"BerSANS" Data Reduction Manual

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INTRODUCTION

1. General features

Small angle neutron scattering (SANS) is an advanced method to investigate materials structures in a length scale between 1 nm and 400 nm. It is applicable to many different systems like metals, alloys, magnetic materials, proteins, macromolecules, and polymers. This leads to a constantly high demand from the international user community to carry out experiments on SANS instruments, for which only a limited amount of beamtime and device responsible manpower are available. The time required for a single SANS measurement is typically short and in most cases varies between five minutes and one hour. This leads to a large number of samples measured and a large amount of raw data produced by each user group, and user groups frequently change with an average beamtime per group of only two to four days. Besides this, the users have a very different scientific background and are often inexperienced with the data processing methods and with the application of computer techniques. Thus, handling this large amount of data under the existing notable time pressure requires special software solutions. The present program package "BerSANS" has been developed as a comfortable, easy-to-use and error-proof software tool to organize the standard data processing procedures in an efficient way, not only to achieve a fast throughput of the user groups, but especially to guarantee reliable and well-documented data evaluation results with a minimum interaction by the device responsible.

2. Programs

A schematic overview of the "BerSANS" program package is shown in Fig.1. The package consists of a set of individual programs each of which is self-sufficient and executes one particular set of operations in numerical data reduction, graphical visualization, or data management. We prefered this way of splitting tasks amongst different programs to one large main program in order to allow clear insight into the intermediate results of different steps of data reduction, as well as to reduce the number of different options per program, thus providing slim menus for easier operation. The integrity of the different programs within the package is provided by using uniform input and output routines, standard dialogue and menu types, and a well-recognisable system of program names. A set of comfort features has been implemented into the input routines of all programs, including repetition functions to recall complete sets of previous input values, and search functions for the selection of input data files by scanning groups of files for certain entries and properties.

The package provides all tools necessary for the data reduction, starting from the two-dimensional raw data files as obtained from the measurement, and ending at the corrected anisotropic or isotropic data files which can then be used for physical interpretation by other programs. Detailed descriptions for the individual programs of the "BerSANS" package are given in the main chapter "Programs" of this manual in alphabetical order.

The programming languages used are Fortran for the numerical programs (anisotropic data reduction No.1 in Fig.1, radial averaging No.2, calculation of beamcenters and transmissions No.3, tool programs No.7), and PV-Wave for the graphic programs (anisotropic plot No.4, isotropic plot No.5, creation of mask files No.6). The programs are fully operational on OpenVMS and UNIX workstations. Due to historical reasons, especially the very limited graphical abilities of the VAX workstations available during the creation days of the "BerSANS" package, most of the user-computer interface has been based on command line communication, with only sparse application of graphical gimmicks. The Fortran programs already run on a minimum hardware basis of VT100 terminal, but a X-Windows terminal is required for the PV-Wave programs. Besides this, the programs have also been tested on PC's with network connection to the host workstation and equipped with commercial "eXcursion" software by Digital Equipment Corporation.

Since different user groups usually have very different degrees of skill concerning the application of data processing methods and computer equipment, is was necessary to design the "BerSANS" program package in a way to provide simple, well-explained, and error-proof program surfaces for

inexperienced users without creating any uncomfortable limitations for experts. This problem was solved by the implementation of very extensive internal error checks, and an online help is available for each input operation which only becomes effective if asked for.

While the inexperienced users normally proceed the data reduction step by step, executing only one of the different programs at a time and then looking at the results, for the experienced users there is the possibility to combine the execution of several programs by writing user-defined command files using the shell programming languages of the particular operating system. Thus, an automatic execution of different data reduction steps at a time can be performed, and tailor-made versions of the programs with their own input-output interfaces can be designed to provide efficient data processing in case of special requirements of the experimental task.
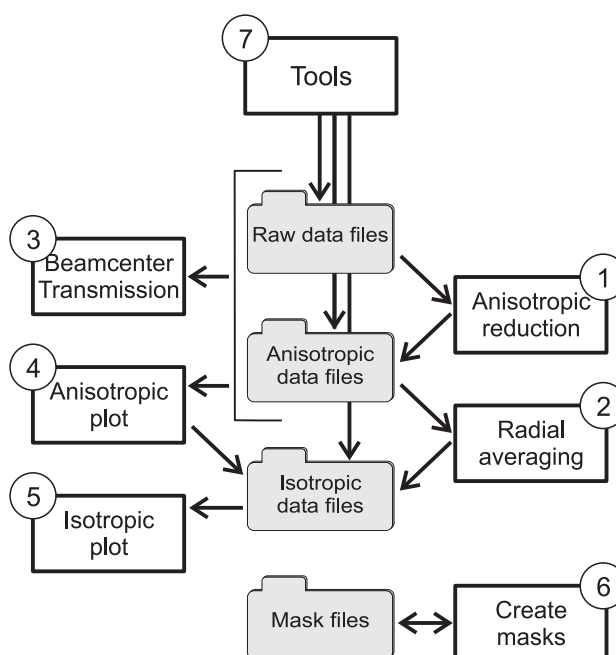
Fig. 1: Schematic overview of the "BerSANS" program package.

3. Files

SANS instruments usually offer a set of different sample environments like sample changers, cradle system, electromagnet, cryomagnet, and high temperature oven. Each of these environments is characterized by special measurement parameters that have to be recorded in the data files. In this situation, it was not considered to be useful to apply a fixed data file format with pre-defined record entries because this would create limitations which might turn out to be of disadvantage during later instrument upgrades. Instead, a flexible data file format was defined for two-dimensional (raw, anisotropic) and one-dimensional (isotropic) data (see Fig.1), as described in detsil in chapter "File Formats". All data files are in ASCII format which allows an easier access to the contents of the files by user-written special programs, or even a direct editing with a standard text editor program if required. These advantages outpoint the only drawback of a larger file size compared to a binary format, since disk space is sufficiently available on most modern computers today.

There are three different types of data files available within the "BerSANS" program package (cf. Fig.1). For efficiency reasons, amongst the two-dimensional data files "raw data" as obtained from the measurement (integer numbers, no explicit values of statistical error) and "anisotropic data" as produced during the data reduction process (real numbers, calculated values of statistical error) are distinguished. As a third data type, "isotropic data" exist which contain one-dimensional scattering information. Each data file contains the data of one single measurement. All types of data files have a uniform system of automatically created file names in the form "Dxxxxxxx.yyy", where "xxxxxxx" is a

7-digit run number which incrementally counts all the data files ever measured on the SANS instrument, and "yyy" is a 3-digit extension nummer which counts the processing steps applied to a certain data file. This extension number starts at "001" for the raw data file, and is automatically incremented by the "BerSANS" programs which create new output files from an input file during different data processing steps. This name system supports easy management of the files during data reduction, and avoids accidental loss of files due to erroneously entered double-defined names.

Besides these data files, other important file types within the "BerSANS" software package are command files which control the numerical data reduction, and mask files for exclusion of selected unwanted detector cells from the data processing. These files are based on the same ASCII line entry format as the data files.

4. How to proceed the data reduction

A) All data files: correction and absolute scaling of the raw data

Step #1: Calculate the transmissions of the samples and of the water used for detector efficiency and geometry correction using programs "SANSTrans" and "SANSTransDo".

Step #2: Calculate the scaling factors for the samples and for water.

Step #3: Perform the anisotropic data reduction using programs "SANSAni" and "SANSAniDo".

Step #4 (optional): Display or print the corrected anisotropic data files with program "SANSAniPlot".

B) Data files with perfect circular symmetry: radial averaging

Step #1: Calculate the beam center for each sample-detector distance using program "SANSArea".

Step #2: Create mask files using program "SANSMask".

Step #3: Perform the full radial averaging using programs "SANSIso" and "SANSIsoDo".

Step #4 (optional): Display or print the resulting isotropic data files with program "SANSIsoPlot".

C) Data files without perfect circular symmetry: cuts and radial sector averaging

For anisotropic data files without circular symmetry, the normal procedure has been finished with A). The following steps can optionally be performed to distill more information from these files:

Step #1: Calculate the beam center for each sample-detector distance using program "SANSArea".

Step #2: Create mask files using program "SANSMask".

Step #3: Perform the radial averaging over limited sectors using programs "SANSIso" and "SANSIsoDo", or create cuts through the anisotropic data files using program "SANSAniPlot".

Step #4 : Display or print the resulting isotropic data files with program "SANSIsoPlot".

D) Additional tool programs: might be helpful for you

To handle the data files: SANSDataPresent, SANSDataDelete

To see and to modify the header information of data files: SANSDataList, SANSDataModify

To communicate with other programsnot capable of the "BerSANS" file format: SANSDataExport, SANSDataImport

Other useful tools: SANSDisplay, SANSInfo, SANSNews

E) Special programs: do not use unless being told so

SANSDataArchive, SANSDataPack, SANSDataUnarchive, SANSDataUnpack, SANSInit

STANDARD MENUS

1. General overview

This chapter contains detailed descriptions of large menus that are identically used in more than one of the programs available within the "BerSANS" program package. Whenever one of these menus appears in a program, the program description will contain a link to the menu description in this chapter. The purpose of an extra description in this special chapter is to avoid endless repetitions of the same description texts in chapter "Programs", making the program descriptions shorter and easier to read. The menus are listed in alphabetical order. The standard format is:

A) Menu name

B) Description

This part contains a short description of what the menu dialogue does. A note indicates whether an on-line help is available.

C) Terminal dialogue

This part gives a very detailed description of all input and output operations that may occur during the execution of the menu. When a menu offers several options, all these options are described but not all of them may become relevant during a single menu dialogue. The **program prompts** appearing on the screen are typed in bold characters. When a menu provides an on-line help, typing "help" at any prompt gives an abbreviated version of the corresponding description in this manual.

D) Calling programs

This part contains the names of the programs which use this menu. The programs are listed in alphabetical order.

File Item Search Menu

Description

All data files of "SANSDRaw", "SANSDAni" and "SANSDIso" types used within the "BerSANS" program package contain the same standard item elements describing the experimental set-up, the properties of the sample, the results of actions done with the files in the past, or input values for actions that will be done with the files in the future. With the option "Search", provided by many programs, you can select a set of files to be used for a particular action by scanning a run number range for certain item values. Only those files within the range are selected that match all conditions.

"help" can be entered at any prompt to get on-line assistance if required.

Terminal dialogue

A menu appears which lists all items that may be present in a data file.

Search item No. n:

or

Search item No. 1 or RETURN for Preset:

Choose the items you want to be present in the data files from the menu list and enter the appropriate item numbers, one on each prompt. To terminate the input sequence, simply press RETURN. You must enter at least one item number. The maximum number of search items is limited to 8.

If the program you're currently running has been executed in the same directory before, the complete input sequence typed for this particular menu during the last run of the program has been stored as a preset and can be recalled by simply pressing RETURN instead of entering an item number for search item number 1.

Depending on the type of the particular item (string or number), you will be prompted for either a string value or for two numeric values. For a detailed description of the items and item types, please refer to chapter "File Formats".

Search string:

Enter the string you want to search for in the specified item.

For item types "word" and "text", a data file will be selected in case of a full equivalence of the strings including upper and lower case matching. Example: A search for sample name "large sample" will not select files with sample names "Large sample" or "large samples".

For item type "comment", a data file will be selected if the search string appears as a substring at any line or position in block "%Comment". Upper and lower case matching is required. Example: A search for comment "sample" will select files with comment "My samples are best", but not files with comment "Your Sample".

For item type "date/time", the string must be in the date/time format of the operating system. A data file will be selected if the search string appears as a substring at any position in the item. Upper and lower case matching is not required. Example: A search for start date of the measurement "jan-199" will select files with start date "15-JAN-1995" and with start date "7-JAN-1994".

For item types "word" and "date/time", no spaces are allowed within the input string. An input containing spaces will be formally accepted by the program but the part following the first space will be cut off.

Search limits <Minimum> [<Maximum>]:

Enter the minimum and maximum limits you want to allow for the specified item, separated by a space. <Minimum> and <Maximum> are two integer numbers for item type "integer", and two real or integer numbers for item type "real", respectively. If <Minimum> is greater than <Maximum> both

numbers are swapped. If <Maximum> is missing it will be set to <Minimum>. A data file will be selected if the relationship "<Minimum> ≤ item value ≤ <Maximum>" holds.

D) Calling programs

This menu is used by programs "SANSAni", "SANSArea", "SANSDataExport", "SANSDataList", "SANSDataModify", "SANSIso", and "SANSTrans".

PROGRAMS

1. General overview

This chapter contains detailed descriptions of all programs available within the "BerSANS" program package. The programs are listed in alphabetical order. The standard format is:

A) Program name

B) Description

This part contains a short description of what the program does. Sometimes a formula is included to illustrate the purpose of a program but no physical background is being discussed. A note indicates whether an on-line help is available.

C) Terminal dialogue

This part gives a very detailed description of all input and output operations that may occur during the execution of the program. When a program offers several options, all these options are described but not all of them may become relevant during a single run of the program. The `command line` to be entered and the `program prompts` appearing on the screen are typed in bold characters. When a program provides an on-line help, typing "help" at any prompt gives an abbreviated version of the corresponding description in this manual.

D) Input requirements

This part summarizes all input data you will be prompted for during the execution of the program. Before running a program, it is recommended to read this part in order to decide if these input data are already available of if any additional preparations have to be made.

E) NOTE

This part gives you special information on technical problems that may occur with particular programs. It is only included in some program descriptions.

SANSAni

Description

This program pre-processes anisotropic data files "Dnnnnnnn.nnn" of "SANSDRaw" and "SANSDAni" types from the current directory interactively and creates a command file "*.SCA" for actual data reduction by the program "SANSAniDo". The created command file can be edited before execution and can also be printed to obtain a complete listing of data and parameters used in data reduction.

"help" can be entered at any prompt to get on-line assistance if required.

Terminal dialogue

Type the command line

SANSAni

No command line parameters are required.

Command file name (no extension):

Enter the name of the command file to be created. Choose any name that is suitable for your own purposes but do not type an extension. The standard extension "*.SCA" will be appended by the program. If you want to copy the file to a DOS or Windows 3.x PC later use a name not longer than 8 characters. You must enter a name.

Minimum output extension:

Enter the minimum extension number for the output data files. Each anisotropic output data file, created by program "SANSAniDo" later, will have the same run number as the last raw or anisotropic input data file used for a particular data type "SampleN". To determine the actual extension number for the output data file, "SANSAniDo" will initially set the extension number to the minimum value entered here. If a data file with this new extension number already exists the program will continue incrementing the extension number until there is no interference with existing files. To use the input extension plus 1 as minimum output extension, simply press RETURN.

Mask file name (no extension):

Enter the name of the mask file to be used to label individual detector cells for exclusion from data reduction but do not type an extension. The standard extension "*.MSK" will be appended by the program. If you do not wish to use a mask file, simply press RETURN. If the input file does not exist or is not a valid mask file you will be prompted for a new input.

Accept this mask file? (Y)/N:

If you entered the name of a valid mask file information on this file is written to the screen. If you agree that this is the file you intended to use, enter "y" (or simply press RETURN) to confirm. If you don't want to use this mask file, enter "n" to choose a new one.

