

Analysis of Nuclear Data using the R-Matrix Code SAMMY

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An overview is presented of the analysis code SAMMY, used for evaluation and analysis of time-of-flight cross section data in the resolved and unresolved resonance regions. Included are brief descriptions of the methods used for generating the theoretical cross sections (R-Matrix theory), for simulating the effect of experimental conditions (such as Doppler- and resolution-broadening, multiple-scattering corrections), and for fitting to the model parameters (Bayes' equations). Emphasis is placed on recent developments such as the inclusion of direct capture contributions to the cross section, the use of an implicit data covariance technique for including all experimental uncertainties, and the development of methodologies for propagating other uncertainties inherent in the correction processes.

Keywords: analysis, R-matrix, resolved resonance region

1. Introduction

Analysis of neutron-induced cross section data in the resolved resonance region requires properly simulating all features of the experiments which produced that data. The underlying cross section must be described by a physically realistic model. Those theoretical cross sections must then be modified to include such real-world effects as finite temperature and scattering within the sample. Finally, a fitting procedure is used to determine which values of the parameters permit the calculated and suitably-modified cross sections to agree with the measured cross sections within experimental uncertainties.

In this report, each of the three aspects of the analysis procedure is described briefly within the context of the author's analysis code SAMMY [1]. While much of this material has appeared in other publications, several new features are reported here, including methods for describing non-compound effects (direct capture) and interference effects involving the radiation channels. Particular emphasis is placed on the

the fitting procedure, in an effort to encourage the use of sophisticated techniques which permit more accurate treatment of uncertainties.

A brief description is also given of the post-processing capabilities in SAMMY, notably, the ability to provide complete resonance parameter and covariance information for the evaluated nuclear data files.

2. Theoretical Cross Sections

Multilevel multi-channel R-matrix theory [2] is the formalism of choice for treatment of most cross sections in the resolved-resonance energy region. Among the approximations permitted, for example, in the evaluated nuclear data files, are single-level and multilevel Breit Wigner and Reich Moore. SAMMY includes options to use any of these three, but the recommended choice is Reich Moore, which is a less-extreme approximation than either of the Breit Wigner forms. Fröhner expressed it well [3],

“Experience has shown that with this approximation [Reich Moore] all resonance cross section data can be described in detail, in the windows as well as in the peaks, even the weirdest multilevel interference patterns ... It works equally well for light, medium-mass and heavy nuclei, fissile and nonfissile.”

Nevertheless, there are situations in which the Reich Moore approximation is not adequate.

(1) R-matrix theory describes *compound* effects, in which the incident particle and the target nucleus combine to form a compound nucleus which then decays to give the outgoing particle and residual nucleus. Some physical phenomena are attributed to *direct* effects, which therefore cannot be described by R-matrix theory. One example of this is low-energy capture in ^{37}Cl [4].

In the case of ^{37}Cl , the treatment of direct capture was accomplished entirely external to the SAMMY analysis. Recently, however, the capability to include a direct capture component within the analysis was added to the SAMMY code. An estimate of the direct capture cross section is made externally and listed in tabular form for input to SAMMY; the code will interpolate between the listed energies as needed. Because the absolute

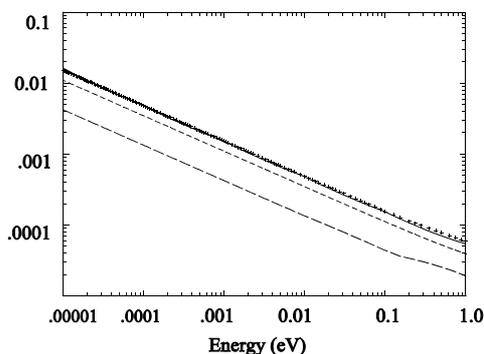


Fig. 1. Capture cross section for ^{19}F . Crosses represent the experimental data, dashed curve is the R-matrix contribution, longer dashes represent the direct capture contribution, and the solid curve gives the sum of the two.

magnitude of the model calculation for the direct component cannot be well known, a constant (energy-independent) coefficient multiplying the direct component may be adjusted during the analysis.

Preliminary results [5] from a new ^{19}F analysis by Leal, with direct capture model calculation by Arbanas, are shown in Fig. 1. In this case the initial value for the coefficient of the direct capture component was unity; after analysis of total and capture data, the value for this coefficient changed to 0.547 (well within the uncertainty of the direct capture model calculation). This value provides a good fit to both capture and total cross section measurements, including thermal values.

