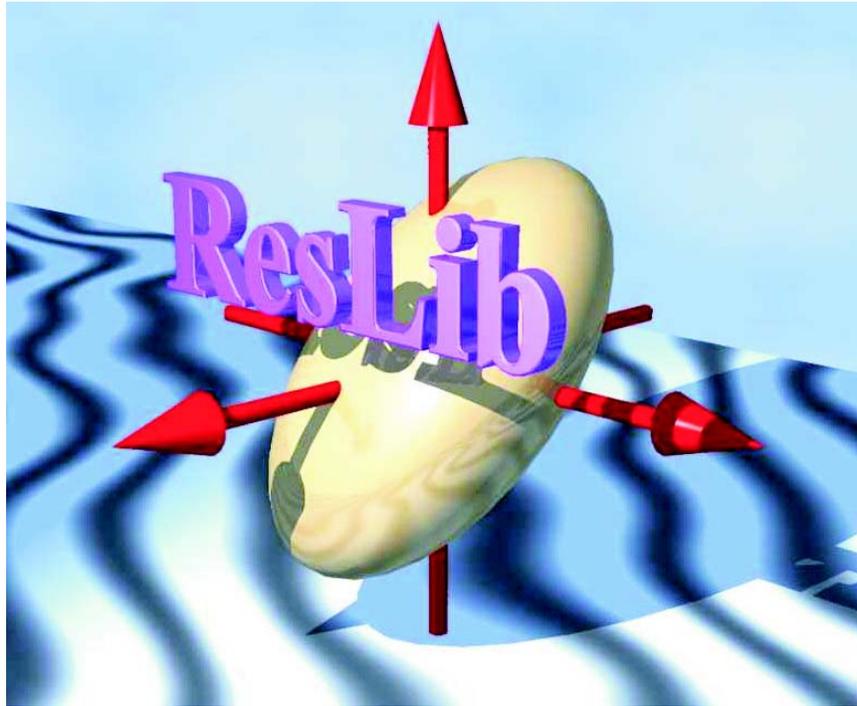


ResLib 3.4



3-axis resolution library for MatLab

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Abstract

Features of the latest *ResLib* release include: 3-axis resolution calculations in the **Cooper-Nathans** and **Popovici** approximations with support for horizontally focusing analyzers, anisotropic sample mosaic, neutron guides, normalization to monitor counts, analyzer reflectivity corrections and data smoothing; numerical convolution of user-supplied cross section functions with calculated experimental resolution, including cross sections written in the **single mode or Lorentzian approximations**; fitting of parameterized model cross sections to experimental data; graphical representation of resolution ellipsoids in 2 and 3 dimensions; spectrometer positioning and and crystallographic utility functions. The present manual provides a detailed description of the functions included in the *ResLib* library and quotes all the essential formulas used in the calculations.

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I. INTRODUCTION

Perhaps the most important aspect of analyzing inelastic neutron scattering data measured using a 3-axis spectrometer is properly taking into account the experimental resolution. Even though one is fairly confident that the Gaussian approximation to the resolution function is accurate, thanks to the Central Limit Theorem, the problem is still quite non-trivial. In general, to properly analyze experimental scans using a parameterized model cross section $S(\mathbf{Q}, \hbar\omega, \mathbf{p})$, one needs to 1) be able to calculate the resolution function at each data point, given the spectrometer configuration and sample parameters, 2) numerically convolute the theoretical cross section with this resolution function; and 3) fit the convoluted cross section to the data. The *ResLib* library is designed to accomplish these tasks.

II. FORMULAS FOR RESOLUTION CALCULATION

ResLib is based on the Gaussian approximation for the resolution function. The measured inelastic neutron scattering intensity is related to the dynamic structure factor through:

$$\frac{d\sigma}{d\Omega dE'} \approx R_0(\mathbf{Q}_0) \int \int \int \int d^4\mathcal{Q} S(\mathcal{Q}) \exp \left[-\frac{1}{2} (\mathcal{Q}^i - \mathcal{Q}_0^i) (\mathcal{Q}^j - \mathcal{Q}_0^j) M_{ij}(\mathbf{Q}_0) \right]. \quad (1)$$

Here $\mathcal{Q} \equiv (Q_x, Q_y, \hbar\omega, Q_z)$ represents a 4-D vector in energy-momentum space, $\mathbf{Q}_0 = \mathbf{k}_i - \mathbf{k}_f$ is the momentum transfer to the sample, and $\hbar\omega_0 = E_i - E_f$ is the energy transfer. In *ResLib* wave vectors are measured in \AA^{-1} , and energy in meV. The coordinate system for components of \mathbf{Q} and M is defined by the scattering vector and the scattering plane. x is chosen along \mathbf{Q}_0 , z is perpendicular to the scattering plane (vertical) and y completes the orthogonal right-handed basis set. Note that in Eq. 1 the usual k_i/k_f scaling factor is included into R_0 .

A. Cooper-Nathans resolution matrix

In the Cooper-Nathans approximation [1, 2] it is assumed that the beam divergences on each arm of the 3-axis spectrometer are determined by the Soller collimators and the mosaic spread of monochromator and analyzer crystals. The most elegant formulas for this approximation are given in [3]. The Soller collimators are described by a diagonal 8×8 matrix with non-zero elements $G_{1,1} = 8 \ln(2)\alpha_1^{-2}$, $G_{2,2} = 8 \ln(2)\alpha_2^{-2}$, $G_{3,3} = 8 \ln(2)\beta_1^{-2}$, $G_{4,4} = 8 \ln(2)\beta_2^{-2}$, $G_{5,5} = 8 \ln(2)\alpha_3^{-2}$, $G_{6,6} = 8 \ln(2)\alpha_4^{-2}$, $G_{7,7} = 8 \ln(2)\beta_3^{-2}$ and $G_{8,8} = 8 \ln(2)\beta_4^{-2}$, where α_i and β_i are the FWHM horizontal and vertical beam divergences in the collimators, starting from the in-pile collimation. η and η' , the horizontal and vertical FWHM mosaic spreads for the monochromator and analyzer crystals, are collected into a diagonal 4×4 matrix with non-zero elements $F_{1,1} = 8 \ln(2)\eta_M^{-2}$, $F_{2,2} = 8 \ln(2)\eta'_M{}^{-2}$, $F_{3,3} = 8 \ln(2)\eta_A^{-2}$, and $F_{4,4} = 8 \ln(2)\eta'_A{}^{-2}$. In addition, the following matrixes are defined. A is a 6×8 matrix with non-zero elements $A_{1,1} = -A_{1,2} = k_i \cot(\theta_M)/2$, $A_{4,5} = -A_{4,6} = k_f \cot(\theta_A)/2$, $A_{2,2} = A_{3,4} = k_i$ and $A_{5,5} = A_{6,7} = k_f$. C is a 6×8 matrix with non-zero elements $C_{1,1} = C_{1,2} = C_{3,5} = C_{3,6} = 1/2$, $C_{2,3} = -C_{2,4} = 1/(2 \sin \theta_M)$ and $C_{4,7} = -C_{4,8} = 1/(2 \sin \theta_A)$. Note that in [3] there is a typo in the definition of matrix C . Finally, B is defined as a 4×6 matrix with the following non-zero elements: $B_{1,1} = B_{2,2} \cos \phi$, $B_{1,2} = -B_{2,1} = \sin \phi$, $B_{1,4} = B_{2,5} = -\cos(\phi - 2\theta_S)$, $B_{1,5} = -B_{2,4} = -\sin(\phi - 2\theta_S)$, $B_{3,3} = -B_{3,6} = 1$,

$B_{4,1} = \frac{\hbar^2}{m} k_i$ and $B_{4,4} = -\frac{\hbar^2}{m} k_f$. In these formulas $2\theta_M$, $2\theta_S$ and $2\theta_A$, are the scattering angles in monochromator, sample and analyzer, respectively and m is the neutron mass. The scattering angles are calculated as:

$$\begin{aligned}\theta_M &= -\arcsin(\tau_M/(2k_i))\epsilon_M, \\ \theta_A &= -\arcsin(\tau_A/(2k_f))\epsilon_A, \\ 2\theta_S &= \arccos[(k_i^2 + k_f^2 - Q^2)/(2k_i k_f)],\end{aligned}\tag{2}$$

where $\epsilon_M = 1$ if the sample scattering direction is opposite to the monochromator scattering directions and -1 otherwise, $\epsilon_A = 1$ if the sample scattering direction is opposite to the analyzer scattering directions and -1 otherwise, and $\tau_M = 2\pi/d_M$ and $\tau_A = 2\pi/d_A$ are the monochromator and analyzer scattering vectors, respectively. The sample rotation angle is given by:

$$\phi = \text{ATAN2}(-k_f \sin 2\theta_S, k_i - k_f \cos 2\theta_S).\tag{3}$$

These matrixes defined, the resolution matrix is given by:

$$\tilde{M}^{-1} = BA(G + C^T FC)^{-1} A^T B^T.\tag{4}$$

The resolution matrix M is obtained from \tilde{M} by switching the 3rd and 4th rows and columns.

B. Popovici resolution matrix

The beam divergences are influenced not only by Soller collimators, but also by the shapes and dimensions of the source, monochromator, sample, analyzer and detector [3]. These shapes are described by the 13×13 covariance matrix S^{-1} . The matrix is cell-diagonal and has the form: $S^{-1} = \{\langle y_0^2 \rangle, \langle z_0^2 \rangle, S_M^{-1}, S_S^{-1}, S_A^{-1} \langle y_4^2 \rangle, \langle z_4^2 \rangle\}$. $\langle y_0^2 \rangle$ and $\langle z_0^2 \rangle$ describe the spatial distribution of the source density perpendicular to the first spectrometer arm in the horizontal and vertical directions, respectively. Similarly, $\langle y_4^2 \rangle$ and $\langle z_4^2 \rangle$ describe the spatial distribution of the detector. S_M^{-1} , S_S^{-1} and S_A^{-1} are the spatial distributions of the monochromator, sample and analyzer densities, respectively. For example,

$$S_S^{-1} = \begin{bmatrix} \langle x^2 \rangle & \langle xy \rangle & \langle xz \rangle \\ \langle yx \rangle & \langle y^2 \rangle & \langle yz \rangle \\ \langle zx \rangle & \langle zy \rangle & \langle z^2 \rangle \end{bmatrix},\tag{5}$$

where x bisects the incident and scattered beams on the sample, z is the vertical axis and y completes an orthogonal coordinate system.