Use "<DataType>"? Range/Search/Continue/(No):

The program now prompts for input data types "Cadmium", "Water", "WaterBackground", "SampleBackground" and "SampleN" (N = 1..50), respectively. The prompt for "WaterBackground" will only appear if you use raw data files of "SANSDRaw" type for "Water".

To select the input mode of data files for the particular data type, enter one of the following options (1) to (4):

Option (1): **Range**

Enter "r" for "Range" if the data files you want to use form a continuous range of run numbers, and if you already know the first and the last run number of this range. Within the range, all files will be

selected that pass the test for a valid data file. This option often provides a faster operation than "Search", and it requires less input typing.

Range limits <FirstRun> <LastRun> [<Extension>]:

Enter the first run number, the last run number, and the extension number of the data file range to be processed, all separated by spaces. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". <LastRun> must be greater or equal <FirstRun>. If <Extension> is missing the default value "1" is assumed. All data files must have the same extension number.

Files will now be processed. For each individual data file, the file name is listed together with the sample name. If an input file does not exist or is not a valid data file the run number is skipped. The numbers of files expected in the entered range and of files actually found are compared.

Accept this selection? (Y)/N:

If you agree that these are the files you intended to use, enter "y" (or simply press RETURN) to confirm. If you don't want to use these data files, enter "n" to choose a new range.

The number of files found will usually be equal to the number of files expected. If it is smaller then some data files have not been found or have not passed the test for a valid file type.

A set of input data files may contain no files at all, may consist of one or more data files of "SANSDRaw" type, or may consist of exactly one data file of "SANSDAni" type. No mixing of "SANSDRaw" and "SANSDAni" data files and no adding of "SANSDAni" data files is permitted.

Add another set of files? Y/(N):

This prompt only appears if the previous set of files entered for the current data type were raw data files of "SANSDRaw" type. Enter "y" to select another set of files for the current data type. This returns you to the ' Range limits <FirstRun> <LastRun> [<Extension>]: ' prompt.

Enter "n" (or simply press RETURN) if you don't want to use this option.

From this point, the terminal dialogue is the same both for option (1) "Range" and for option (2) "Search".

If the current data type is any other than "Cadmium", the program now tries to read the transmission of this data type from the last data file of the set automatically. If this data file contains a transmission value it will be written to the screen, if not you will be prompted to enter it.

Transmission of "<DataType>":

Enter the transmission value. Any real number will be accepted.

If the current data type is "Water" or "SampleN", the program now tries to read the scaling factor of this data type from the last data file of the set automatically. If this data file contains a scaling factor value it will be written to the screen, if not you will be prompted to enter it.

Scaling factor of "<DataType>":

Enter the scaling factor value. Any real number will be accepted.

If the current data type is "SampleN", the program now tries to read the attenuation factor and the scattering probability of this data type from the last data file of the set automatically. If this data file contains an attenuation factor value and a scattering probability value, these will be used, if not default values of "1.0" for the attenuation factor and of "0.0" for the scattering probability will be assumed. Since these two parameters only need to be modified from the defaults in very rare cases, the values used for them are only written to the screen for information, but there is no extra prompt for them. To modify them, you must edit the command file directly.

This ends option (1) "Range" and returns you to the ' Use "<DataType>"? ' prompt.

Option (2): **Search**

Enter "s" for "Search" if the data files you want to use do not form a continuous range of run numbers, or if you are not certain about the limits of the range. With this option, you can select the files used for data reduction by scanning a run number range for certain item values. Only those files within the range are selected that match all conditions. This option provides a slower operation than "Range" if the run number range to be scanned is large, and it requires more input typing.

Range limits <FirstRun> <LastRun> [<Extension>]:

Enter the first run number, the last run number, and the extension number of the data file range to be scanned, all separated by spaces. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". <LastRun> must be greater or equal <FirstRun>. If <Extension> is missing the default value "1" is assumed. All data files must have the same extension number.

A menu appears which lists all items that may be present in a data file. For a detailed description of this menu, please refer to "File Item Search Menu" in chapter "Standard Menus".

Files will now be processed. For each individual data file that matches all conditions, the file name is listed together with the sample name. If an input file does not exist or is not a valid data file the run number is skipped. If you choose an item that is not present in a particular data file it will be treated as "no matching". The numbers of files expected in the entered range and of files actually found are compared.

Accept this selection? (Y)/N:

If you agree that these are the files you intended to use, enter "y" (or simply press RETURN) to confirm. If you don't want to use these data files, enter "n" to choose a new range.

The number of files found and the number of files expected may differ considerably, depending on the size of the scan range entered.

A set of input data files may contain no files at all, may consist of one or more data files of "SANSDRaw" type, or may consist of exactly one data file of "SANSDAni" type. No mixing of "SANSDRaw" and "SANSDAni" data files and no adding of "SANSDAni" data files is permitted.

Add another set of files? Y/(N):

This prompt only appears if the previous set of files entered for the current data type were raw data files of "SANSDRaw" type. Enter "y" to select another set of files for the current data type. This returns you to the ' Range limits <FirstRun> <LastRun> [<Extension>]: ' prompt.

Enter "n" (or simply press RETURN) if you don't want to use this option.

From this point, the terminal dialogue will be the same as for option (1) "Range", starting from the ' Transmission of "<DataType>": ' prompt.

Option (3): **Continue**

Enter "c" for "Continue" to use a special option that has been designed for quickly processing data from measurements like temperature, pressure or magnetic field scans where different environment conditions are applied to the same sample. To use this option, the measurement must be organized in a way that there is always the same number of data files for each state of the sample.

After typing "c", for the current "SampleN" data type the same number of runs and the same extension number like for the preceding "SampleN-1" data type will be used. Like in options (1) "Read" and (2) "Search", the program now tries to read the transmission, the scaling factor, the attenuation factor and the scattering probability of "SampleN" from the last data file directly. But in contrast to these two former cases, if this data file does not contain a transmission and/or a scaling factor the program will not prompt you to enter a number, and if this data file does not contain an attenuation factor and/or a scattering probability the program will not assume a default. Instead, the missing values will be replaced with the values used for "SampleN-1" automatically. This saves you from typing the same

redundant numbers again and again. The run number range for "SampleN" starts with the run following the last run of the preceding "SampleN-1" data type. Example: "Sample2" covered runs 17 to 19 with extension number 1. Choosing option "Continue" for "Sample3" selects runs 20 to 22 with extension number 1. If run 22 contains a transmission, a scaling factor, an attenuation factor, and a scattering probability, these values are used for "Sample3". If one or more of them are missing, they are automatically replaced with the appropriate values either read from run 19 or entered from the keyboard for "Sample2" before.

This option is only available for a "SampleN" data type and after an initial "Range" command setting the starting point, the step width for continuation and the default extension number.

Files will now be processed. For each individual data file, the file name is listed together with the sample name. If an input file does not exist or is not a valid data file the run number is skipped. The numbers of files expected in the entered range and of files actually found are compared.

Accept this selection? (Y)/N:

If you agree that these are the files you intended to use, enter "y" (or simply press RETURN) to confirm. If you don't want to use these data files, enter "n" to choose a new range. In this case, you will be prompted for limits and extension number of the run number range like in option (1) above, but the program uses the same transmission, scaling factor, attenuation factor and scattering probability like for the preceding sample. Please note that this action sets new initial values for the starting point, the step width for continuation and the default extension number for option "Continue", but leaves the transmission, the scaling factor, the attenuation factor and the scattering probability unchanged.

The number of files found will usually be equal to the number of files expected. If it is smaller then some data files have not been found or have not passed the test for a valid file type.

A set of input data files may contain no files at all, may consist of one or more data files of "SANSDRaw" type, or may consist of exactly one data file of "SANSDAni" type. No mixing of "SANSDRaw" and "SANSDAni" data files and no adding of "SANSDAni" data files is permitted.

This ends option (3) "Continue" and returns you to the ' Use "<DataType>"? ' prompt for the next sample directly. Please note that unlike options (1) "Range" and (2) "Search", no addition of another set of data files for the same sample is supported.

Option (4): **No**

Enter "n" for "No" (or simply press RETURN) if you don't want to use the specified data type.

Choosing this option for "Cadmium", "Water", "WaterBackground" or "SampleBackground" returns you to the ' Use "<DataType>"? ' prompt directly.

If the current data type is "SampleN", option "No" terminates the input sequence for a set of samples "Sample1" to "SampleN-1" for which the sample background selected before (or no sample background if you skipped the appropriate input) will be used. Please note that this option is not available for "Sample1" because at least one sample is required for a useful operation.

Another sample background? Y/(N):

Enter "y" to choose another sample background, which will be valid for all following samples until you change the background again. Use this option if you measured your samples with different background conditions (e.g. some samples in a holder and some other samples in a quartz cell) but with the same "Cadmium", "Water" and "WaterBackground" files. In this case, you won't have to type in all these files again. Typing "y" ends option "No" and returns you to the ' Use "SampleBackground"? ' prompt.

If you want to change the data files used for "Cadmium", "Water" or "WaterBackground" you must execute this program again.

Enter "n" (or simply press RETURN) if you don't want to use another sample background. The output command file "*.SCA" will now be written, including all data required to proceed the actual data reduction, and must be executed using the program "SANSAniDo".

Execute the command file now? Y/(N):

Enter "y" to start this execution now.

Enter "n" (or simply press RETURN) to run the program "SANSAniDo" later. You may then print or edit the command file first to verify and possibly to correct it's content before execution.

Input requirements

Run numbers of the data files to be processed for each data type must be known, or the item values in the data files must be set in a way that the files corresponding to one particular data type can be identified by a unique combination of these item values.

The transmissions of water, water background and sample background (if used) and of the samples must be determined first using programs "SANSTrans" and "SANSTransDo". The transmission values can either be written into the input data files before running this program using program "SANSDataModify", or can be entered directly while this program is running.

The scaling factors of water (if used) and of the samples must be calculated first. The scaling factor values can either be written into the input data files before running this program using program "SANSDataModify", or can be entered directly while this program is running.

To use the defaults of "1.0" for the attenuation factor and of "0.0" for the scattering probability, no extra action needs to be taken. Individual values different from these defaults can be written into the input data files before running this program using program "SANSDataModify".

If you intend to mask data explicitly the mask file "*.MSK" must be created first using the program "SANSMask", or an appropriate pre-defined mask file must be chosen.

NOTE

If a message "This program can only handle up to ... data files." appears please consult the device responsible.

SANSAniDo

Description

This program processes anisotropic data files "Dnnnnnnn.nnn" of "SANSDRaw" and "SANSDAni" types from the current directory by executing an anisotropic command file "*.SCA" of "SANSCAni" type created interactively with the program "SANSAni". All required information is included in the command file and in the data files themselves.

Data reduction is done for each detector cell (i,j) individually. Raw data intensities $I_{ij-Measured}$ coming from input files of "SANSDRaw" type are first corrected by the program for detector deadtime τ according to the formula

$$I_{ij-Corrected} = \frac{I_{ij-Measured}}{1 - \frac{\tau}{t} \sum_{i,j} I_{ij-Measured}} \tag{1}$$

In this equation, I represents each of the input data types "Cadmium", "Water", "WaterBackground", "SampleBackground", and "Sample", respectively, and t is the total measurement time used for the appropriate input data type. The detector deadtime τ has been experimentally determined, and is written into the "Deadtime" item in block "%Default" of the command file by the program "SANSAni" automatically. This value can be modified before execution of the command file. However, it is strongly recommended to use the pre-defined value only, unless you really know what you are doing.

After this correction, intensities are normalized to the individual monitor values recorded in the data files. Anisotropic data coming from input data files of "SANSDAni" type are considered as already being corrected for deadtime and normalized. The implicit masking of invalid and masked cells included both in input data files of "SANSDRaw" and "SANSDAni" types is transferred to the output data file.

In the standard case, the program calculates the absolute scattering cross-section dσ/dΩ from the corrected and normalized intensities of the input data types "Cadmium" (Cd), "Water" (W), "WaterBackground" (WB), "SampleBackground" (SB), and "Sample" (S) for each cell (i,j) according to the formula

$$\left(\frac{d\sigma}{d\Omega}\right)_{ij} = \frac{\left(\frac{S_{ij} - Cd_{ij}}{T(S)}\right) * A(S) - \left(\frac{SB_{ij} - Cd_{ij}}{T(SB)}\right) * (1 - p(S))}{\left(\frac{W_{ij} - Cd_{ij}}{T(W)}\right) - \left(\frac{WB_{ij} - Cd_{ij}}{T(WB)}\right)} * \frac{ScalingFactor(W)}{ScalingFactor(S)} \tag{2}$$

where T are the transmissions of these input data types, and A ($A \geq 1$) and p ($0 \leq p \leq 1$) are the attenuation factor and the scattering probability of data type "Sample", respectively. The absolute output error Δ(dσ/dΩ) is calculated from the errors of the input data types "Cadmium" (ΔCd), "Water" (ΔW), "WaterBackground" (ΔWB), "SampleBackground" (ΔSB), and "Sample" (ΔS) according to the formula

$$\Delta\left(\frac{d\sigma}{d\Omega}\right)_{ij} = \sqrt{\left(\frac{\partial \frac{d\sigma}{d\Omega}}{\partial Cd} \Delta Cd_{ij}\right)^2 + \left(\frac{\partial \frac{d\sigma}{d\Omega}}{\partial W} \Delta W_{ij}\right)^2 + \left(\frac{\partial \frac{d\sigma}{d\Omega}}{\partial WB} \Delta WB_{ij}\right)^2 + \left(\frac{\partial \frac{d\sigma}{d\Omega}}{\partial SB} \Delta SB_{ij}\right)^2 + \left(\frac{\partial \frac{d\sigma}{d\Omega}}{\partial S} \Delta S_{ij}\right)^2} \tag{3}$$

using the partial derivatives of equation (2).

A special alternate version of the data reduction formula (2)

$$\left(\frac{d\sigma}{d\Omega}\right)_{ij} = \frac{\left(\dfrac{S_{ij} - Cd_{ij}}{T(S)}\right)*A(S) - \left(\dfrac{SB_{ij} - Cd_{ij}}{T(SB)}\right)*(1 - p(S))}{W_{ij}} * \frac{ScalingFactor(W)}{ScalingFactor(S)} \tag{4}$$

is available in the program which allows a simultaneous input of raw data files of "SANSDRaw" type for "Sample", "SampleBackground" and "Cadmium", and a pre-corrected anisotropic data file of "SANSDAni" type for "Water", avoiding a subtraction of "Cadmium" from the corrected "Water" which would occur if equation (2) was used. This alternate formula (4) is automatically applied instead of formula (2), if the command file contains one or more "Cadmium" files, exactly one corrected (not raw data) "Water" file, and no "WaterBackground" file. The absolute output error is calculated using the same equation (3) like in the standard case.

Terminal dialogue

Type the command line

SANSAniDo <CommandFileName>

Parameter is the name of the command file to be executed. <CommandFileName> is a string compatible to the requirements of the operating system, without extension. The standard extension "*.SCA" will be appended by the program. Only a proper command line is accepted.

Information on the command file and the mask file used by the program is written to the screen. If an input file does not exist or is not a valid command file or mask file the program aborts.

