

## SKAT2MAUD help file (ver. 0.20120727)

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### 0. Acknowledgements

I would like to thank MAUD team and SKAT team for creation of a great software and great instrument; without these SKAT2MAUD would have never existed (as its name implies).

I especially would like to express my earnest gratitude to *Dr. Klaus Ullemeyer* (Kiel University, Kiel, Germany), *Dr. Vyacheslav Sumin*, *Dr. Gizo Bokuchava*, and *Igor Papushkin* (Joint Institute for Nuclear Research, Dubna, Russia) for their support and suggestions to improve this program.

I will also be grateful to you if you cite a very first work where SKAT2MAUD has been applied during data analysis:

Wenk H.-R., Vasin R.N., Kern H., Matthies S., Vogel S.C., Ivankina T.I. Revisiting elastic anisotropy of biotite gneiss from the Outokumpu scientific drill hole based on new texture measurements and texture-based velocity calculations. // Tectonophysics. 2012. V. 570-571. P. 123-134.

### 1. General

SKAT2MAUD is software designed to convert standard datafiles of different neutron diffraction instruments of Frank Laboratory of Neutron Physics of Joint Institute for Nuclear Research in Dubna, Russia into the format suitable for processing them with a program MAUD. I am not related to MAUD in any way and for more info on it the user is advised to visit the official website at <http://www.ing.unitn.it/~maud/>.

SKAT2MAUD is written on C++ and it uses WinAPI functions to work with files and folders. It has been tested on different PC under different operation systems. It seems to be working fine under Microsoft Windows XP Professional, Microsoft Windows 7 Home Premium x64, Microsoft Windows 7 Professional x64 and Ubuntu 12.04 (using Wine 1.4). Main program does not need any additional programs installed, or any libraries or files (well, except for this help file in case you need it).

Here is some info on the data conversion speed. On Intel Core i7-2600 with 16 Gb DDR3-1333 (CL9) and 1 Tb WD Caviar Black 'WD1002FAEX' HDD working under Microsoft Windows 7 Professional x64 the processing of all 1368 SKAT datafiles (data conversion, normalization, creation of MAUD script and protocol file) takes less than 10 seconds. On AMD Athlon64 3200+ with 1 Gb DDR-400 (CL3) and 120 Gb Seagate Barracuda 7200.7 under Microsoft Windows XP Professional the processing of all 1368 SKAT datafiles takes less than 20 sec., and under Ubuntu 12.04 (+ Wine 1.4) – 5-6 min.

If you feel that SKAT2MAUD does something wrong/unexpected, or works too slow, or you need some new functions/instruments added, please, contact me:

Roman Vasin

Frank Laboratory of Neutron Physics,  
Joint Institute for Nuclear Research,

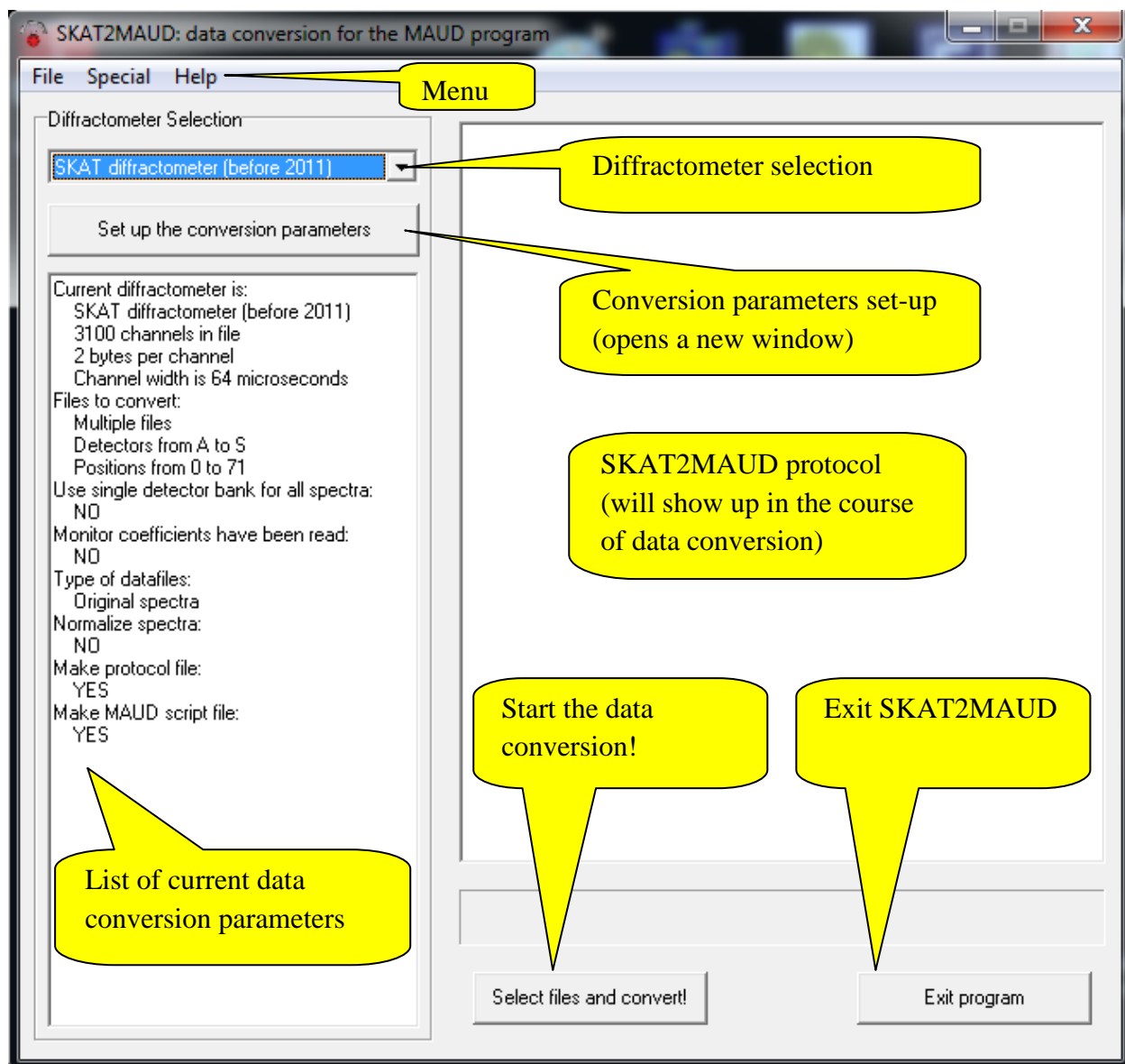
Joliot-Curie 6, 141980 Dubna,  
Moscow Region, RUSSIA  
Phone: +74962164789  
Fax: +74962165882  
e-mail: [olddragon@mail.ru](mailto:olddragon@mail.ru)

## 2. Version history

Current version of SKAT2MAUD is 0.20120727. It is one and only at the moment.

## 3. Main window and data conversion process

Here is how the SKAT2MAUD main window looks like:



Main menu consists of three items: **File**, **Special**, and **Help**.

**File** menu has only one item **Exit** that closes the SKAT2MAUD program.

**Special** menu currently has only one item **SKAT sum**. See the details on what it does below (section 5 of this help file).

**Help** menu has two items. First is another **Help** that opens your default .doc-file viewer and shows this help file. Second is **About** that shows a message window with short info on SKAT2MAUD and my contact info.

Left part of the SKAT2MAUD main window contains a **Diffractometer Selection** panel that has three elements.

First, there is a combo box there which contains a drop-down list of diffractometers. There a user may choose an appropriate diffraction instrument used to obtain diffraction spectra that should be converted.

Below it there is a button **Set up the conversion parameters**. Clicking it should open a new window that is unique for each diffractometer. There a user may adjust some of the data conversion parameters. See the details on this below (section 4 of this help file).

Third element here is a text panel containing the list of current data conversion parameters. Check it prior to starting the data conversion!

Right part of the SKAT2MAUD main window contains a huge text panel where the data conversion protocol will appear. Below there is a progress bar showing the data conversion progress. In the right lower corner there is **Exit program** button that closes the SKAT2MAUD program.

**Select files and convert!** button opens two dialog windows one after another.

First, a user will be prompted to select data files to convert. For the SKAT diffractometer a user can select only one file (multiselect is disabled!) and, depending on the conversion parameters (**Single file** or **Multiple files** option has been selected in SKAT setup window), only this data file or all the data files with the same name located in the same folder will be converted. Note that in the case of SKAT **Multiple files** conversion SKAT2MAUD will try to convert all the data files with the same name within the selected range of detectors and sample positions located in the same folder; if some files are missing SKAT2MAUD will write a corresponding error message (see below in this section) to the protocol but will not stop the data conversion (it will proceed to the next file than to the next etc.)! For the FSD diffractometer the multiselect option is active and a user can select any number of files for the data conversion. Still, all the files should be located in the same folder.

Important info!!!