(2) In certain compound nuclear states, interference effects occur between particle and capture channels [6]; examples are $^{12}\text{C}(a,\gamma)$, $^{15}\text{N}(p,\gamma)$, $^{21}\text{Ne}(p,\gamma)$, and $^{22}\text{Ne}(n,\gamma)$. In such a situation, the capture widths cannot be treated in an average manner (as is the case in the Reich Moore approximation); instead, at least one gamma width must be treated explicitly, on the same footing with particle widths. Ideally this situation is represented by the full (unapproximated) R-matrix. Nevertheless, it is possible for a Reich-Moore implementation (such as that in SAMMY) to be made to mimic the full R-matrix with a high degree of accuracy. This is accomplished by setting the Reich-Moore capture width to a very small (but non-zero) value, and defining one reaction channel to be the true capture channel.

A simple example of this is shown in Fig. 2, which compares the Reich-Moore calculation with two pseudo-full-R-matrix calculations for a fictitious nuclide. When the reaction channel (gamma channel) and the incident channel (neutron channel) have the same sign, a large interference dip is observed in the calculation. Parameter values used for this example are given in Table 1.

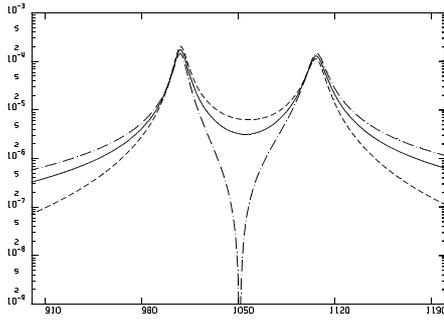


Fig. 2. Comparison of Reich-Moore with full R-matrix when capture channel can interfere with neutron channel. The solid line is Reich Moore, the dot-dash line is fake full R-matrix # 1, and the dashed line is fake full R-matrix # 2. [See Table 1 for details.] Clearly Reich-Moore is inadequate to describe large interference effects involving the capture channel.

Table 1. R-matrix parameter values used to create Fig. 2.

	Energy (MeV)	Γ_γ (eV)	Γ_n (eV)	$\Gamma_{reaction}$ (eV)
Reich Moore	1.0	1.0	10 000	
	1.1	1.1	11 000	
fake full R-matrix # 1	1.0	10^{-8}	10 000	1.0
	1.1	10^{-8}	11 000	1.1
fake full R-matrix # 2	1.0	10^{-8}	10 000	1.0
	1.1	10^{-8}	11 000	-1.1

3. Simulation of Experimental Conditions

Various effects can cause a measurement to be different from the quantity which an experiment purports to measure. Perhaps the best known of these is Doppler broadening, which occurs because the sample nuclei are at finite (non-zero) temperature. Resolution broadening is caused by the finite size of the neutron-producing target, of the detector

system, and of the time-intervals over which the counts are measured. Scattering of neutrons within the sample, prior to the reaction of interest, is another noticeable experimental effect. These three effects will be briefly described in this section; readers interested in more detail or in learning about other effects are referred to the SAMMY users' guide [1].

3.1 Doppler broadening

In its simplest form, Doppler broadening can be simulated by assuming that the nuclei within the sample behave as if they formed a free gas. This Doppler effect is illustrated in Fig. 3, in which the measured cross section appears to be much broader than the "true" cross section, which is a tall narrow resonance.

One common approximation to the free-gas model (FGM) of Doppler broadening is the high-energy Gaussian approximation (HEGA), of historical significance prior to the advent of modern computer systems because it could be combined analytically with Breit-Wigner cross sections to give reasonable first-order approximations to the Doppler-broadened cross section in many situations. Today, use of this approximation is strongly discouraged: Breit Wigner approximations are known to be inadequate for many nuclides;

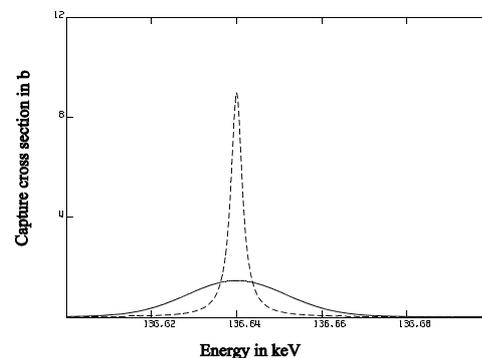


Fig. 3. Doppler broadening. The dotted curve represents the unbroadened resonance, and the solid curve shows the result of Doppler broadening at 300 K.

hence, even HEGA must be calculated numerically. HEGA, therefore, has no advantage over FGM.