The following screen listing of data files processed is grouped into separate blocks. The first block always contains one set of files for each data type "Cadmium", "Water" and "WaterBackground" respectively, which are valid for all samples. This block is followed by one or more blocks that all start with a set of files for data type "SampleBackground" and only contain those data types "SampleN" that refer to these particular background data.

For each individual data file, the file name is listed together with the sample name during processing. Please note that this sample name is taken from the data file directly. The sample name included in the corresponding line of the command file is only a comment, so editing the name in the command file will have no effect on the screen output. If you use the original command file as created by the program "SANSAni" without subsequent editing this fact is not important for you.

If an input file does not exist or is not a valid data file the program aborts.

After a set of input data files for a data type "SampleN" has been processed an output data file of "SANSDAni" type is written. The run number for this output file will always be the last run number of the input data files used. To determine the actual extension number for the output data file, the extension number is initially set to the minimum output extension entered in program "SANSAni". If a data file with this new extension number already exists the program will continue incrementing the extension number until there is no interference with existing files. In this case, a warning will be displayed on the screen.

Most item values that describe the sample and the experimental set-up are copied from the last processed file of a data type "SampleN" to the output file directly. There is no check if these values are the same in the whole set of input data files used for the particular sample. For details, please refer to the description of the "SANSDAni" file format. Item values from other data types ("Cadmium" etc.) are never used.

A set of input data files may contain no files at all, may consist of one or more data files of "SANSDRaw" type, or may consist of exactly one data file of "SANSDAni" type. No mixing of "SANSDRaw" and "SANSDAni" data files and no adding of "SANSDAni" data files is permitted. The program "SANSAni" automatically verifies this upon creation of the command file but if you edit the command file before execution you have to respect this condition, otherwise the program aborts.

After each execution of a command file, a listing of input data file names and data reduction parameters actually used and of output data file names actually created is appended to the end of the

command file. This automatic recording of log information increases the size of the command file by adding comment lines which do not affect later executions. If you do not wish to add this log information to the command file you can disable this feature by editing the file and changing entry "Logging=YES" in block "%File" to "Logging=NO". However, it is strongly recommended to leave this feature enabled since it provides you with a complete printer-ready recording of the work you've done.

Input requirements

The command file "*.SCA" must be created first using the program "SANSAni". The mask file and the data files that were used during this creation must be present.

NOTE

If a message "Command file is too long." appears please consult the device responsible.

SANSAniPlot

Description

This program creates 2-dimensional contour plots and 1-dimensional profile cuts of anisotropic data files "Dnnnnnnn.nnn" of "SANSDRaw" and "SANSDAni" types. The graphics output can optionally be printed on paper or saved as a PostScript file. A mask file "*.MSK" can be used to hide unwanted detector cells in the output.

"help" can be entered at any prompt to get on-line assistance if required.

Terminal dialogue

Type the command line

SANSAniPlot

No command line parameters are required.

A graphics window for the contour plot will be opened displaying the square area, with the co-ordinates (0,0) in the lower left corner and the co-ordinates (<DetectorSize>-1,<DetectorSize>-1) in the upper right corner. Each tick mark on the axis represents four detector cells. If a data file contains information on a beam center, during some options the position of this beam center is displayed as a cross "+". On the bottom line of the contour plot window, the current mask file name and the current data file name are displayed.

Actions taken by this program neither modify the original data file nor the original mask file. Masking unwanted detector cells only affects the screen display, the print or graph file output, and the writing of profile cut files, and mainly serves as a tool for "beauty corrections" of this output for further processing or for publication.

On some computer types, the keyboard input remains permanently directed to the DECterm window where you typed the command line to start the program. You can enter commands even while a graphics window is highlighted, and you only have to highlight the DECterm window explicitly by a mouse click if the graphics window hides a part of the DECterm window that you want to see. In contrast, on some other computer types the input will be always directed to the currently highlighted window. Therefore, no keyboard input is recognized by the program when a graphics window is highlighted. To enter any keyboard input, the DECterm window must be highlighted first by a mouse click. Since after the start of the program the contour plot window is always highlighted automatically, on this computer type this has to be your first action before entering any command from the PC keyboard.

The main menu appears which lists all options provided by the program.

Read Levels Table Print Save maskFile Implicit Explicit Cut mOde Vms Quit
Option? R/L/T/P/S/F/I/E/C/O/V/Q:

Enter one of the following options (1) to (12):

Option (1): **Read**

Enter "r" for "Read" to read an anisotropic data file "Dnnnnnnn.nnn" of "SANSDRaw" or "SANSDAni" type.

Data file <Run> [<Extension>] or Next:

Enter the run number and the extension number of the data file to be read, separated by a space. <Run> is a positive integer number between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". If <Extension> is missing the default value "1" is assumed. Or enter "n" to read the next existing run number with the same extension as before. "Next" is only available

after an initial input of a correct data file specification setting the starting point for continuation. It does not require a continuous range of run numbers but increments the last run number loaded until a new data file has been found. To avoid an infinite loop in case no other data file follows, the maximum size of a gap allowed between two run numbers is limited to 100. If you do not wish to read a data file, simply press RETURN.

If the input file does not exist or is not a valid data file you will be prompted for a new input. If you entered the name of a valid data file, information on this file is written to the screen, the new data are displayed in the contour plot window, and the data file name in the contour plot window is updated.

If the data file was read as "Next", the levels for the contour plot of the data remain unchanged. Otherwise, the levels are re-defined automatically in equidistant steps between the minimum and maximum intensities of the new data file.

Option (2): **Levels**

Enter "l" for "Levels" to change the contour plot levels for the data file. Intensities within a data file may extend over many decades. You may find it necessary to experiment with different level values to reveal all details in the measured data.

An information on the intensity range covered by the current data, and on the contour plot levels currently defined is written to the screen.

Up to 6 levels or Auto:

Enter up to 6 real or integer numbers, all separated by spaces. The numbers must be in the range between "Minimum" and "Maximum" values of the data intensity. The input values will be sorted in ascending order, and redundant inputs of the same value will be removed. Or enter "a" to set the contour plot levels automatically. The data are displayed in the contour plot window with the new contour plot levels. If you do not wish to change the current levels, simply press RETURN.

Please note that automatic scaling using option "a" will be performed using only those data cells that are currently neither implicitly nor explicitly masked. This means that the contour plot levels calculated before and after a change of options (7) "Implicit" or (8) "Explicit" may differ, depending on the intensity of the cells added to or removed from the current anisotropic plot by these two options.

Option (3): **Table**

Enter "t" for "Table" to display a sub-area of the data file as a table. After selecting the center point of the desired sub-area, a table is written to the screen displaying a square sub-area of 11 by 11 cells, centered symmetrically around the selected center point. The numbers in the top line and in the left column of the table represent the X and Y co-ordinates of the displayed cells, respectively. If the center point has been selected very close to the edge of the detector area, it is shifted automatically to a distance of 5 cells from the edge in order to obtain a fixed table size.

The numbers in the table usually represent the original content of the detector cells. Optionally, these numbers can also be normalized to an integer range of "0".."10000", where "0" corresponds to the minimum intensity in the selected sub-area, and "10000" corresponds to the maximum intensity in the selected sub-area. This may be useful for some applications. The minimum, maximum and average intensities of the data file sub-area displayed in the table are always given in absolute values.

For original intensities from data files of "SANSDRaw" type and for normalized intensities from all data file types, the output format of the numbers is "I6". For original intensities from data files of "SANSDAni" type, the output format is "F6.2". All numbers which are too large for these output formats are displayed as "******".

Depending on the setting of option (10) "mOde", the selection of the center point can be done either using the mouse, or using the keyboard.

a) Selecting the center point using the mouse:

Click with the mouse into the contour plot window. Three numbers in the lower right corner of the contour plot window display the current (X,Y) cursor position and the data intensity at this position. Move the mouse to the cell you want to select as the center point for the table. Click the LEFT mouse button to create a table of original intensities. Click the RIGHT mouse button to create a table of normalized intensities.

To end this option and return to the main menu, press the LEFT and RIGHT mouse buttons together at the same time until the menu appears. Now click on the DECterm window once again to redirect the keyboard input to that window.

b) Selecting the center point using the keyboard:

You will be prompted for the co-ordinates of the center point.

Sub-area co-ordinates <X-Mid> <Y-Mid> [Normalized]:

Enter two integer numbers between "0" and "<DetectorSize>-1", separated by a space. Enter an additional "n" on the same input line to display normalized intensities instead of the original ones. To end this option and return to the main menu, simply press RETURN.

Option (4): **Print**

Enter "p" for "Print" to print the contour plot (see Fig.1). This option is only available if a data file has been read in before.

Graphics layout type? (1)/2/3:

Enter "1" (or simply press RETURN) to print the plain contour lines.

Enter "2" to add labels to the printed contour lines. This option is only recommended for pictures which do not have a too complex structure, because otherwise the labels may overlap and become unreadable.

Enter "3" to enhance the printed contour plot with up to 6 different grey shadings that fill the areas between the contour lines. This option provides a slower operation than "1" and "2" but gives a better understanding of the actual intensity distribution.

A menu appears which lists all available printers and their locations.

Printer number:

Enter the number of the printer to be used. To select the printer marked as "default", simply press RETURN. Depending on the load of the computer and the network and on the complexity of the picture, the printing may require up to a few minutes.

The printed page contains some additional information on the sample, the experimental set-up and the processing done with the data file so far, read from the data file. If the data file contains a comment, the number of comment lines printed depends on the space available at the bottom of the page.

If "explicit masking" using a mask file was enabled, the output block "Processing information" contains the name of this mask file. If "implicit masking" was enabled, this block contains the name of the last mask file that has been used in the past to add an implicit mask to the data file. If the presence of implicitly masked cells has been detected but no corresponding mask file name has been found in the data file, the implicit mask file name is set to "UNKNOWN".
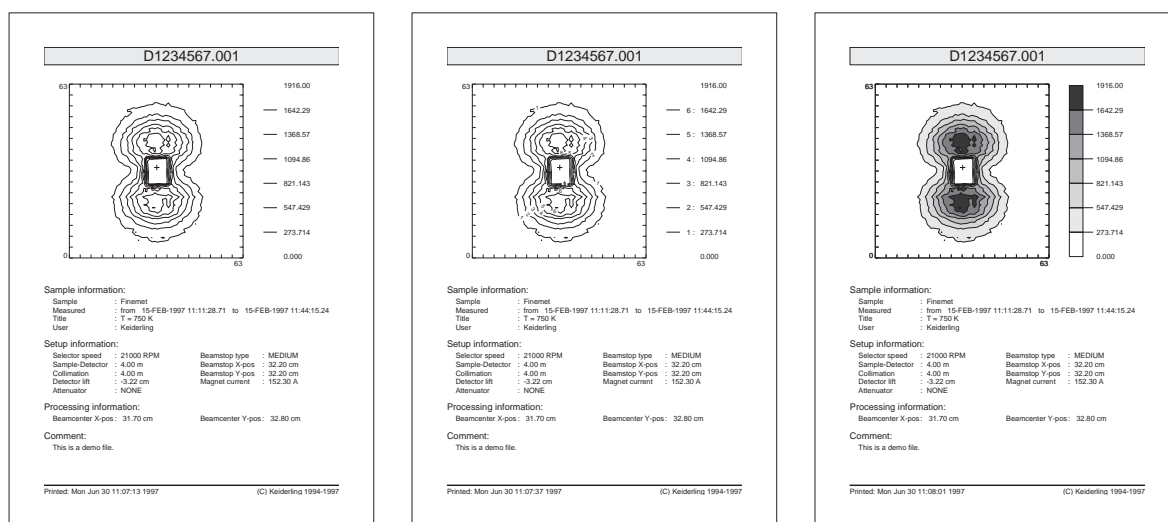
Fig.1: Printer output pages created using graphics layout types "1", "2" and "3" (left to right).

Option (5): **Save**

Enter "s" for "Save" to save the contour plot as an "Encapsulated PostScript" graph file, ready for import into common text or graphics programs which support this file format, e.g. "Microsoft Word" or "CorelDraw!" (see Fig.2). This option is only available when a data file has been read in before.

Output file name (no extension):

Enter the name of the output file but do not type an extension. The standard extension "*.EPS" will be appended by the program. If you do not wish to save a graph file, simply press RETURN.

There is no check whether a graph file of the same name already exists in the current directory. If a file exists it will be overwritten without a warning.

Graphics layout type? (1)/2/3/4/5/6/7/8:

Enter "1" (or simply press RETURN) to create a graph file containing the plain contour lines.

Enter "2" to create a graph file containing the plain contour lines, plus an intensity scale.

Enter "3" to add labels to the contour lines. This option is only recommended for pictures which do not have a too complex structure, because otherwise the labels may overlap and become unreadable.

Enter "4" to add labels to the contour lines, plus an intensity scale. This option is only recommended for pictures which do not have a too complex structure, because otherwise the labels may overlap and become unreadable.

Enter "5" to enhance the created graph file with up to 6 different grey shadings that fill the areas between the contour lines. This option provides a slower operation than "1" to "4" but gives a better understanding of the actual intensity distribution.

Enter "6" to enhance the created graph file with up to 6 different grey shadings that fill the areas between the contour lines, plus an intensity scale. This option provides a slower operation than "1" to "4" but gives a better understanding of the actual intensity distribution.

Enter "7" to produce the same result as "5", but with color shadings instead of grey shadings.

Enter "8" to produce the same result as "6", but with color shadings instead of grey shadings.