Input (for **Select files and convert!**):

- 1) For SKAT: binary file/s (either little- or big-endian; a user MUST select a correct option), 3100 2-bytes (unsigned) integer numbers per file (6200 bytes total in file).  
In case of the multiple data file conversion data files should have extension .xyy, where x is a letter (A to S) and yy is a number (00-71).
- 2) For FSD: binary file/s, 3900 4-bytes integer numbers per file (15600 bytes total in file).

Output:

ASCII text file/s in standard GSAS (.gda) format (see GSAS and GSAS manual at <http://www.ccp14.ac.uk/solution/gsas/>). Note, that a user can adjust this file format by simply editing it in any text editor, changing, e.g., detector bank number, TOF channel width, etc. Feel free to do this at your own risk!

After the data files to convert have been selected second dialog window will pop up requesting to select the output folder to store the converted files. If a user presses **Cancel** at this moment the output folder will be set to be the same as the (input) folder where all the original data files are. And the data file conversion will begin.

Once the data file conversion begins two things will happen. First, a data conversion protocol will appear in the protocol text panel and second, the progress bar below the protocol text panel will be showing a data conversion progress.

When the data conversion is completed a message window will appear saying exactly that "Data conversion is completed!" Please, do not close the main window (or change any of the data conversion parameters) before that happens!

I advise to check out some of the last lines in the protocol text panel (the ones just before the "SKAT2MAUD protocol file end at *time*"). SKAT2MAUD will warn a user if it encounters

missing data files/data files with “wrong” names; data files with unexpectedly high intensity values (e.g., this could happen if wrong data format is selected for the SKAT data conversion); if it could not create a file to write data into it (e.g., a user does not have rights to write into the selected output folder); etc. In that case a user is advised to look for the text string “!!!ERROR!!!” in the protocol to identify the exact problem with the data conversion.

If no problems have been recognized during the data conversion SKAT2MAUD will report that “Program encountered no errors!” Note, that this merely means the absence of machine-recognizable errors, and not that a user selected correct files/chosen correct data conversion options.

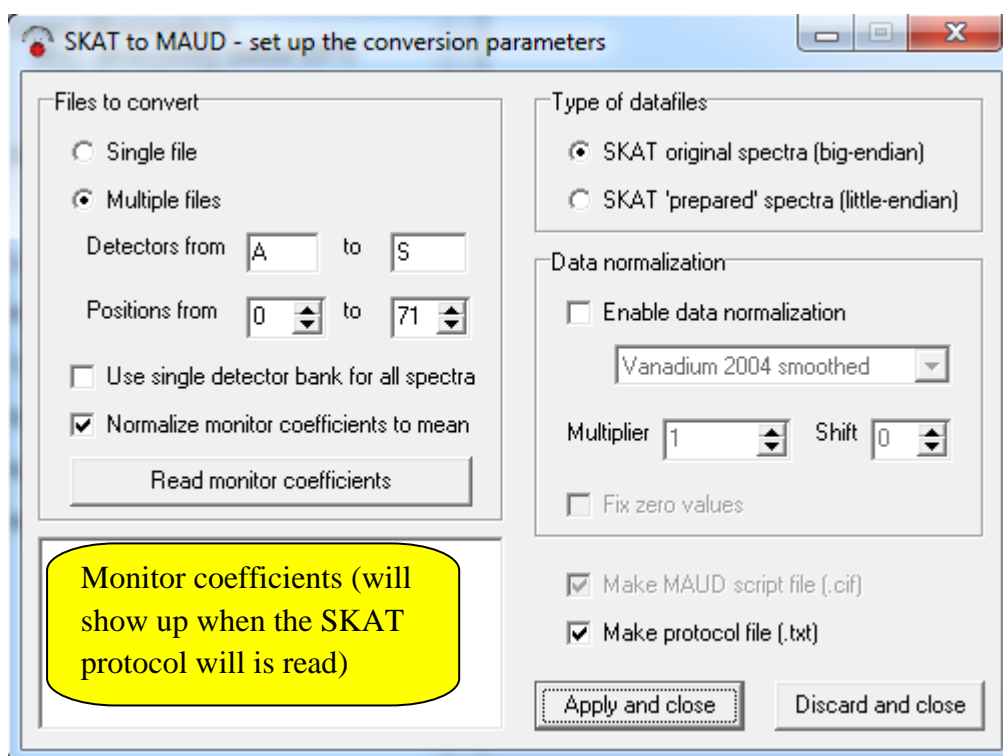
A couple of words about the **MAUD script file**. This file (for now) is only created for the SKAT diffractometer. It contains all the converted data file names, pole figure angles and monitor coefficients and it should be imported into MAUD by selecting Datasets->Datafiles tab->Script import... With this, all the converted data files will be loaded into MAUD with correct pole figure angles and monitor coefficients, saving a user a great deal of time.

