

ifm_0403.pxp

Version 2004 – 03

Neutron Interferometry Data Analysis, Script for Igor Pro 4.04

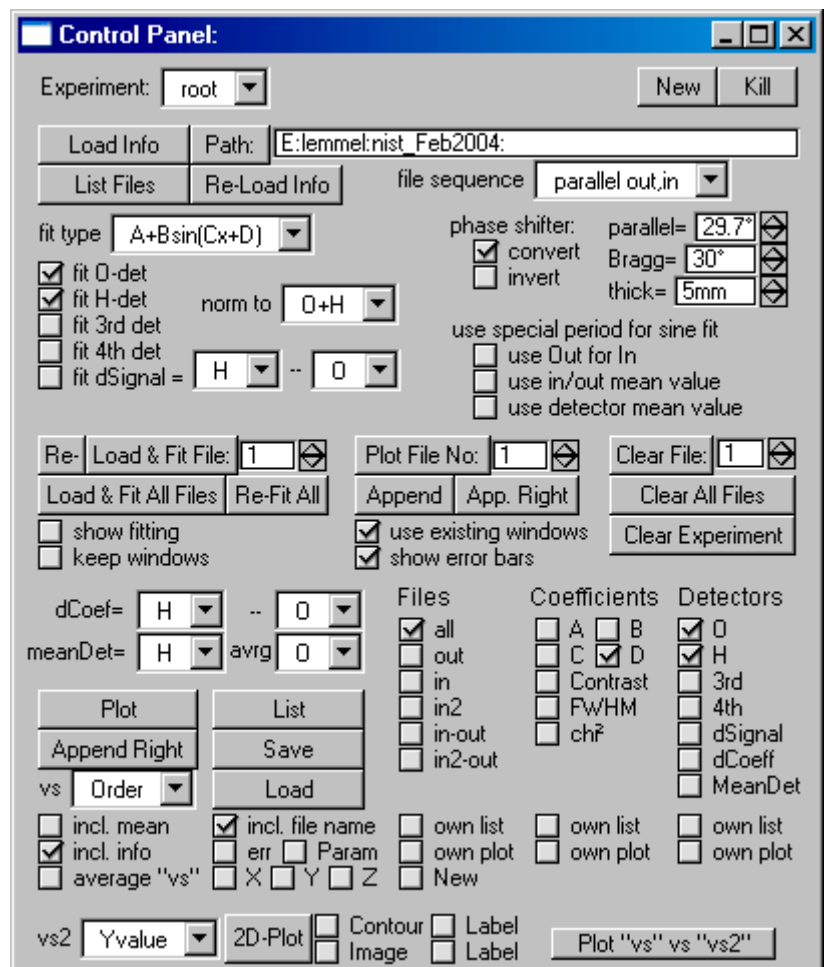
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Features:

- loading of data files (ILL ascii files and NIST excel files)
- plotting of data files
- automatic fitting
 - sine fit for interferograms
 - gauss fit for adjustment scans
- post processing of the fit parameters
- generating plots and tables

User's Guide

Start Igor and load IFM.pxp. If you don't see this window, select the menu command "Windows – Panel Macros – Control". (Note that the Procedure Window must be closed, otherwise Igor does not execute macros.)



Select Data

Experiment

In Igor 4.04 it is not possible to open multiple Igor Experiments simultaneously. Therefore the IFM script was built to maintain multiple sets of data, now referred to as "Experiments". The root experiment contains global control data. Always click on **New** to make a new experiment for your own data. The currently displayed experiment serves as a template for the new one. Click on **Kill** to delete an experiment.

Path

Select the path to your data directory.

Load Info

Select either an ILL info file (*.inf)

Format: ASCII file with tab separated columns containing data file name, order number and up to four changing parameters (loaded as "Param", "Xvalue", "Yvalue", "Zvalue"), e.g.

```
r2p1_drehserie11_1_out.dat  1.000000  111.000032
r2p1_drehserie11_1_in.dat  1.000000  111.000032
r2p1_drehserie11_2_out.dat  2.000000  111.099907
r2p1_drehserie11_2_in.dat  2.000000  111.099907
r2p1_drehserie11_3_out.dat  3.000000  111.199782
r2p1_drehserie11_3_in.dat  3.000000  111.199782
```

or a NIST excel file (*.xls). The values of the "OuterLoop" (if present) are loaded as "Param".