For all types "1" to "8", the beam center of the data file will be displayed if present.
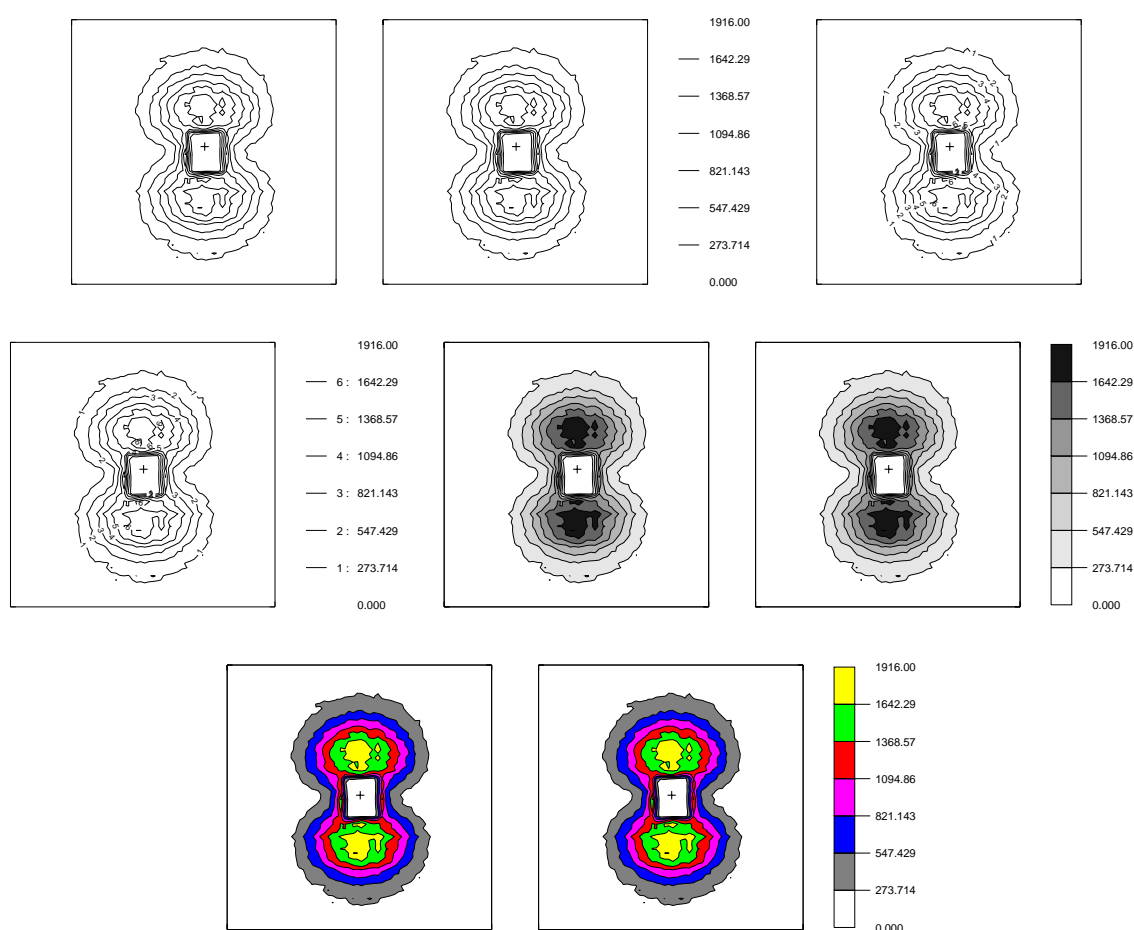
Fig.2: Graph files created using graphics layout types "1" to "3" (first line, left to right), "4" to "6" (second line, left to right), and "7" to "8" (third line, left to right).

Option (6): `maskFile`

Enter "f" for "maskFile" to read a mask from a file.

Mask file name (no extension):

Enter the name of the mask file to be read but do not type an extension. The standard extension "*.MSK" will be appended by the program. If you do not wish to read a mask file, simply press RETURN.

If the input file does not exist or is not a valid mask file you will be prompted for a new input. If you entered the name of a valid mask file, information on this file is written to the screen, and the mask file name in the contour plot window is updated.

Please note that masked detector cells will only disappear from the graphics output when explicit masking has been enabled using option (8) "Explicit". If explicit masking is disabled when reading a mask file, there will be no visible changes in the contour plot.

Option (7): `Implicit`

Enter "i" for "Implicit" to hide or expose cells that are implicitly masked in the data file. This option is only available when an implicit mask has been detected in the data file. When a cell is masked, the intensity value of this cell is temporarily set to zero in the program, without modifying the original data file.

This option works in a toggle mode: Entering "i" while implicit masking is disabled sets it to the enabled state, and vice versa. The default setting after the start of the program is "disabled".

When you read a new data file containing an implicit mask, the setting of this option remains the same as before. When you read a new data file which does not contain an implicit mask, this option is automatically reset to "disabled".

Option (8): **Explicit**

Enter "e" for "Explicit" to hide or expose cells that are explicitly masked by the mask file. This option is only available when a mask file has been read in before. When a cell is masked, the intensity value of this cell is temporarily set to zero in the program, without modifying the original data file. Thus, if the initial intensity of a cell is already zero, using this option causes no visible changes of the graphics output for this particular cell.

This option works in a toggle mode: Entering "e" while explicit masking is disabled sets it to the enabled state, and vice versa. The default setting after the start of the program is "disabled".

Option (9): **Cut**

Enter "c" for "Cut" to create a 1-dimensional profile cut through the anisotropic data file, displaying the intensity I vs. the scattering vector Q. The profile cut always covers a line from the cell at the beam center to a cell at the detector edge, containing all cells touched by this line in between. This yields a non-equidistant distribution of data points. The number of data points in the profile cut and the Q-values of these data points depend on the beam center co-ordinates and the cut angle used. This option is only available when a data file has been read in before.

The profile cut is displayed as a curve in a separate graphics window which will be opened after the first cut has been created, and then remains permanently open until option "Cut" will be ended. On the right margin of the profile cut window, the cut angle for the current curve is displayed.

The wavelength and the sample-detector distance are required to scale the scattering vector Q on the "X"-axis of the profile cut in absolute units of "nm^{-1}". If the appropriate items "Lambda" and "SD" are present in the data file, the program automatically uses these values, and displays them for verification. If these items are not present, the program prompts for them.

Wavelength [nm]:

and / or

Sample-Detector distance [m]:

Enter the required values. Any real or integer numbers will be accepted. These values cannot be modified later, but remain valid until a new data file has been read in.

The co-ordinates of the beam center are required to determine the starting point of the profile cut. If the appropriate items "BeamcenterX" and "BeamcenterY" are present in the data file, the program automatically uses these values, and displays them for verification. If these items are not present, the program prompts for them.

Beam center co-ordinates <X> <Y>:

Enter two real numbers between "0" and "<DetectorSize>-1", separated by a space. They are used as initial values and can be modified later. The initial beam center position is displayed as a cross "+" in the contour plot window.

A menu appears which lists all "Cut" sub-options provided by the program.

**Beamcenter Angle X-axis Y-axis Table Write Print Save End
Option? B/A/X/Y/T/W/P/S/E:**

Enter one of the following sub-options (9-1) to (9-9):

Sub-option (9-1): **Cut│Beamcenter**

Enter "b" to change the co-ordinates of the beam center.

Beam center co-ordinates <X> <Y>:

Enter two real numbers between "0" and "<DetectorSize>-1", separated by a space. The symbol "+" for the beam center in the contour plot window will be shifted to the new position. If the profile cut window has already been opened, it will be erased.

Sub-option (9-2): **Cut│Angle**

Enter "a" to define the cut angle relative to the beam center. Depending on the setting of option (10) "mOde", this can be done either using the mouse, or using the keyboard.

a) Defining the angle using the mouse:

Click with the mouse into the contour plot window. Two numbers in the lower right corner of the contour plot window display the angle of the current cursor position relative to the beam center and the data intensity at this position. Move the mouse to the angle you want to select, and click the LEFT mouse button. A line from the beam center through the haircross cursor to the detector edge will be drawn, and a profile cut of the data intensities along this line will be calculated and displayed as a curve in the profile cut window. If no profile cut has been created before, the profile cut window will be opened at this point. Since this is a time-consuming process, it may require up to a few seconds, depending on the load of the computer and the network.

The profile cut will be drawn with the current settings for types and ranges of the axis. The number of data points actually visible in the profile cut window will be written to the screen. If an axis has been defined in a way that some data points cannot be displayed because they are outside the axis limits or invalid for the current axis types (e.g. a negative value on a logarithmic axis), the numbers of these additional data points will be written to the screen, too. The sum of these three numbers yields the total number of data points present in the profile cut. If no data points fit to the current axis settings, the profile cut window will be erased and remains blank.

If implicit and/or explicit masking has been enabled in the program before, the masked cells will be omitted from the profile cut. If the profile cut does not contain any data points because all relevant cells are masked, a message will be written to the screen, and the profile cut window will be erased and remains blank.

Instead of clicking the LEFT mouse button, you can alternatively click the RIGHT mouse button to round the selected angle to steps of 5 deg. This feature is very useful for a quick selection of frequently used standard angles like "0.0 deg", "45.0 deg" etc. because with this option it is sufficient to position the mouse in a range of ±2.5 deg around the desired value, instead of trying to move it by fractions of a degree.

To end this sub-option and return to the cut menu, press the LEFT and RIGHT mouse buttons together at the same time until the menu appears. Now click on the DECterm window once again to redirect the keyboard input to that window.

b) Defining the angle using the keyboard:

You will be prompted for the cut angle.

Profile angle [deg]:

Enter one real or integer number between "0.0" and "359.9". To end this sub-option and return to the cut menu, simply press RETURN. The profile cut will be drawn exactly in the same way as described for using the mouse.

<u>Sub-option (9-3)</u>: `Cut|X-axis`

Enter "x" to format the horizontal "X"-axis of the plotted profile cut displaying the scattering vector Q. The current settings of the "X"-axis will be written to the screen. The default settings after the start of the program are "Logarithmic" and "Automatic scaling".

`Axis type:`

Choose an axis type from the menu list and enter the appropriate number. If you do not wish to change the current axis type, simply press RETURN.

`Axis range <Minimum> <Maximum> or Auto:`

Enter two real or integer numbers, separated by a space. Or enter "a" to set the axis range automatically according to the Q-range of the individual profile cut. If you do not wish to change the current range settings, simply press RETURN.

If any of the settings for axis type or axis range have been changed, and a profile cut is currently displayed in the profile cut window, it will be redrawn with these new settings. The number of data points actually visible in the profile cut window will be written to the screen. If the axis has been defined in a way that some data points cannot be displayed because they are outside the axis limits or invalid for the current axis type (e.g. a negative value on a logarithmic axis), the numbers of these additional data points will be written to the screen, too. If no data points fit to the current axis settings, the profile cut window will be erased and remains blank.

If the axis range is invalid for the current axis type (e.g. a negative minimum on a logarithmic axis), a message will be written to the screen, and you will be prompted for new axis settings. Please note that this error message may also appear when you only selected a new axis type, but did not enter a new axis range. In this case, a range setting from the last application of this sub-option incompatible with the current axis type may still be in effect.

The new settings will be used to display all following profile cuts until they are modified again.

<u>Sub-option (9-4)</u>: `Cut|Y-axis`

Enter "y" to format the vertical "Y"-axis of the plotted profile cut displaying the intensity I. The default settings after the start of the program are "Logarithmic" and "Automatic scaling". The terminal dialogue will be performed exactly in the same way as described for sub-option (9-3) "Cut | X-axis".

<u>Sub-option (9-5)</u>: `Cut|Table`

Enter "t" for "Table" to display a sub-area of the data file as a table. This is exactly the same as main menu option (3) "Table" described above. It only re-appears in this sub-menu to enable the display of a table while working with cuts.

<u>Sub-option (9-6)</u>: `Cut|Write`

Enter "w" to write the current profile cut to an isotropic data file. This sub-option is only available when a profile cut is displayed in the profile cut window.

`Minimum output extension:`

Enter the minimum extension number for the output data file. The isotropic output data file will have the same run number as the anisotropic input data file used. To determine the actual extension number for the output data file, the program will initially set the extension number to the minimum value entered here. If a data file with this new extension number already exists the program will continue incrementing the extension number until there is no interference with existing files. In this case, a warning will be displayed on the screen. To use the input extension plus 1 as minimum output extension, simply press RETURN.

Most item values that describe the sample and the experimental set-up are copied from the input file to the output file directly while some other item values are taken from the program. For details, please refer to the description of the "SANSDIso" file format.

Sub-option (9-7): **Cut│Print**

Enter "p" to print the current profile cut together with a thumbnail picture of the contour plot (see Fig.3). This sub-option is only available when a profile cut is displayed in the profile cut window.

A menu appears which lists all available printers and their locations.

Printer number:

Enter the number of the printer to be used. To select the printer marked as "default", simply press RETURN. A printed output similar to the pictures currently shown in the profile cut window and in the contour plot window will be created. Depending on the load of the computer and the network and on the complexity of the picture, the printing may require up to a few minutes.

The printed page contains some additional information on the sample, the experimental set-up and the processing done with the data file so far, read from the data file. If the data file contains a comment, the number of comment lines printed depends on the space available at the bottom of the page.

If "explicit masking" using a mask file was enabled, the output block "Processing information" contains the name of this mask file. If "implicit masking" was enabled, this block contains the name of the last mask file that has been used in the past to add an implicit mask to the data file. If the presence of implicitly masked cells has been detected but no corresponding mask file name has been found in the data file, the implicit mask file name is set to "UNKNOWN".

Fig.3: Printer output page.

Sub-option (9-8): **Cut│Save**

Enter "s" to save the current profile cut and/or the contour plot with the profile line as an "Encapsulated PostScript" graph file, ready for import into common text or graphics programs which support this file format, e.g. "Microsoft Word" or "CorelDraw!" (see Fig.4). This sub-option is only available when a profile cut is displayed in the profile cut window.

Output file name (no extension):

Enter the name of the output file but do not type an extension. The standard extension "*.EPS" will be appended by the program. If you do not wish to save a graph file, simply press RETURN.

There is no check whether a graph file of the same name already exists in the current directory. If a file exists it will be overwritten without a warning.

Graphics layout type? (1)/2/3:

Enter "1" (or simply press RETURN) to create a graph file containing the profile cut with a labelled curve together with a thumbnail picture of the contour plot showing the profile line. A file similar to the pictures currently shown in the profile cut window and in the contour plot window will be created.

Enter "2" to create a graph file containing only the contour plot showing the profile line. A file similar to the picture currently shown in the contour plot window will be created.

To create graph files containing only the curve from the profile cut, write the curve to an isotropic data file with sub-option (9-6) "Cut | Write", and load that file into program "SANSIsoPlot" which offers different graphics layout types for isotropic data files.
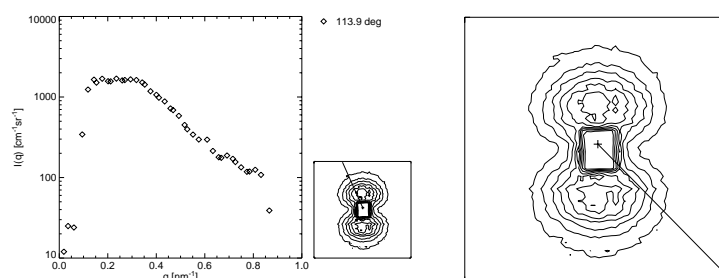

Fig.4: Graph files created using graphics layout types "1" to "2" (left to right).

Sub-option (9-9): **Cut|End**

Enter "e" to end option "Cut", close the profile cut window, and return to the main menu.

On some computers, after closing the profile cut window the contour plot window may change to "strange" colors. If this happens just click on the contour plot window once with the mouse, and the original colors will be restored.

Option (10): **mOde**

Enter "o" for "mOde" to toggle the input mode for options (3) "Table" and (9) "Cut" between mouse input and keyboard input. The default setting after the start of the program is "mouse". Choosing option "keyboard" instead of "mouse" is recommended especially for morning work after heavy consumption of German beer.

Option (11): **Vms**

Enter "v" for "VMS" to obtain a temporary command prompt of the VMS operating system. From this prompt, any DCL command can be executed while the program "SANSAniPlot" is still present in the background. To return to "SANSAniPlot", type "logout". You will find the program exactly as you left it.

All commands will be executed in a spawned child process with it's own process environment. As a result of this, your actions will not affect the proper work of "SANSAniPlot" as long as you do not delete or rename any files used by the program. Please note that due to this separate process environment, the DCL commands "SET DEFAULT" and "CD" cannot be used to change the default directory the program works in, since the result of this action is lost as soon as you leave the child process with "logout" and return to "SANSAniPlot".

