# AGS, A Computer Code for Uncertainty Propagation in Time-Of-Flight Cross Section Data

C. Bastian[1], A. Borella[1,2], F. Gunsing[2], J. Heyse[1], S. Kopecky[1], G. Noguere[3], P. Siegler[1] and P. Schillebeeckx[*1]
[1]EC-JRC-IRMM, Retieseweg 111, B-2440 Geel, Belgium
[2]CEA DAPNIA/SPhN, F-91911 Gif-sur-Yvette CEDEX, France
[3]CEA SPRC/LEPH, F-13108 Saint Paul lez Durance, France

**Abstract**

In this paper, the AGS (**A**nalysis of **G**eneric TOF_**S**pectra) system is described. The AGS system has been developed to transform count rate spectra of time of flight measurements in an efficient and convenient way into experimental observables, which can be used as input for nuclear reaction model fitting codes. It is explained how the covariance matrix can be broken down in an uncorrelated and a correlated part. The latter may in turn be expressed as the product of a rectangular matrix with its own transpose. We describe how this representation is used to propagate uncertainties starting from uncorrelated uncertainties due to counting statistics and to store the full covariance information with reduced storage space.

***KEYWORDS: TOF-measurements, total and partial cross sections, uncertainty propagation, covariance matrix, data analysis***

## 1. Introduction

The output of multi-channel data acquisition systems widely used in experimental physics often consists of counting histograms. The histograms or spectra undergo various mathematical transformations to obtain data to which a theoretical model is applied. The Analysis of Generic TOF_Spectra (AGS) package [1] has been developed for this purpose at the Institute for Reference Materials and Measurements in Geel (B). The system, consisting of a set of stand-alone C programs, has been developed to transform count rate spectra in an efficient and convenient way into a final observable, transmission factor or partial reaction yield, which can be used for model fitting. Although the package is tailored for neutron time-of-flight (TOF) measurements, it can in principle be used for any application involving spectrum transformations. The package performs a full propagation of uncertainties, starting from the uncorrelated uncertainties due to counting statistics. The final output includes a complete covariance matrix accounting for both correlated and uncorrelated uncertainty components. In the AGS system the covariance matrix is split in two parts, separating the uncorrelated and correlated components [1,2]. The uncorrelated part can be represented as a diagonal matrix, while the correlated part may be expressed as the product of a rectangular matrix with its own

[*] Corresponding author, Tel. + 32 (0)14 571 475, Fax. ++32 (0)14 571 862, E-mail: peter.schillebeeckx@cec.eu.int

transpose. This structure results in a substantial reduction of space for data storage and provides a convenient input structure suitable for subsequent data analysis involving nuclear reaction models.

## 2. Experimental Observables in Cross Section Measurements

High resolution cross section measurements are mostly performed at time-of-flight facilities such as the GELINA facility at the IRMM [3], the ORELA facility at the ORNL [4] and the n_TOF facility at CERN [5]. At such facilities, neutrons are produced by the impact of a short pulse of high-energy charged particles on a neutron producing target, providing a white neutron spectrum. Energy dependent cross section measurements are based on the time-of-flight technique, in which the neutron energy is determined by its time needed to travel a certain distance before it is detected.

The experimental observables of a total and a partial TOF cross section measurement are the transmission factor and the partial reaction yield, respectively. These observables are the input to nuclear reaction model codes such as the resonance shape analysis codes REFIT [6] and SAMMY [7] or statistical models implemented in e.g. FITACS [8].

The transmission factor is that fraction of the neutron beam that traverses the sample without any interaction. Experimentally the transmission factor $T_{exp}$ is obtained from the ratio of a sample-in measurement $C_{in}$ and sample-out measurement $C_{out}$, both corrected for their respective background contribution $B_{in}$ and $B_{out}$:

$$T_{exp} = N_T \frac{C_{in} - B_{in}}{C_{out} - B_{out}} \quad (1),$$

where $N_T$ is a normalization constant. The experimental spectra in Eq. 1 are all corrected for losses due to the dead time in the detector and electronics chain. In an ideal experiment, without any broadening due to resolution effects, the experimental observed transmission factor is a direct measure of the total Doppler-broadened cross section $\sigma_t$:

$$T_{\exp} = e^{-n_t \sigma_t} \quad (2),$$

where $n_t$ is the target thickness.