At this point no actual data is loaded but just the list of data files names.

List Files

Display a list of all data files (or excel data sheets)

Re-Load Info

Re-load the info/excel file in case you have added more data files/excel sheets.

file sequence

Specifies the sequence of data files for sample in/out scans .

parallel	The In and Out scans where taken simultaneously by moving the sample in and out for each phase shifter position.
serial	The In and Out scans where taken one after the other.
out,in	file 1 = out, file2 = in, file 3 = out, etc.
out,in1,in2	file 1 = out, file 2 = sample in beam I, file 3 = sample in beam II, file 4 = out, etc.
in,out	file 1 = in, file 2 = out, file3 = in etc.
out,in,...out	file 1 = out, file 2 = in, etc. and the last file is out again. For excel files, the first out scan is expected in a data sheet named "Data Sheet 0".

Select Fit Options

fit type

Chose either sinusoidal " $A+B\sin(Cx+D)$ " or gaussian " $A+B\exp(-(x-C)^2/D^2)$ ".

[x] fit ... det

Select the detector curves to be fitted. The meaning of "3rd" and "4th" depends on your data files. "3rd" usually contains O+H.

"dSignal" can be defined as any difference between two of the real data curves.

norm to

The data can be normalized to O+H or Monitor. This is done right after loading, before fitting.

phase shifter angle

[x] convert If ticked the phase shifter angle ϵ will be converted to the optical path length

$$D = \text{thick} / (\cos(\text{bragg} + (\epsilon - \text{parallel})) - \cos(\text{bragg} - (\epsilon - \text{parallel})))$$

parallel = phase shifter angle where the phase shifter is in parallel position.

Bragg = Bragg angle

thick = thickness of the phaseshifter

[x] invert Invert the phase shifter angle. This results in an inverted phase shift. It is needed to compare measurements with different positions of the phase shifter (before or after the mirror plate).

use special period for sine fit

[x] use Out for In: Use the period of your sample-out scan for the sample-in scan (which may have a lousy contrast)

[x] use in /out mean value: Fit In and Out data separately, average over the periods and re-fit

[x] use detector mean value: Average the period over all selected detectors and re-fit.

Note that the error calculation may not be correct if one of this options is ticked because the fit routine assumes that a constant fit parameter has an exact value without error.

Load & Fit File:

Select a single data file from an Open File Dialog. The file is loaded at the the given position within the file list and the selected fits are performed. If you select an excel file only the first data sheet is loaded.

Re- (Load & Fit File:)

Same as above without the Open File Dialog. The file name for the given file number must have been specified before.

Load & Fit All Files

All data files / excel sheets given in the file list (see List Files) are loaded from the disk and the selected fits are performed.

Re-Fit All

Recalculate the fits after changing the fit options. Note that you must also re-load the data if you have changed the normalization or the phase shifter conversion.

If you want to load data without fitting deselect all checkboxes "fit ...-det".

[x] show fitting

Displays a plot showing the fitting process.

[x] keep windows

Keep all fitting plots in separate windows. Otherwise each plot overwrites the previous one.

Plot Measurements

Plot File No.

All detectors selected on the bottom right side of the Control Panel are plotted for the selected data file.

Append

The plot is added to the currently selected graphics window

Append Right

The plot is added to the currently selected graphics window but the vertical axis is displayed on the right side. It can be scaled independently.

[x] use existing windows

If selected, only one graphics window will be created. Every new plot overwrites the old one.

Clear File:

deletes the data of the given file

Clear All Files

deletes all file data

Clear Experiment

deletes all file data and all fit parameters. Similar to **Kill + New** experiment.

Analyzing Fit Results

The fit parameters of all files in the current experiment can be plotted or listed in a table. Use the checkboxes to select which fit coefficients for which detector curves and for which files types you want to see.

Files

Chose "all" if you have no sample in/out measurement. Otherwise select the files you want to evaluate. Select "in-out" to evaluate the difference between sample in and sample out parameters (e.g. phase shift).

Coefficients

The parameters A to D refer to the formula given in the fit type. The Contrast is valid only for sine fits, the FWHM is valid only for gaussian fits.