Option (12): **Quit**

Enter "q" for "Quit" to terminate the program.

Input requirements

If you intend to use an existing mask file "*.MSK" to mask the data for the graphics output, the file name of that mask file must be known.

NOTE

If you want to run this program from a PC with "eXcursion" software or from a X Windows terminal for the first time, you may have to redirect the graphics output using command file "SANSDisplay" first before starting this program. If still a message "Unable to open X Windows display." appears please consult the device responsible. If you run this program on a workstation with directly connected screen, execution of command file "SANSDisplay" is not necessary.

When a part of a graphics window that was previously hidden by another window is exposed, the damaged part will usually be restored by the window manager system automatically. Since this transfer of graphical bitmap data is a time-consuming process it may require up to a few seconds, depending on the load of the computer and the network. If this restoration fails or produces unusual colors, type "new" on the main menu prompt to redraw the graphics window from the program.

If a message "Internal error." appears please consult the device responsible.

SANSArea

Description

This program calculates the number of counts and the center of gravity for sub-areas of anisotropic data files "Dnnnnnnn.nnn" of "SANSDRaw" and "SANSDAni" types from the current directory and writes the results to the screen and optionally into an ASCII file. The output is formatted as a table of right-justified fields separated by spaces.

"help" can be entered at any prompt to get on-line assistance if required.

Terminal dialogue

Type the command line

SANSArea <FirstRun> <LastRun> [<Extension>]

Parameters are the first run number, the last run number, and the extension number of the data file range to be processed, all separated by spaces. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". <LastRun> must be greater or equal <FirstRun>. If <Extension> is missing the default value "1" is assumed. All data files must have the same extension number. Only a proper command line is accepted.

Apply "Search" option to the data file range? Y/(N):

To select the input mode of data files to be processed, enter one of the following options (1) or (2):

Option (1): **No**

Enter "n" for "No" (or simply press RETURN) if you want to use the complete run number range you entered in the command line. Within this range, all files will be selected that pass the test for a valid data file. This option often provides a faster operation than "Yes", and it requires less input typing.

From this point, the terminal dialogue will be the same as for option (2) "Yes", starting from the ' Enter <X-Min> <X-Max> <Y-Min> <Y-Max> or Mask: ' prompt.

Option (2): **Yes**

Enter "y" for "Yes" if you only want to use individual files from the run number range you entered in the command line. With this option, you can select the files to be listed by scanning this run number range for certain item values. Only those files within the range are selected that match all conditions. This option provides a slower operation than "No" if the run number range to be scanned is large, and it requires more input typing.

A menu appears which lists all items that may be present in a data file. For a detailed description of this menu, please refer to "File Item Search Menu" in chapter "Standard Menus".

From this point, the terminal dialogue is the same both for option (1) "No" and for option (2) "Yes".

Enter <X-Min> <X-Max> <Y-Min> <Y-Max> or Mask:

or

Enter <X-Min> <X-Max> <Y-Min> <Y-Max> or Mask or RETURN for Preset:

To proceed the calculations for a plain rectangular area, enter the co-ordinates of the rectangle corners. Enter four integer numbers between "0" and "<DetectorSize>-1", all separated by spaces. <X-Max> must be greater or equal <X-Min>, and <Y-Max> must be greater or equal <Y-Min>.

Instead of this rectangular area, you can also use a mask file created with program "SANSMask". In this case, all cells within the detector area that are not masked will be used for the calculation, while masked cells are considered as "zero intensity". There are no limitations for the arrangement of masked and unmasked cells in the mask file. To choose this option, enter "m" instead of the four numbers. You will be prompted for the name of the mask file.

`Mask file name (no extension):`

Enter the name of the mask file to be used but do not type an extension. The standard extension "*.MSK" will be appended by the program. If you do not wish to use a mask file, simply press RETURN. If the input file does not exist or is not a valid mask file you will be prompted for a new input.

`Accept this mask file? (Y)/N:`

If you entered the name of a valid mask file information on this file is written to the screen. If you agree that this is the file you intended to use, enter "y" (or simply press RETURN) to confirm. If you don't want to use this mask file, enter "n" to choose a new one.

To terminate the input sequence on the ' Enter <X-Min> <X-Max> <Y-Min> <Y-Max> or Mask: ' prompt, simply press RETURN. You must enter at least one area or file name. The maximum number of areas is limited to 5 which gives a full output printer page in 132-column mode. If you are more interested in a well-readable screen output you should not enter more than 3 areas.

If this program has been executed in the same directory before, the complete input sequence typed for this particular menu during the last run of the program has been stored as a preset and can be recalled by simply pressing RETURN instead of entering co-ordinates or a mask file name for area number 1.

`Output file name:`

Enter the name of the output file where the results found by the program will be written to. Choose any name and extension that are suitable for your own purposes. If you want to copy the file to a DOS or Windows 3.x PC later use a name not longer than 8 characters and an extension not longer than 3 characters. If you do not wish to use an output file, simply press RETURN. The output to the screen will work in both cases.

Files will now be scanned. If an input file does not exist or is not a valid data file the run number is skipped. The numbers of files expected in the entered range and of files actually found are compared.

If the number of counts in a sub-area is zero, no calculation of the center of gravity can be performed. In this case, the center co-ordinates (Mid-X,Mid-Y) are displayed as "*****".

Input requirements

Run numbers of the data files to be processed must be known, or the item values in the data files must be set in a way that the files can be identified by a unique combination of these item values.

If you intend to use a mask file "*.MSK" this file must be created first using the program "SANSMask", or an appropriate pre-defined mask file must be chosen.

N<small>OTE</small>

If a message "Can't create preset file ..." appears please consult the device responsible.

SANSDataArchive

Description

This command file initializes an empty TK50 tape and copies as many temporarily archived raw data files "*.BCK" to the tape for final archiving as the tape storage capacity allows. Normally it will be used by the device responsible only.

Terminal dialogue

The command file copies all backup files "*.BCK" from the directory "SANS$PACKEDDATA" to the tape drive. A tape has a maximum storage capacity of 180000 blocks (90 MB). Before using the command file apply the VMS command **dir SANS$PACKEDDATA:*.bck/size** to make sure that the source directory contains the required amount of backup files to fill a complete tape. The total size of the backup files displayed should be as close as possible to a value of 175000 blocks. If the total size is considerably smaller do not proceed the archiving until more raw data have been measured. If the total size exceeds a value of 177000 blocks exclude redundant backup files from processing by temporarily renaming their extensions.

Insert an EMPTY tape in the tape drive and type the command line

SANSDataArchive <VolumeLabel>

Parameter is the label of the tape volume used. <VolumeLabel> is a VMS compatible string of exactly 6 characters. Choose a name which consists of the characters "BCK" followed by a 3-digit number denoting the current tape. Invalid command line parameters may cause unexpected results.

The command file first initializes the tape by re-writing the tape header. After this action, any content of the tape will be lost. Then the backup files are copied to the tape and read back to give a screen listing of the tape content. Processing a tape requires approximately 1 hour.

This command file is only available on the host node of the "BerSANS" program package.

Input requirements

The source directory "SANS$PACKEDDATA" must be prepared according to the description.

SANSDataDelete

Description

This command file deletes data files "Dnnnnnnn.nnn" from the current directory.

Terminal dialogue

Type the command line

SANSDataDelete <FirstRun> <LastRun> [<FirstExtension> [<LastExtension>]]

Parameters are the first run number, the last run number, the first extension number and the last extension number of the data file range to be deleted, all separated by spaces. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <FirstExtension> and <LastExtension> are two positive integer numbers between "1" and "999". <LastRun> must be greater or equal <FirstRun>, and <LastExtension> must be greater or equal <FirstExtension>. If <LastExtension> is missing it will be set to <FirstExtension>. If both <FirstExtension> and <LastExtension> are missing the default values "1" are assumed. Invalid command line parameters may cause unexpected results.

Execute this operation? Y/(N):

The run number and extension number ranges entered in the command line are repeated once again. If you are *REALLY* sure that these are the data files you intended to delete, enter "y" to confirm. If you don't want to delete these data files, enter "n" (or simply press RETURN) to cancel this operation.

Remember that data files that once have been deleted can *NEVER* be restored again. There is no "Undelete" utility available on the multi-user system.

Input requirements

First and last run number and first and last extension number of the file range to be deleted must be known.

SANSDataExport

Description

This program converts "BerSANS" data files "Dnnnnnnn.nnn" from the current directory to data files of external formats.

"help" can be entered at any prompt to get on-line assistance if required.

Terminal dialogue

Type the command line

SANSDataExport <FirstRun> <LastRun> [<Extension>]

Parameters are the first run number, the last run number, and the extension number of the data file range to be converted, all separated by spaces. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". <LastRun> must be greater or equal <FirstRun>. If <Extension> is missing the default value "1" is assumed. All data files must have the same extension number. Only a proper command line is accepted.

Apply "Search" option to the data file range? Y/(N):

To select the input mode of data files to be converted, enter one of the following options (1) or (2):

Option (1): **No**

Enter "n" for "No" (or simply press RETURN) if you want to use the complete run number range you entered in the command line. Within this range, all files will be selected that pass the test for a valid data file. This option often provides a faster operation than "Yes", and it requires less input typing.

From this point, the terminal dialogue will be the same as for option (2) "Yes", starting from the ' Conversion option: ' prompt.

Option (2): **Yes**

Enter "y" for "Yes" if you only want to use individual files from the run number range you entered in the command line. With this option, you can select the files to be converted by scanning this run number range for certain item values. Only those files within the range are selected that match all conditions. This option provides a slower operation than "No" if the run number range to be scanned is large, and it requires more input typing.

A menu appears which lists all items that may be present in a data file. For a detailed description of this menu, please refer to "File Item Search Menu" in chapter "Standard Menus".

From this point, the terminal dialogue is the same both for option (1) "No" and for option (2) "Yes".

A menu appears which lists all conversion options available.

Conversion option:

or

Conversion option or RETURN for Preset:

Choose a conversion option from the menu list and enter the appropriate number. You must enter an option.

If this program has been executed in the same directory before, the complete input sequence typed for this particular menu during the last run of the program has been stored as a preset and can be recalled by simply pressing RETURN instead of entering an option number.

Files will now be converted. If an input file does not exist or is not a valid "BerSANS" data file of the required type, the run number is skipped. The numbers of files expected in the entered range and of files actually found are compared.

The following options (1) to (4) are available:

Option (1): `Anisotropic data: "D00nnnnn.0ee" => "Znnnnn.Zee"`

This option converts anisotropic "BerSANS" data files of "SANSDRaw" and "SANSDAni" types to "Z-file" format used by the ILL Ghosh software.

Since the "Z-file" format only supports 5-digit run numbers and 2-digit extension numbers, the first two digits of the "BerSANS" run number and the first one digit of the "BerSANS" extension number must be omitted by the program. Example: "BerSANS" data files "D1234567.890" and "D0034567.090" will both be converted to "Z34567.90".

Item values and counts are copied as character strings. There is no check if they are actually numbers. Errors (if present) will be transferred to the Z-file with their absolute value only, i.e. an implicit mask contained in the "BerSANS" data file (by adding a negative sign to the error value) will be removed. If a format error occurs in the errors, a message will be displayed, and the run number is skipped.

The standard structure of the Z-file can only carry limited additional information on the measurement in a coded form. Therefore, all other relevant items contained in the "BerSANS" data file will be lost.

Option (2): `Isotropic data: "D00nnnnn.0ee" => "nnnnnXee.PDH"`

This option converts isotropic "BerSANS" data files of "SANSDIso" type to "PDH-file" format used by the Glatter software.

Since the "PDH-file" format only supports file names of 8 characters, the first two digits of the "BerSANS" run number and the first one digit of the "BerSANS" extension number must be omitted by the program. Example: "BerSANS" data files "D1234567.890" and "D0034567.090" will both be converted to "34567X90.PDH". For the symbolic character "X", see general description below.

Data points that have been masked in the "BerSANS" data file (by adding a negative sign to the error value) will not be transferred to the PDH-file. If a format error occurs in the data points themselves or in an item essential for the standard structure of the PDH-file, a message will be displayed, and the run number is skipped.

The standard structure of the PDH-file can only carry limited additional information on the measurement in a coded form. Therefore, all relevant items contained in the "BerSANS" data file will added as a comment at the end of the PDH-file. These item values are copied as character strings. There is no check if they are actually numbers.

Option (3): `Isotropic data: "D00nnnnn.0ee" => "nnnnnXee.EPW"`

This option converts isotropic "BerSANS" data files of "SANSDIso" type to "EPW-file" format used by the PC program "EasyPlot".

Since the "EPW-file" format only supports file names of 8 characters, the first two digits of the "BerSANS" run number and the first one digit of the "BerSANS" extension number must be omitted by the program. Example: "BerSANS" data files "D1234567.890" and "D0034567.090" will both be converted to "34567X90.EPW". For the symbolic character "X", see general description below.

Data points that have been masked in the "BerSANS" data file (by adding a negative sign to the error value) will not be transferred to the EPW-file. If a format error occurs in the data points, a message will be displayed, and the run number is skipped.

The standard structure of the EPW-file cannot carry any additional information on the measurement. Therefore, all relevant items contained in the "BerSANS" data file will added as comment at the beginning of the EPW-file. These item values are copied as character strings. There is no check if they are actually numbers.

Option (4): **Isotropic data: "D00nnnnn.0ee" => "nnnnnXee.PRN"**

This option converts isotropic "BerSANS" data files of "SANSDIso" type to "PRN-file" format used by the PC program "PeakFit".

Since the "PRN-file" format only supports file names of 8 characters, the first two digits of the "BerSANS" run number and the first one digit of the "BerSANS" extension number must be omitted by the program. Example: "BerSANS" data files "D1234567.890" and "D0034567.090" will both be converted to "34567X90.PRN". For the symbolic character "X", see general description below.

Data points that have been masked in the "BerSANS" data file (by adding a negative sign to the error value) will not be transferred to the PRN-file. If a format error occurs in the data points, a message will be displayed, and the run number is skipped.

The standard structure of the PRN-file cannot carry data errors or any additional information on the measurement. Therefore, the errors and all items contained in the "BerSANS" data file will be lost.

Option (5): **Isotropic data: "D00nnnnn.0ee" => "nnnnnXee.DAT"**

This option converts isotropic "BerSANS" data files of "SANSDIso" type to a general "DAT-file" format usable for all PC programs supporting a simple three-column data file structure but no comment lines, e.g. "PlotIt".

Since the "DAT-file" format only supports file names of 8 characters, the first two digits of the "BerSANS" run number and the first one digit of the "BerSANS" extension number must be omitted by the program. Example: "BerSANS" data files "D1234567.890" and "D0034567.090" will both be converted to "34567X90.DAT". For the symbolic character "X", see general description below.

Data points that have been masked in the "BerSANS" data file (by adding a negative sign to the error value) will not be transferred to the DAT-file. If a format error occurs in the data points, a message will be displayed, and the run number is skipped.