Partial cross sections are more difficult to determine compared to total cross sections. Experimentally one records the emitted particles or gamma rays resulting from the interaction in the sample. The experimental response $C_r$ can be directly linked to the so-called partial reaction yield $Y_r$, which is the fraction of the neutron beam that undergoes a partial reaction in the sample. The determination of the partial reaction yield requires an additional measurement of the neutron flux and the experimental observed partial reaction yield is obtained from the ratio between the response of the partial measurement $C_r$ and the neutron flux $\varphi_n$:

$$Y_{r,exp} = N_r \frac{1}{\varepsilon_r} \frac{C_r - B_r}{\varphi_n} \quad (3),$$

where $B_r$ is the background contributions and $\varepsilon_r$ is the efficiency to detect a partial reaction event. Since in most cases the absolute neutron flux is not known and only the shape of the energy dependence can be accurately determined, the normalization factor $N_r$ is introduced. In a

first approximation, neglecting resolution and multiple scattering effects, the reaction yield is related to the reaction cross section $\sigma_r$ by:

$$Y_r = (1 - e^{-n_t \sigma_t}) \frac{\sigma_r}{\sigma_t} \quad (4),$$

where $\sigma_t$ is the total cross section and $n_t$ the target thickness.

The neutron flux can be determined by measurements of a standard reaction, such as the $^{10}B(n,\alpha)$ reaction, for which the cross section $\sigma_\varphi$ is well known. The shape of the neutron flux can be deduced from the experimental response $C_n$:

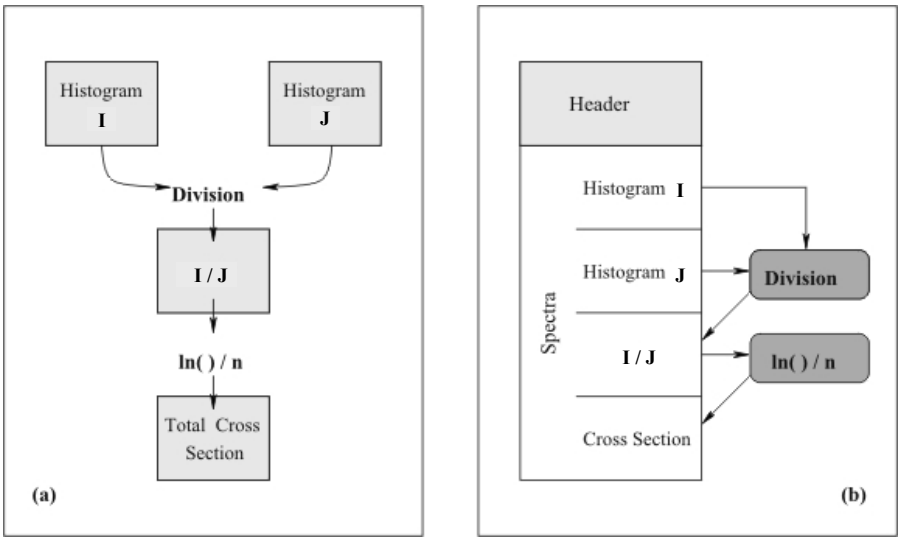
$$\varphi_n = N_\varphi \frac{C_n - B_n}{(1 - e^{-n\sigma_t})\,\sigma_n} \quad (5),$$

where $B_n$ is the background contribution to the flux measurements and $N_\varphi$ is a normalization factor which accounts for the target thickness and the detection efficiency, which in most cases is energy independent.

## 3. The AGS system

The discussion in section 2 shows that the reduction of the experimental observables depends on the reaction under investigation and the experimental set-up. However, most of the data reduction processes may be broken down conceptually in a sequence of "standard" operations or corrections, as shown in Fig. 1. In order to realize such an execution scheme and handle the uncertainty propagation during the operations on the spectra in a convenient way, the AGS code has been developed. The simplified case in Fig. 1 illustrates how the total cross section is deduced from a transmission measurement.

**Figure 1**: Breakdown of a reduction task of transmission measurement data for the determination of the total cross section (a) and the implementation in the AGS system (b).



Breaking down the reduction task into pre-programmed steps allows to identify intermediate and final results as spectra. In the AGS concept, every reduction operation reads operand spectra from and appends result spectra to the same file, which finally contains all the intermediate and final results of a reduction task, including their full covariance matrix. All spectra manipulations such as dead time correction, linear combination of spectra, background fitting and subtraction, calculation of self-shielding factors, projection of spectra on different time axes, reading of ENDF data files and spectra interpolation are included.