Detectors

In addition to the fittable detector curves you can select "dCoeff" and "meanDet".

dCoeff=

Can be defined as the difference of the fit parameters of any two detectors.

meanDet=

Can be defined as the weighed mean value of the fit parameters of any two detectors.

[x] own list, [x] own plot

For each checkbox column you can chose if the selected options are listed/plotted together in one single window or in different ones.

Plot

Creates a plot of the selected fit parameters. The checkbox "use existing window" below the "Plot File No." button also applies here.

Append Right

The plot is added to the currently selected graphics window with the vertical axis on the right side for independent scaling.

vs Order/Time/Param/Xvalue/Yvalue/Zvalue: Chose the type of the horizontal axis. Param, X, Y and Z refer to the values listed in the info file.

[x] incl. mean: the mean value of all plotted points is calculated and displayed in the plot

[x] incl. info: the name of the info/excel file is displayed in the top right corner

[x] average "vs": e.g. plot vs. Param: If you have more than one file per Param value, the mean value is calculated and displayed as a textbox for each Param value.

List

Creates a table showing all selected parameters.

[x] incl. file name: Creates a column with the data file names.

[x] err: Each parameter column is followed by a column with its error.

[x] Param, X, Y, Z: Creates additional columns with the selected parameters.

Save

Save all selected parameters in an ASCII file. If you enter a new file name the Igor Wave Names are saved in the first line. If the file already exists the data will be appended. This feature allows to combine the results of different experiments. Each of the selected file types (in/out/in-out/...) will be stored in a different ASCII file.

Load

Loads a previously saved ASCII file.

2D-Plot

Makes a Contour or Image Plot versus the parameters selected in "vs" and "vs2".

Plot "vs" vs "vs2":

plots the parameter selected in "vs" versus the parameter selected in "vs2".

Examples

Interferometer Adjustment (Bragg Peak)

- create a new experiment by clicking on **New**
- deselect all **fit ...-det** options
- deselect **phase shifter angle: convert**
- **Load & Fit File: 1**
- chose you rocking curve (excel or ascii file) which is for example a rough scan
- select the **Detectors O, H and 3rd** (3rd usually contains the sum of O+H)
- **Plot File No: 1**

Let's assume you have made another scan which is a fine scan of the peak region.

- select **fit type: $A+B\exp(-(x-C)^2/D^2)$**
- select **fit 3rd det** (sum of O+H)
- **Load & Fit File: 2** and chose the data file of the second scan
- **Plot File No: 2**
- If you want to see both plots besides each other make sure that **use existing windows** is deselected.

Now display the values of the fit parameters:

- **Files: all**
- **Coefficients: C** (center of gaussian) and **FWHM** (full width at half maximum)
- **Detectors: 3rd**
- **List**

Plot both scans in one graphics window

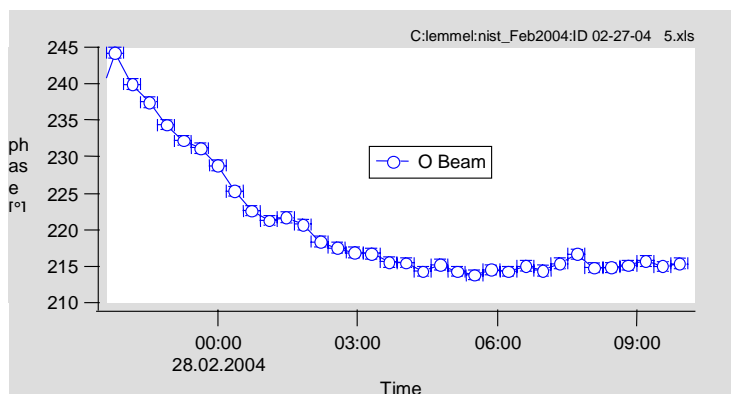
- **Plot File No: 1**
- **Append, 2**
- If both files have different vertical scalings (e.g. because of different measuring times per point) use **Append Right** instead of **Append**. Now each axis can be scales independently. Double click on one axis, select the tab **Axis Range** and enter the range.