For the symbolic character "X" separating the run number from the extension number in the file names of isotropic output data files, either a letter "C", "S", "F", "N", "M", "A", or "U" will appear. This letter indicates whether the isotropic data file has been created from an anisotropic data file in the past as a "C"ut with program "SANSAniPlot", by radial averaging over a limited "S"ector or by "F"ull radial averaging with program "SANSIsoDo", or as the "N"uclear, "M"agnetic or "A"dded nuclear + magnetic scattering component of a $\sin^2(\psi)$-fit with program "SANSIsoDo". This information is taken from item "ContentY" in the data file as described in chapter "File Formats - SANSDIso". If no value for this item is available in the data file, the creation method is "U"nknown. The variable separation letter only serves for easy recognition of the origin of the file, but does not affect the content of the file itself.

Input requirements

Run numbers of the data files to be converted must be known, or the item values in the data files must be set in a way that the files can be identified by a unique combination of these item values.

NOTE

If a message "Can't create preset file ..." appears please consult the device responsible.

If a message "Can't create output file name for run ... / extension ..." appears, the last 5 digits of the run number and/or the last 2 digits of the extension number may be zero, e.g. "D1200000.001" or "D1234567.100". For the external data file name using only this part of the original run number and extension number, this would yield a run number of "0" and/or a extension number of "0" which is not permitted.

SANSDataImport

Description

This program converts data files of external formats from the current directory to "BerSANS" data files "Dnnnnnn.nnn".

"help" can be entered at any prompt to get on-line assistance if required.

Terminal dialogue

Type the command line

SANSDataImport <FirstRun> <LastRun> [<Extension>]

Parameters are the first run number, the last run number, and the extension number of the data file range to be converted, all separated by spaces. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". <LastRun> must be greater or equal <FirstRun>. If <Extension> is missing the default value "1" is assumed. All data files must have the same extension number. Only a proper command line is accepted.

A menu appears which lists all conversion options available.

Conversion option:

or

Conversion option or RETURN for Preset:

Choose a conversion option from the menu list and enter the appropriate number. You must enter an option.

If this program has been executed in the same directory before, the complete input sequence typed for this particular menu during the last run of the program has been stored as a preset and can be recalled by simply pressing RETURN instead of entering an option number.

Some external file formats only support a smaller number of digits for the run number and the extension number than the "BerSANS" program package. If the run number range entered in the command line is not suitable for the particular input data type selected the program aborts.

Files will now be converted. If an input file does not exist, the run number is skipped. The numbers of files expected in the entered range and of files actually found are compared.

The following options (1) to (2) are available:

Option (1): **Raw data: "Znnnnn.Z01"+"Hnnnnn.Z01" => "D00nnnnn.001"**

This option converts raw data files of "Z-file" format used by the ILL Ghosh software plus header files to "BerSANS" raw data files of "SANSDRaw" type. This combination has been used to record measured raw data at the HMI until spring 1996.

All item values for the output file are taken from the header file, except "Sum" which is taken from the Z-file, and "Sum/Time", "Sum/Moni1", "Sum/Moni2" and "Sum/Moni3" which are re-calculated using the new "Sum" value. Besides "Sum", from the Z-file only the counts are used. Item values and counts are copied as character strings. There is no check if they are actually numbers, and there is no check if they are the same in the header file and in the Z-file.

The errors of a raw data file are expected to be the square root of the counts. Additional errors that may be included in the Z-file are omitted.

To convert a run successfully, both the Z-file and the header file must be present and are expected to have a correct structure. There is only a rough check for severe errors. If such an error has been

detected or one of the two files is missing, a message will be displayed, and the run number is skipped.

Option (2): **Anisotropic data: "Znnnnn.Zee" => "D00nnnnn.0ee"**

This option converts anisotropic data files of "Z-file" format used by the ILL Ghosh software to "BerSANS" data files. If the Z-file has the extension "*.Z01" it is expected to contain raw data, and the result will be of "SANSDRaw" type. In all other cases, the result will be of "SANSDAni" type.

Item values, counts and errors (if present) are copied as character strings. There is no check if they are actually numbers. Since the Z-files only contain little additional information on the measurement, the "BerSANS" data files created will only contain a limited number of item values. If this should cause any problems during further processing of these files with the "BerSANS" program package, more item values can be written into the converted data files using program "SANSDataModify" if known from other sources.

If the Z-file is of raw data type "*.Z01", the errors are expected to be the square root of the counts, and additional errors that may be included in the Z-file are omitted. If the Z-file is of anisotropic data type "*.Zee", it may or may not contain calculated errors, depending on the source of the file. If calculated errors are present they are copied to the "BerSANS" data file created. If no errors are present, due to compatibility requirements of the "BerSANS" program package, a constant dummy error value is assigned to all cells in the "BerSANS" data file created.

Input data files are expected to have a correct structure. There is only a rough check for severe errors. If such an error has been detected, a message will be displayed, and the run number is skipped.

Input requirements

Run numbers of the data files to be converted must be known.

N<small>OTE</small>

If a message "Can't create preset file ..." appears please consult the device responsible.

SANSDataList

Description

This program scans data files "Dnnnnnnn.nnn" from the current directory for selected items and writes the item values found to the screen and optionally into an ASCII file. The output is formatted as a table of right-justified fields separated by commas.

"help" can be entered at any prompt to get on-line assistance if required.

Terminal dialogue

Type the command line

SANSDataList <FirstRun> <LastRun> [<Extension>]

Parameters are the first run number, the last run number, and the extension number of the data file range to be listed, all separated by spaces. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". <LastRun> must be greater or equal <FirstRun>. If <Extension> is missing the default value "1" is assumed. All data files must have the same extension number. Only a proper command line is accepted.

Apply "Search" option to the data file range? Y/(N):

To select the input mode of data files to be listed, enter one of the following options (1) or (2):

Option (1): **No**

Enter "n" for "No" (or simply press RETURN) if you want to use the complete run number range you entered in the command line. Within this range, all files will be selected that pass the test for a valid data file. This option often provides a faster operation than "Yes", and it requires less input typing.

From this point, the terminal dialogue will be the same as for option (2) "Yes", starting from the ' List item No. n: ' prompt.

Option (2): **Yes**

Enter "y" for "Yes" if you only want to use individual files from the run number range you entered in the command line. With this option, you can select the files to be listed by scanning this run number range for certain item values. Only those files within the range are selected that match all conditions. This option provides a slower operation than "No" if the run number range to be scanned is large, and it requires more input typing.

A menu appears which lists all items that may be present in a data file. For a detailed description of this menu, please refer to "File Item Search Menu" in chapter "Standard Menus".

From this point, the terminal dialogue is the same both for option (1) "No" and for option (2) "Yes".

A menu appears which lists all items that may be present in a data file.

List item No. n:

or

List item No. 1 or RETURN for Preset:

Choose the items you want to see in the data files from the menu list and enter the appropriate item numbers, one on each prompt. To terminate the input sequence, simply press RETURN. You must enter at least one item number. The maximum number of list items is limited to 8 which gives a full

output printer page in 132-column mode. If you are more interested in a well-readable screen output you should not enter more than 5 items.

If this program has been executed in the same directory before, the complete input sequence typed for this particular menu during the last run of the program has been stored as a preset and can be recalled by simply pressing RETURN instead of entering an item number for list item number 1.

For a detailed description of the items, please refer to chapter "File Formats".

`Output file name:`

Enter the name of the output file where the item values found by the program will be written to. Choose any name and extension that are suitable for your own purposes. If you want to copy the file to a DOS or Windows 3.x PC later use a name not longer than 8 characters and an extension not longer than 3 characters. If you do not wish to use an output file, simply press RETURN. The output to the screen will work in both cases.

Files will now be scanned. If an input file does not exist or is not a valid data file the run number is skipped. The numbers of files expected in the entered range and of files actually found are compared.

In most cases, a data file does not include all possible items. If you choose an item that is not present in a particular file the output field will be blank.

Input requirements

Run numbers of the data files to be listed must be known, or the item values in the data files must be set in a way that the files can be identified by a unique combination of these item values.

NOTE

If a message "Can't create preset file ..." appears please consult the device responsible.

SANSDataModify

Description

This program modifies item values in data files "Dnnnnnnn.nnn" from the current directory, adds new items to the files or deletes existing items.

"help" can be entered at any prompt to get on-line assistance if required.

Terminal dialogue

Type the command line

SANSDataModify <FirstRun> <LastRun> [<Extension>]

Parameters are the first run number, the last run number, and the extension number of the data file range to be listed, all separated by spaces. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". <LastRun> must be greater or equal <FirstRun>. If <Extension> is missing the default value "1" is assumed. All data files must have the same extension number. Only a proper command line is accepted.

Apply "Search" option to the data file range? Y/(N):

To select the input mode of data files to be modified, enter one of the following options (1) or (2):

Option (1): **No**

Enter "n" for "No" (or simply press RETURN) if you want to use the complete run number range you entered in the command line. Within this range, all files will be selected that pass the test for a valid data file. This option often provides a faster operation than "Yes", and it requires less input typing.

Files will now be scanned. For each individual data file, the file name is listed together with the sample name. If an input file does not exist or is not a valid data file the run number is skipped. The numbers of files expected in the entered range and of files actually found are compared.

Accept this selection? (Y)/N:

If you agree that these are the files you intended to modify, enter "y" (or simply press RETURN) to confirm. If you don't want to modify these data files, enter "n" to abort the program.

The number of files found will usually be equal to the number of files expected. If it is smaller then some data files have not been found or have not passed the test for a valid file type.

From this point, the terminal dialogue will be the same as for option (2) "Yes", starting from the ' Modify item No. n: ' prompt.

Option (2): **Yes**

Enter "y" for "Yes" if you only want to use individual files from the run number range you entered in the command line. With this option, you can select the files to be listed by scanning this run number range for certain item values. Only those files within the range are selected that match all conditions. This option provides a slower operation than "No" if the run number range to be scanned is large, and it requires more input typing.

A menu appears which lists all items that may be present in a data file. For a detailed description of this menu, please refer to "File Item Search Menu" in chapter "Standard Menus".

Files will now be scanned. For each individual data file that matches all conditions, the file name is listed together with the sample name. If an input file does not exist or is not a valid data file the run number is skipped. If you choose an item that is not present in a particular data file it will be treated as

"no matching". The numbers of files expected in the entered range and of files actually found are compared.

Accept this selection? (Y)/N:

If you agree that these are the files you intended to modify, enter "y" (or simply press RETURN) to confirm. If you don't want to modify these data files, enter "n" to abort the program.

The number of files found and the number of files expected may differ considerably, depending on the size of the scan range entered.

From this point, the terminal dialogue is the same both for option (1) "No" and for option (2) "Yes".

A menu appears which lists all items that may be modified, inserted or deleted in a data file.

Modify item No. n:

or

Modify item No. 1 or RETURN for Preset:

Choose the items you want to modify in the data files from the menu list and enter the appropriate item numbers, one on each prompt. To terminate the input sequence, simply press RETURN. You must enter at least one item number. The maximum number of modify items is limited to 8.

If this program has been executed in the same directory before, the complete input sequence typed for this particular menu during the last run of the program has been stored as a preset and can be recalled by simply pressing RETURN instead of entering an item number for modify item number 1.

Depending on the type of the particular item (string or number), you will be prompted for either a string value or for a numeric value. For a detailed description of the items and item types, please refer to chapter "File Formats".

New string:

Enter the string you want to define as the new value for the specified item.

For item type "word", no spaces are allowed within the string. Input characters beyond the first space will be formally accepted but removed by the program. Upper and lower case remain significant. To delete the entire item, simply press RETURN.

For item type "text", the string may include spaces. Upper and lower case remain significant. To delete the entire item, simply press RETURN.

For item type "comment", the string may include spaces. Upper and lower case remain significant. This is the only item type where the new string does not replace the existing item value but will be appended to the block "%Comment" as a new line. You can add more than one comment line to the data files by choosing this item repeatedly. You cannot use this program to remove comment lines from data files, pressing RETURN will take no effect.

For item type "date/time", the string must be in the date/time format of the operating system. No spaces are allowed within the string. Input characters beyond the first space will be formally accepted but removed by the program. The string will be converted to upper case. To delete the entire item, simply press RETURN.

New number:

Enter the number you want to define as the new value for the specified item. The input will be written to the files exactly the way you type it, including decimal places and exponents. A check for a valid number will be proceeded. Since no spaces are allowed within a number, input characters beyond the first space will be formally accepted but removed by the program. To delete the entire item, simply press RETURN.

For all item types, leading spaces are removed from the input.

Files will now be modified. The numbers of files expected in the entered range and of files actually modified are compared.

All lines within the input data files that are not subject to modifications are copied to the output data files without any changes. Consequently, all user-specific blocks, items and comment lines are preserved. The program only deletes completely blank lines from the files.

Each output file has the same run number and extension number as the related input file. On a VMS operating system, the original input file will be retained with its VMS version number ";n", and the output file will automatically obtain an incremented VMS version number ";n+1". On a UNIX operating system, the output file replaces the original input file, and the original input file will be lost.

Input requirements

Run numbers of the data files to be modified must be known, or the item values in the data files must be set in a way that the files can be identified by a unique combination of these item values.

NOTE

If a message "This program can only handle up to ... data files.", "Block ... is too long." or "Can't create preset file ..." appears please consult the device responsible.

SANSDataPack

Description

This command file compresses groups of anisotropic raw data files "Dnnnnnnn.001" from the current directory into a backup file "*.BCK" for temporary archiving. Normally it will be used by the device responsible only.

Terminal dialogue

Type the command line

SANSDataPack <FirstRun> <LastRun>

Parameters are the first run number and the last run number of the data file range to be packed, separated by a space. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <LastRun> must be greater or equal <FirstRun>. All data files must have extension number "1". Invalid command line parameters may cause unexpected results.

The command file first copies the selected raw data files from the current directory to a scratch area. If an input file does not exist the run number is skipped. Then the VMS "Backup" utility is applied to compress the files into a single backup file which is stored in the directory "SANS$PACKEDDATA". The file name for this backup file is generated automatically by joining <FirstRun> and <LastRun> with an underscore "_" and appending the standard extension "*.BCK".

Input requirements

First and last run number of the file range to be compressed must be known.

SANSDataPresent

Description

This command file lists data files "Dnnnnnnn.nnn" that are present and not present in the current directory.

Terminal dialogue

Type the command line

SANSDataPresent <FirstRun> <LastRun> [<FirstExtension> [<LastExtension>]]

Parameters are the first run number, the last run number, the first extension number and the last extension number of the data file range to be scanned, all separated by spaces. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <FirstExtension> and <LastExtension> are two positive integer numbers between "1" and "999". <LastRun> must be greater or equal <FirstRun>, and <LastExtension> must be greater or equal <FirstExtension>. If <LastExtension> is missing it will be set to <FirstExtension>. If both <FirstExtension> and <LastExtension> are missing the default values "1" are assumed. Invalid command line parameters may cause unexpected results.

Files will now be processed. If a data file has been found the name of this file is written to the left column on the screen, and if it has not been found it is written to the right column. The numbers of files found and of files not found are compared.

Input requirements

First and last run number and first and last extension number of the file range to be scanned must be known.

SANSDataUnarchive

Description

This command file decompresses finally archived groups of anisotropic raw data files "Dnnnnnnn.001" from a TK50 tape into the current directory. Normally it will be used by the device responsible only.