### 3.1 The AGS file format

A general TOF-spectrum of m channels consists of a 2-column matrix **X** of m TOF-boundaries and of a vector **Y** of m values. In Ref. 2 it is shown that the covariance matrix for **Y** can be built using a vector **U** of m uncorrelated uncertainties and a matrix $\mathbf{S_a}$ of m x p correlated uncertainties, where p is the number of common sources of uncertainties. The covariance matrix **C** may be broken down in an uncorrelated and correlated part [1,2]:

$$\mathbf{C} = \mathbf{U} + \mathbf{S_a}\ \mathbf{C_a}\mathbf{S_a}^{\mathbf{t}} \tag{5},$$

where **U** is a diagonal matrix which contains the uncorrelated uncertainties and of which only the diagonal has to be stored as a vector of length m. The correlated part results from the common sources of uncertainties due to the parameters **a** involved in the data reduction process. This part is deduced from the covariance matrix $\mathbf{C_a}$ and the sensitivity matrix $\mathbf{S_a}$. The elements of the sensitivity matrix $\mathbf{S_a}$ are the partial derivatives with respect to the parameters **a**. Since a covariance matrix is symmetric and positive definite, a Cholesky decomposition can be performed and the matrix $\mathbf{C_a}$ can be expressed as [1,2]:

$$\mathbf{C_a} = \mathbf{T_a}\ \mathbf{T_a}^{\mathbf{t}} \tag{6},$$

where $\mathbf{T_a}$ is a lower triangular matrix. Combining Eq. 5 and 6, the covariance matrix **C** becomes:

$$\mathbf{C} = \mathbf{U} + \mathbf{ST_a}\ \mathbf{ST_a}^{\mathbf{t}} \tag{7},$$

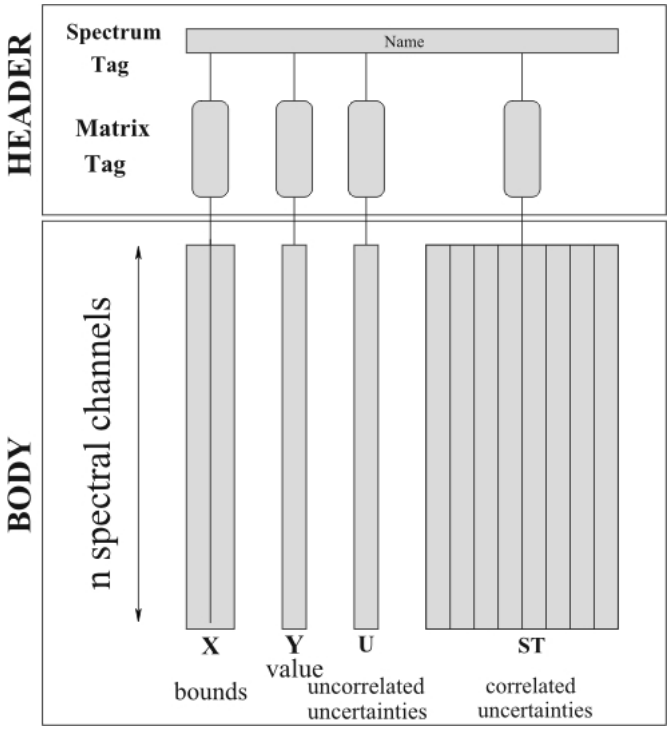
with $\mathbf{ST_a}$ a matrix containing p vectors of length m:

$$\mathbf{ST_a} = \mathbf{S_a}\ \mathbf{T_a} \tag{8}.$$

The number p expresses the number of common sources of uncertainties and depends on the number of operations applied to an originally uncorrelated spectrum.

Fig. 2 illustrates how every part **X**, **Y**, **U** or **ST** of a spectrum is stored in the body of an AGS file. The matrix tag and spectrum tag in the header of the file hold information about the data type and structure. In practice, m is typically 3 x $10^4$ and p is in the order of 10. Therefore, the number of elements of the covariance matrix which need to be stored are reduced by a factor 1000. In addition, such a data structure allows a full documentation of the propagation of uncertainties through every step of the data analysis.

