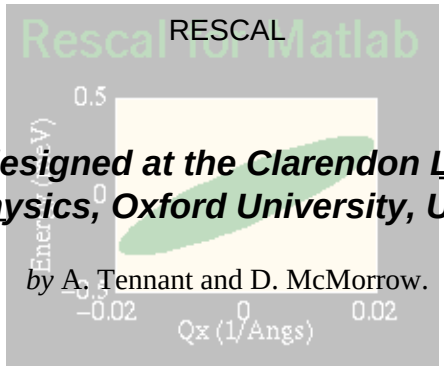

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by A. Tennant and D. McMorrow.

Rescal for Matlab: a computational package for calculating neutron TAS resolution functions.

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Introduction

RESCAL for MATLAB is a comprehensive and integrated set of MATLAB programs which (1) calculate the resolution function of a neutron triple−axis spectrometer, (2) simulate scans using a 4D Monte Carlo convolution for a user−defined dispersion and line−shape, and (3) fit data within the MFIT environment for Matlab. Because Matlab is optimised for linear algebraic operations, it has been possible to write the code for **RESCAL for MATLAB** more concisely and transparently than would be possible with a conventional language like Fortran. The code is machine independent in that it will work equally well on any platform running Matlab and also has the advantage of *not* requiring compilation. **RESCAL for MATLAB** makes use of Matlab's powerful graphics and has been designed to be *entirely windows and menu driven*. The spectrometer parameters can be entered either from a file or interactively in the control windows. This makes learning how to use **RESCAL** easy. The main features of **RESCAL for MATLAB** are listed below:

Choice of resolution methods

- **Cooper−Nathans method** : calculate resolution function from angular elements of spectrometer such as collimators but neglect spatial effects such as size of sample.
- **Popovici method**: calculates resolution function including spatial effects.

Interactive windows and menus

- Save/read parameters to/from a file.
- Enter parameters interactively in windows.
- Choose operations such as open file, print, and resolution method from pull−down menus.

Display calculated resolution parameters and ellipsoid projections

- Calculates resolution parameters such as Bragg widths, vanadium widths and phonon widths.
- Resolution widths and relevant parameters are written to a rescal figure which can be printed out.
- Plot of resolution ellipsoid projections is included in the figure.

Simulation of scans

- 4D Monte Carlo convolution of resolution ellipsoid with dispersion.
- User−defined dispersion and line−shape.
- Scan, dispersion and line width entered in parameter windows.

Fitting scans

For a guide to installing and starting up rescal use the hyperlink Installing and Starting RESCAL for MATLAB. If you have any queries or comments please mail us at the address below. (c) A. Tennant D. McMorrow November 29 1995

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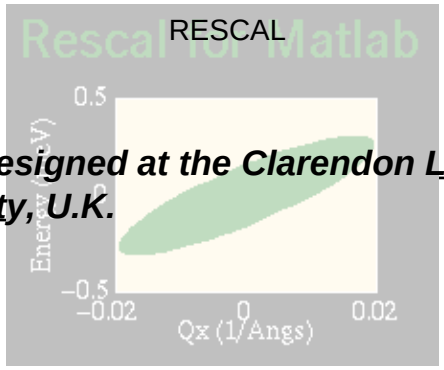

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Installing and Starting RESCAL for MATLAB

RESCAL for MATLAB requires the installation of MATLAB to work. If matlab is installed already then a copy of the set of programs **RESCAL for MATLAB** need to be ftp'ed from the main Oxford Neutron Group server onto a working directory named "RESCAL". As this program has just been developed a request for **RESCAL for MATLAB** should be made directly to the e−mail address below. Once installed the program is easy to run. Start up "matlab" in the new RESCAL directory then at the matlab prompt simply type "rescal". Two parameter windows will appear into which all the spectrometer parameters can be entered. Printing is supported for postscript laser printers but the rc_prt.m file needs to be configured for the specific printer queue of your computer. To do this you must edit the rc_prt.m file which creates a postscript file of temp.ps by modifying the line **!print/queue=clps4_av6 temp.ps** to be **!print_your_queue temp.ps**