Additional matrices are defined and contain the distances L_0 , L_1 , L_2 and L_3 from the source to the monochromator, from the monochromator to the sample, from the sample to the analyzer and from the analyzer to the detector, respectively. Additional parameters are the horizontal and vertical curvature radii ρ and ρ' , for the monochromator and analyzer crystals. T is a 4×13 matrix with the following non-zero elements: $T_{1,1} = -1/(2L_0)$, $T_{1,3} = \cos \theta_M(1/L_1 - 1/L_0)/2$, $T_{1,4} = \sin \theta_M(1/L_0 + 1/L_1 - 2/(\rho_M \sin \theta_M))/2$, $T_{1,6} = \sin \theta_S/(2L_1)$, $T_{1,7} = \cos \theta_S/(2L_1)$, $T_{2,2} = -1/(2L_0 \sin \theta_M)$, $T_{2,5} = (1/L_0 + 1/L_1 - 2 \sin \theta_M/\rho'_M)/(2 \sin \theta_M)$, $T_{2,8} = -1/(2L_1 \sin \theta_M)$, $T_{3,6} = \sin \theta_S/(2L_2)$, $T_{3,7} = -\cos \theta_S/(2L_2)$, $T_{3,9} = \cos \theta_A(1/L_3 - 1/L_2)/2$, $T_{3,10} = \sin \theta_A(1/L_2 + 1/L_3 - 2/(\rho_A \sin \theta_A))/2$, $T_{3,12} = 1/(2L_3)$, $T_{4,8} = -1/(2L_2 \sin \theta_A)$, $T_{4,11} = (1/L_2 + 1/L_3 - 2 \sin \theta_A/\rho'_A)/(2 \sin \theta_A)$ and $T_{4,13} = -1/(2L_3 \sin \theta_A)$. D is defined as an 8×3 matrix with non-zero elements $D_{1,1} = -1/L_0$, $D_{1,3} = -\cos \theta_M/L_0$, $D_{1,4} = \sin \theta_M/L_0$, $D_{3,2} = D_{1,1}$, $D_{3,5} = -D_{1,1}$, $D_{2,3} = \cos \theta_M/L_1$, $D_{2,4} = \sin \theta_M/L_1$, $D_{2,6} = \sin \theta_S/L_1$, $D_{2,7} = \cos \theta_S/L_1$, $D_{4,5} = -1/L_1$, $D_{4,8} = -D_{4,5}$, $D_{5,6} = \sin \theta_S/L_2$, $D_{5,7} = -\cos \theta_S/L_2$, $D_{5,9} = -\cos \theta_A/L_2$, $D_{5,10} = \sin \theta_A/L_2$, $D_{7,8} = -1/L_2$, $D_{7,11} = -D_{7,8}$, $D_{6,9} = \cos \theta_A/L_3$, $D_{6,10} = \sin \theta_A/L_3$, $D_{6,12} = 1/L_3$, $D_{8,11} = -D_{6,12}$ and $D_{8,13} = D_{6,12}$. Note that [3] contains numerous typos in the definition of matrix T and D . The resolution matrix M in the Popovici approximation is given by:

$$\tilde{M}^{-1} = BA \left[\{D(S + T^T FT)^{-1} D^T\}^{-1} + G \right]^{-1} A^T B^T \quad (6)$$

C. Normalization factors

1. Normalization to source flux

The normalization of the measured intensity by the intensity of the neutron source in the Cooper-Nathans approximation is given by:

$$R_0 = \frac{k_f}{k_i} \frac{\pi^2 (k_i^3 \cot \theta_M)(k_f^3 \cot \theta_A)}{(16 \sin \theta_M \sin \theta_A)} \sqrt{\frac{\det(F)}{\det(G + C^T FC)}} \times (2\pi)^{-2} \sqrt{\det(M)}. \quad (7)$$

The factor $(2\pi)^{-2} \sqrt{\det(M)}$ is included to comply with the resolution function normalization convention used in Eq. 1 above and [2]. As mentioned above, the k_f/k_i factor is included

in the normalization coefficient. The expression for R_0 in the Popovici approximation in [3] does not include the effect of Soller collimators. If these are correctly taken into account, R_0 becomes:

$$R_0 = \frac{k_f \pi^2 (k_i^3 \cot \theta_M) (k_f^3 \cot \theta_A)}{k_i (16 \sin \theta_M \sin \theta_A)} \sqrt{\frac{\det(F)}{\det([D(S + T^T F T)^{-1} D^T]^{-1} + G)}} \times (2\pi)^{-2} \sqrt{\det(M)}. \quad (8)$$

2. Normalization to monitor counts

The monitor is typically positioned between the 2nd Soller collimator and the sample. In the Cooper-Nathans approximation the flux on the monitor is straightforward to calculate, since the resolution function is simply a product of transmission functions for each spectrometer component. Including the $1/k_i$ monitor sensitivity correction, the count rate on the monitor is proportional to:

$$R_{\text{mon}} = \frac{1}{k_i} \frac{\pi (k_i^3 \cot \theta_M)}{(2 \sin \theta_M)} \sqrt{\frac{\det(f)}{\det(g + c^T f c)}}. \quad (9)$$

In this formula is the matrices g , f and c are primary minors of matrices G , F and C , of sizes 4×4 , 2×2 and 2×4 , respectively.

In the Popovici approximation the monitor rate will depend on the dimensions and position of the monitor on the second spectrometer arm. To estimate the count rate, one has to define the following matrices. The matrix s is similar to S and is defined as $s^{-1} = \{\langle y_0^2 \rangle, \langle z_0^2 \rangle, S_M^{-1}, \langle y_{\text{mon}}^2 \rangle, \langle z_{\text{mon}}^2 \rangle\}$. Here $\langle y_{\text{mon}}^2 \rangle$ and $\langle z_{\text{mon}}^2 \rangle$ describe the spatial distribution of the monitor perpendicular to the second spectrometer arm, in the horizontal and vertical directions, respectively. L_{mon} being the distance from the monochromator to the monitor, the transformation matrices t and d are of dimension 4×7 and 2×7 , respectively, and have the following non-zero elements: $t_{1,1} = -1/(2L_0)$, $t_{1,3} = \cos(\theta_m)(1/L_{\text{mon}} - 1/L_0)/2$, $t_{1,4} = \sin(\theta_m)(1/L_0 + 1/L_{\text{mon}} - 2/(\rho_M \sin(\theta_m)))/2$, $t_{1,7} = 1/(2L_{\text{mon}})$, $t_{2,2} = -1/(2L_0 \sin(\theta_m))$, $t_{2,5} = (1/L_0 + 1/L_{\text{mon}} - 2 \sin(\theta_m)/\rho'_M)/(2 \sin(\theta_m))$, $d_{1,1} = -1/L_0$, $d_{1,3} = -\cos(\theta_m)/L_0$, $d_{1,4} = \sin(\theta_m)/L_0$, $d_{3,2} = d_{1,1}$, $d_{3,5} = -d_{1,1}$, $d_{2,3} = \cos(\theta_m)/L_{\text{mon}}$, $d_{2,4} = \sin(\theta_m)/L_{\text{mon}}$, $d_{2,6} = 0$, $d_{2,7} = 1/L_{\text{mon}}$, and $d_{4,5} = -1/L_{\text{mon}}$. The monitor rate is then proportional to:

$$R_{\text{mon}} = \frac{1}{k_i} \frac{\pi (k_i^3 \cot \theta_M)}{(2 \sin \theta_M)} \sqrt{\frac{\det(f)}{\det([d(s + t^T f t)^{-1} d^T]^{-1} + g)}}. \quad (10)$$

In either the Popovici or Cooper-Nathans case, to normalize the measured intensity to monitor counts, the factor R_0 in Eq. 1 is to be modified: $R_0 \rightarrow R_0/R_{\text{mon}}$.

3. Analyzer reflectivity

The prefactor R_0 can include the effect of analyzer reflectivity. The effective reflectivity in the Gaussian model differs from the actual reflectivity of the analyzer crystal. To compensate for this effect, R_0 is corrected so that the integral reflectivity of the effective Gaussian matches the integral reflectivity of an ideal crystal. The reflectivity curve of an ideal crystal can be taken from [4]. In particular, for a PG(002) analyzer, at $E_f < 5.5$ meV, where no parasitic (hkl) reflections interfere with the reflected (002) peak [5], this approximation is expected to be valid within a few percent [6]. At higher final neutron energies this approach can not be considered valid, as the Shapiro-Chesser effects become important [5]. In *ResLib* the optional reflectivity correction is done following [7].

D. Focusing analyzer

ResLib provides a means of calculating the Cooper-Nathans resolution function in the case of a multi-blade horizontally focusing analyzer. The central analyzer blade is positioned to reflect at nominal \mathbf{k}_f . The remaining blades are aligned to reflect at the same $|k_f|$ as the central blade. Energy resolution is actually improved, because the narrow blades provide additional collimation. Wave vector resolution is of course broadened. The effect can be taken into account through an approximation proposed by C. L. Broholm. Eq. ?? for the resolution matrix is replaced with:

$$\begin{aligned}
 \tilde{M}^{-1} &= BP^{-1}B^T, & (11) \\
 P_{i,j} &= \left[\left(A(G + C^TFC)^{-1} * A^T \right)^{-1} \right]_{i,j} \text{ for } i, j \neq 4, 5, \\
 P_{5,5} &= 12 / (k_f \alpha_f)^2, \\
 P_{4,4} &= 12 [\tan \theta_A / (\eta_A k_f)]^2, \\
 P_{4,5} &= (P^{-1})_{5,4} = 0,
 \end{aligned}$$

where α_f is the angular size of the analyzer as seen from the sample. When calculating the prefactor R_0 , the FWHM horizontal beam divergence in the 3rd Soller collimator α_3 in the

definition of matrix G is to be replaced by $\frac{\sqrt{8 \ln 2}}{\sqrt{12}} \alpha_f$.

E. Sample mosaic

The effect of sample mosaic can be included in the resolution calculation following [8]. The matrix M and the prefactor R_0 are modified as follows:

$$R_0 \rightarrow R_0 \left[1 + \frac{1}{8 \ln 2} (|Q_0| \eta_S)^2 M_{4,4} \right]^{-1/2} \left[1 + \frac{1}{8 \ln 2} (|Q_0| \eta'_S)^2 M_{2,2} \right]^{-1/2}, \quad (12)$$

$$(M^{-1})_{2,2} \rightarrow (M^{-1})_{2,2} + (|Q_0| \eta_S)^2 / (8 \ln 2), \quad (13)$$

$$(M^{-1})_{4,4} \rightarrow (M^{-1})_{4,4} + (|Q_0| \eta'_S)^2 / (8 \ln 2). \quad (14)$$

Here η_S and η'_S are the FWHM of horizontal and vertical sample mosaic spreads, respectively.