Surprising though it seems, the FGM provides a fairly accurate representation of reality for most samples. Occasionally, however, solid-state effects are observed in measured cross sections (primarily at low energies). SAMMY therefore now contains an option for a crystal-lattice model (CLM) of Doppler broadening, borrowed from Naberejnev [7] who in turn borrowed it from MacFarlane [8].

3.2 Resolution broadening

Unlike Doppler broadening, resolution broadening is highly experiment- and site-dependent. The resolution function appropriate for use with capture data taken at the Oak Ridge Electron Linear Accelerator (ORELA), for example, bears little resemblance to the resolution function appropriate for transmission data taken at the Gelina facility in Geel.

Among the options available in SAMMY for resolution broadening are (1) a simple Gaussian plus exponential tail (RSL), (2) a realistic resolution function appropriate for ORELA data (the Oak Ridge resolution function, ORR), (3) a realistic function designed for data from the Gaerttner LINAC at Rensselaer Polytechnic Institute (RPI), (4) a straight-line energy-average from E to $E - \Delta$ (DEX, for use primarily with charged-particle data), and (5) a user-defined resolution function (UDR, implemented in SAMMY but not yet completely reliable). In addition, it is possible to use combinations of RSL plus DEX plus one of ORR, RPI, or UDR.

Readers interested in more detail on any of these options are referred to the SAMMY users' guide [1].

3.3 Multiple-scattering corrections

For analyses of capture measurements, one important experimental effect is the multiple-scattering correction: When a neutron reaches the sample, it is often first scattered by one or more of the nuclei in the sample before it is finally captured by yet another nucleus. At each scattering, the neutron loses energy. What may therefore be seen in the measurement is not only the resonance peak, but also an additional (smaller) peak at a higher energy; the center of this single-scattering peak corresponds to 90-degree scattering with the exact position determined by kinematics alone. Double- and higher-multiple-scattering peaks also may be visible in the data.

Analytic calculation of the full multiple-scattering correction is not practical, since each additional scattering introduces an additional six-fold embedded integration. The single-scattering correction can be calculated with high accuracy for specific geometries. Double- and higher-multiple-scattering corrections can be calculated with modest accuracy using crude approximations to decouple the integrations.

Figure 4 illustrates this phenomenon for the 1.15-keV resonance in ^{56}Fe [9]. Here the single-scattering peak is obvious both in the measured data and in the calculated values (double-plus scattering is not visible in this example). Proper treatment of the multiple-scattering effects may be even more important where the effect is not obvious: A resonance may be sufficiently broad that the peak is buried within the resonance, thus distorting its true shape. A second resonance may be located at the position of the single-scattering peak, thus giving a wrong impression of the magnitude and shape of that resonance.

Greater detail on this subject, including equations, examples, and a discussion of implementation issues, for both single- and double-plus scattering, can be found in [10].

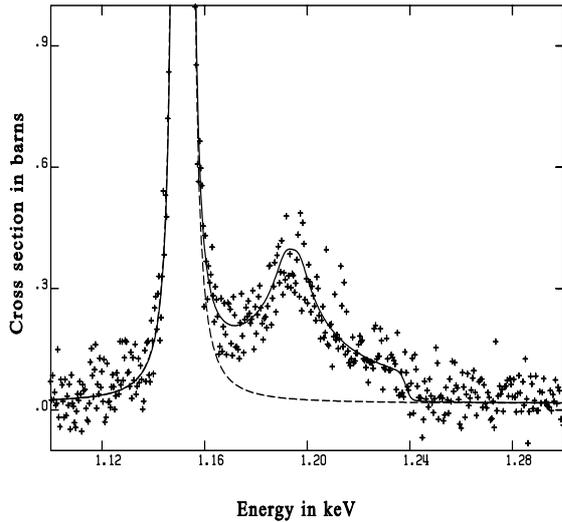


Fig. 4. The 1.15-keV ^{56}Fe resonance in natural iron capture data of R. Spencer et al. Dashed curve is SAMMY calculation without self-shielding or single-scattering correction; solid curve includes those corrections.