Series of contrast scans with empty interferometer

- create a new experiment
- **Load Info**, chose your info or excel file
- **fit type: $A+B\sin(Cx+D)$**
- select **fit O-det, fit H-det**
- **norm to: O+H**
- **phase shifter angle:** select **convert** and enter the parallel position, bragg angle and phase shifter thickness
- **Load & Fit All Files**

Now plot the phase development over time

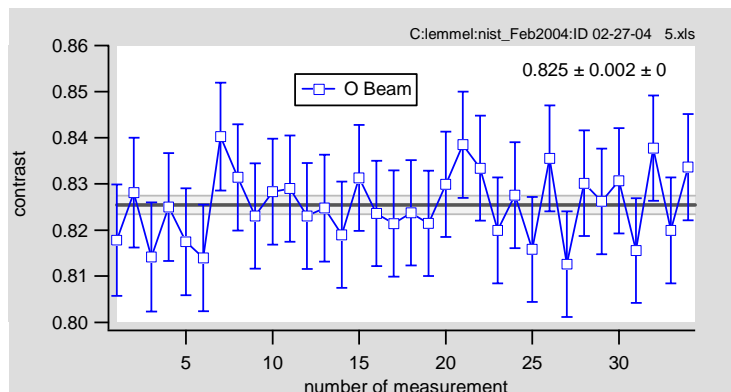
- **Files: all**
- **Coefficients: D (phase)**
- **Detectors: O**
- **vs: Time**
- **Plot**



Now plot the contrast with mean value

- **Files: all**
- **Coefficients: Contrast**
- **Detectors: O**
- **vs: Order**
- **[x] incl. mean**
- **Plot**

The mean value is indicated by a black line with a gray error bar.



Scanning the interferometer blades

Assume you have scanned your interferometer blade to find place with the best contrast. Create a new experiment and load the info file. If you click on List it should look like this:

File_Name	Order	Yvalue	Zvalue
mean value	0		
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 1	1	-5	-3
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 2	2	-4	-3
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 3	3	-3	-3
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 4	4	-2	-3
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 5	5	-1	-3
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 6	6	0	-3
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 7	7	1	-3
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 8	8	2	-3
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 9	9	3	-3
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 10	10	4	-3
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 11	11	5	-3
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 12	12	-5	-1.5
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 13	13	-4	-1.5
E:\lemmel:nist_Feb2004:ID 02-06-04 6.xls;Data Sheet 14	14	-3	-1.5
etc.	etc.	etc.	etc.

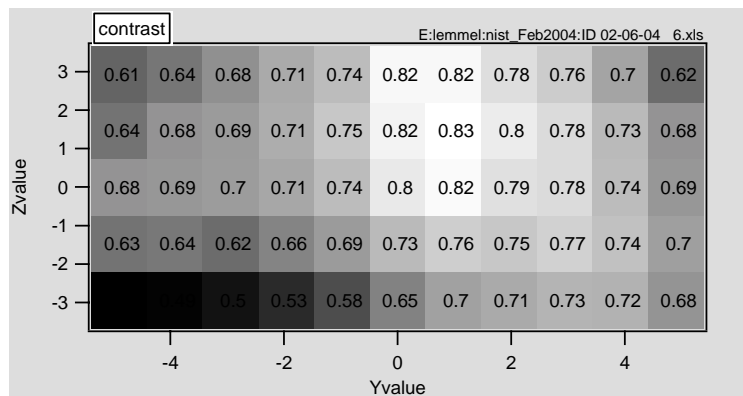
Fit a sine curve in each contrast scan as described in the previous example.

Now display the results:

- **Files: all**
- **Coefficients: Contrast**
- **Detectors: O**

Besides the **2D-Plot** button select

- **Image**
- **Image Label**
- Click on **2D-Plot**

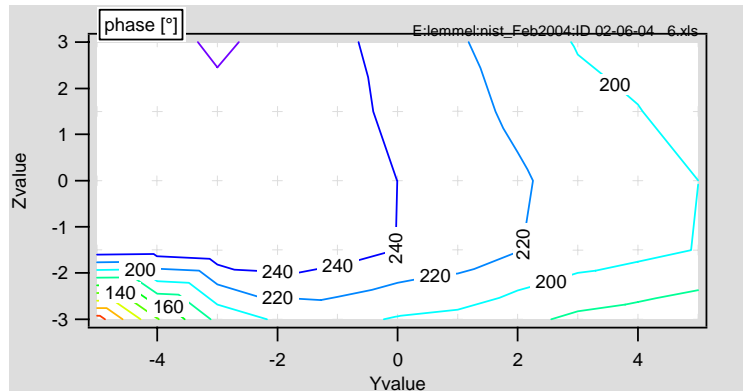


Example for another plot type:

- **Files: all**
- **Coefficients: D (phase)**
- **Detectors: O**

Besides the **2D-Plot** button select

- **Contour**
- **Contour Label**
- Click on **2D-Plot**



Both plot types can also be combined.