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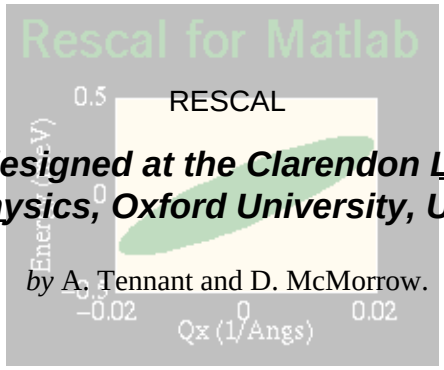

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Resolution Methods

RESCAL for MATLAB offers a choice of methods for calculating the resolution function of a neutron triple−axis spectrometer on the control bar of the parameter window, see Interactive windows and menus. The choices are:

- **Cooper−Nathans method** : (*M.J. Cooper and R. Nathans, Acta Cryst. A29, 160−169.*) calculates the resolution function from angular elements of spectrometer such as collimators, and neglect spatial effects such as size of sample.
- **Popovici method**: (*M. Popovici, Acta Cryst. A31, 507 (1975)*) calculates resolution function including spatial effects (source, monochromator,sample,analyser and detector shapes and dimensions), focussed monochromators and analysers, and waveguides.

The reason for offering a choice is that the spatial components are often not important or are perhaps unknown. Or, phenomenological parameters for an instrument may have been developed some time ago based on the Cooper−Nathans method which are known to give the correct resolution widths with this method. In other cases however spatial focussing effects play an important role, or it may be that a focussed monochromator or analyser was used and needs to be accounted for in the resolution calculation. For these cases the Popovici method is used. This method is chosen by default on starting RESCAL for MATLAB. Both methods use interactive windows and menus for entering parameters either by file or directly with an extra window being started up for spatial parameters in the case of the Popovici method. The Popovici method is identical with the Cooper−Nathans method when the lateral spatial sizes such as detector width are made much larger than the spectrometer distances and flat monochromator/analysers are chosen. This provides a check on the two calculations. Both methods have been tested against similar fortran implementations of the respective methods (RESCAL at the ILL for the Cooper−Nathans method, and RESTRAX at the ILL for the Popovici method) and are in agreement.

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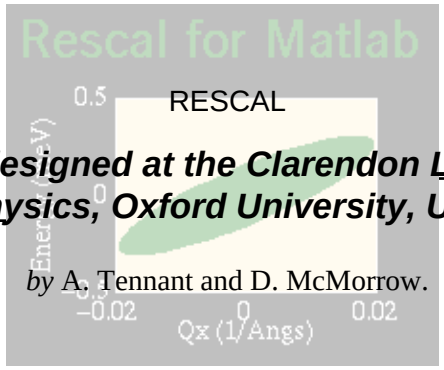