F. Guide collimators

The neutron beam is often collimated not by slit- or blade-type collimation devices, but by a neutron guide. The key difference is that in this case the beam divergence is dependent on the neutron energy. The critical reflection angle Θ_c of the guide is inversely proportional to the wavenumber of the neutron: $\Theta_c = \theta \lambda$, where θ is a characteristic of the material the guide is made of. For convenience, guides are characterized by their so-called m -value, which is defined as $m = \theta / \theta_0$, $\theta_0 = 0.1^\circ \text{\AA}^{-1}$ being the critical angle for natural Ni. Isotopic ^{58}Ni has a slightly higher critical angle, with $m = 1.2$. Super-mirror guides can have $m = 2$ or higher. The angular transmission of a guide has a roughly rectangular profile of width 2Θ . The corresponding angular standard deviation is $\Theta / \sqrt{3}$. Thus, a neutron guide acts as a collimator with a FWHM divergence of $m\theta_0 \lambda \sqrt{8 \ln 2} / \sqrt{3}$.

G. Coordinate systems

All the formulas above describe the resolution matrix in the coordinate system defined by the scattering vector and the scattering plane. x is chosen along \mathbf{Q}_0 , z is vertical and y completes the orthogonal right-handed basis set. This coordinate system is referred to as the Q -system in the text below. The *ResLib* function used to calculate resolution parameters in this coordinate system is `ResMat.m`.

ResLib also provides a means to calculate the resolution matrix in a coordinate system (S -system) coupled to the sample. The S -system is defined by two (h, k, l) reciprocal-space vectors in the sample. The axis x is chosen along the 1st orienting vector, y is normal to x in the scattering plane and is in the direction of the second vector, and z completes the orthogonal right-handed basis set. The *ResLib* function `ResMatS.m` performs all the calculations in the S -system.

H. Smoothed data

In certain cases it is useful to bin or smooth collected data before proceeding with the data analysis. This is particularly true for very large data sets, such as those collected using area-sensitive detectors. Smoothing consists of folding the measured intensity with a custom smoothing kernel, such as a Π -shaped function of a Gaussian. Of course, the effective resolution of the measurement is modified by this procedure and is equal to a convolution of the smoothing kernel and the actual spectrometer resolution. *ResLib* can handle the special case of a Gaussian resolution kernel at the level of `ResMatS.m`. The resolution matrix is modified by the 4×4 smoothing matrix σ as follows:

$$\Sigma_{1,1} = 8 \ln 2 / \sigma_x^2,$$

$$\Sigma_{2,2} = 8 \ln 2 / \sigma_y^2,$$

$$\Sigma_{3,3} = 8 \ln 2 / \sigma_E^2,$$

$$\Sigma_{4,4} = 8 \ln 2 / \sigma_z^2,$$

$$M^{-1} \rightarrow \Sigma^{-1} + M^{-1}, \tag{15}$$

$$R_0 \rightarrow \frac{\sqrt{\det(\Sigma^{-1} + M^{-1})}}{\sqrt{\det(M^{-1})}} R_0. \tag{16}$$

Here σ_x, σ_y and σ_z , are the smoothing Gaussian FWHM along the three components of the scattering vector and σ_E is the smoothing Gaussian FWHM along the energy axis.

III. *RESLIB* FUNCTIONS FOR RESOLUTION CALCULATION

A. *ResMat.m*

This function calculates the resolution matrix M and the prefactor R_0 in the Q coordinate system (see definition above).

```
function [R0,M]=ResMat(Q,W,EXP)
```

INPUT ARGUMENTS:

- Q is the wave vector transfer in \AA^{-1} .
- W is the energy transfer in meV.
- **EXP** is a structure that contains all the information on the experimental setup and the required method of resolution calculation. See the detailed description below.

OUTPUT ARGUMENTS:

- **R0** is the normalization prefactor as defined above.
- **M** is a 4×4 resolution matrix as defined above.

DEPENDENCIES: *ResMat.m* uses the utility functions *CleanArgs.m* and *GetTau.m*.

ResMat.m can be used to simultaneously calculate resolution matrices for several scattering vectors, energies, and experimental setups. The input arguments Q , W and **EXP** can be vectors of the same length N , in which case **R0** will be returned as a vector of length N and **M** will be a $4 \times 4 \times N$ array. If some of the input arguments are scalars, they will be automatically replicated into vectors of appropriate length.

The fields of the structure **EXP** are defined as follows:

- **EXP.method** selects the computation method. If **EXP.method**=0 or the field is left undefined, a Cooper-Nathans calculation is performed. For a Popovici calculation set **EXP.method**=1.
- **EXP.moncor** selects the type of normalization used to calculate R_0 . If **EXP.moncor**=1 or the field is left undefined, R_0 is calculated in normalization to monitor counts (Section II C 2). $1/k_i$ monitor efficiency correction is included automatically. To normalize R_0 to source flux (Section II C 1), use **EXP.moncor**=0.

- `EXP.mono` is a structure that describes the monochromator:
 - `EXP.mono.tau` is the monochromator reciprocal lattice vector in \AA^{-1} . Instead of a numerical input one can use one of the following keyword strings: `'PG(002)'`, `'PG(004)'`, `'Ge(111)'`, `'Ge(220)'`, `'Ge(311)'`, `'Be(002)'` or `'PG(110)'`.
 - `EXP.mono.mosaic` is the monochromator mosaic in minutes of arc.
 - `EXP.mono.vmosaic` is the vertical mosaic of monochromator in minutes of arc. If this field is left unassigned, an isotropic mosaic is assumed.
- `EXP.ana` is a structure that describes the analyzer and contains fields as in `EXP.mono` plus the following optional fields:
 - `EXP.ana.thickness` is the analyzer thickness in cm for ideal-crystal reflectivity corrections (Section II C 3). If no reflectivity corrections are to be made, this field should remain unassigned or set to a negative value.
 - `EXP.ana.Q` is the kinematic reflectivity coefficient for this correction. It is given by $Q = \frac{4|F|^2}{V_0} \frac{(2\pi)^3}{\tau^3}$, where V_0 is the unit cell volume for the analyzer crystal, F is the structure factor of the analyzer reflection, and τ is the analyzer reciprocal lattice vector. For PG(002) $Q = 0.1287$. Leave this field unassigned or make it negative if you don't want the correction done.
 - `EXP.horifoc` is a flag that is set to 1 if a horizontally focusing analyzer is used (Section II D). In this case `EXP.hcol(3)` (see below) is the angular size of the analyzer, as seen from the sample position. If the field is unassigned or equal to -1, a flat analyzer is assumed. Note that this option is *only available with the Cooper-Nathans method*.
- `EXP.hcol(1:4)` are the horizontal Soller collimations in minutes of arc (FWHM beam divergence) starting from the in-pile collimator. In case of a horizontally-focusing analyzer `EXP.hcol(3)` is the angular size of the analyzer, as seen from the sample position. If the beam divergence is limited by a neutron guide, the corresponding element of `EXP.hcol` is the negative of the guide's m -value. For example, for a 58-Ni guide ($m=1.2$) before the monochromator, `EXP.hcol(1)` should be -1.2.

- `EXP.vcol(1:4)` are the vertical Soller collimations in minutes of arc (FWHM beam divergence) starting from the in-pile collimator. If the beam divergence is limited by a neutron guide, the corresponding element of `EXP.vcol` is the negative of the guide's m -value. For example, for a 58-Ni guide ($m=1.2$) before the monochromator, `EXP.vcol(1)` should be -1.2.
- `EXP.dir1` defines the scattering direction in the monochromator. This field is equal to 1 or left unassigned if the scattering direction in the monochromator is opposite to that in the sample. Set this field to -1 if the sample and monochromator scattering directions are the same.
- `EXP.dir2` defines the scattering direction in the analyzer. This field is equal to 1 or left unassigned if the scattering direction in the analyzer is opposite to that in the sample. Set this field to -1 if the sample and analyzer scattering directions are the same.
- `EXP.mondir` defines the scattering angle in the monochromator which is positive (counter-clockwise) if this field is absent or positive, and negative (clockwise) otherwise [10].
- `EXP.efixed` is the fixed incident or final neutron energy, in meV.
- `EXP.infin` is a flag set to -1 or left unassigned if the final energy is fixed, or set to +1 in a fixed-incident setup.
- `EXP.sample` is a structure that describes the sample. It contains the following fields:
 - `EXP.sample.mosaic` is the FWHM sample mosaic in the scattering plane in minutes of arc. If this field is left unassigned, no sample mosaic corrections (section II E) are performed.
 - `EXP.sample.vmosaic` is the vertical sample mosaic in minutes of arc. If this field is left unassigned, isotropic mosaic is assumed.

Additional fields in the structure `EXP` are needed for Popovici calculations:

- A series of fields contains information on the linear dimensions of spectrometer components. For each object the “sizes” along a the given coordinate axis x are defined as

$\sqrt{\langle x^2 \rangle}$. For a rectangular shape of width A along the x axis, for example, the correct input would be $A/\sqrt{12}$. For a spherical object of diameter D , the input would be $D/4$.

- `EXP.beam.width` is the width of the source in length units.
 - `EXP.beam.height` is the height of source in length units.
 - `EXP.detector.width` is the width of detector in length units.
 - `EXP.detector.height` is the height of detector in length units.
 - `EXP.mono.width` is the width of the monochromator crystal.
 - `EXP.mono.height` is the height of monochromator crystal.
 - `EXP.mono.depth` is the thickness of monochromator crystal.
 - `EXP.ana.width` is the width of analyzer.
 - `EXP.ana.height` is the height of analyzer.
 - `EXP.ana.depth` is the thickness of analyzer.
 - `EXP.monitor.width` is the width of the monitor. This field is only used in `EXP.moncor=1`.
 - `EXP.monitor.height` is the height of the monitor. This field is only used in `EXP.moncor=1`.
- `EXP.sample.shape` is a matrix describing the sample shape. This is a 3×3 matrix similar to the matrix S_S in section 5. A crucial difference is that `EXP.sample.shape` is defined in the Q coordinate system used in `ResMat.m`. The two matrices are related by a rotation around the vertical axis, which `ResMat.m` performs automatically in the course of its calculations.
 - `EXP.arms(1:5)` are distances between the source and monochromator, monochromator and sample, sample and analyzer, analyzer and detector, and monochromator and monitor, respectively. The 5th element is only needed if `EXP.moncor=1`.
 - `EXP.mono.rv` is the vertical curvature radius of the monochromator crystal. Use a large value for a flat monochromator.
 - `EXP.mono.rh` is the horizontal curvature radius of the monochromator

- `EXP.ana.rv` is the vertical curvature radius of the analyzer
- `EXP.ana.rh` is the horizontal curvature radius of the analyzer

B. `ResMatS.m`

This function is very similar to `ResMat.m`, and calculates the resolution matrix M and the prefactor R_0 , but works in the S coordinate system.

```
function [R0,M]=ResMatS(H,K,W,L,EXP)
```

INPUT ARGUMENTS:

- `H`, `K` and `L` specify the wave vector transfer and are given in reciprocal-lattice units.
- `W` is the energy transfer in meV.
- `EXP` is a structure that contains all the information on the experimental setup and the required method of resolution calculation. It requires all the fields as for `ResMat.m` plus additional fields described below.

