaled. The reason for this is that the central peak values of the FFT are extremely high compared with the interesting data. Therefore, the display will load with nominal values that often produce a good display, but this will depend heavily on your SNR and incident light levels. Typical maximum values range from 100's for very high signals, down to 1E-5 for weak signals.

7. All done

That's it. We hope your HES1000 performs as you hope and delivers the capability you require. If you have any problems, we'll be happy to help.

Appendix A: Troubleshooting

If you follow the instructions provided you should not experience any problems. However, should a problem occur please check out this section for advice on how to fix it. If nothing in here helps, then please contact us and we'll try to resolve the problem as quickly as possible.

Problem: When I run the software the 'Run' button is disabled

Cause 1: Spectrometer connected before installing software

Solution: Remove the Unknown Device from Windows Device Manager

1. Open Windows Device Manager. This is done through the Control Panel. If you are unsure how to get to this check out the Windows help.
2. Locate the Other Devices option and expand the Other Devices selection by clicking on the "+" sign to the immediate left.
3. Locate the unknown device (marked with a large question mark). Right-click on the Unknown Device listing and select the Uninstall or Remove option.
4. Click the OK button to continue. A warning box appears confirming the removal of the Unknown Device. Click the OK button to confirm the device removal.
5. Disconnect the HES spectrometer USB cable connecting from your computer.
6. Uninstall the software (if you have already installed it)
7. Reinstall the software

Cause 2: The software has not recognized the HES is connected

Solution: Confirm the HES spectrometer is connected by the USB cable

Cause 3: The USB port has become 'jammed'

Solution: USB ports frequently become jammed if devices are plugged/unplugged frequently or software crashes. The easiest way to solve this is to reboot the PC but often closing the software, unplugging then reinserting the USB cable and then restarting the software will do the job.

Problem: When I run the software, it can't find HES1000.ini and stops working

Cause: The file has either not been installed properly, moved or corrupted

Solution: Copy the file from the installation stick/location into the installed directory

Appendix B: Calibration

Though your HES spectrometer is calibrated at ISI, like all spectrometers this calibration can drift over time due to several reasons, such as environmental conditions.

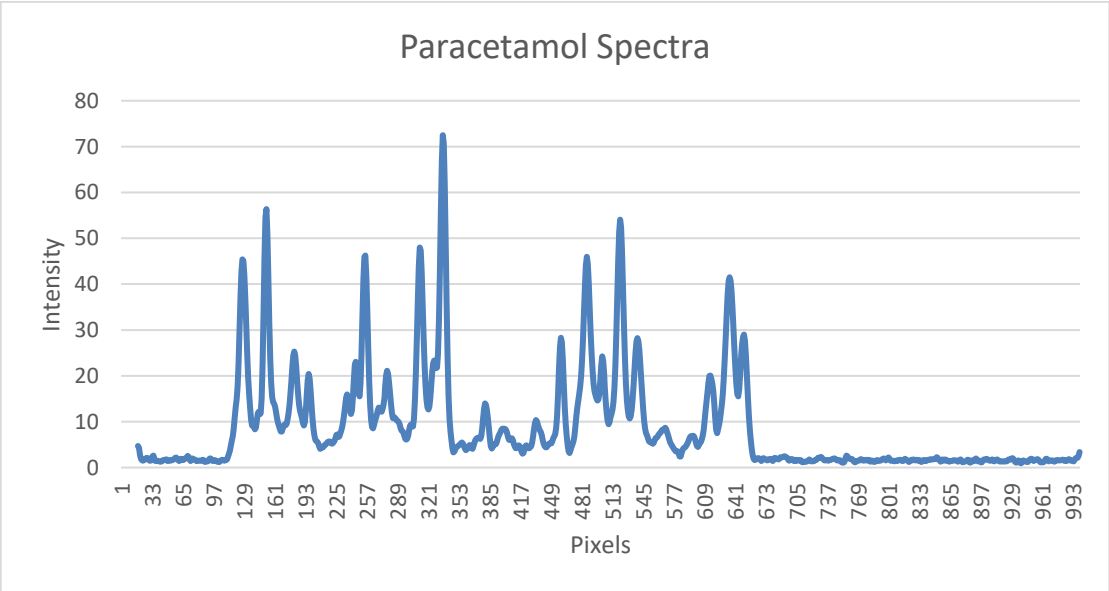
As the HES spectrometer is based around diffraction gratings the only coefficient likely to ever need changing (assuming correct use) is the Littrow Wavelength. This is the wavelength of incident light that will be reflected straight back.