RESCAL

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Parameter Windows and Menus

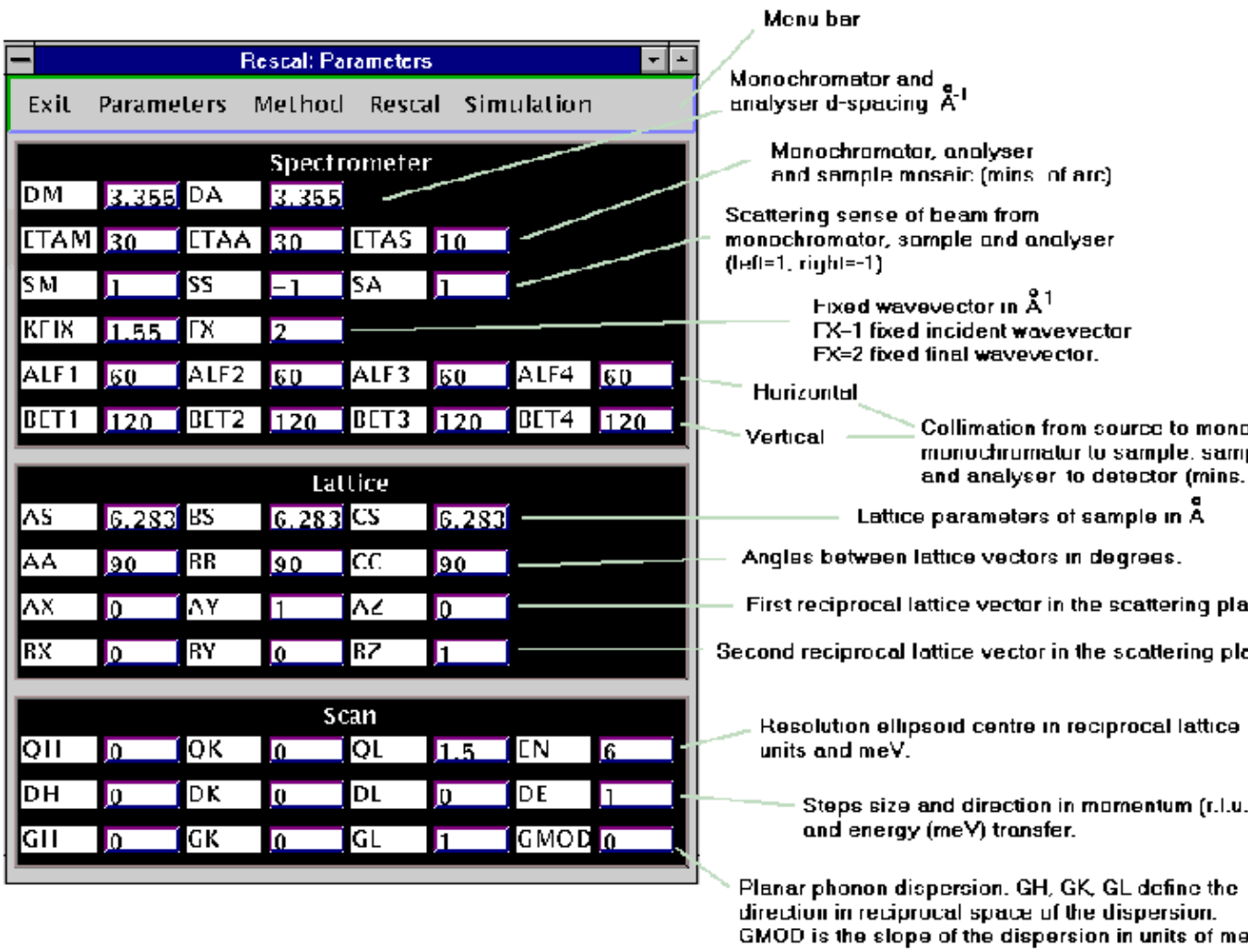
RESCAL for MATLAB makes use of MATLAB's powerful graphics and windowing systems. The spectrometer parameters can be entered either from a file or interactively in the control windows. This makes learning how to use **RESCAL for MATLAB** fairly easy. This web page gives a run down on the parameter windows that appear on startup, and what each parameter corresponds to.

On starting up **RESCAL for MATLAB** two windows appear, one entitled "Rescal: Parameters", and the other "Rescal: Instrument". The window "Rescal: Parameters" contains spectrometer parameters such as collimators and d−spacings that are common to both the Cooper−Nathans and Popovici resolution methods. The other window that appears "Rescal:Instrument" contains parameters such as monochromator dimensions and curvatures which are specific to the Popovici method. The reason that both windows appear on startup is that the Popovici method is the default setting. If the Cooper−Nathans method is selected from the pull−down menu entitled **method** on the menu bar on "Rescal: Parameters" then the "Rescal: Instrument" disappears as it is not needed. To aid in explaining what each part of the two parameter windows do, screen shots of both windows are given below.

The "Rescal: Parameters" Window

The "Rescal: Parameters" window is shown below. It consists of a title bar in blue, then underneath that a menu bar in grey followed by three sets of parameter boxes "Spectrometer", "Lattice", and "Scan". Each individual parameter box has a label such as DM (for monochromator d−spacing) and an explanation of the labels and units used are provided in the figure below. A parameter is entered or changed simply by clicking on the parameter box with the left mouse button and entering the new value from the keyboard.