OUTPUT ARGUMENTS and vectorization are similar to those for `ResMat.m`.

DEPENDENCIES: `ResMatS.m` requires `ResMat.m`, `StandardSystem.m`, `GetLattice.m`, `star.m`, `scalar.m`, `CleanArgs.m`, `GetTau.m` and `modvec.m` to function properly.

The function `ResMatS.m` requires the following additional fields in structure `EXP`:

- `EXP.sample.a` is the a lattice constant of the sample in Å.
- `EXP.sample.b` is the b lattice constant of the sample in Å.
- `EXP.sample.c` is the c lattice constant of the sample in Å.
- `EXP.sample.alpha` is the α lattice angle of the sample in degrees of arc.
- `EXP.sample.beta` is the β lattice angle of the sample in degrees of arc.
- `EXP.sample.gamma` is the γ lattice angle of the sample in degrees of arc.
- `EXP.orient1(1:3)` are Miller indexes of the first reciprocal-space orienting vector for the S coordinate system, as explained in Section II G.

- `EXP.orient2(1:3)` are Miller indexes of the second reciprocal-space orienting vector for the S coordinate system, as explained in Section II G.
- `EXP.sample.shape` is similar to the corresponding field used with `ResMat.m`, but defines the sample shape in the S coordinate system.
- `EXP.Smooth` defines the smoothing parameters as explained in Section II H. Leave this field unassigned if you don't want this correction done.
 - `EXP.Smooth.E` is the smoothing FWHM in energy (meV). A small number means “no smoothing along this direction”.
 - `EXP.Smooth.X` is the smoothing FWHM along the first orienting vector (x_0 axis) in \AA^{-1} .
 - `EXP.Smooth.Y` is the smoothing FWHM along the y axis in \AA^{-1} .
 - `EXP.Smooth.Z` is the smoothing FWHM along the vertical direction in \AA^{-1} .

C. `MakeExp.m`

This function is an example of creating the `EXP` structure for use with `ResMat.m` and `ResMatS.m`. The user is encouraged to make copies of this m-file and edit them to generate particular experimental setups. The function takes no arguments and returns a `ResMatS`-compatible structure `EXP`.

IV. CRYSTALLOGRAPHY UTILITY FUNCTIONS

ResLib contains several routines for crystallographic calculations “free of charge”. These are `star.m`, `scalar.m`, `modvec.m`, `angle.m`, `angle2.m`, `gtensor.m`, `vector.m`, and `reciprocate.m`. They are particularly useful in user-supplied prefactor and background functions used with `ConvRes.m` and `ConvResSMA.m` (see below).

A. `star.m`

Given direct-space lattice parameters, this function calculates reciprocal-space lattice parameters (or vice-versa).

```
function [V,Vstar,rlattice]=star(lattice)
```

INPUT ARGUMENTS:

- `lattice` is a structure that contains the direct or reciprocal-space lattice parameters (note the difference with the structure `EXP.sample` described above!):
 - `lattice.a` is the a or a^* lattice constant in \AA or \AA^{-1} .
 - `lattice.b` is the b or b^* lattice constant in \AA or \AA^{-1} .
 - `lattice.c` is the c or c^* lattice constant in \AA or \AA^{-1} .
 - `lattice.alpha` is the α or α^* lattice constant in *radians*.
 - `lattice.alpha` is the β or β^* lattice constant in *radians*.
 - `lattice.gamma` is the γ or γ^* lattice constant in *radians*.

OUTPUT ARGUMENTS: `V` and `Vstar` are the direct (reciprocal) and reciprocal (direct) unit cell volumes depending on whether direct or reciprocal lattice parameters are put in. `rlattice` has the same structure as `lattice`, but contains reciprocated cell parameters.

VECTORIZATION: The function can be used to simultaneously reciprocate several sets of lattice parameters. For N calculations *each field of `lattice`* should be a vector of length N or a scalar (if identical values are assumed for a particular cell constant). `V` and `Vstar` and the fields of `rlattice` will then be vectors of length N .

DEPENDENCIES: `star.m` is a stand-alone function.

B. `scalar.m`

Calculate the scalar product of two vectors defined by their fractional cell coordinates. Alternatively, calculates the scalar product of two reciprocal vectors defined by their Miller indexes.

```
function s=scalar(x1,y1,z1,x2,y2,z2,lattice)
```

INPUT ARGUMENTS:

- `lattice` is as in `star.m`. It contains all the lattice parameters for this calculation. Alternatively, it contains reciprocal-lattice parameters.
- `x1`, `y1`, `z1` are fractional cell coordinates of the first vector. Alternatively, they define the Miller indexes of the first reciprocal-lattice vector.
- `x2`, `y2`, `z2` are fractional cell coordinates of the second vector. Alternatively, they define the Miller indexes of the second reciprocal-lattice vector.

OUTPUT ARGUMENTS: The returned value is the scalar product of the two vectors.

VECTORIZATION: The function can be used to simultaneously calculate several scalar products. For N calculations, `x1–z2` are vectors of length N or scalars. Correspondingly, each field of `lattice` should be a vector of length N or a scalar. The returned value will be a vector of length N as well.

DEPENDENCIES: `scalar.m` is a stand-alone function that does not rely on any other components in *ResLib*.

C. `modvec.m`

Very similar to `scalar.m`, but takes only one vector for input and returns its modulus.

```
function m=modvec(x,y,z,lattice)
```

DEPENDENCIES: `modvec.m` relies on `scalar.m`.

D. `angle.m`

Calculate the angle between two vectors in real or reciprocal space.

```
function phi=angle(x1,y1,z1,x2,y2,z2,lattice)
```

INPUT ARGUMENTS: As is `scalar.m`.

OUTPUT ARGUMENTS: The returned value is angle, in radians, between the two vectors.

VECTORIZATION: As is `scalar.m`.

DEPENDENCIES: `angle.m` relies on `scalar.m` and `modvec.m`.

E. `angle2.m`

Calculate the angle between a real-space and a reciprocal-space vector.

```
function phi=angle2(x,y,z,h,k,l,lattice)
```

INPUT ARGUMENTS:

- `lattice` is as in `star.m`. It contains all the lattice parameters for this calculation.
- `x`, `y`, `z` are fractional cell coordinates of the first vector, that is defined in real space.
- `h`, `k`, `l` are Miller indexes of the second vector that is defined in reciprocal space.

OUTPUT ARGUMENTS: The returned value is angle, in radians, between the two vectors.

VECTORIZATION: As is `scalar.m`.

DEPENDENCIES: `angle.m` relies on `scalar.m` and `modvec.m`.

F. `gtensor.m`

Calculate the metric tensor for a set of crystallographic parameters.

```
function g=gtensor(lattice)
```

INPUT ARGUMENTS:

- `lattice` is as in `star.m`.

OUTPUT ARGUMENTS: `g` is the 3×3 metric tensor.

VECTORIZATION: The function can be used to simultaneously calculate several metric tensors. For N calculations, `lattice` is a vector of length N . Correspondingly, `g` is a $3 \times 3 \times N$ array.

DEPENDENCIES: `gtensor.m` is a stand-alone function.

G. `vector.m`

Calculate the scalar product of two vectors defined by their fractional cell coordinates. Alternatively, calculates the scalar product of two reciprocal vectors defined by their Miller indexes.

```
function s=scalar(x1,y1,z1,x2,y2,z2,lattice)
```

INPUT ARGUMENTS:

- `lattice` is as in `star.m`. It contains all the lattice parameters for this calculation. Alternatively, it contains reciprocal-lattice parameters.
- `x1`, `y1`, `z1` are fractional cell coordinates of the first vector. Alternatively, they define the Miller indexes of the first reciprocal-lattice vector.
- `x2`, `y2`, `z2` are fractional cell coordinates of the second vector. Alternatively, they define the Miller indexes of the second reciprocal-lattice vector.

OUTPUT ARGUMENTS: The returned value is the scalar product of the two vectors.

VECTORIZATION: The function can be used to simultaneously calculate several scalar products. For N calculations, `x1–z2` are vectors of length N or scalars. Correspondingly, each field of `lattice` should be a vector of length N or a scalar. The returned value will be a vector of length N as well.

DEPENDENCIES: `scalar.m` is a stand-alone function that does not rely on any other components in *ResLib*.

H. `reciprocate.m`

Calculate the reciprocal-space coordinates (Miller indexes) of a vector defined by its fractional cell coordinates, or vice versa.

```
function [h,k,l]=reciprocate(x,y,z,lattice)
```

INPUT ARGUMENTS:

- `lattice` is as in `star.m` and contains crystallographic lattice parameters. `x`, `y` and `z` are fractional cell coordinates of a vector. Alternatively `lattice` contains reciprocal lattice parameters and `x`, `y` and `z` define a reciprocal-space vector.

OUTPUT ARGUMENTS: `h`, `k` and `l` are reciprocal-space coordinates of the input real-space vector (or real-space coordinates of the input reciprocal-space vector).

VECTORIZATION: As is `scalar.m`.

DEPENDENCIES: `reciprocate.m` calls `gtensor.m`.

I. `GetLattice.m`

This function extracts the lattice parameter from an experimental setup structure (such as used by `ResMatS`) and returns the direct and reciprocal lattice parameters in the form used by `scalar.m`, `star.m`, etc.

```
function [lattice,rlattice]=GetLattice(EXP)
```

INPUT ARGUMENTS:

- `EXP` is a structure of type used with `ResMatS.m`. The fields actually used are: `EXP.sample.a`, `EXP.sample.b`, `EXP.sample.c`, `EXP.sample.alpha`, `EXP.sample.beta`, `EXP.sample.gamma`.

OUTPUT ARGUMENTS: `lattice` and `rlattice` are structures containing the direct and reciprocal space lattice parameters, respectively. They are in the form described above for use with `star.m`.

VECTORIZATION: if `EXP` is a vector of length N , then *each field in `lattice` and `rlattice`* will be a vector of length N .

DEPENDENCIES: `GetLattice.m` is a standalone function.