If necessary the plot can be mirrored.

Double click on the axis. In the dialog box select **Axis Range** and **Reverse axis**.

Series of scans with sample in and out

- select the **file sequence** depending on your measurements
- repeat the steps of the previous example to load and fit the data

Plot the contrast you got with and without sample:

- **Files: out and in**
- **Coefficients: Contrast**
- **Detectors: O**
- **Plot**

Plot the phase shift between sample in and sample out:

- **Files: in-out**
- **Coefficients: D (phase)**
- **Detectors: O, H**
- select **incl mean** to display the mean value in the plot
- **Plot**

Plot the weighed mean value of the phase shift in beam O and H:

- define **dCoef = O avrg H**
- **Detectors: dCoeff**
- **Plot**

Display mean values and errors:

- select **incl. error**
- **List**

The first line always contains the mean value \bar{x} of the whole column. The first element of the error column contains the the statistical error $\bar{\sigma}_{stat}$ of the mean value. In order to check if the single values are grouped nicely around the mean value a kind of weighed standard deviation $\bar{\sigma}_{dev}$ is calculated (S. Brandt, Datenanalyse, 1999 Spektrum Akademischer Verlag). It is stored in an additional element appended to the error column. If this value exceeds the statistical error the difference is called systematic error $\bar{\sigma}_{sys}$. Otherwise $\bar{\sigma}_{sys}$ is set to zero. The mean values displayed in the plots are given as $\bar{x} \pm \bar{\sigma}_{stat} \pm \bar{\sigma}_{sys}$.

$$\bar{x} = \frac{\sum_i \frac{x_i}{\sigma_i^2}}{\sum_i \frac{1}{\sigma_i^2}} \quad \bar{\sigma}_{stat} = \sqrt{\frac{1}{\sum_i \frac{1}{\sigma_i^2}}} \quad \bar{\sigma}_{dev} = \sqrt{\frac{\sum_i \frac{(x_i - \bar{x})^2}{\sigma_i^2}}{(N-1) \cdot \sum_i \frac{1}{\sigma_i^2}}} \quad \bar{\sigma}_{sys} = \max(0, \bar{\sigma}_{dev} - \bar{\sigma}_{stat})$$

Scans with changing sample parameter

Assume

- you have a changing sample parameter, e.g. sample angle
- one series of scans (=experiment) consists of one pair of in/out scans per sample angle
- you have done several series and want to calculate the average result for each sample angle.

First combine all experiments to one:

With ILL info files:

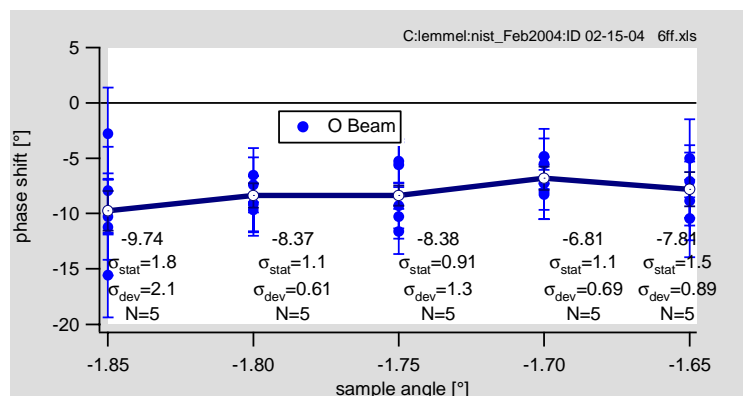
- copy the contents of all info files into a single one

With NIST excel files:

- copy all data sheets into one excel file
- rename all copied sheets to "Data Sheet n ", with a continuous counter n
- make the sheet "Global Variables" visible. Click on "Extras – Macros – Visual Basic Editor". Select the sheet "Global Variables" and set the property "Visible" to "xlSheet Visible". Close the Visual Basic Editor. Select the sheet "Global Variables" and change the field "B2" to the number of data sheets.