The **menu bar** consists of five choices: **Exit**: to exit the RESCAL for MATLAB program **Parameters**: a pull down menu which gives the choice of opening a parameter file or saving existing parameters in a new file. **Method**: a pull down menu giving choice of resolution methods, Cooper−Nathans or Popovici. **Rescal**: executes the calculation and plot of resolution widths and various projections of the resolution ellipsoid. **Simulation**: executes the simulation which generates new parameter windows for the simulation parametrs, dispersion &c.



The "Rescal: Instrument" Window

The "Rescal: Instrument" window is shown below. It consists of a title bar in blue, then underneath that a menu bar in grey followed by the parameter box. The **menu bar** has a single option "parameters" for opening and saving parameter files.

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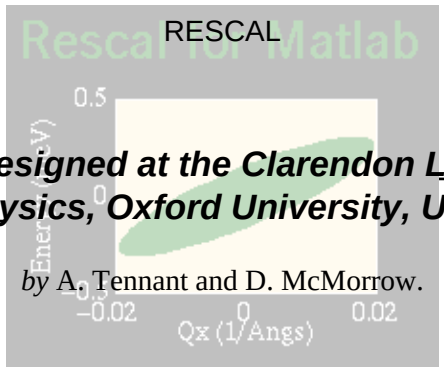

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Graphical Output of Resolution Calculation

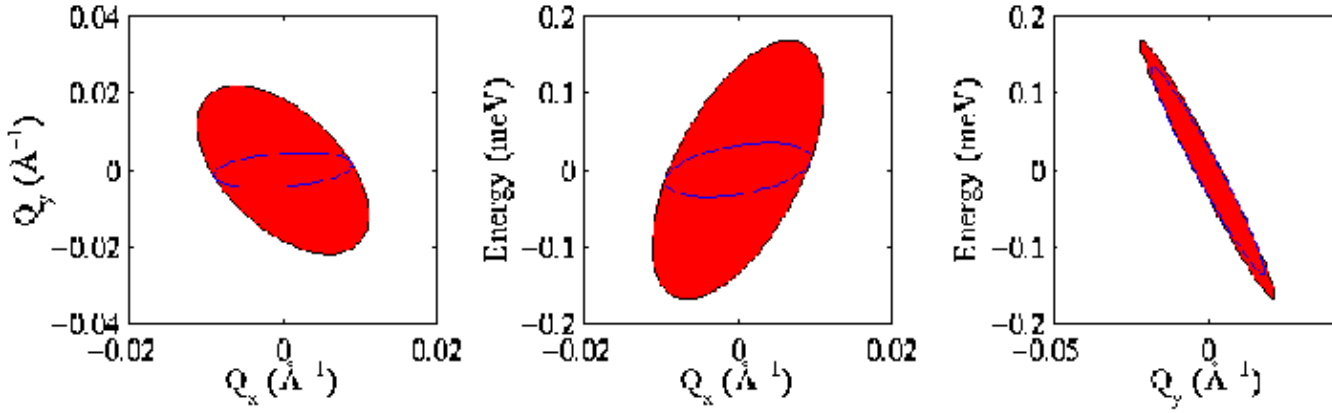
The **rescal** option on the "Rescal: Parameters" window menu bar executes the calculation of the resolution ellipsoid. A figure is generated which has:

a pull−down print menu as well as output showing method used spectrometer parameters lattice parameters Bragg widths: Qx−radial width, Qy−transverese width, Qz−vertical width, V−vanadium width, and DEE−energy width all expressed as FWHM and units of Ang−1 or meV. resolution volumes: R0−total volume, Vi−volume before sample, Vf−after−sample volume. dispersion surface and scan parameters phonon width: full width half maximum of a scan DQ through the dispersion surface GQ in units of Ang−1, meV or a mixture of both. three projections of the resolution ellipsoid onto the Qx−Qy, Qx−Energy, and Qy−Energy planes where Qx is the radial direction i.e. along the direction of momentum transfer Q and Qy is the transverse direction i.e. perpendicular to Q in the scattering plane.