## 4. Diffractometer setup

This section covers the adjustment of different data conversion options in different windows appearing once a user presses a **Set up the conversion parameters** button in the main SKAT2MAUD window.

### 4.1. SKAT (before 2011)

Here is how the SKAT diffractometer setup window looks like:



A user may select/change different data conversion options here.

In the **Files to convert** panel it is possible to select either **Single file** option (all the other elements of the panel will become inactive in this case) or **Multiple files** option. In the first case, only single data file would be converted (it is useful if a user wants to convert only, e.g., sum spectrum). In the second case all the data files with the same name within the selected range of detectors and sample positions located in the same folder would be converted. A user may select a range of detectors and sample positions for the multiple files conversion via **Detectors from... to...** and **Positions from... to...** fields. SKAT2MAUD accepts detector names from A to S

(either capital and lower-case letters) and sample positions from 0 to 71. “**from**” position or detector not necessarily should be lower than “**to**” position or detector, e.g., it is possible to input a range as **Positions from 54 to 10**. SKAT2MAUD will later convert this to **Positions from 10 to 54** by itself.

Checking a **Use single detector bank for all spectra** option will result in that all the converted data files will have the same detector bank number in the header (to be exact, they all will be assigned to bank number 1, which is detector A).

Checking a **Normalize monitor coefficients to mean** option will result in that the normalized to their mean value monitor coefficients (within the selected range of sample positions) would be written to the MAUD script file. E.g., if monitor coefficients read 80000, 100000, 120000 their mean value would be 100000 and normalized monitor coefficient values written to the MAUD script file would be 0.8, 1, 1.2.

Pressing **Read monitor coefficients** button will open a dialog window where a user can select a standard SKAT protocol file to read monitor coefficients from it. Once the file is read a user should check a text panel below the button. If file has been read successfully then a list of sample positions and corresponding monitor coefficients will appear there.

Important info!!!

Input (for **Read monitor coefficients**):

A standard SKAT protocol file (ASCII text, with .txt extension) that looks like this:

```
24Oct01 10:59 1003921178 tofa: open_prot 26db2.txt
24Oct01 10:59 1003921181 tofa: user lebit_leiss
24Oct01 10:59 1003921184 tofa: file 26db2
24Oct01 10:59 1003921186 tofa: sample quartzite_26d_b2
24Oct01 10:59 1003921189 tofa: time 900
24Oct01 10:59 1003921197 unipa: condition monitor_count test
24Oct01 11:00 1003921200 unipa: start
24Oct01 11:00 1003921200 Unipa has been started
24Oct01 11:00 1003921203 motor: phi
24Oct01 11:00 1003921206 motor: find 11
24Oct01 11:00 1003921208 phi at 1C = -9.0000 deg
24Oct01 11:00 1003921212 motor: setpos 0.
24Oct01 11:20 1003922408 tofa: expo #.$00
24Oct01 11:20 1003922408 900.105 4359 61596 60837 26db2.$00
24Oct01 11:35 1003923311 motor: move -5.0
24Oct01 11:35 1003923314 phi at -5.0000 deg
24Oct01 11:35 1003923314 tofa: expo #.$01
24Oct01 11:35 1003923315 900.107 4344 61615 60867 26db2.$01
```

.....

SKAT2MAUD will be looking for strings like the ones highlighted in green.

In the **Type of datafiles** panel a user must select the type of files to convert: big-endian (that’s SKAT original data files) or little-endian (these are the files ‘prepared’/‘byte swapped’ by the program GeoTOF).

In the **Data normalization** panel a user can **Enable data normalization**. If this option is checked the data files will be normalized to the selected effective (vanadium) spectrum. Currently two vanadium spectra are available. One is **Vanadium 1999 smoothed**, and the other is **Vanadium 2004 smoothed**. These are sum vanadium spectra collected in 1999 and 2004 correspondingly; they are smoothed by Savitzky–Golay procedure (60 points per window, polynomial order is 3) to get good normalization on the tail of spectra and stored in SKAT2MAUD.

By changing a **Multiplier value** (integer number from 1 to 100000) a user can adjust the overall “intensity” of the resulting normalized spectrum (here multiplier is basically a value to which the resulting spectrum will be multiplied). Note that the resulting spectrum will also be multiplied onto the maximum intensity values of the vanadium spectrum, so selecting too high multiplier values is not recommended because in an unlucky case the intensity value of the resulting spectrum may reach  $10^9$  which is the limit for the .gda file (there each number may have only 8 digits).