V. CARTESIAN COORDINATES OF VECTORS.

ResLib contains several routines for crystallographic calculations involving cartesian coordinates of vectors defined in the *S*-system. These are `StandardSystem.m`, `R2S.m` and `S2R.m`. They are particularly useful in user-supplied prefactor and background functions used with `ConvRes.m` and `ConvResSMA.m` (see below).

A. `StandardSystem.m`

Based on a structure `EXP` of type used by `ResMatS.m` constructs the standard basis set of the *S* coordinate system, as defined in Section II G.

```
[x,y,z,lattice,rlattice]=StandardSystem(EXP)
```

INPUT ARGUMENTS:

- `EXP` is a structure of type used with `ResMatS.m`. The fields actually used are: `EXP.sample.a`, `EXP.sample.b`, `EXP.sample.c`, `EXP.sample.alpha`, `EXP.sample.beta`, `EXP.sample.gamma`, `EXP.orient1` and `EXP.orient2`.

OUTPUT ARGUMENTS:

- `x(1:3)` are Miller indexes of the first unit length basis vector for the *S* system.
- `y(1:3)` are Miller indexes of the second unit length basis vector for the *S* system.
- `z(1:3)` are Miller indexes of the third unit length basis vector for the *S* system.
- `lattice` is a structure containing lattice parameters for the sample in `EXP`. It is of the same form as used by `star.m`, `modvec.m`, `scalar.m`, etc..
- `rlattice` is a structure containing reciprocal lattice parameters for the sample in `EXP`. It is of the same form as used by `star.m`, `modvec.m`, etc.

VECTORIZATION: If `EXP` is a vector of length N , then `x`, `y` and `z` are $3 \times N$ matrices and the fields of `sample` and `rsample` are vectors of length N .

DEPENDENCIES: `StandardSystem.m` relies on `star.m`, `GetLattice.m`, `scalar.m` and `modvec.m`.

B. R2S.m

Given cartesian coordinates of a vector in the S-system, calculate its reciprocal-space coordinates (Miller indexes).

```
function [H,K,L,q]=R2S(qx,qy,qz,EXP)
```

INPUT ARGUMENTS:

- EXP is as in `StandardSystem.m`.
- qx, qy, qz are cartesian coordinates of a vector in the S-system defined by the parameters of EXP.

OUTPUT ARGUMENTS: H, K and L are reciprocal-space coordinates of the input vector. q is the vector's absolute value.

VECTORIZATION: As is `scalar.m`.

DEPENDENCIES: R2S.m relies on `StandardSystem.m`, `GetLattice.m`, `star.m`, `scalar.m` and `modvec.m`.

C. S2R.m

Given reciprocal-space coordinates of a vector, calculates its cartesian coordinates in the S-System.

```
function [qx,qy,qz,q]=S2R(H,K,L,EXP)
```

The syntax and usage is similar to `S2R.m`

VI. CONVOLUTION WITH RESOLUTION FUNCTION: GENERAL 4-D CONVOLUTION

In many cases it is convenient to break down the parameterized model cross section function $S(\mathbf{Q}, \omega, \mathbf{p})$ into a sum of partial contributions of several excitation “modes”:

$$S(\mathbf{Q}, \omega, \mathbf{p}) = \sum_{m=1}^{N_m} S_m(\mathbf{Q}, \omega, \mathbf{p}). \quad (17)$$

To save numerical computation time, each partial contribution can be further broken down into a product of a “slowly” and “rapidly” varying components:

$$S_m(\mathbf{Q}, \omega, \mathbf{p}) = P_m(\mathbf{Q}, \omega, \mathbf{p}) \tilde{S}_m(\mathbf{Q}, \omega, \mathbf{p}). \quad (18)$$

Here the “slow” prefactor $P_m(\mathbf{Q}, \omega, \mathbf{p})$ is expected to be almost constant within the volume of the resolution ellipsoid, and therefore does not need to be numerically folded with the resolution function. Typical examples are polarization factors and magnetic form factors. For the “fast” part of the cross section $\tilde{S}_m(\mathbf{Q}, \omega, \mathbf{p})$ there is no escape and a full convolution has to be performed numerically in four dimensions. With the “slow” prefactor and an additional background function $B(Q)$, Equation 1 becomes:

$$\begin{aligned} \frac{d\sigma}{d\Omega dE'} &\approx B(Q_0) + R_0(Q_0) \sum_{m=1}^{M_m} \{P_m(\mathbf{Q}_0, \omega_0, \mathbf{p}) \times \\ &\times \int \int \int \int d^4\mathcal{Q} S(\mathcal{Q}) \exp \left[-\frac{1}{2} (\mathcal{Q}^i - \mathcal{Q}_0^i) (\mathcal{Q}^j - \mathcal{Q}_0^j) M_{ij}(\mathcal{Q}_0) \right] \}. \end{aligned} \quad (19)$$

Given the above definitions and by a substitution of integration variables Equation 19 can be rewritten as:

$$\begin{aligned} \frac{d\sigma}{d\Omega dE'} &\propto B(Q_0) + R_0(Q_0) \frac{1}{\sqrt{\det(M)}} \times \\ &\times \sum_{m=1}^{N_m} \left\{ P_m(\mathbf{Q}_0, \omega_0, \mathbf{p}) \int_{-\pi/2}^{\pi/2} d\phi_1 \int_{-\pi/2}^{\pi/2} d\phi_2 \int_{-\pi/2}^{\pi/2} d\phi_3 \int_{-\pi/2}^{\pi/2} d\phi_4 \tilde{S}_m(\mathbf{Q}, \omega, \mathbf{p}) \times \right. \\ &\times \left. \frac{\exp \left(-\frac{1}{2} \tan^2 \phi_1 - \frac{1}{2} \tan^2 \phi_2 - \frac{1}{2} \tan^2 \phi_3 - \frac{1}{2} \tan^2 \phi_4 \right)}{\cos^2 \phi_1 \cos^2 \phi_2 \cos^2 \phi_3 \cos^2 \phi_4} \right\}, \end{aligned} \quad (20)$$

where the new variables are defined as:

$$Q_x - Q_{0,x} = -\frac{1}{\sqrt{\tilde{M}_{11}}} \tan \phi_1,$$

$$\begin{aligned}
Q_y - Q_{0,y} &= -\frac{1}{\sqrt{\tilde{M}_{22}}} \tan \phi_2 - \frac{\tilde{M}_{12}}{\tilde{M}_{22}\sqrt{\tilde{M}_{11}}} \tan \phi_1, \\
\omega - \omega_0 &= -\frac{1}{M_{33}} \tan \phi_3 - \frac{M_{23}}{M_{33}\sqrt{\tilde{M}_{22}}} \tan \phi_2 - \frac{\left(\frac{M_{13}}{M_{33}} - \frac{M_{23}}{M_{22}} \frac{\tilde{M}_{12}}{\tilde{M}_{22}}\right)}{\sqrt{\tilde{M}_{11}}} \tan \phi_1, \\
Q_z - Q_{0,z} &= -\frac{1}{\sqrt{M_{44}}} \tan \phi_4, \\
\tilde{M}_{11} &= M_{11} - \frac{M_{13}^2}{M_{33}} - \frac{\tilde{M}_{12}^2}{\tilde{M}_{22}}, \\
\tilde{M}_{12} &= M_{12} - \frac{M_{13}M_{23}}{M_{33}}, \\
\tilde{M}_{22} &= M_{22} - \frac{M_{23}^2}{M_{33}}.
\end{aligned}$$

If this integral is evaluated numerically by sampling of integrand in a set of points uniformly distributed in ϕ -space, the sampling points will be distributed according to a Lorenzian in (\mathbf{Q}, ω) -space. The widths of the 4D-Lorenzian will be determined by the resolution ellipsoid. More points will get sampled near the resolution center, and less on the "tails". This allows one to achieve much better results with fewer sampling points.

A. `ConvRes.m`

Numerically convolutes a user-supplied cross section function (defined in separate m-files) with the resolution function in a given set of points in (\mathbf{Q}, ω) -space. This process requires laborious calculations and one always has to compromise between computation times and accuracy. The sharper the intrinsic features of the cross section, the more difficult it is to get an accurate result. In particular, if the cross section has a singular form (energy δ -function), straightforward 4D convolution doesn't work at all. A work-around is to artificially introduce some intrinsic width in the excitations. A much better approach is to use `ConvResSMA.m`, described below. In fact, try to use `ConvResSMA.m` whenever possible, as it is much faster than `ConvRes.m`. `ConvRes.m` implements two algorithms of numerical integration. The "fixed-sampling" method samples the "fast" cross section on a fixed grid in ϕ -space. Alternatively, the Monte Carlo algorithm can be used, eliminating any "structured" artifacts (a common problem with fixed sampling), but introduces "noise". MC is good for simulations, but the irreproducible "noise" will confuse many least-squares fitting routines. For an example of use see `ConvDemo.m`.

```
function conv=ConvRes(sqw,pref,H,K,L,W,EXP,METHOD,ACCURACY,p)
```

INPUT ARGUMENTS:

- 'sqw' is the name of the user-supplied “fast” model cross section. It must be defined in a separate m-file. The requirements for this function are specified below.
- 'pref' is the name of the user-supplied “slow” cross section prefactor and background function. It must be defined in a separate m-file. The requirements for this function are specified below. If this argument is set to [], the prefactors for all modes will be assumed to be unity, and the background will be zero for all data points.
- H, K, L and W specify the wave vector and energy transfers at which the convolution is to be calculated (i.e., define \mathcal{Q}_0). H, K and L are given in reciprocal lattice units, and W in meV.
- EXP is a structure that contains all the information on the experimental setup. It has the form used with ResMatS.m, as described above.
- METHOD is a string that specifies which 4D-integration method to use, and ACCURACY determines the number of sampling points in the integration. The following options are available:
 - METHOD='fix': Sample the cross section on a fixed grid of points uniformly distributed in ϕ -space. If this option is chosen, $2*\text{ACCURACY}(1)+1$ points are sampled along ϕ_1 , ϕ_2 and ϕ_3 , and $2*\text{ACCURACY}(2)+1$ along ϕ_4 (vertical direction).
 - METHOD='mc': 4D Monte Carlo integration. The cross section is sampled in $1000*\text{ACCURACY}$ randomly chosen points, uniformly distributed in ϕ -space.
- p is a parameter that is passed on, without change, to sqw and pref.

OUTPUT ARGUMENTS: conv is the calculated value of the cross section, folded with the resolution function, at the give \mathcal{Q}_0 position.

VECTORIZATION: The code is vectorized with respect to H, K, L, W and EXP. It can be used to simultaneously calculate convolutions at several \mathcal{Q}_0 -points or even for several experimental setups. Any vectors among H, K, L, W and EXP must be of the same length. If any of these are scalars, they will be automatically replicated into vectors of appropriate

length. For input vectors of length N the result is, correspondingly, a length- N row-vector of convolution values.