A screen shot of the output figure is given below.

Method:	Popovici's			
Spectrometer:	DM = 3.355	DA = 3.355		
	ETAM= 30.000	ETAA= 30.000	ETAS= 10.000	
	SM = 1.000	SS = −1.000	SA = 1.000	
	KFIX= 1.550	FX = 2.000		
	ALF1= 60.000	ALF2= 60.000	ALF3= 60.000	ALF4= 60.000
	BET1=120.000	BET2=120.000	BET3=120.000	BET4=120.000
Lattice:	AS = 6.283	BS = 6.283	CS = 6.283	
	AA = 90.000	BB = 90.000	CC = 90.000	
	AX = 0.000	AY = 1.000	AZ = 0.000	
	BX = 0.000	BY = 0.000	BZ = 1.000	
	QH = 0.000	QK = 0.000	QL = 1.500	EN = 6.000
Bragg widths:	Qx = 0.017	Qy = 0.009	Qz = 0.031	V = 0.337 DEF
Normalisation:	R0 =6.519e−03	Vi =1.302e−04	Vf =1.642e−04	
Dispersion:	DH = 0.000	DK = 0.000	DL = 0.000	DE = 1.000
	GH = 0.000	GK = 0.000	GL = 1.000	GMOD= 0.000

Phonon Width: 0.337 (meV, 1/Angs or a mixture of both)



Source:	Width = 10.000	Height = 10.000		
Guide:	Hor. Div.= 7.000	Ver. Div.= 12.000		
Sample:	Depth = 0.500	Width = 3.000	Height = 0.500	
Detector:	Width = 2.600	Height = 4.000		
Monochromator:	Thickness= 0.300	Width = 16.000	Height = 20.000	
Analyser:	Thickness= 0.300	Width = 10.000	Height = 4.000	
Distances:	L0 = 300.000	L1 = 140.000	L2 = 106.000	L3 = 40.000
Distances:	ROMH = 0.000	ROMV = 0.050	ROAH = 0.000	ROAV = 0.000

Unit vector projection axes in terms of AS BS CS: Qx = 0.00 0.00 1.00 Qy = 0.00 −1.00 0.00

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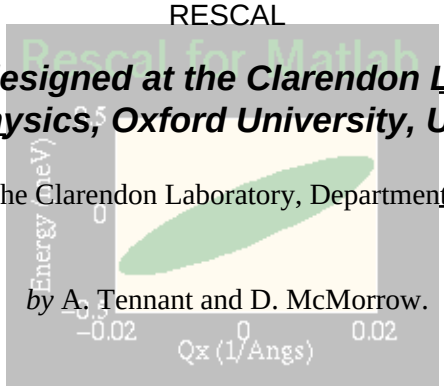

Monte Carlo simulations of scans for neutron triple−axis spectrometers.

One of the options on the menu bar of the "Rescal: Parameters" window is labelled "**simulation**". Clicking on it causes an *extra window* to a appear entitled "**Rescal: Simulation**". In order to make a simulation, a dispersion and line−shape need to be defined. At the moment the program is set up for sinusoidal dispersions with an energy gap at the zone centre. The current line−shape is Lorentzian and a detailed balance and 1/energy structure factor for antiferromagnetic line−shapes has been included. Details of how to modify the program are given in the final section of this web page. The simulation takes full account of the changes in the resolution at each point in the scan and also corrects for changes in resolution volume, counts by monitor etc.

Entering parameters for the simulation

Parameters defining the scan, dispersion, and linewidth are given in the "**Rescal: Simulation**" window generated on clicking on the "**simulation**" button on the menu bar of the "Rescal: Parameters" window. The "Rescal: Simulation" window (a screen−shot will be added later) consists of a title bar ("Rescal: Simulation"), menu bar with options

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- Exit: exits out of the simulation level of **RESCAL for MATLAB** and closes the "Rescal: Simulation" window and plot.
- Parameters: a pull−down menu giving the choice of "Get Parameters" or "Save Parameters" which allows the user to read/save *simulation* parameters from/to a file.
- Run: which runs the specified simulation. The 4D Monte Carlo convolution is calculated and displayed on a new figure (screen−shot to be added) along with plot of unconvoluted line−shape.