Another adjustable number is **Shift** (integer number from -10 to 10) which effectively shifts the vanadium spectrum. E.g., if a shift of 5 is selected then the intensity value in the 1<sup>st</sup> TOF channel of the data file will be divided onto the intensity value in the 6<sup>th</sup> (1+5) TOF channel of the vanadium spectrum; intensity in the 2<sup>nd</sup> channel of the data file will be divided onto the intensity in the 7<sup>th</sup> channel of the vanadium spectrum; etc. If a shift of -5 is selected then the intensity value in the 6<sup>th</sup> TOF channel of the data file will be divided onto the intensity value in the 1<sup>st</sup> (6-5) TOF channel of the vanadium spectrum; etc.

Checking **Fix zero values** option eliminates all the zero values on all the converted spectra. After the data normalization all the zero intensity values on each spectrum will be substituted with minimum non-zero intensity value on the same spectrum.

Changing **Make MAUD script file (.cif)** option is not possible for now. It is always on and MAUD script file will always be created in the process of data conversion.

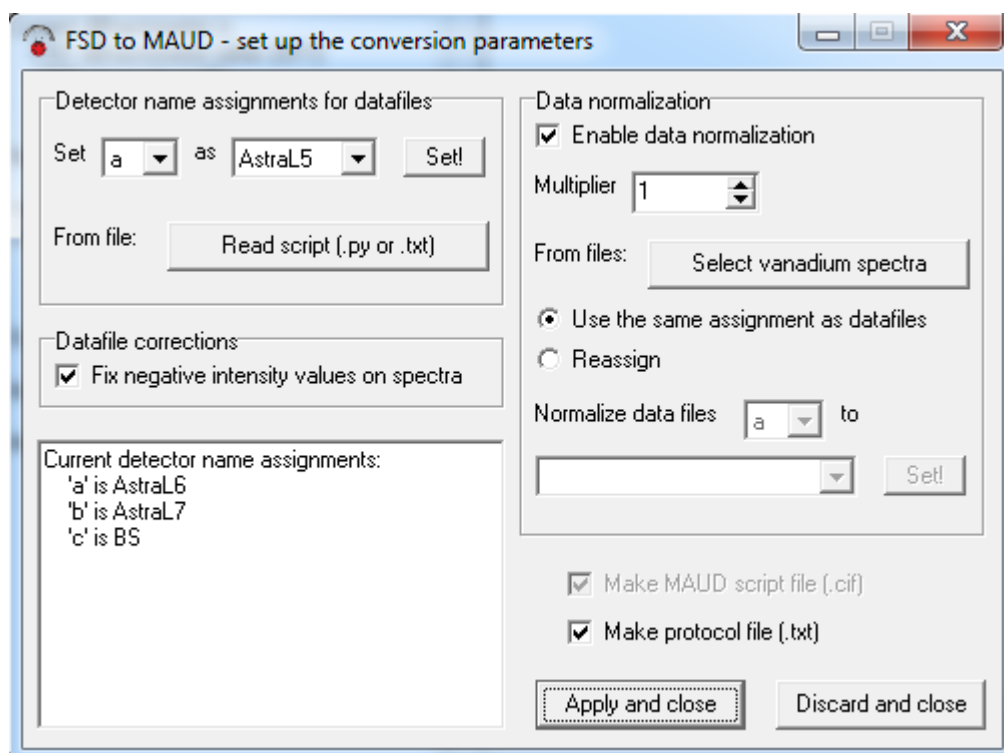
Checking **Make protocol file (.txt)** option results in that the SKAT2MAUD protocol file (plain text) will be saved into conversion output folder. If the option is not checked that it is only possible to check the data conversion protocol in the corresponding panel of the main SKAT2MAUD window.

## 4.2. SKAT (after 2011)

This is not yet implemented! Intended use for this variant is the data conversion of data collected on the multi-ring SKAT diffractometer.

## 4.3. FSD (after 2011)

Here is how the FSD diffractometer setup window looks like:



A user may select/change different data conversion options here.

In the **Detector name assignments for datafiles** panel a user is to select assignment of data files to a certain detector. Different data files are recognized by the last letter of the data file name. E.g., a data file ALO040\_c.H “has” a letter “c”. The assignment could be done manually (by selecting an appropriate letter and corresponding detector name and pressing **Set!** button). In this case only 3 letters could be assigned (a, b, c). Also it is possible to read the assignment from the file by pressing **Read script (.py or .txt)** button. A dialog window will appear where a user can select a script containing all the assignments (up to 15 letters, from a to o). It is possible then to change some of assignments manually. Current detector name assignments are shown in the text panel in the down left corner of the window.

Important info!!!