DEPENDENCIES: To properly function `ConvRes.m` requires the following m-files from *ResLib*: `ResMatS.m`, `ResMat.m`, `StandardSystem.m`, `GetLattice.m`, `star.m`, `scalar.m`, `modvec.m`, `GetTau.m`, `CleanArgs`.

The “fast” cross section functions are defined in a separate user-supplied m-file that must be of the form: `function s=sqw(H,K,L,W,p)`. The arguments H , K and L specify the scattering vector in rec. lattice units, and W is the energy transfer in meV. p is an additional parameter that can be anything: a number, an array, a structure, or a cell array. See `SqwDemo.m` for an example. The function `sqw` must be vectorized, i.e., if H , K , L and W are vectors of length N , the output should be a vector of values of the same length. Even when some of the input arguments are vectors of length N , others may be scalars, and in this case should be treated as equivalents on length- N vectors of constant values. `sqw` can return several partial contribution to the cross section. For N_m modes and N data points the output argument must be a $N_m \times N$ matrix.

The “slow” cross section prefactors p and background b are defined in a separate user-supplied m-file that must be of the form: `function [p,b]=pref(H,K,L,W,p,EXP)`, or, if no background is to be calculated: `function p=pref(H,K,L,W,p,EXP)`. `pref` is similar to `sqw` function, except that it has direct access to experimental conditions and must list `EXP` as its argument. See `PrefDemo.m` for an example. If `sqw` returns several partial contributions to the cross section, `pref` is expected to do the same: for N_m modes and N data points the output argument p must be a $N_m \times N$ matrix. The background is calculated separately for each data point, so b is a length- N vector. For a flat background b can be a scalar. Note that b is truly the “raw” background. It is applied to the result *after* all the convolutions, summation over multiple modes, and scaling factors.

VII. CONVOLUTION WITH RESOLUTION FUNCTION: SINGLE MODE APPROXIMATION AND VOIGT PROFILES

In many cases the “fast” dynamic structure factor can be broken written as:

$$\tilde{S}_m(\mathbf{Q}, \omega, \mathbf{p}) = s_m(\mathbf{Q}, \mathbf{p})\delta(\omega - \omega_m(\mathbf{Q}, \mathbf{p})). \quad (21)$$

Here $s_m(\mathbf{Q}, \mathbf{p})$ is the intensity of the m -th excitation branch, and $\omega_m(\mathbf{Q}, \mathbf{p})$ is its dispersion relation. `ConvRes.m` becomes unusable in this case, as it can not handle infinitely sharp features of the cross section. The solution is to eliminate the δ -functions analytically, also reducing a laborious 4-D numerical convolution to a much faster 3-D convolution.

Equation 21 can be generalized to the case when each mode is characterized by some intrinsic Lorentzian energy-width $\Gamma_m(\mathbf{Q}, \mathbf{p})$:

$$\tilde{S}_m(\mathbf{Q}, \omega, \mathbf{p}) = \frac{1}{\pi} s_m(\mathbf{Q}, \mathbf{p}) \frac{\Gamma_m(\mathbf{Q}, \mathbf{p})}{\Gamma_m(\mathbf{Q}, \mathbf{p})^2 + [\omega - \omega_m(\mathbf{Q}, \mathbf{p})]^2} \quad (22)$$

While a convolution of a Gaussian and a Lorentzian (so-called Voigt function) can not be computed analytically, some very efficient numerical approximations are available [9].

The ϕ -transformation is performed only in 3 dimensions in either case. Exact expressions used in *ResLib* are as follows: Equation 1 is rewritten as:

$$\begin{aligned} \frac{d\sigma}{d\Omega dE'} &\approx B(\mathbf{Q}_0) + R_0(\mathbf{Q}_0) \frac{1}{\sqrt{\tilde{M}_{11}\tilde{M}_{22} - \tilde{M}_{12}^2}\sqrt{\tilde{M}_{33}}} \times \\ &\times \sum_{m=1}^{N_m} \left\{ P_m(\mathbf{Q}_0, \omega_0, \mathbf{p}) \int_{-\pi/2}^{\pi/2} d\phi_1 \int_{-\pi/2}^{\pi/2} d\phi_2 \int_{-\pi/2}^{\pi/2} d\phi_3 \tilde{S}_m(\mathbf{Q}, \mathbf{p}) V(\tilde{\omega}_m(\mathbf{Q}, \mathbf{p}), \tilde{\Gamma}_m(\mathbf{Q}, \mathbf{p})) \times \right. \\ &\times \left. \frac{\exp\left(-\frac{1}{2}\tan^2\phi_1 - \frac{1}{2}\tan^2\phi_2 - \frac{1}{2}\tan^2\phi_3\right)}{\cos^2\phi_1 \cos^2\phi_2 \cos^2\phi_3} \right\}, \quad (23) \end{aligned}$$

where the new variables are defined as:

$$\begin{aligned} \tilde{\Gamma}_m(\mathbf{Q}, \mathbf{p}) &= \frac{1}{\sqrt{\tilde{M}_{33}}}\Gamma_m(\mathbf{Q}, \mathbf{p}), \\ \tilde{\omega}_m(\mathbf{Q}, \mathbf{p}) &= \omega - \omega_m(\mathbf{Q}, \mathbf{p}) + \frac{M_{13}Q_x + M_{23}Q_y}{\sqrt{\tilde{M}_{33}}}, \\ V(x, y) &\equiv \frac{1}{\pi} \int dt \exp(-t^2) \frac{y}{y^2 + (t-x)^2}, \\ Q_y - Q_{0,y} &= \frac{\sqrt{\tilde{M}_{11}}}{\sqrt{\tilde{M}_{11}\tilde{M}_{22} - \tilde{M}_{12}^2}} \tan\phi_2, \end{aligned}$$

$$\begin{aligned}
Q_x - Q_{0,x} &= \frac{1}{\sqrt{\tilde{M}_{11}}} \tan \phi_1 - \frac{\tilde{M}_{12}}{\sqrt{\tilde{M}_{11}} \sqrt{\tilde{M}_{11} \tilde{M}_{22} - \tilde{M}_{12}^2}} \tan \phi_2, \\
Q_z - Q_{0,z} &= -\frac{1}{\sqrt{M_{44}}} \tan \phi_4, \\
\tilde{M}_{11} &= M_{11} - \frac{M_{13}^2}{M_{33}}, \\
\tilde{M}_{12} &= M_{12} - \frac{M_{13} M_{23}}{M_{33}}, \\
\tilde{M}_{22} &= M_{22} - \frac{M_{23}^2}{M_{33}}.
\end{aligned}$$

A. ConvResSMA.m

Handles user-supplied cross section functions written in the single-mode form. Having one dimension less to deal with, it is much faster than `ConvRes.m` and should be used in its stead whenever possible. For an example of use see `ConvDemo.m`.

```
function conv=ConvResSMA(sqw,pref,H,K,L,W,EXP,METHOD,ACCURACY,p)
```

INPUT ARGUMENTS:

- `'sqw'` is the name of the user-supplied “fast” model single-mode cross section. It must be defined in a separate m-file. The requirements for this function are listed below.
- `'pref'`, `H`, `K`, `L`, `W`, `p`, and `EXP` have exactly the same meaning and form as for `ConvRes.m`.
- `METHOD` is a string that specifies which 3D-integration method to use, and `ACCURACY` determines
 - `METHOD='fix'`: Sample the cross section on a fixed grid of points uniformly distributed in ϕ -space. If this option is chosen, $2*\text{ACCURACY}(1)+1$ points are sampled along ϕ_1 and ϕ_2 , and $2*\text{ACCURACY}(2)+1$ along ϕ_3 (vertical direction).
 - `METHOD='mc'`: 3D Monte Carlo integration. The cross section is sampled in $1000*\text{ACCURACY}$ randomly chosen points, uniformly distributed in ϕ -space.

OUTPUT ARGUMENTS: See output arguments for `ConvRes.m`.

VECTORIZATION: See vectorization of `ConvRes.m`.

DEPENDENCIES: To properly function `ConvResSMA.m` requires the following m-files from *ResLib*: `ResMatS.m`, `ResMat.m`, `StandardSystem.m`, `GetLattice.m`, `GetTau.m`, `star.m`, `scalar.m`, `modvec.m`, `CleanArgs`.

The user-supplied single mode cross section `sqw` is defined in a separate m-file. It must have the form: `function [w0,S,HWHM]=sqw(H,K,L,p)`. The input arguments are as those for the cross section function for `ConvRes.m`. See `SMADemo.m` for an example. For N_m modes and N data points the output arguments are $N_m \times N$ matrices. For mode m at i -th reciprocal-space point $(H(i),K(i),L(i))$, $s(m,i)$ is the mode intensity, $w0(m,i)$ is its energy in meV, and $HWHM(m,i)$ is its Lorentzian energy half-width. If $HWHM(m,i)=0$, the mode is assumed to have a δ -function energy profile at this point.

VIII. LEAST-SQUARES FITTING OF CONVOLUTED CROSS SECTIONS

A. `FitConv.m`

This function provides Levenberg-Marquardt least squares fitting of convoluted cross sections to experimental data. The algorithm is exactly as in NR 15.5. Analytic derivatives are not supported in the current version. This function calls `ConvRes.m` for convolution calculations at each iteration step. An example of use is given in `FitDemo.m`. The function call has the following form:

```
function [pa,dpa,chisqN,sim,CN,PQ,nit,kvg,details] =  
FitConv(H, K, L, W, EXP, Iobs, dIobs, sqw, pref, pa, ia, METHOD, ACCURACY,  
nitmax, tol, dtol)
```

INPUT ARGUMENTS:

- `'sqw'`, `'pref'`, `METHOD` and `ACCURACY` are exactly as in `ConvRes.m`.
- `H`, `K`, `L`, `W`, `EXP` are vectors that contain the wave vector components, energy transfers, and experimental conditions for each experimental data point. They all must be of the same length or scalars. See `ConvRes.m` for more details.
- `Iobs`, `dIobs` are vectors of the same length as `H-EXP`, and contain the observed scattering intensities and error bars for each data point, respectively.
- `pa` is the initial guess for parameter values. This should be a 1-dimensional array of the form accepted as the parameter `p` by the `sqw` and `pref` functions.
- `ia` (optional) - a list with zero elements corresponding to fixed parameters and ones for parameters that should be varied. This array should be of the same size as `pa`. The default value is `ia=ones`.
- `nitmax` (optional)- the maximum number of iterations allowed before the program exits. The default value is `nitmax=20`.
- `tol` (optional)- the convergence criterion: convergence declared when χ^2 decreases by a relative amount less than `tol`. The default value is `tol=0.001`.