The single-scattering treatment used in SAMMY was developed by this author with significant input from F. G. Perey. The ideas for the approximations incorporated into SAMMY's double-plus scattering treatment were borrowed from M. Moxon [11], but programmed independently.

4. Fitting Procedure

A fitting procedure is used to determine which set of parameter values provide the best fit of theoretical calculation to measured data. The procedure employed in SAMMY is Bayes' method, sometimes described as "generalized least squares." For more details on the use of Bayes' method, see [12].

A derivation of Bayes' Equations is given in the SAMMY manual [1], and will not be repeated here; instead we quote the results. Let P represent the parameter values and M the associated covariance matrix, D represent the experimental data to be fitted and V the associated covariance matrix, T represent the

theoretical value calculated at the initial parameter values P , and G represent the partial derivatives of the theory with respect to the parameters (G is sometimes called the sensitivity matrix). Primes indicated the updated posterior values. In matrix form, Bayes' Equations can be written as

$$\begin{aligned} P' - P &= M' Y \\ M' &= (M^{-1} + W)^{-1} \\ Y &= G' V^{-1} (D - T) \\ W &= G' V^{-1} G \end{aligned} \quad (1)$$

where the last two lines define Y and W . Setting M^{-1} to zero in the second line of Eq. (1) gives the more familiar Least Squares equations.

4.1 Implicit data covariance method

The data covariance matrix V required for both Bayes' method and Least Squares is, in practice, usually approximated by its diagonal components. There are several reasons for this: (1) V is very large, as it is an N -by- N matrix where N (the number of data points) can be thousands or even hundreds of thousands. (2) Extra effort is required to accurately estimate V . (3) Many analysis codes are not equipped to work with the full off-diagonal data covariance matrix.

While the SAMMY code is able to make use of the full data covariance matrix, an alternative methodology is available which is both easier and more accurate. This alternative, which is denoted the "Implicit Data Covariance (IDC) method," makes use of the mathematical structure of V to simplify the computation effort involved in the solution of Bayes' equations.

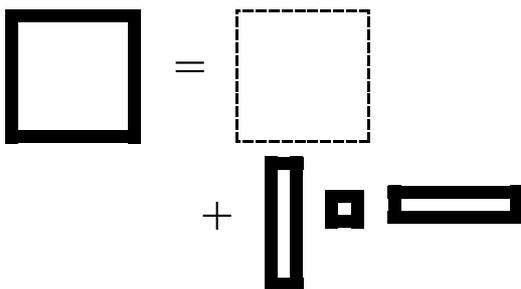
The data covariance matrix V is derived as the sum of two contributions to the data uncertainties, statistical and systematic. The statistical contribution comes directly from the measurement process, and is usually described by Poisson statistics (so that the uncertainty on K measured counts is the square root of K).

This contribution is diagonal (that is, it does not give correlations between two different data points).

The systematic contribution comes from those features of the experiment which are common to all data points. (Fröhner denotes these “common errors”.) The so-called data-reduction process is this: the measured (“raw”) data are modified (“reduced”) to be more closely related to the quantity of physical interest. For example, raw counts must often be normalized (divided by a number related to the duration of the experiment). The data-reduction parameter (normalization) has an uncertainty, and the process of dividing the raw data by this number gives rise to correlations between the modified data points.

Let v be the statistical contribution to the data covariance matrix. The systematic contribution is the product of the sensitivity matrix X (partial derivative of the reduced data with respect to the data-reduction parameter) times the data-reduction-parameter covariance matrix Q times the transpose of X . In matrix form, the data covariance matrix is

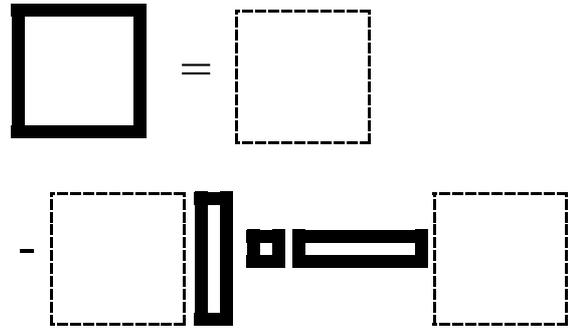
$$V = v + XQX^t, \quad (2)$$



where the boxes are used to indicate the relative size of the matrices; solid outlines indicate full off-diagonal matrices, and dashed outlines indicate diagonal matrices. The relative sizes are best considered to be logarithmic: there are possibly thousands (or hundreds of thousands) of data points, and very few (on the order of 10) data-reduction parameters.