If you feel that the calibration has drifted, then you can adjust this by clicking on the 'Tools>Calibrate>Adjust Coeffs' menu item. Any changes you make cannot be undone, so please make notes of previous calibration coefficients in case of a problem. This will be saved into the configuration file and used going forward. If this file becomes corrupt it be reloaded from the installation stick or a copy requested from ISI (info@is-instruments.com).

It should be noted that if the instrument is to be used for Raman measurements the Littrow wavelength of the spectrometer and the Raman laser wavelength will need to be entered.

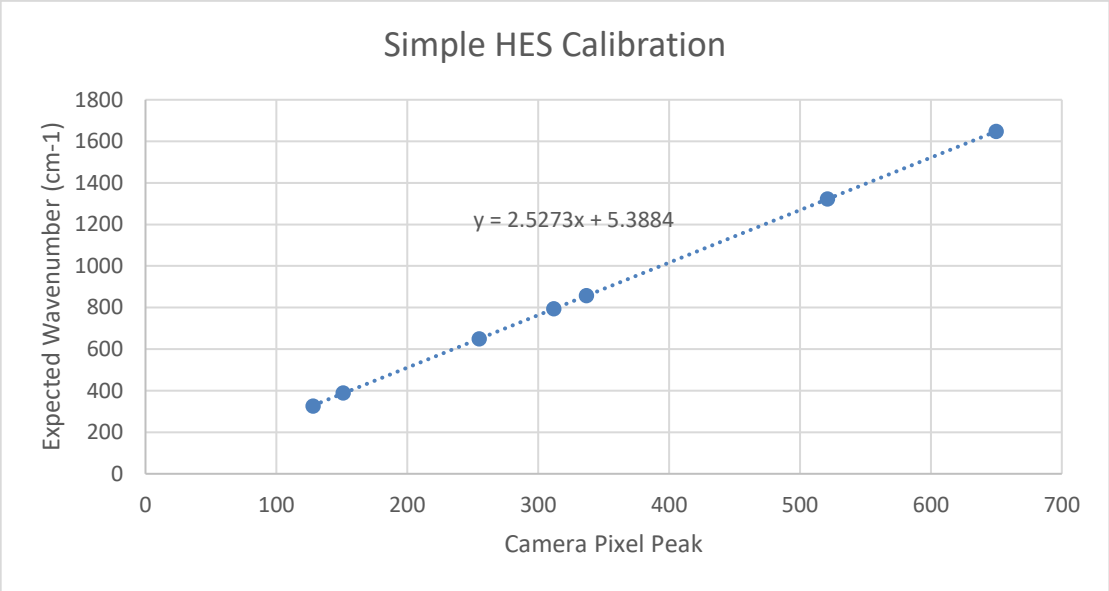
If your system is fitted with an alignment option (detailed in the operator guide) then adjustment of this will require an update of the calibration coefficients. This is most likely to affect the Littrow wavelength (the wavelength at which the Littrow condition applies for each grating).

The value for the Littrow wavelength can be determined either by trial and error adjustment to match known calibration peaks, or by plotting the position of the known calibration peaks from an output spectrum (in pixel space) against the expected wavenumber. For example, if a paracetamol spectrum were used…



Pixel Peak	Expected Wavenumber (cm-1)
128	326
151	389
255	650
312	795
337	857
521	1323
650	1647

Now plot the Pixel peaks vs expected wavenumber and use a linear fit to determine the gradient and intercept:



The gradient (2.53 in the example above) is the wavenumber resolution obtained by the system per pixel. The intercept (5.4 in the example above) is the Littrow wavelength (λ_L) expressed as a Raman shift (Δw in cm-1) from the excitation wavelength (λ_0).

$$\Delta w = \left(\frac{1}{\lambda_0} - \frac{1}{\lambda_L}\right)$$

So…

$$\lambda_L = \frac{1}{\left(\frac{1}{\lambda_0} - \Delta w\right)}$$

Therefore, in the example above:

$$\lambda_L = 785.31\ nm$$

This can then be entered as the new Littrow wavelength in the calibration coefficients. The other coefficient should not be adjusted without first consulting IS-Instruments.

Appendix C: Apodisation

Apodisation is a technique to apply a window function to an image. This sets all values to zero outside this window area. It is commonly used to improve data quality and suppress noise effects, especially in Fourier transform spectrometers. By default, apodisation is enabled in this software using a Hanning window. Several window functions are available. Some are described below.

Hanning (Hann) Window

If *y* represents the output sequence **Windowed X**, the Hanning Window obtains the elements of *y* using

$$y_i = 0.5x_i[1 - \cos w]$$

for *i* = 0, 1, 2, …, *n* – 1,

where *n* is the number of elements in **X**.