Evaluation:

- Load the combined experiment with **Load Info**
- Click **List Files** if you want to verify if each file has the correct Param value
- **Load & Fit All Files**
- **Detectors: O, Coefficients: D, Files: in-out** (for example)
- select **vs: Param**
- select **average "vs"**
- **Plot**



longterm evaluation of the empty phase

Assume you have done many series of scans and you want to evaluate the long term development of the empty interferometer phase. The idea is to select the data in each experiment and save it to a common text file. Finally load this text file into a new experiment.

- select the first experiment. Let's assume it consists only of empty interferometer scans.
- therefore select **Files: all**
- **Coefficients: D** (phase)
- **Detectors: O, H**
- select **incl. error**
- **Save.** You will be asked for a text file. If this file already exists the data will be appended. If you want to overwrite the file you have to delete it first.
- select the second experiment. Let's assume it contains sample-in and sample-out data.
- select Files: out because we want to collect only the empty phases. If you select more than one in/out types you will be asked for a different file name for each of them.
- **Coefficients: D** (phase)
- **Detectors: O, H**
- select **incl. error**
- **Save.** Enter the same file name as before. Ignore the message saying the file will be overwritten. In fact the data will be appended.
- ... (continue with other experiments) ...
- create a new experiment
- **Load.** Enter the same file name as before.
- **Files: all**
- **Coefficients: D** (phase)
- **Detectors: O, H**
- **Plot**, e.g. vs Time

using two vertically separated beams

Once we prepared two vertically separated neutron beams going through the interferometer. The lower one should keep track of the empty phase and the upper one contained the sample. The O detector measured only the upper beam, the H detector only the lower beam. In order to calculate the phase difference between the O and H detectors I created the option **dCoeff = H - O**. However, the phase drift was different in the upper and lower beams and the method couldn't be used.

Data Structures

Data arrays in Igor are called "waves". The waves and variables of each experiment are stored in separate data folders. To see this, select the menu command "Data – Data Browser". In addition each experiment has a subfolder called "ctrl" containing the control panel settings.

Waves for each experiment

Waves running over all loaded files [0,1,...number of files]. The first element [0] does not specify a file but is reserved for the mean value.

File_Name	data file name
Order	scan number
Timestamp	mean date & time of the scan, (begin + end)/2
Duration	(end – begin)/2, shown as horizontal error bars in plots versus time
Param	user defined parameter per scan
Xvalue	user defined parameter per scan
Yvalue	user defined parameter per scan

Data waves loaded from the data files:

$\langle n \rangle \in \{1, \dots, \text{number of files}\}$

Std_Phase $\langle n \rangle$	x-axis of the scan		
DataMon $\langle n \rangle$	Monitor		
Data0 $\langle n \rangle$	O detector	Err_Data0 $\langle n \rangle$	$\sqrt{\text{Data0}\langle n \rangle}$
DataH $\langle n \rangle$	H detector	Err_DataH $\langle n \rangle$	$\sqrt{\text{DataH}\langle n \rangle}$
Data3rd $\langle n \rangle$	3rd detector	Err_Data3rd $\langle n \rangle$	$\sqrt{\text{Data3rd}\langle n \rangle}$
Data4th $\langle n \rangle$	4th detector	Err_Data4th $\langle n \rangle$	$\sqrt{\text{Data4th}\langle n \rangle}$
DatadSignal $\langle n \rangle$	user def. difference	Err_DatadSignal $\langle n \rangle$	$\sqrt{\text{DatadSignal}\langle n \rangle}$

Fit results:

$\langle n \rangle \in \{1, \dots, \text{number of files}\}$

$\langle \text{det} \rangle \in \{0, \text{H}, \text{3rd}, \text{4th}, \text{dSignal}\}$

$\langle \text{coeff} \rangle \in \{\text{CoeffA}, \text{CoeffB}, \text{CoeffC}, \text{CoeffD}, \text{Contr}, \text{FWHM}, \text{Chi2}\}$

fit_Data $\langle \text{det} \rangle \langle n \rangle$	curve showing the fit
$\langle \text{coeff} \rangle _ \langle \text{det} \rangle$	fit parameter
Err_ $\langle \text{coeff} \rangle _ \langle \text{det} \rangle$	fitting error