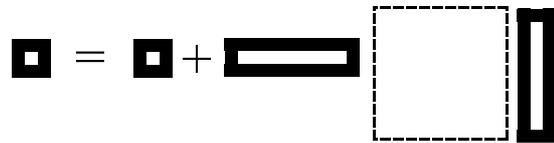
The inverse of V can be formally derived as

$$\begin{aligned} V^{-1} &= (v + XQX^t)^{-1} \\ &= v^{-1} - v^{-1}X \\ &\quad (Q^{-1} + X^t v^{-1} X)^{-1} X^t v^{-1} \\ &= v^{-1} - v^{-1}XZ^{-1}X^t v^{-1} \end{aligned} \quad (3)$$



where Z is defined by

$$Z = Q^{-1} + X^t v^{-1} X \quad (4)$$



From Eq. (3) and (4), it is clear that one could find the inverse of V without explicitly generating V or inverting this large matrix. In addition, from Bayes' Equations [Eq. (1)], it is also clear that there is no need to explicitly generate or store even the inverse of V . Instead, only the quantities Y and W are required:

$$\begin{aligned} Y &= G^t V^{-1} (D-T) \\ &= G^t v^{-1} (D-T) \\ &\quad - G^t v^{-1} X Z^{-1} X^t v^{-1} (D-T) \end{aligned} \quad (5)$$

and

$$\begin{aligned} W &= G^t V^{-1} G \\ &= G^t v^{-1} G \\ &\quad - G^t v^{-1} X Z^{-1} X^t v^{-1} G \end{aligned} \quad (6)$$

For the “box” version of these equations, please see reference [12].

Equations (5) and (6) appear on the surface to be much more complicated than the original expressions in Eq. (1). However, each element appearing in the longer equations is either diagonal or of small dimensions. Hence these forms are actually easier to calculate than are the original versions. That is, the arrays to be stored are significantly smaller, and the computation time is not much longer than required for the (incorrect) diagonal-only approximation. In addition to these expected results, tests have also shown that the IDC method is numerically better behaved than the full data covariance matrix method.

These assertions are illustrated with an example taken from SAMMY test case tr140. The data are a limited energy range from a ^{129}I measurement [13]; the full data set contains 32,660 data points. Figure 5 shows the data along with a SAMMY fit, and Table 2 describes the various choices for including the data covariance matrix.

Table 2. Statistics re IDC runs.
[1245 experimental data points;
9 data-reduction parameters;
655 resonances;
9 varied parameters in these runs;]

Description of run	cpu time, Bayes solver	total cpu time (sec)	array size
a statistical errors only	0.03	14	254 K
b statistical + common, diagonal	0.03	14	254 K
c explicit data cov matrix	16.46	59	1800 K
d IDC	0.06	14	267 K

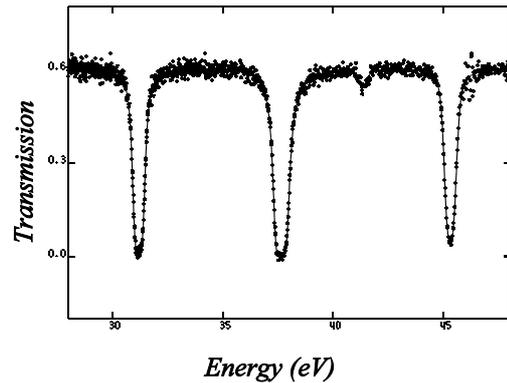


Fig. 5. Test Case tr140: ^{129}I transmission data (+) and SAMMY fit (solid curve) using Implicit Data Covariance method.

Equivalent results were obtained by the two runs which properly included the data covariance matrix (runs c and d). However, in order to obtain those results via the explicit data covariance method, it was necessary to take special care to write the matrix elements with many significant digits. (In general, too few significant digits in a covariance matrix will either give erroneous results or cause the matrix to be non-positive-definite.)