Input (for **Read script (.py or .txt)**):

A FSD script-like file (ASCII text, with .txt or .py extension) that looks like this:

```
#Detectors:
```

```
#DSP1-a-BS
```

```
#DSP2-b-AstraL5
```

```
#DSP3-c-AstraL6
```

```
.....
```

Possible letters are a, b, c..., o and possible detector names are BS for backscattering detector and AstraL1, AstraL2..., AstraL7, AstraR1, AstraR2..., AstraR7 for corresponding Astra detectors.

In the **Datafile corrections** panel a single option is available. It is **Fix negative intensity values on spectra**. If checked SKAT2MAUD will add an absolute of a minimum (negative) intensity value on the spectrum to each intensity value on this spectrum (it is like adding a constant background). Thus a minimum intensity value on each “fixed” spectrum will be 0.

In the **Data normalization** panel a user can **Enable data normalization**. If this option is checked the data files will be normalized to the selected effective (vanadium) spectra. Pressing a **Select vanadium spectra** button will show a dialog window where a user can select any number (multiselect is active!) of vanadium spectra to normalize data files. Vanadium files would be automatically assigned (if **Use the same assignment as datafiles** option is active) to corresponding data files using the last letter of the file name (e.g., if three vanadium spectra selected: VAN042\_a.D, VAN042\_b.D, and VAN042\_c.D, data file ALO040\_c.H would be automatically assigned to be normalized to the vanadium spectrum VAN042\_c.D, etc.). To change this “normalization assignment” a user can select the option **Reassign**, select an appropriate letter and corresponding vanadium file name and press **Set!** button In the **Data normalization** panel.

Current “normalization assignments” are also shown in the text panel in the down left corner of the window

By changing a **Multiplier value** (integer number from 1 to 100000) a user can adjust the overall “intensity” of the resulting normalized spectrum (here multiplier is basically a value to which the resulting spectrum will be multiplied). Note that the resulting spectrum will also be multiplied onto the maximum intensity values of the vanadium spectrum, so selecting too high multiplier values is not recommended because in an unlucky case the intensity value of the resulting spectrum may reach  $10^9$  which is the limit for the .gda file (there each number may have only 8 digits).

Changing **Make MAUD script file (.cif)** option is not possible for now. Despite it is always on here, SKAT2MAUD for now does not create a MAUD script file for FSD diffractometer.

Checking **Make protocol file (.txt)** option results in that the SKAT2MAUD protocol file (plain text) will be saved into conversion output folder. If the option is not checked that it is only

possible to check the data conversion protocol in the corresponding panel of the main SKAT2MAUD window.

#### 4.4. Generic diffractometer (TEST!!!)

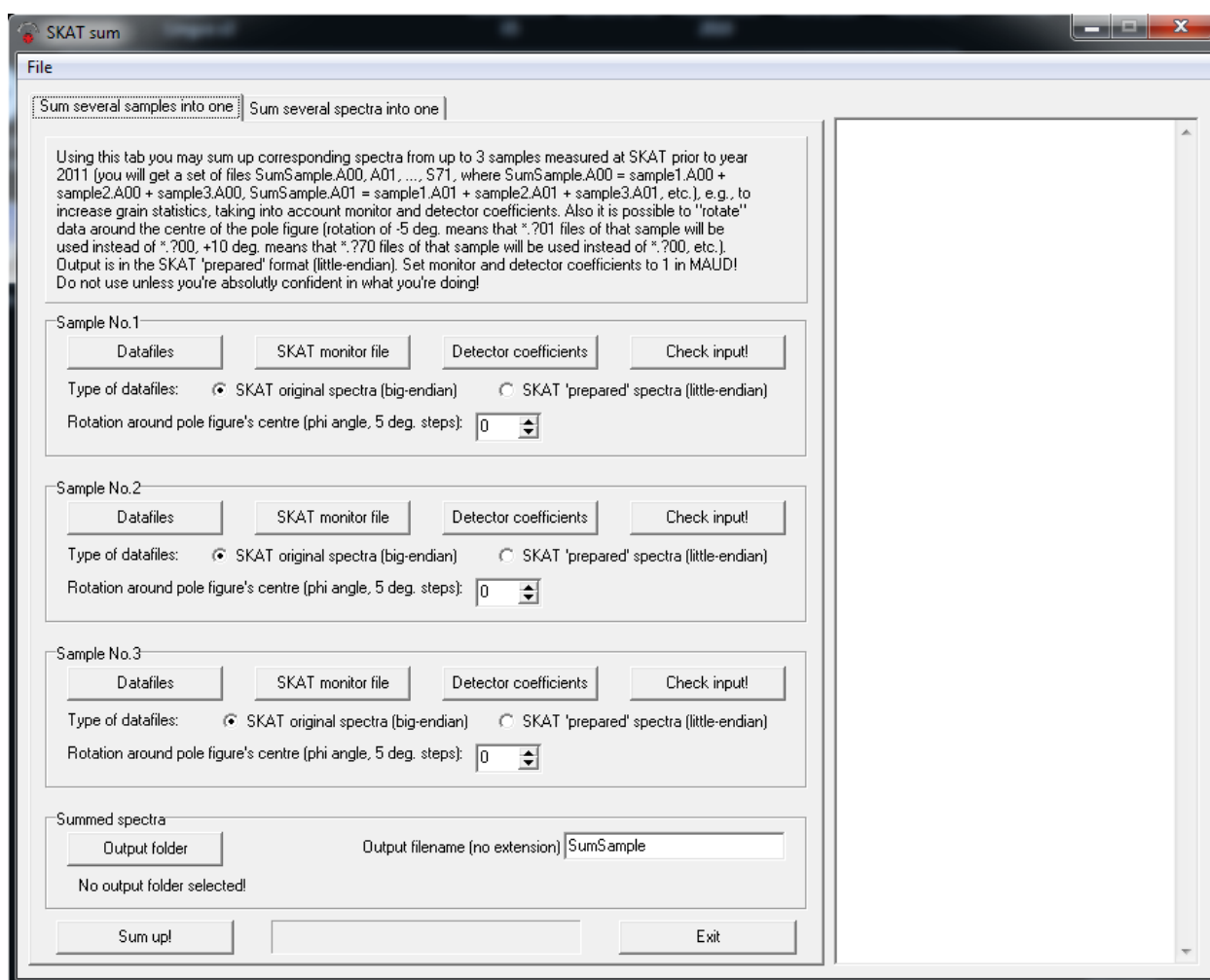
This option is there for the test purposes only. Don't use it.