Terminal dialogue

Insert the data archive tape in the tape drive and type the command line

SANSDataUnarchive <VolumeLabel> <BackupFileName> <FirstRun> <LastRun>

or

SANSDataUnarchive <VolumeLabel> <BackupFileName> **all**

Parameters are the label of the tape volume used, the name of the backup file on the tape volume to be unarchived, and the first and last run number of the data file range to be unpacked, all separated by spaces. <VolumeLabel> is a VMS compatible string of exactly 6 characters written on the label sticker of the tape. <BackupFileName> is a VMS compatible string with the extension ".BCK" indicating the run number range contained in the file. It can be taken from the content listing of the tape. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <LastRun> must be greater or equal <FirstRun>. Invalid command line parameters may cause unexpected results.

Depending on the command line parameters used, the command file either extracts a certain run number range from the backup file, or unpacks all data files contained. It first copies the selected backup file from the tape to a scratch area. Then unpacking is proceeded using the VMS "Backup" utility. The unpacked raw data files will be written to the current directory. Processing a backup file may require up to 30 minutes, depending on the position of the file on the tape.

This command file is only available on the host node of the "BerSANS" program package.

Input requirements

The name of the backup file "*.BCK" and optionally the first and last run number of the file range to be decompressed must be known.

SANSDataUnpack

Description

This command file decompresses temporarily archived groups of anisotropic raw data files "Dnnnnnnn.001" from a backup file "*.BCK" into the current directory. Normally it will be used by the device responsible only.

Terminal dialogue

Type the command line

SANSDataUnpack <BackupFileName> <FirstRun> <LastRun>

or

SANSDataUnpack <BackupFileName> **all**

Parameters are the name of the backup file and the first and last run number of the data file range to be unpacked, all separated by spaces. <BackupFileName> is a VMS compatible string with the extension ".BCK" indicating the run number range contained in the file. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <LastRun> must be greater or equal <FirstRun>. Invalid command line parameters may cause unexpected results.

Depending on the command line parameters used, the command file either extracts a certain run number range from the backup file, or unpacks all data files contained. The backup file is expected to reside in the directory "SANS$PACKEDDATA" (where it is stored by the packing tool "SANSDataPack" automatically), and the unpacked raw data files will be written to the current directory. Unpacking is proceeded using the VMS "Backup" utility.

Input requirements

The name of the backup file "*.BCK" and optionally the first and last run number of the file range to be decompressed must be known.

SANSDisplay

Description

This command file defines the graphics output device for all PV-Wave programs of the "BerSANS" program package when used on a PC with "eXcursion" software or on a X Windows terminal. It has to be executed once for each DECterm window in which you want to run the programs "SANSAniPlot", "SANSIsoPlot" or "SANSMask". Executing the command file for the same DECterm window repeatedly will have no negative effects on the system. If you run the programs on a workstation with directly connected screen, execution of this command file is not necessary.

Terminal dialogue

Type the command line

SANSDisplay <NodeName>

Parameter is the node name of the PC or X Windows terminal you are currently working on. <NodeName> is a string written on a label sticker on the device, e.g. "NIALWI".

Input requirements

None.

SANSInfo

Description

This command file displays an overview of the "BerSANS" program package content and gives a short description of each program, including the command line parameters expected.

Terminal dialogue

Type the command line

SANSInfo [<ProgramName>]

<ProgramName> is the name of the particular program from the "BerSANS" program package. If <ProgramName> is missing or invalid a list of all program names available will appear.

If you don't know the exact name of a program, type **SANSInfo** first to find the proper name, and then type **SANSInfo** <ProgramName> again to obtain the requested information.

Input requirements

None.

SANSInit

Description

This command file defines the system environment for all parts of the "BerSANS" program package. It is executed automatically whenever you log in to the system. Normally there will be no need to run it again unless "strange things" happen which cause some definitions of logical names or symbols to be lost. Executing the command file repeatedly will have no negative effects on the system.

Terminal dialogue

Type the command line

SANSInit

No command line parameters are required.

Input requirements

None.

NOTE

If the symbol "SANSInit" is lost, try: **@DISK$SYSTEM:[BERSANS.COM]SANSInit**

SANSIso

Description

This program pre-processes anisotropic data files "Dnnnnnnn.nnn" of "SANSDRaw" and "SANSDAni" types from the current directory interactively and creates a command file "*.SCI" for radial averaging by the program "SANSIsoDo". As a special option, magnetic scattering patterns can be splitted into a nuclear and a magnetic scattering component. The created command file can be edited before execution and can also be printed to obtain a complete listing of data and parameters used in data reduction.

"help" can be entered at any prompt to get on-line assistance if required.

Terminal dialogue

Type the command line

SANSIso

No command line parameters are required.

Command file name (no extension):

Enter the name of the command file to be created. Choose any name that is suitable for your own purposes but do not type an extension. The standard extension "*.SCI" will be appended by the program. If you want to copy the file to a DOS or Windows 3.x PC later use a name not longer than 8 characters. You must enter a name.

A menu appears which lists the current default values of all items and settings that are required for radial averaging. If this program has been executed in the same directory before, the values entered during the last run of the program have been stored as a preset and are offered as the new default automatically. If no appropriate preset has been found, all items are set to standard values.

Item No. or "0" to redraw:

Choose the items you want to change from the menu list and enter the appropriate item numbers, one on each prompt. To terminate the input sequence, simply press RETURN. Enter "0" to redraw the list of current item values. You can change each item value as often as you want to.

Depending on the type of the particular item (string or number), you will be prompted either for a string value or for a numeric value. For a detailed description of the items and item types, please refer to chapter "File Formats".

Items: **Lambda, SD, BeamcenterX, BeamcenterY**

For these items, you will be prompted for a number:

New number:

Enter the number you want to define as the new value for the specified item. A check for a valid number will be proceeded, and the decimal places of the number will be rounded as shown in the menu.

Item: **UseDefault**

For this item, you will be prompted for a keyword:

Yes or No:

Enter "y" for "YES" or "n" for "NO".

The block "%Commands" of the command file created by this program will feature a list of the individual values for items "Lambda", "SD", "BeamcenterX" and "BeamcenterY" taken directly from the

input data files if present there. With the standard setting "UseDefault=NO", the values for these four items entered in this menu will only serve as a substitute for those data files which do not contain these individual values themselves. You can force the program "SANSIsoDo" to override all individual values existing for these four items with the defaults entered above by setting "UseDefault=YES". Please note that the program "SANSIsoDo" will also use the appropriate default value automatically if an individual value contained in the block "%Commands" of the command file is not a syntactically correct number, which may happen if you edit the command file carelessly.

Item: **`RadialSteps`**

For this items, you will be prompted for a number:

`New number:`

Enter the number you want to define as the new value for the item. A check for a valid number will be proceeded, and the decimal places of the number will be rounded as shown in the menu.

The item "RadialSteps" [cells] defines the interval of distances between the beam center and the co-ordinates of detector cell centers that will be reduced into a single point of the one-dimensional output file. If you choose a small value of "RadialSteps" you will obtain a larger number of output data points, but at the cost of an increased statistical error since each output data point will represent a smaller number of detector cells, and vice versa. The recommended standard value is "RadialSteps = 1 cell".

Items: **`Sectors, SectorStart, SectorInc, SectorWidth`**

For these items, you will be prompted for a number:

`New number:`

Enter the number you want to define as the new value for the specified item. A check for a valid number will be proceeded, and the decimal places of the number will be rounded as shown in the menu.

For an isotropically scattering sample, you will normally proceed the radial averaging using full circles on the detector. However, in case of an anisotropically scattering sample you may wish to limit the angular range of radial averaging to certain sectors along preferred directions from the beam center. This can be done via items "Sectors" defining the number of sectors to be processed, "SectorStart" [deg] defining the center angle of the first sector, "SectorInc" [deg] defining the increment steps for following sector centers relative to the preceding sector center, and "SectorWidth" [deg] defining the width of each sector. One of these "sectors" always covers two circular sectors of the full circle with an angular width of "SectorWidth" each, positioned symmetrically on opposite sides of the beam center. Gaps between the sectors and an overlap of sectors are allowed. For each sector, a separate isotropic output file will be created. Fig.1 gives an example of a set of these item settings and the results arising from it. You can add more limitations of the detector area used for radial averaging (e.g. to use only one of the two symmetrical circular sectors covered by one "sector") by creating an appropriate mask file.

Instead of this method of radial averaging over sectors, you can alternately use the program "SANSAniPlot" to create one-dimensional cuts through an anisotropic data file directly.

To proceed a full radial averaging for an isotropically scattering sample, use "Sectors=1", "SectorStart=0", "SectorInc=0" and "SectorWidth=180".
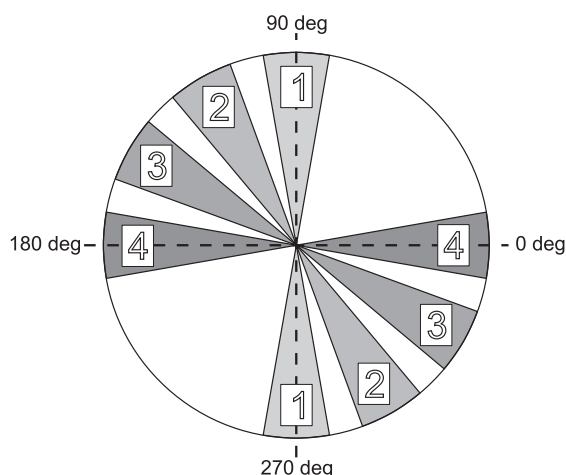
Fig.1: Example for a radial averaging procedure using item values "Sectors=4", "SectorStart=90", "SectorInc=30" and "SectorWidth=20". Four isotropic output files with the same run number as the anisotropic input file and with incrementing extension numbers will be created.

Item: **MaskFile**

For this item, you will be prompted for a file name:

Mask file name (no extension):

Enter the name of the mask file to be used to label individual detector cells for exclusion from radial averaging but do not type an extension. The standard extension "*.MSK" will be appended by the program. If you do not wish to use a mask file, simply press RETURN. If the input file does not exist or is not a valid mask file you will be prompted for a new input.

Accept this mask file? (Y)/N:

If you entered the name of a valid mask file information on this file is written to the screen. If you agree that this is the file you intended to use, enter "y" (or simply press RETURN) to confirm. If you don't want to use this mask file, enter "n" to choose a new one.

Item: **ImplicitMask**

For this item, you will be prompted for a keyword:

Yes or No:

Enter "y" for "YES" or "n" for "NO".

This item defines whether an implicit mask (coded as "Error < 0") that may be present in some of the anisotropic input data files of "SANSDAni" type should be used for radial averaging of these files. In contrast, invalid cells (coded as "Error = 0") are never used for radial averaging. If you choose "ImplicitMask=YES" and select an additional explicit mask file, both the implicit and the explicit masks will be combined by a logical "OR" operation: if a cell is masked in one or both of the two input masks it will be masked in the resulting mask, too. The setting of this item will have no effect on processing raw data files of "SANSDRaw" type since these files never contain an implicit mask.

If implicit masking of an anisotropic data file has been performed before with program "SANSAni", the name of the last mask file used for this operation may still be contained in that data file. This file name only serves as a reminder for the user. The programs "SANSIso" and "SANSIsoDo" will not require access to that explicit mask file again since the content of that mask file is already part of the data file.

Item: **CalcMode**

The item "CalcMode" defines the parameter, as a function of which the radially averaged intensity in the isotropic output data files will be calculated, see Fig.2.

A menu appears which lists all available calculation modes.

Calculation mode:

Enter "1" to calculate the intensity as a function of the scattering vector Q [nm^{-1}]. This is the standard setting.

Enter "2" to calculate the intensity as a function of the scattering angle 2θ [deg]. This option is only relevant for instrument maintenance and for the rare case of analyzing Bragg peaks. In this case, the value for "Lambda" in the listed menu will not be used.

Enter "3" to calculate the intensity as a function of the radial distance R [cells] from the beam center on the detector. This option is only relevant for instrument maintenance. In this case, the values for "Lambda" and "SD" in the listed menu will not be used.
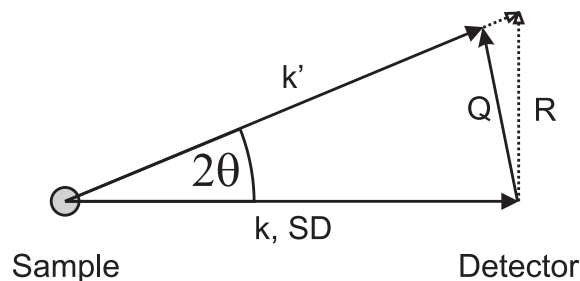
Scattering vector: Q = k' - k; |k'| = |k|

$$Q = \frac{4\pi}{\lambda} * \sin\theta \qquad 2\theta = \arctan\left(\frac{R}{SD}\right)$$

Fig.2: Scattering vector Q, scattering angle 2θ and radial distance R in the small angle scattering geometry. The vectors k, k' and Q are all in the same plane.

Item: **MagFit**

The item "MagFit" defines whether a splitting of the anisotropic input data I into a nuclear scattering component I_{Nuc} and a magnetic scattering component I_{Mag} according to the formula

$$I(x,\psi) = I_{Nuc}(x) + \sin^2(\psi) * I_{Mag}(x) \; ; \; x = Q \,|\, 2\theta \,|\, R \tag{1}$$

as shown in Fig.3 should be performed. This fit option is only useful if the anisotropic data files have been measured on magnetic samples and in a homogeneous magnetic field, so that the validity of a $\sin^2(\psi)$-fit can be assumed. Technically, the fitting procedure will also work with all other non-magnetic data without producing an error message, but the results for I_{Nuc} and I_{Mag} obtained from such fits will have no physical relevance.

A menu appears which lists all available fitting modes.

Fitting mode:

Enter "1" to perform no $\sin^2(\psi)$-fit. This is the standard setting.

Enter "2" to perform the $\sin^2(\psi)$-fit for data that have been measured in a sample environment equipped with a magnet which produces a horizontally orientated magnetic field.

Enter "3" to perform the $\sin^2(\psi)$-fit for data that have been measured in a sample environment equipped with a magnet which produces a vertically orientated magnetic field.

The numerical procedure is the same for both options "2" and "3". The only difference is the definition of the origin direction "0 deg" for the angle ψ relative to the detector area (see Fig.1). This direction "0 deg" will always be parallel to the magnetic field, and thus will be located on the right side of the detector for "MagFit=HORIZONTAL", and on the top side of the detector for "MagFit=VERTICAL". For information which option "2" or "3" should be used for your particular experimental set-up, ask the device responsible.