4.2 Propagating uncertainties on non-varied parameters

During the course of an analysis, it is often expedient to treat parameters as exact even when they are measured quantities rather than absolutes. For example, the pulse width for the neutron beam is known to within some uncertainty, but might be treated as constant for purposes of resolution broadening. Nevertheless the uncertainty associated with that quantity should be propagated throughout the analysis process and thus reflected in the final results.

A scheme for doing that will soon be incorporated into SAMMY. Currently there are two options for variables in the code:

- (1) Treat the variable as exact; do not vary. In this case any uncertainty associated

with this value is not propagated through the analysis process, and therefore is not reflected in the final resonance-parameter covariance matrix.

(2) Treat the variable as one of the fitting parameters in solving Bayes' Equations. In this case the initial uncertainty for the variable is reflected in the final covariance matrix. In addition, the value of this variable is refined, and the uncertainty associated with this variable is (probably) decreased, based on information inherent in the experimental data being analyzed.

A third option will be added:

(3) Generate the partial derivatives, and propagate the uncertainties in a manner similar to the implicit data covariance methodology. In this case the uncertainty associated with this variable will be included in the final results, but no additional information about this variable and its uncertainty will be obtained from analysis of these data.

4.3 Sequential vs. simultaneous analyses

There are many advantages to using Bayes' method rather than least squares, not the least of which is the ability of Bayes' Equations to "remember" earlier results. Because the prior covariance matrix is assumed to be finite (rather than infinite, as is the case with least squares), the output parameter covariance matrix from analysis of one data set can be used as input to the analysis of another unrelated data set. Results from such sequential analyses of multiple data sets are, in principle, equivalent to results from simultaneous analysis of all data sets.

Unfortunately, the reality is somewhat different from the principle. Sequential is exactly equivalent to simultaneous only if the theory is exactly linear with respect to the parameters of that theory – a *proviso* that R-matrix parameters clearly violate.

For this reason, it is the intention of this author to restructure the SAMMY code to provide an option for truly simultaneous analyses of several data sets. Examination of the expressions for Y and W [see Eq. (1)] shows that they may be rewritten as

$$\begin{aligned} Y &= \sum_i G_i^t V_i^{-1} (D_i - T_i) \\ W &= \sum_i G_i^t V_i^{-1} G_i \quad , \end{aligned} \quad (7)$$

where i represents the individual data sets. It is therefore possible to treat each data set separately, calculating Y_i and W_i and storing these values until calculations are completed for all data sets. The summed quantities Y and W are then formed, and Bayes' Equations are solved to give the new parameter values and covariance matrix that reflect the best fit to all data sets.

Changes to incorporate this option into SAMMY are underway. Because this requires significant changes both internal to the code and to the input, it may be some time before this option is fully functional.

Currently, simultaneous analyses can be accomplished in a limited, awkward fashion entailing several separate SAMMY runs; no iteration to account for non-linearities is possible. To date, this option has been used primarily as a means of retroactively producing an approximate resonance covariance matrix for inclusion in the evaluated nuclear data files (ENDF) [14].

5. Post-Processing

In the previous section, a technique for retroactively producing approximate resonance covariance matrices was mentioned. Such retroactive calculations are necessary because many of the current evaluations in ENDF do not contain any covariance information for the resonance region. Assuming input to the code is complete, SAMMY automatically produces

the resonance-parameter covariance matrix along with the parameter values, for both the resolved and the unresolved resonance region. With the insertion of simple input commands, the analyst can request SAMMY to output the covariance matrix into appropriate ENDF formats.

For some nuclides such as ^{235}U , the complete covariance matrix is prohibitively large and cannot be stored in ENDF formats. A proposed addition to the ENDF formats will make it possible to store these large matrices in approximate form, as uncertainties plus abbreviated correlation coefficients. Information regarding this proposal is available from this author.

6. Summary

Three essential requirements for analysis of neutron-induced time-of-flight cross section data have been discussed: formalism for calculation of cross section, mathematical description of experimental effects, and fitting procedure. Post-processing options, notably the capability of producing resonance-parameter covariance matrices in ENDF formats, were also discussed.

Use of the IDC (Implicit Data Covariance) method was stressed as a practical and viable alternative to the incorrect but often-used method of ignoring off-diagonal data covariances in the fitting procedure.

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