### 5. Special: SKAT sum

A user have access there through the **Special->SKAT sum** menu. The new window has two tabs: **Sum several samples into one** and **Sum several spectra into one**. The latter one is empty for now.

**File** menu has only one item **Exit** that closes the SKAT sum window.

Here is how a **Sum several samples into one** tab looks like:



It's functions are completely described in the text panel in the top part of the window. A user can sum up corresponding spectra from up to 3 samples measured at SKAT prior to year 2011.

Below there are three similar panels for three samples.

Pressing the **Datafiles** button will result in a dialog window appearance where a user will be prompted to select one data file of this sample. Note, that all the data files of a sample should be located in the same folder. Also, if data file for a sample No.1 is not selected the summation will fail.

Pressing **SKAT monitor file** button will open a dialog window where a user can select a standard SKAT protocol file to read monitor coefficients from it.



Important info!!!

Input (for **SKAT monitor file**):

A standard SKAT protocol file (ASCII text) that looks like this:

```
24Oct01 10:59 1003921178 tofa: open_prot 26db2.txt
24Oct01 10:59 1003921181 tofa: user lebit_leiss
24Oct01 10:59 1003921184 tofa: file 26db2
24Oct01 10:59 1003921186 tofa: sample quartzite_26d_b2
24Oct01 10:59 1003921189 tofa: time 900
24Oct01 10:59 1003921197 unipa: condition monitor_count test
24Oct01 11:00 1003921200 unipa: start
24Oct01 11:00 1003921200 Unipa has been started
24Oct01 11:00 1003921203 motor: phi
24Oct01 11:00 1003921206 motor: find 11
24Oct01 11:00 1003921208 phi at 1C = -9.0000 deg
24Oct01 11:00 1003921212 motor: setpos 0.
24Oct01 11:20 1003922408 tofa: expo #,$00
24Oct01 11:20 1003922408 900.105 4359 61596 60837 26db2.$00
24Oct01 11:35 1003923311 motor: move -5.0
24Oct01 11:35 1003923314 phi at -5.0000 deg
24Oct01 11:35 1003923314 tofa: expo #,$01
24Oct01 11:35 1003923315 900.107 4344 61615 60867 26db2.$01
```

.....

SKAT2MAUD will be looking for strings like the ones highlighted in green.

Pressing **Detector coefficients** button will open a dialog window where a user can select a file containing detector coefficients. This file could either be a MAUD analysis file (.par) or GeoTOF detector coefficients file (.det).

Important info!!!