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the final component of the "Rescal: Simulation" window is the set of parameter boxes. This consists of nine parameters describing the scan

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- Hstart, Kstart, Lstart & Estart: starting point values of H,K,L & E, in r.l.u. and meV respectively, for the scan.
- Hend, Kend, Lend & Estart: final values of H,K,L & E, in r.l.u. and meV respectively, for the scan.
- NSC: number of points in the scan including the starting and finishing points.

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a parameter for the number of Monte Carlo points in the integration

---

- NMC: number of Monte Carlo points in the integration (typically of order 3000).

---

ten parameters describing the dispersion of the excitations

- Hzb, Kzb, Lzb & Egap: these are the (H,0,0), (K,0,0), (L,0,0) zone−boundary energies and energy gap at the zone−centre respectively (all in meV).
- Hzero, Kzero & Lzero: the three r.l.u. coordinates of the zone−centre point.
- Hphase, Kphase & Lphase: these are the parameters defining the repetition rate of the sinusoidal dispersion in the principle directions (H,K,L). The values are 2 for an antiferromagnetic repitition and 1 for a ferromagnetic repetition.

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and the final two parametrs are

- Gamma: the full−width−half−maximum (FWHM) of the Lorentzian line−shape.
- T(K): temperature in degrees Kelvin.

Modifying the dispersion and line−shape

As remarked earlier, the program has been set up to calculate scattering for a sinusoidal dispersion and Lorentzian line−shape. Both of these can be tailored for specific purposes. The dispersion and lineshape are defined in the macro mc_sqw.m. This consists of a definition of *wq* − the dispersion as a function of Q(r.l.u.) − and *s* − the scattering from the line−shape. The definitions of *wq* and *s* are self evident form mc_sqw.m, however there is a fundamental difference in the definition of the functions from that using Fortran. Matlab uses matrices as it's basic unit rather than scalars. Because of this *wq* and *s* should be viewed as array equalities and functions. One ramification of this is that the normal arithmetic operators (+,−,*,/,^) are matrix operations and other operators between scalars and matrices or element−by−element operations must be prfixed by a dot i.e. .*,./ or .^.

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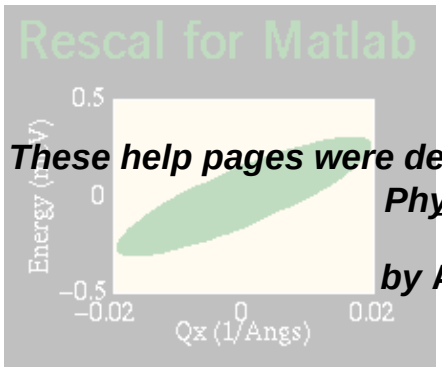

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***by* A. Tennant and D. McMorrow.**

Fitting with MFIT and RESCAL for MATLAB.

RESCAL for MATLAB has been linked in with the MFIT environment for MATLAB. This is an extension of the Monte Carlo simulation method in **RESCAL for MATLAB**. When the trix2.m file is loaded into MFIT and chosen as the fitting function, the **RESCAL for MATLAB** parameter windows appear. Spectrometer parameters can be chosen from files or entered interactively. A window is generated for the fitting and dispersion parameters. The file trixsqw.m, which must be in the MFIT and RESCAL path, defines the line−shape in the same way as mc_sqw.m for the simulation. At the moment this is defined as a Lorentzian line shape − see simulation for the meaning of parameters. Fitting on some machines can be significantly speeded up by compiling a C routine for the Monte Carlo convolution with the dispersion into Matlab. This requires building a MEX−file which consists of a dispersion and cross−section, portable random number generator, and gateway routine. Fitting takes a couple of minutes on a DEC 3000 Alpha. As well as triple−axis fitting, MFIT also provides a number of other fitting functions such as Gaussians. Used in this way MFIT and **RESCAL for MATLAB** provide a comprehensive platform for analysing neutron triple−axis data.

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