Hamming Window

If *y* represents the output sequence **Windowed X**, the Hamming Window obtains the elements of *y* from

$$y_i = x_i[0.54 - 0.46 \cos w]$$

for *i* = 0, 1, 2, …, *n* – 1,

where *n* is the number of elements in the input sequence **X**.

Blackman-Harris Window

If *y* represents the output sequence **Windowed X**, the Blackman-Harris Window obtains the elements of *y* using the following formula:

$$y_i = x_i[0.42323 - 0.49755\cos w + 0.07922 \cos 2w]$$

for $i = 0, 1, 2, \ldots, n-1$

where n is the number of elements in $\mathbf{X}$ and $w = \frac{2\pi i}{n}$.

Exact Blackman Window

If *y* represents the output sequence **Windowed X**, the Exact Blackman Window obtains the elements of *y* using the following formula:

$$y_i = x_i\left[\frac{7938}{18608} - \frac{9240}{18608}\cos w + \frac{1430}{18608}\cos 2w\right]$$

for $i = 0, 1, 2, \ldots, n-1$

where n is the number of elements in $\mathbf{X}$ and $w = \frac{2\pi i}{n}$.

Blackman Window

If *y* represents the output sequence **Windowed X**, the Blackman Window obtains the elements of *y* using the following formula:

$$y_i = x_i[0.42 - 0.50\cos w + 0.08\cos 2w]$$

for $i = 0, 1, 2, \ldots, n-1$

where n is the number of elements in $\mathbf{X}$ and $w = \frac{2\pi i}{n}$.

Flat Top Window

If *y* represents the output sequence **Windowed X**, the Flat Top Window obtains the elements of *y* using the following formula:

$$\begin{aligned} y_i = x_i[&0.21557895 \\ &- 0.41663158\cos w + 0.277263158\cos 2w \\ &- 0.083578947\cos 3w + 0.006947368\cos 4w] \end{aligned}$$

for $i = 0, 1, 2, \ldots, n-1$

where n is the number of elements in $\mathbf{X}$ and $w = \frac{2\pi i}{n}$.

Appendix D – File Format

Example files are partly reproduced below:

Spectrum file (.spec/.pspec)

ISI HES1000	
150914_125024.185	Time YYMMDD_hhmmss.ms
Exp: 1.000000	Exposure in seconds
Littrow: 784.800000	Littrow wavelength
Laser: 785.000000	Laser wavelength
Cal: 14.950000	Calibration coeff
Window: 1	Window (Apodising used)
Averaging: None: 1	Averaging type & number

Header – this includes the date and time, configuration and calibration information plus the contents of the 'Save Notes'

[data]

784.800000	-9.7342	
784.971578	-6.949066	
785.143232	-4.163908	
785.314961	-1.378749	
785.486764	1.406409	2.964024
785.658643	4.191568	1.692935
785.830598	6.976726	0.258375
786.002627	9.761885	0.486264
786.174732	12.547043	0.446257
786.346912	15.332202	0.180656
786.519168	18.117360	0.218201
786.691499	20.902518	0.149626
786.863905	23.687677	0.177486

Data section

Contains three columns each of data

Wavelength (nm), wavenumber(cm^{-1}), relative intensity/power

Image File (.hes) & Dark Image file (.dark)

ISI HES1000

150914_125024.185 — Time YYMMDD_hhmmss.ms

Exp: 1.000000 — Exposure in seconds

Littrow: 784.800000 — Littrow wavelength

Laser: 785.000000 — Laser wavelength

Cal: 14.950000 — Calibration coeff

Window: 1 — Window (Apodising used)

Averaging: None: 1 — Averaging type & number

Header – this includes the date and time, configuration and calibration information plus the contents of the 'Save Notes'

[data]

531	530	532	532	530							
532	531	531	533	533							
532	533	533	533	533							
533	533	533	533	533							
533	535	534	534	534	535	535	534	534	537	536	537
537	537	538	539	537	540	541	543	544	545	543	546
547	547	547	551	551	554	556	560	559	563	561	562
567	569	571	573	574	574	580	580	586	589	590	591
594	600	600	600	604	603	601	610	609	617	609	616
616	619	619	618	616	622	627	628	630	633	639	636
639	643	654	660	655	658	655	664	660	669	676	668
671	681	674	675	687	695	687	693	700	699	696	699

….

Data section

This will be multiple columns corresponding to the rows and columns of the pixels in the detector