Input (for **Detector coefficients**):

1) A standard MAUD analysis file (.par) (ASCII text) that looks like this:

```
data_global
_audit_creation_date 'Mon Oct 12 15:11:53 PDT 1998'
_audit_creation_method 'Maud, version 2.3'
_audit_update_record 'Last update Tue May 24 18:06:47 MSD 2011'
_computing_structure_refinement 'Maud, version 2.3'
_refine_ls_R_factor_all 0.4260389
.....
loop_
_inst_inc_spectrum_scale_factor
1.2161942E-6 #min -10000 #max 10000
0.8904439E-6 #min -10000 #max 10000
1.0883708E-6 #min -10000 #max 10000
1.1132917E-6 #min -10000 #max 10000
1.1327876E-6 #min -10000 #max 10000
0.976434E-6 #min -10000 #max 10000
1.1152169E-6 #min -10000 #max 10000
9.977559E-7 #min -10000 #max 10000
0.9632112E-6 #min -10000 #max 10000
1.0105699E-6 #min -10000 #max 10000
1.1580913E-6 #min -10000 #max 10000
1.0047807E-6 #min -10000 #max 10000
```

```
1.0993804E-6 #min -10000 #max 10000
1.063578E-6 #min -10000 #max 10000
1.1561499E-6 #min -10000 #max 10000
1.1297467E-6 #min -10000 #max 10000
9.4812685E-7 #min -10000 #max 10000
1.1697674E-6 #min -10000 #max 10000
1.1312835E-6 #min -10000 #max 10000
```

#end\_subordinateObject\_Multibank Incident Spectrum

.....

- 2) GeoTOF detector coefficients file (.det) (ASCII text) that looks like this (S-detector first):

```
0.86787 ;s
0.89965 ;r
0.86220 ;q
0.85725 ;p
0.90848 ;o
0.71750 ;n
0.87476 ;m
0.81501 ;l
0.93404 ;k
0.84145 ;j
0.78682 ;i
0.67578 ;h
0.97963 ;g
0.76200 ;f
0.98438 ;e
0.96122 ;d
0.93089 ;c
0.65638 ;b
1.00000 ;a
```

- 3) GeoTOF detector coefficients file (.det) (ASCII text) that looks like this (A-detector first):

```
1.00000 ;A
0.72948 ;B
0.89498 ;C
0.91503 ;D
0.92873 ;E
0.80357 ;F
0.91792 ;G
0.81950 ;H
0.79294 ;I
0.83443 ;J
0.94994 ;K
0.82631 ;L
0.90378 ;M
0.87337 ;N
0.95281 ;O
0.92615 ;P
0.78112 ;Q
0.96190 ;R
```

0.92792 ;S

SKAT2MAUD will be looking for strings like the ones highlighted in green.

In case of a MAUD analysis file SKAT2MAUD will correctly handle values with E multiplier and also values with error values given (e.g., 1.913752(1.5090359E-5)).

In case of a GeoTOF (.det) file SKAT2MAUD will recognize the order of the detector coefficients in the file by the letter in the first row (either ;A or ;S, case does not matter, ;a and ;s is also acceptable).

Pressing **Check input** button will show up selected data file for this sample, and also monitor and detector coefficients in the text panel in the right side of the window.

For each sample a **Type of datafiles** should be chosen by a user: big-endian (that's SKAT original data files) or little-endian (these are the files 'prepared'/'byte swapped' by the program GeoTOF).

Also it is possible to "rotate" data around the center of the pole figure with the steps of 5 degrees (e.g., rotation of -5 deg. means that \*.?01 files of that sample will be used during the summation instead of \*.?00, +10 deg. means that \*.?70 files of that sample will be used instead of \*.?00, etc.).

In the **Summed spectra** panel a user can select the folder to put in the summed spectra by pressing **Output folder** button and selecting some folder in the dialog window. By default the folder with the data files of the first sample is used.

Also a user can select a file name for the summed spectra in the textbox **Output filename (no extension)**. As it says, please don't put an extension there as it should be assigned automatically for each summed data file.

Pressing **Sum Up!** Button will start the summation and the progress bar between **Sum Up!** and **Exit** buttons will be showing a summation progress.

Important info!!!

Input (for **Sum Up!**):

Binary file/s (either little- or big-endian; a user MUST select a correct option), 3100 2-bytes (unsigned) integer numbers per file (6200 bytes total in file).

Data files should be in the same folder and should have extension .xyy, where x is a letter (A to S) and yy is a number (00-71).

Output:

Binary file/s, little-endian (SKAT 'prepared' format), 3100 2-bytes (unsigned) integer numbers per file (6200 bytes total in file).

Set monitor and detector coefficients to 1 in MAUD (everything is already accounted for during the summation)!

Finally, **Exit** button closes the SKAT sum window.