**Figure 2**: Layout of the AGS file format.




### 3.2 The AGS commands

The AGS reduction operations are implemented as a set of independent programs coded in the C-language. Each program operates on a single file, the AGS file, which contains all spectra and associated information. A sequence of these commands can be conveniently put in a shell script in order to automize the full data reduction process.

The first operation in an AGS reduction sequence is mostly `ags_mpty` which creates an empty AGS file. Usually it is followed by `ags_get` operations to import experimental data into AGS format. Most AGS commands read spectra from and write spectra to an AGS file. Besides channel-to-channel arithmetics, they also perform dynamic spectrum condensation, bin averaging, dead time correction, conversion of time of flight to energy bounds, and least squares fitting. All operations propagate the covariance data on the basis of the sensitivity coefficients. Read-only operations are available to survey an entire AGS file and to examine any spectrum in it, either numerically or graphically. A flexible output operation allows to export final results as ASCII text files. The header of an AGS file holds the sequence of commands which created it. This information can be used by a special operation to create a shell script reproducing the reduction sequence. The most important commands are summarized in Table 1.

Table 1. The most important AGS commands, subdivided into three categories

| | ***Write only commands*** |
|---|---|
| `ags_mpty` | Create an empty AGS file |
| `ags_getA` | Import spectra from another AGS file |
| `ags_getE` | Import/interpolate evaluated data from an ENDF file |
| `ags_getXY` | Import histogram data from an ASCII file |
| | ***Read/Write commands : Operations on spectra*** |
| `ags_addval` | Add a constant value to all Y-values of a spectrum |
| `ags_avgr` | Average Y values per channel |
| `ags_func` | Calculates the Y values for a special function |
| `ags_idtc` | Determine the dead time correction of a TOF-spectrum |
| `ags_divi` | Divide a spectrum by another |
| `ags_mult` | Multiply a spectrum with another |
| `ags_lico` | Linear combination of n spectra with n constants |
| `ags_ener` | Build energy from TOF X-vector |
| `ags_fit` | Non-linear fit of spectra |
| `ags_fxyp` | User-programmed function |
| | ***Read Only commands*** |
| `ags_edit` | Edit constants and scalers attached to a spectrum |
| `ags_list` | List Y values of spectra with common X values |
| `ags_putX` | Export final result to an ASCII file |
| `ags_scan` | Scan the contents of an AGS file |

A new option in SAMMY has been implemented in order to introduce the covariance representation of AGS (see Figure 2) instead of an explicit very large covariance matrix. The AGS representation is also numerically more stable, not only because of the problems related to storage and inversion of very large matrices, but also to avoid round-off errors. The `ags_putX` command includes various options for the output format. One of the options produces an output which includes the covariance information that can be used as input for the SAMMY code. The SAMMY test case Tr140 [7] includes the AGS representation of the covariance matrix for the iodine measurements performed by G. Noguere et al. [9].

In Tab. 2 a script or sequence of AGS commands is given that can be used to deduce the transmission factor starting from raw sample-in and sample-out spectra following the scheme of Figure 1. In this script dead time correction are performed on the TOF-spectra and the transmission factor is obtained from the division of the background corrected sample-in and sample-out spectra. Similar scripts have been defined for the analysis of partial cross section measurements.

Table 2. A simplified shell script containing a sequence of AGS operations to deduce the transmission factor

```
# create ags-file
ags_mpty TRFAK

# read sample out
scaler=TOout,CMout
ags_getXY TRFAK /SCALER=$scaler /FROM=spout.his /ALIAS=SOUT

# read sample in
scaler=TOin,CMin
ags_getXY TRFAK /SCALER=$scaler /FROM=spin.his /ALIAS=SIN /LIKE=A01SOUT

# dead time correction
dtcoef=DTCOEF
ags_idtc TRFAK,A01SOUT /DTIME=$dtcoef /LPSC=1
ags_idtc TRFAK,B01SIN /DTIME=$dtcoef /LPSC=1

# normalize to central monitor
ags_avgr TRFAK,C01SOUT /CMSC=2
ags_avgr TRFAK,D01SIN /CMSC=2

#calculate background contribution
ags_func TRFAK /FUN=f01 /PARFILE=PAROUT /ALIAS=SBOUT /LIKE=A01SOUT
ags_func TRFAK /FUN=f01 /PARFILE=PARIN /ALIAS=SBIN /LIKE=A01SOUT

#subtract background
ags_lico TRFAK,E01SOUT,G01SBOUT /ALIAS=SOUTNET /PAR=1.0,-1.0
ags_lico TRFAK,F01SIN,H01SBIN /ALIAS=SINNET /PAR=1.0,-1.0

#create transmission factor
ags_divi TRFAK,I01SOUTNET,J01SINNET
```