Make dCoeff

$\langle \text{coeff} \rangle \in \{\text{CoeffA}, \text{CoeffB}, \text{CoeffC}, \text{CoeffD}\}$

$\langle \text{coeff} \rangle _ \text{dCoeff}$	user defined difference between the coefficients of two detectors
Err_ $\langle \text{coeff} \rangle _ \text{dCoeff}$	error

Splitting fit results in sample In and sample Out

$\langle \text{det} \rangle \in \{0, \text{H}, \text{3rd}, \text{4th}, \text{dSignal}, \text{dCoeff}\}$

$\langle \text{coeff} \rangle \in \{\text{CoeffA}, \text{CoeffB}, \text{CoeffC}, \text{CoeffD}, \text{Contr}, \text{FWHM}, \text{Chi2}\}$

$\langle \text{inout} \rangle \in \{\text{Out}, \text{In1}, \text{In2}\}$

$\langle \text{header} \rangle \in \{\text{File_Name}, \text{Order}, \text{Timestamp}, \text{Duration}, \text{Param}, \text{Xvalue}, \text{Yvalue}\}$

<inout>_<header>
 <inout>_<coeff>_<det>
 Err_<inout>_<coeff>_<det>

sequence	Order
parallel	<inout>_Order = {1, 2, 3, ...}
serial out, in	Out_Order = { 1, 2, 3, ...} In1_Order = { 1.5, 2.5, 3.5, ...}
serial out, in1, in2	Out_Order = { 1, 2, 3, ...} In1_Order = { 1.33, 2.33, 3.33, ...} In2_Order = { 1.67, 2.67, 3.67, ...}
serial in, out	Out_Order = { 1.5, 2.5, 3.5, ...} In1_Order = { 1, 2, 3, ...}
serial out,in, ...out	Out_Order = { 0.5 1.5, 2.5, 3.5, ...} In1_Order = { 1, 2, 3, ...}
etc.	

Calculating the difference between sample In and sample Out

<det> ∈ {0, H, 3rd, 4th, dSignal, dCoeff}

<coeff> ∈ {CoeffA, CoeffB, CoeffC, CoeffD, Contr, FWHM, Chi2}

<in> ∈ {In1, In2}

<header> ∈ {File_Name, Order, Timestamp, Duration, Param, Xvalue, Yvalue}

<in>Out_<header> = ...

	<Out> := Out_<coeff>_<det>={o1, o2, o3, ...} <In> := <in>_<coeff>_<det>={i1,i2,i3,...} <InOut> := <in>Out_<coeff>_<det>
sequence	
parallel	<InOut> = <In> - <Out> Err_<InOut> = sqrt(Err_<In> ² + Err_<Out> ²)
serial out, in, ... out	<InOut> = { i1 - (o1+o2)/2, i2 - (o2+o3)/2, ...} Err_<InOut> = { sqrt(erri1 ² + ((erro1+erro2)/2) ² , ...}
serial out, in	<Out> = { o1, o2, o3, ...} <In> = { i1, i2, i3, ...} <InOut> = { i1-o1, i1-o2, i2-o2, ...} Err_<InOut> = ... todo...

Calculating MeanDet

<coeff> ∈ {CoeffA, CoeffB, CoeffC, CoeffD}

<inout> ∈ {"", Out, In1, In2, In1Out, In2Out}

<inout>_<coeff>_meanDet = ...

Err_<inout>_<coeff>_meanDet = ...

... to be continued ...

Programmer's Guide

Control Waves

There are global control waves stored in the root data folder. To see these waves start the "Show_Control_Waves" in the Macro menu. (Note that the procedure window must be closed, otherwise Igor doesn't execute the macro.)

DetectorNames, InoutNames, CoeffNames

contain wave name fragments which are used by the program to assemble the wave names for all kinds of detectors, coefficients and file types.

DetectorColorR, -G, -B

Colors representing distinct detectors in the plots.

CoeffMarkerOut, -In1, -In2.

Markers representing distinct coefficients and in/out types in the plots

CoeffAxis0

Meaning of the fit parameters for sine fits

CoeffAxis1

Meaning of the fit parameters for gaussian fits

CoeffAxis0inout

Meaning of the fit parameter differences for sine fits

.... to be continued ...