- `dtol` (optional)- parameter for relative change in numerical derivatives, default `dtol=1e-5`.

OUTPUT ARGUMENTS:

- `pa, dpa` - refined parameters and error bars.
- `chi2N` - χ^2 normalized by degrees of freedom.
- `CN` - normalized correlation matrix - includes varying parameters only (in order).
- `PQ` - probability that χ^2 exceeds that observed.
- `nit` - number of iterations to convergence.
- `kvg` - convergence flag:
 - `kvg= 0` did not converge due to too many iterations `nit` \geq `nitmax`
 - `kvg= 1` converged normally
 - `kvg= 2` questionable convergence (final $\lambda > 1 \cdot 10^{-3}$)
- `sim` - (optional) fitted value of convoluted cross section at input points
- `details` - optional output structure with fields:
 - `chisq` -raw χ^2
 - `DF` -degrees of freedom
 - `Ndata` -number of data points
 - `Npar` -total number of parameters
 - `Nvar` -number of parameters varied
 - `C` -raw covariance matrix
 - `final_lamda` -final value of λ used in the fitting process
 - `yf` -fitted values of function at input points

DEPENDENCIES: To properly function `FitConv.m` requires the following m-files from *ResLib*: `ConvRes.m`, `ResMatS.m`, `ResMat.m`, `GetTau.m`, `StandardSyssem.m`, `star.m`, `modvec.m`, `scalar.m`, `CleanArgs`.

B. FitConvSMA.m

This function is very similar to `FitConv.m`, but uses single-mode cross sections as in `ConvResSMA.m`. The function call has the following form:

```
function [pa,dpa,chisqN,sim,CN,PQ,nit,kvg,details] =  
FitConvSMA(H, K, L, W, EXP, Iobs, dIobs, sqw, pref, pa, ia, METHOD,  
ACCURACY, nitmax, tol, dtol)
```

INPUT ARGUMENTS:

- 'sqw', 'pref', METHOD and ACCURACY are exactly as in `ConvResSMA.m`
- Other parameters as in `FitConv.m`.

DEPENDENCIES: To properly function `FitConvSMA.m` requires the following m-files from *ResLib*: `ConvResSMA.m`, `ResMatS.m`, `ResMat.m`, `GetTau.m`, `StandardSystem.m`, `star.m`, `modvec.m`, `scalar.m`, `CleanArgs`.

C. FitConvBoth.m

This function fits a sum of a "standard" and single mode-type cross sections to the data. This is very useful when the scattering contains both a singular and a diffuse part. The function call has the following form:

```
function [pa,dpa,chisqN,sim,CN,PQ,nit,kvg,details]=  
FitConvBoth(H, K, L, W, EXP, Iobs, dIobs, sqw, pref, sma, smapref, pa, ia,  
METHOD, ACCURACY, SMACCURACY, nitmax, tol, dtol)
```

INPUT ARGUMENTS:

- 'sma', 'smapref', METHOD, and SMACCURACY are exactly as in `ConvResSMA.m`.
- 'sma', 'pref', and ACCURACY are as in `ConvRes.m`.
- Other parameters as in `FitConv.m`.

DEPENDENCIES: To properly function `FitConvBoth.m` requires the following m-files from *ResLib*: `ConvResSMA.m`, `ConvRes.m`, `ResMatS.m`, `ResMat.m`, `GetTau.m`, `StandardSystem.m`, `star.m`, `modvec.m`, `scalar.m`, `CleanArgs`.

IX. GRAPHIC REPRESENTATIONS OF RESOLUTION ELLIPSOIDS

It is often very helpful to visualize resolution ellipsoids for each point in an inelastic scan, see how they change from one point to the next, and try to understand how they are oriented relative to the dispersion surface in the system under investigation. Also, while the resolution matrix contains all the information on the instrumental resolution at a given point, parameters such as resolution volume, projected energy width, Bragg peak width, etc., are much more useful in planning actual measurements. *ResLib* provides two routines for visualizing resolution ellipsoids and calculating the most relevant resolution parameters.

A. `ResPlot.m`

This function plots projections and sections of resolution ellipsoids for a user-defined scan, and calculates a bunch of relevant resolution characteristics for the center-point of the scan. As an option, it also plots the dispersion relation calculated from a user-supplied single-mode cross section function, of the type used by `ConvResSMA.m`. The projection and section planes for resolution ellipsoids are defined by the orienting vectors specified in `EXP`. By changing these one can get projections and sections with any desired reciprocal-space planes. An example of use can be found in `PlotDemo.m`.

```
function ResPlot(H,K,L,W,EXP,SMA,SMAp)
```

INPUT ARGUMENTS:

- `H`, `K`, `L`, `W`, `EXP` are vectors that contain the wave vector components, energy transfers, and experimental conditions for each experimental data point. They all must be of the same length or scalars. See `ConvRes.m` for more details. `ResPlot.m` is designed to work with a single scan, measured in a particular experimental setup. Therefore, calculations for all scan points will be performed using experimental conditions for the center-point of the vector `EXP` (center of scan).
- `SMA` (optional) is the name of a single-mode cross section function to be used for plotting the dispersion relation.
- `SMAp` (optional) - parameters to be passed to the cross section function `SMA`.

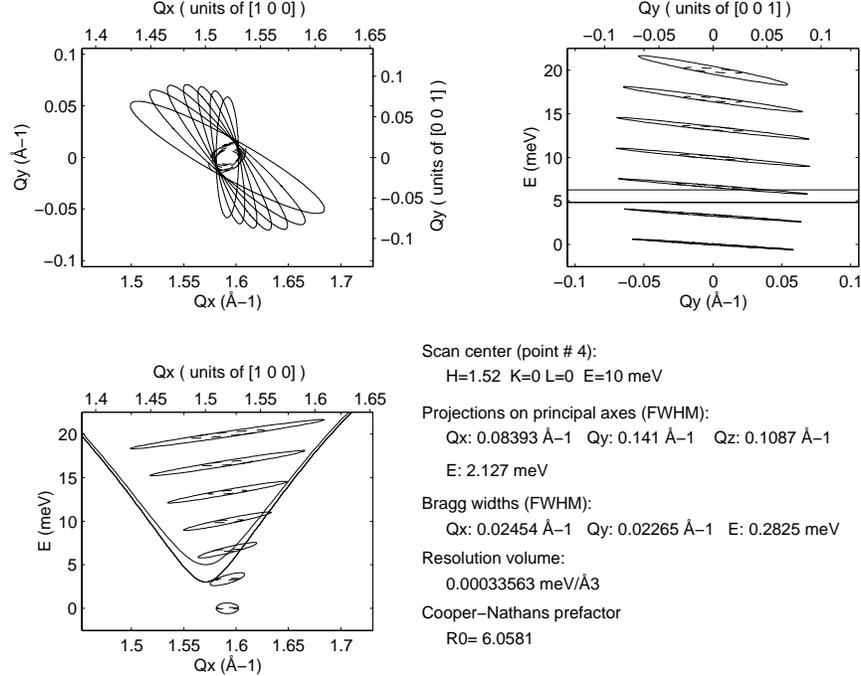


FIG. 1: *Upper left*: projection onto the scattering plane (large ellipses) and constant-energy sections (inner ellipses). *Lower left*: $Q_x - E$ projections and sections. Additional lines (here: parabola) show the dispersion of the two branches defined in the single mode cross section function. The Q_y and Q_z values for this dispersion curve are taken for the mid-point in the scan. *Upper right*: $Q_y - E$ projections and sections. Additional lines (here: straight lines) show the dispersion of the two branches defined in the single-mode cross section function. The Q_x and Q_z values for this dispersion curve are taken for the mid-point in the scan.

OUTPUT: All the information is sent to the current figure. A typical output looks like this:

DEPENDENCIES: To properly function `ResPlot.m` requires the following m-files from `ResLib`: `ResMatS.m`, `ResMat.m`, `GetTau.m`, `StandardSystem.m`, `star.m`, `modvec.m`, `scalar.m`, `CleanArgs`.

B. ResPlot3D.m

This function is similar to `ResPlot.m` but plots a very neat 3D representation of resolution ellipsoids, projections and dispersion surfaces. See `Plot3DDemo.m` for an example of use.

function `ResPlot3D (H,K,L,W,EXP,RANGE,EllipsoidStyle,XYStyle,XEStyle,`

YESTyle, SMA, SMap, SXg, SYg)

INPUT ARGUMENTS:

- H, K, L, W, EXP are as in `ResPlot.m`.
- RANGE defines the range of momentum and energy transfer to use in the plot. RANGE must be of the form [Qxmin, Qxmax, Qymin, Qymax, Emin, Emax], in \AA^{-1} and meV, respectively.
- EllipsoidStyle (optional) is the color of resolution ellipsoids in the plot. Default is EllipsoidStyle='red'.
- XYStyle (optional) - line style to use for the projection onto the scattering plane, in the format used with MatLab's plot command (something like 'r--' for a red dashed line). Use the value 'none' to suppress projections.
- XEStyle (optional) - line style to use for the projection onto the $Q_x - E$ plane, in the format used with MatLab's plot command. Use the value 'none' to suppress projections.
- YEStyle (optional) - line style to use for the projection onto the $Q_y - E$ plane, in the format used with MatLab's plot command. Use the value 'none' to suppress projections.
- SMA and SMap (both optional) are as in `ResPlot.m`.
- SXg and SYg (both optional) define the 2D grid of Q_x and Q_y values for plotting the dispersion surfaces. They must be of the same form as used in MatLab's surf command, and as generated by meshgrid. A good example of use is given in `Plot3Ddemo.m`. If omitted, the dispersion surface is plotted of a 40×40 grid within the boundaries specified by the first 4 elements of RANGE.

OUTPUT: All the information is sent to the current figure.

DEPENDENCIES: To properly function `ResPlot3D.m` requires the following m-files from *ResLib*: `ResMatS.m`, `ResMat.m`, `GetTau.m`, `StandardSysem.m`, `star.m`, `modvec.m`, `scalar.m`, `CleanArgs`.