### 3.3 Some examples

The AGS package is routinely used for the analysis of transmission [9,10], capture [11] and fission [12] cross section measurements at GELINA. Using AGS the impact of the various sources of uncertainties can be verified through each step of the reduction process. Ref. [11] gives a detailed discussion on the correlated and uncorrelated uncertainty components of the $^{232}$Th(n,$\gamma$) capture cross section measurements in the unresolved resonance region.

For transmission measurements the correlated uncertainty components mainly result from the background correction which is mostly determined from a least square fit through black resonance points. For partial cross section measurements the largest contribution to the correlated uncertainty component is due to the normalization (factor $N_r$ in Eq. 3).

## 4. Summary

The AGS package, which was especially developed for the data reduction of total and partial cross section measurements at TOF-facilities, has been described. The package includes a special representation of the covariance matrix which results in a substantial reduction of the required storage space. Using the AGS system the impact of the various uncertainty components can be analyzed and documented.

At present the AGS system was only used for the analysis of data obtained at GELINA. The package has been updated regularly to meet specific user needs. The source code of the package is available for general use and we would encourage the use of it for the production of experimental nuclear reaction cross section data with the conservation of the full covariance matrix. This seems an essential step to us in order to produce in subsequent analyses consistent and reliable covariance information in evaluated data libraries.

## References


1) C. Bastian, *AGS, a set of UNIX commands for neutron data reduction*, Proc. Int. Conf. On Neutron Research and Industry, Crete, Greece, 1996, The international society for optical engeneering Vol. 2867, 611 (1997).
2) C. Bastian, *General procedures and computational methods for generating covariance matrices*, Proc. Int. Symposium On Nuclear Data Evaluation Methodology, Brookhaven National Laboratory, 12-16 October 1992, Ed. Charles L.Dunford, ISBN 981-02-1285-2, p. 642
3) A. Bensussan and J.M. Salome, GELINA, a modern accelerator for high resolution neutron time of flight experiments, Nucl. Instr. Meth., **A489**, 346 (2002)
4) Oak Ridge Linear Accelerator, http://www.phy.ornl.gov/nuclear/orela/
5) n_TOF facility, http://www.cern.ch/ntof
6) M.C. Moxon and J.B. Brisland, *Geel REFIT a least-squares fitting program for resonance analysis of neutron transmission and capture data*, AEA-InTec-0530, AEA Technology, October 1991
7) N. M. Larson, *Updated Users' Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes=Equations*, ORNL/TM-9179/R7, Oak Ridge National Laboratory (2006).
8) F.H. Fröhner, *Evaluation of the unresolved resonance range of $^{238}U$*, Nucl. Sci. & Eng. **103**, 119 (1989)
9) G. Noguere, O. Bouland, A. Brusegan, P. Schillebeeckx, P. Siegler, A. Leprêtre, N. Herault an dthe n-TOF collaboration, *Neutron capture and total cross sections of Iodine-127 and Iodine-129*, accepted for publication in Phys. Rev. C
10) F. Gunsing, A. Leprêtre, C. Mounier, C. Raepsaet, A. Brusegan and E. Macavero, *Neutron resonance spectroscopy of $^{99}Tc$ from 3 eV to 150 keV*, Phys. Rev. **C61** , 054608, (2000)
11) A. Borella, K. Volev, A. Brusegan, P. Schillebeeckx, F. Corvi, N. Koyumdjieva, N. Janeva, and A.A. Lukyanov, *Determination of the $^{232}Th(n,\gamma)$ cross section from 4 to 140 keV at GELINA* , Nucl. Sci. & Eng., **152**, 1(2006)
12) J. Heyse, C. Wagemans, L. De Smet, O. Serot, J. Wagemans and J. Van Gils, *High resolution measurement of the $^{234}U(n,f)$ cross section in the neutron energy range from 0.5 eV up to 100 keV*, submitted to Nucl. Sci. & Eng.