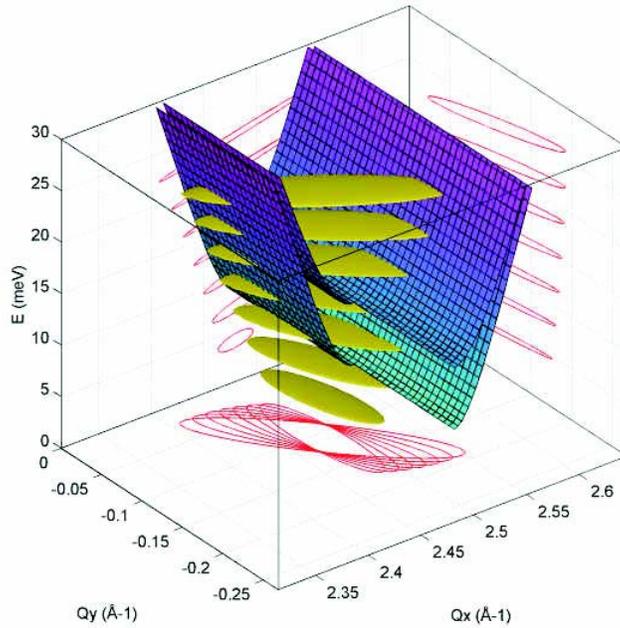


FIG. 2: A typical image generated by ResPlot3D.m.

X. MISCELLANEOUS FUNCTIONS

A. CleanArgs.m

Reshapes input arguments to be row-vectors and makes sure they are same length.

function [N,X,Y,Z,...]=CleanArgs(x,y,z,...)

ARGUMENTS: N is the length of the longest input argument. If any input arguments is a scalar, they are replicated to produce vectors of length N. In any case, the output arguments X, Y,... are row-vectors of length N.

DEPENDENCIES: CleanArgs.m is a stand-alone function that does not rely on any other components in *ResLib*.

B. GetTau.m

Returns τ -values ($2\pi/d$) for common monochromator crystals.

function TAU=GetTau(tau)

ARGUMENTS: If tau is numerical, it is simply copied to the output argument TAU. If tau

is a string such as ‘PG002’ or ‘Si111’, the returned value is the reciprocal vector of the corresponding monochromator crystal.

DEPENDENCIES: This is a stand-alone function.

C. Rebin.m

A simple routine to rebin, average and merge data sets.

```
function [yb,dyb,x1b,x2b...]=Rebin(y,dy,x1,x2,...,[b1,b2...])
```

INPUT ARGUMENTS: Vector y is the data set (dependent variable), vector dy contains the standard deviations (error bars), vectors x_1, \dots are the independent variables, and the scalars b_1, \dots are the bin sizes for each independent variable. All vectors must be of the same length or scalars.

OUTPUT ARGUMENTS: Vector y_b is the binned data (dependent variable), vector dy_b contains the corresponding standard deviations (error bars), and vectors x_{b1}, \dots are the independent variables in the binned data set.

DEPENDENCIES: `Rebin.m` is a stand-alone function that does not rely on any other components in *ResLib*.

D. SpecGoTo.m

Calculate the shaft angles of a 3-axis spectrometer for a given momentum and energy transfer.

```
function [M1,M2,S1,S2,A1,A2]=SpecGoTo(H,K,L,E,EXP)
```

INPUT ARGUMENTS: H, K, L, E, EXP contain the wave vector components, energy transfer, and experimental conditions, as described above.

OUTPUT ARGUMENTS: M_1 and M_2 are the rotation and scattering angle for the monochromator crystal *in radians*. S_1 and S_2 are the rotation and scattering angle for the sample. A_1 and A_2 are the rotation and scattering angle for the analyzer crystal.

VECTORIZATION: Input arguments can be vectors of the same length or scalars. The output arguments will then be vectors, accordingly.

DEPENDENCIES: To properly function `SpecGoTo.m` requires the following m-files from *ResLib*: `CleanArgs.m`, `R2S.m`, `StandardSystem.m`, `GetLattice.m`, `GetTau.m`.

E. SpecWhere.m

Calculate the energy and momentum transfer in a 3-axis spectrometer given the shaft angles.

```
function [H,K,L,E,Q,Ei,Ef]=SpecWhere(M2,S1,S2,A2,EXP)
```

INPUT ARGUMENTS: EXP is as in SpecGoTo.m. M2 is the scattering angle for the monochromator crystal. S1 and S2 are the rotation and scattering angle for the sample. A2 is the rotation and scattering angle for the analyzer crystal. All angles are in *radians*.

OUTPUT ARGUMENTS: H, K, L, E, Q, Ei, Ef are the wave vector components, energy transfer, wave vector transfer, incident energy and final energy.

VECTORIZATION: Input arguments can be vectors of the same length or scalars. The output arguments will then be vectors, accordingly.

DEPENDENCIES: To properly function SpecWhere.m requires the following m-files from *ResLib*: CleanArgs.m, S2R.m, StandardSystem.m, GetLattice.m, GetTau.m.

F. Spurions.m

This function is used to detect potential spurious scattering and false peaks in the neutron data. The normal scattering process involves neutrons of initial energy E_i , scattered from the sample with the momentum transfer (h, k, l) and energy transfer $\hbar\omega$, and detected at a final energy E_f . In practice, the following spurious processes will also contribute to the detector counts:

- Higher-order scattering in the monochromator crystal adds neutrons of energies $4E_i$, $9E_i$, etc., to the incident beam. Similarly, the detector will also detect neutrons with energies $4E_f$, $9E_f$, etc. Any combination of these incident and final energies, if scattered by the sample, will be detected as spurious scattering. The danger of this happening is particularly large if the process corresponds to elastic scattering in the sample (e.g., $4E_i = 9E_f$, $E_i = 4E_f$, etc.).
- A inelastic scattering event may occur due to phonons in the monochromator or analyzer (thermal diffuse scattering). Though very weak, such events will produce strong spurious scattering or sharp false peaks, if by accident the beam gets scattered elastically in the sample.

- Both mechanisms described above can be realized by powder scattering from an Al sample holder, rather than the sample itself. Beware!

`Spurions.m` calculates momentum and energy transfer at sample position for each type of spurious scattering scenarios. The result is displayed on the screen.

```
function Spurions(H,K,L,E,EXP)
```

INPUT ARGUMENTS: H, K, L, E, EXP contain the wave vector components, energy transfer, and experimental conditions.

OUTPUT ARGUMENTS: None.

VECTORIZATION: This function is *not* vectorized.

DEPENDENCIES: To properly function `Spurions.m` requires the following m-files from *ResLib*: `SpecWhere.m`, `SpecGoTo.m`, `CleanArgs.m`, `S2R.m`, `R2S.m`, `GetTau.m`, `StandardSystem.m`, `GetLattice.m`.

XI. NEW FEATURES IN RESLIB 3.4

ResLib 3.4 is **fully backward compatible** with any code written for *ResLib* 3.1. The new features in version 3.4 are:

- User-supplied background functions can be used in the fitting process. See `ConvRes.m`.
- Support for arbitrary monochromator scattering direction in `ResMat.m` and its derivatives.
- Support for beam collimation defined by neutron guides. See `ResMat.m`.
- New crystallographic functions: `gtensor.m`, `angle.m`, `angle2.m`, `reciprocate.m`, `vector.m`, `GetLattice.m`.
- Two new functions for easy conversion between reciprocal-space and cartesian coordinates `R2S.m` and `S2R.m`.
- New function `Rebin.m` for binning data sets.
- New spectrometer “positioning” and “where” functions `SpecGoTo.m` and `SpecWhere.m`.
- New function `Spurions.m` helps detect spurious peaks.

Changes to the manual since version 3.1 and 3.2 are shown in **dark blue** and dark red text, respectively.

XII. DOWNLOADS, PACKAGING, INSTALLATION AND FEEDBACK

A. File download

The most recent version of all *ResLib* files are available here for download as a .zip archive from <http://nsmc1.ssd.ornl.gov/~zhelud/reslib/>.

B. Packaging

- `ResMat.m` - calculate Cooper-Nathans resolution matrices.

- `ResMatS.m` - same thing, in a coordinate system defined by the scattering vector.
- `ConvRes.m` - convolute a user-defined cross-section function with the resolution.
- `ConvResSMA.m` - convolute a user-defined single-mode cross-section with the resolution.
- `FitConv.m` - fit convoluted cross section to experimental data.
- `FitConvSMA.m` - fit convoluted SMA cross section to experimental data.
- `FitConvBoth.m` - fit convoluted sum of "standard" and SMA cross sections to experimental data.
- `ResPlot.m` - 2-D visualization of resolution ellipsoids and dispersion.
- `ResPlot3D.m` - 3-D visualization of resolution ellipsoids and dispersion.
- `scalar.m` - scalar product of vectors defined by fractional cell coordinates or Miller indexes.
- `modvec.m` - length of vectors defined by fractional cell coordinates or Miller indexes.
- `star.m` - calculate reciprocal-lattice parameters, unit cell volume and reciprocal volume.
- `StandardSystem.m` - calculate components of standard sample-centered orthonormal basis set.
- `MakeExp.m` - Example of setting up a structure that contains details on experimental conditions for use with `ResMat`, `ConvRes` and other functions.
- `SqwDemo.m` - example of a user cross section function for use with `ConvRes`.
- `SMADemo.m` - example of a user single-mode cross section function for use with `ConvResSMA`.
- `PrefDemo.m` - example of a "slowly prefactor" function for use with `ConvRes`, `SqwDemo`, `ConvResSMA` and `SMADemo`.
- `ConvDemo.m` - a demo script of the convolution routines.

- `FitDemo.m` - a demo script of the fitting routines.
- `PlotDemo.m` - a demo script of `ResPlot`
- `Plot3DDemo.m` - a demo script for `ResPlot3D`
- `Demo.dat` - an actual data set used in `FitDemo`
- `ResLib.m` - list of functions supplied in *ResLib* for use with the MatLab `help` command.
- `Manual.pdf` - this file.
- `ResLib.jpg` - *ResLib* logo in JPEG format.

C. Installation

Uncompress the archive to a separate new directory and add it to your MatLab path by using the `addpath` command. Run the `ConvDemo` script to see that *ResLib* works on your system. Run the `PlotDemo` and `Plot3DDemo` scripts to get some nice graphics. Change to the directory where the files are installed (to have `Demo.dat` in the current directory) and try `FitDemo`.

D. Feedback

The author welcomes any comments, questions, suggestion and bug reports sent by e@mail to `zhelud@bigfoot.com`.

XIII. CREDITS

Many ideas and entire code fragments are borrowed from IDL routines written at Johns Hopkins University by Collin L. Broholm and Igor Zaliznyak (now at BNL). Levenberg-Marquardt algorithm based on C Numerical Recipes, as adapted for MatLab by Stephen E. Nagler (ORNL). Voigt function by A. N. Maurellis. The library was originally developed at Brookhaven National Laboratory, but is now maintained at Oak Ridge National Laboratory.

XIV. DISCLAIMER

There obviously is no guarantee that the above routines work right. 3-axis resolution calculations are a tricky business and have on many occasions led to incorrect interpretation of experimental data, outright wrong publications, and destruction of glorious careers of young neutron scatterers. Use these m-files freely... at your own risk.

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