The output of the $\sin^2(\psi)$-fit will be the two components I_{Nuc} and I_{Mag} as a function of the scattering vector Q, the scattering angle 2θ, or the radial distance R from the beam center on the detector, respectively, as defined by item "CalcMode".
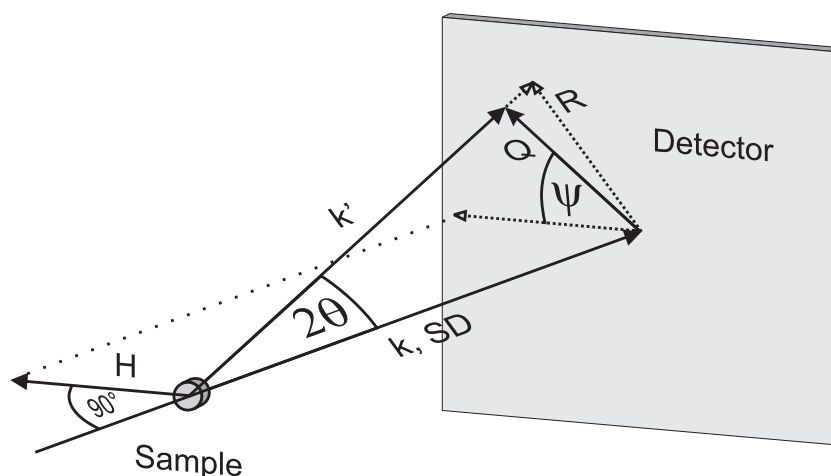

Fig.3: Scattering geometry for magnetic measurements compatible with a $\sin^2(\psi)$-fit. Due to the condition of elastic scattering (i.e. |k'| = |k|), the angle ψ between the scattering vector Q and the field direction H is in a plane which is not parallel to the detector plane. The definition of scattering vector Q, scattering angle 2θ and radial distance R from the beam center remains the same as in Fig.2.

From this point, the terminal dialogue continues after the final pressing of "RETURN" to accept all item values.

`Range limits <FirstRun> <LastRun> [<Extension>]:`

Enter the first run number, the last run number, and the extension number of the data file range to be scanned, all separated by spaces. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". <LastRun> must be greater or equal <FirstRun>. If <Extension> is missing the default value "1" is assumed. All data files must have the same extension number.

`Minimum output extension:`

Enter the minimum extension number for the output data files. Each isotropic output data file, created by program "SANSIsoDo" later, will have the same run number as the anisotropic input data file used. To determine the actual extension number for the output data file, "SANSIsoDo" will initially set the extension number to the minimum value entered here. If a data file with this new extension number already exists the program will continue incrementing the extension number until there is no interference with existing files. To use the input extension plus 1 as minimum output extension, simply press RETURN.

If you perform radial averaging for more than one sector per file, for each sector a separate output file will be created featuring the same run number as the input file and incrementing extension numbers determined according to the scheme described above.

If you requested an additional splitting of the scattering patterns into a nuclear and a magnetic component, the program "SANSIsoDo" will first create the one or more output files containing the normal radially averaged intensity for the one or more sectors, as described above. After that, three extra output files will be created containing the nuclear component I_{Nuc}, the magnetic component I_{Mag}, and the sum of the two components $I_{Nuc}+I_{Mag}$, respectively. These three files will also have the same run number as the anisotropic input data file, and they will use the next three extension numbers after the last of the normal radially averaged output files. There is no way to produce only the $\sin^2(\psi)$-fitted output files for I_{Nuc}, I_{Mag} and $I_{Nuc}+I_{Mag}$ without creating at least one radially averaged output file before.

`Apply "Search" option to the data file range? Y/(N):`

To select the input mode of data files to be processed, enter one of the following options (1) or (2):

Option (1): **`No`**

Enter "n" for "No" (or simply press RETURN) if you want to use the complete run number range you entered above. Within this range, all files will be selected that pass the test for a valid data file. This option often provides a faster operation than "Yes", and it requires less input typing.

From this point, the terminal dialogue will be the same as for option (2) "Yes", starting from the ' Accept this selection? ' prompt.

Option (2): **`Yes`**

Enter "y" for "Yes" if you only want to use individual files from the run number range you entered above. With this option, you can select the files to be processed by scanning this run number range for certain item values. Only those files within the range are selected that match all conditions. This option provides a slower operation than "No" if the run number range to be scanned is large, and it requires more input typing.

A menu appears which lists all items that may be present in a data file. For a detailed description of this menu, please refer to "File Item Search Menu" in chapter "Standard Menus".

From this point, the terminal dialogue is the same both for option (1) "No" and for option (2) "Yes".

Files will now be scanned. For each individual data file that matches all conditions, the file name is listed together with the sample name. If an input file does not exist or is not a valid data file the run number is skipped. If you choose an item that is not present in a particular data file it will be treated as "no matching". The numbers of files expected in the entered range and of files actually found are compared.

`Accept this selection? (Y)/N:`

If you agree that these are the files you intended to use, enter "y" (or simply press RETURN) to confirm. If you don't want to use these data files, enter "n" to choose a new range.

`Add another set of files? Y/(N):`

Enter "y" to select another set of files to be radially averaged with the same default values. This returns you to the ' Range limits <FirstRun> <LastRun> [<Extension>]: ' prompt.

If you want to change the default values you must execute this program again.

Enter "n" (or simply press RETURN) if you don't want to use this option. The output command file "*.SCI" will now be written, including all data required to proceed the actual data reduction, and must be executed using the program "SANSIsoDo". Please note that this option is not available when no input data files have been selected because at least one data file is required for a useful operation.

`Execute the command file now? Y/(N):`

Enter "y" to start this execution now.

Enter "n" (or simply press RETURN) to run the program "SANSIsoDo" later. You may then print or edit the command file first to verify and possibly to correct it's content before execution.

Input requirements

Run numbers of the data files to be processed must be known, or the item values in the data files must be set in a way that the files can be identified by a unique combination of these item values.

The beam center co-ordinates must be determined first using program "SANSArea". The "BeamcenterX" and "BeamcenterY" values can either be written into the input data files before running this program using program "SANSDataModify", or can be entered directly while this program is running.

If you intend to mask data explicitly the mask file "*.MSK" must be created first using the program "SANSMask", or an appropriate pre-defined mask file must be chosen.

SANSIsoDo

Description

This program radially averages anisotropic data files "Dnnnnnnn.nnn" of "SANSDRaw" and "SANSDAni" types from the current directory by executing an isotropic command file "*.SCI" of "SANSCIso" type created interactively with the program "SANSIso". The program also performs an additional splitting of magnetic scattering patterns into a nuclear and a magnetic scattering component if requested. All required information is included in the command file and in the data files themselves.

For the normal radial averaging, the unmasked detector cells are first sorted into groups of cells with their centers [R(k),Angle(k)] relative to the beam center falling into the same radial range

$$n * RadialSteps \leq R(k) < (n+1) * RadialSteps \tag{1}$$

and into the same angular range

$$SectorCenter - 0.5 * SectorWidth \leq Angle(k) < SectorCenter + 0.5 * SectorWidth \tag{2}$$

or into the angular sector located symmetrically to this angular range on the other side of the beam center. For each of these groups, the program then calculates the averaged absolute output intensity $I_n(R_n=const)$ from the individual cell intensities I(k) of all cells within this particular group as the weighted mean according to the formula

$$I_n = \frac{\sum_k p(k) * I(k)}{\sum_k p(k)} \tag{3}$$

and the absolute output error $\Delta I_n(R_n=const)$ from the individual cell errors $\Delta I(k)$ according to the formula

$$\Delta I_n = \frac{\sqrt{\sum_k \left(p(k) * \Delta I(k) \right)^2}}{\sum_k p(k)} \tag{4}$$

using weight factors

$$p(k) = \frac{1}{\Delta I(k)^2} \tag{5}$$

Each value of R_n together with the corresponding intensity $I_n(R_n)$ and the error $\Delta I_n(R_n)$ yields one data point for the isotropic output data file. Depending on the setting of item "CalcMode", the value of the radial distance R_n from the beam center may finally be transformed for the output into the scattering vector Q or the scattering angle 2θ if required, as shown in Fig.2 in the description of program "SANSIso".

For the splitting of magnetic scattering patterns into a nuclear and a magnetic scattering component, the unmasked detector cells are only sorted into groups of cells with their centers [R(k),Angle(k)] relative to the beam center falling into the same radial range as given by equation (1) above, but not into different angular ranges. For this sorting procedure, the same value of item "RadialSteps" as for the normal radial averaging will be used, while the values for items "Sector", "SectorStart", "SectorInc" and "SectorWidth" are omitted. Each of these cell groups now represents a ring on the detector for which the radial distance R from the beam center can be assumed as a constant value. This reduces the general equation for the intensity distribution of a magnetic scattering pattern

$$I(R,\psi) = I_{Nuc}(R) + \sin^2(\psi) * I_{Mag}(R) \tag{6}$$

to the equation of a straight line in the form

$$y = b + x * m \tag{7}$$

for each of the cell groups. The independent variable $x = \sin^2(\psi)$ for a cell with the intensity $y = I(R,\psi)$ within a group is determined by the angle ψ between the scattering vector Q and the field direction H, being different for each cell, as shown in Fig.3 in the description of program "SANSIso". For each cell group n, the program then performs a standard least-squares linear regression, yielding the slope $m_n = I_{n,Mag}(R_n{=}\text{const})$ and the y-intercept $b_n = I_{n,Nuc}(R_n{=}\text{const})$ for this cell group, and performs the corresponding standard error calculation for $\Delta I_{n,Nuc}(R_n)$ and $\Delta I_{n,Mag}(R_n)$.

Each value of R_n together with the corresponding intensity $I_{n,Nuc}(R_n)$ and the error $\Delta I_{n,Nuc}(R_n)$ yields one data point for the isotropic output data file containing the nuclear scattering component, and the same value of R_n together with the corresponding intensity $I_{n,Mag}(R_n)$ and the error $\Delta I_{n,Mag}(R_n)$ yields one data point for the isotropic output data file containing the magnetic scattering component. Depending on the setting of item "CalcMode", the value of the radial distance R_n from the beam center may finally be transformed for the output into the scattering vector Q or the scattering angle 2θ if required, in the same way as for the normal radial averaging.

The definition of a linear regression line requires at least two data points, and the error calculation for slope and y-intercept of this line requires at least three data points. Thus, only cell groups containing at least three cells will be considered for the $\sin^2(\psi)$-fit. Cell groups containing less cells will be omitted without a message.

However, within a group of detector cells with R_n = const the intensities of the cells as a function of their corresponding angles ψ may not perfectly fit to the straight line defined by equation (7). Therefore, for each linear regression (i.e. for each data point in the three isotropic output data files for I_{Nuc}, I_{Mag} and $I_{Nuc}{+}I_{Mag}$) the program calculates a correlation coefficient C_n to measure how well the line fitted to the data actually does approximate the data. This large amount of correlation information cannot be written to the screen anymore in a readable form. Therefore, these correlation coefficients will be written only into the output data files for I_{Nuc}, I_{Mag} and $I_{Nuc}{+}I_{Mag}$ as comment lines, together with the number of detector cells N_n that were available for the $\sin^2(\psi)$-fit within each cell group. Since one fit always yields one value $I_{n,Nuc}$ and one value $I_{n,Mag}$ at the same time, the corresponding C_n and N_n are the same for both values, and will be written into the three output data files in duplicate. For short on-screen information, only the average and the standard deviation of this set of correlation coefficients will be displayed.

To be sure that the anisotropic input data file you have processed actually can be described by equation (6) for a magnetic scattering pattern, you should edit or print one of the three isotropic output data files for I_{Nuc}, I_{Mag} or $I_{Nuc}{+}I_{Mag}$, and check the values of the correlation coefficients there. If the input data file is suitable for a $\sin^2(\psi)$-fit and only affected by minor statistical errors, all correlation coefficients should be well above 0.9. If they are much smaller for most of the data points, the input data file will most probably not represent a magnetic scattering pattern, and the results obtained for I_{Nuc} and I_{Mag} will have no physical relevance. It may also happen that there is a good correlation over a large range of data points, and a bad correlation only at the detector edge and around the beamstop. In this case, the input data file in general represents a suitable magnetic scattering pattern, but the masking of unwanted detector cells may not be sufficient in these areas, the number of unmasked cells available for the $\sin^2(\psi)$-fit may be too small here, or the statistical errors may be too large here.

For the splitting of magnetic scattering patterns into a nuclear and a magnetic scattering component, a mask file must always be used, even if the calculation is only performed as a preliminary data test. Otherwise, in most cases an unmasked beamstop area will distort even a good magnetic scattering pattern so severely that the program might crash.

Terminal dialogue

Type the command line

SANSIsoDo <CommandFileName>

Parameter is the name of the command file to be executed. <CommandFileName> is a string compatible to the requirements of the operating system, without extension. The standard extension "*.SCI" will be appended by the program. Only a proper command line is accepted.

Information on the command file and the mask file used by the program is written to the screen. If an input file does not exist or is not a valid command file or mask file the program aborts.

For each individual data file, the file name is listed together with the sample name during processing. Please note that this sample name is taken from the data file directly. The sample name included in the corresponding line of the command file is only a comment, so editing the name in the command file will have no effect on the screen output. If you use the original command file as created by the program "SANSIso" without subsequent editing this fact is not important for you.

If an input file does not exist or is not a valid data file the program aborts.

After an input data file has been processed, one output data file or a set of output data files of "SANSDIso" type are written, depending on the number of angular sectors used for radial averaging and on the request of a $\sin^2(\psi)$-fit. The run number for the output file(s) will always be the run number of the input data file used. To determine the actual extension number(s) for the output data file(s), the extension number is initially set to the minimum output extension entered in program "SANSIso". If a data file with this new extension number already exists the program will continue incrementing the extension number until there is no interference with existing files. In this case, a warning will be displayed on the screen. If radial averaging is performed for more than one sector per file, for each output file the center angle of the corresponding sector is written to the screen. If an additional splitting into a nuclear and a magnetic component has been requested, for the first two additional output files containing the separated components I_{Nuc} and I_{Mag} a note "NUC" or "MAG" is written to the screen, and for the third additional output file containing the sum $I_{Nuc}+I_{Mag}$ a note "ADD" is written to the screen.

If the current sector or the complete data file do not contain any unmasked valid detector cells, no output file will be created, and a message will be displayed on the screen.

Most item values that describe the sample and the experimental set-up are copied from the input file to the output file(s) directly while some other item values are taken from the command file. For details, please refer to the description of the "SANSDIso" file format.

After each execution of a command file, a listing of input data file names and data reduction parameters actually used and of output data file names actually created is appended to the end of the command file. This automatic recording of log information increases the size of the command file by adding comment lines which do not affect later executions. If you do not wish to add this log information to the command file you can disable this feature by editing the file and changing entry "Logging=YES" in block "%File" to "Logging=NO". However, it is strongly recommended to leave this feature enabled since it provides you with a complete printer-ready recording of the work you've done.

Input requirements

The command file "*.SCI" must be created first using the program "SANSIso". The mask file and the data files that were used during this creation must be present.

NOTE

If a message "Invalid parameter in block "%Default"." appears one of the following relationships required for the values in this block of the command file may not hold: RadialSteps > approx. 0.1 cells; SectorInc > 0 deg; SectorWidth > 0 deg.

SANSIsoPlot

Description

This program displays and edits 1-dimensional isotropic data files "Dnnnnnnn.nnn" of "SANSDIso" type. The graphics output can optionally be printed on paper or saved as a PostScript file.

"help" can be entered at any prompt to get on-line assistance if required.

Terminal dialogue

Type the command line

SANSIsoPlot

No command line parameters are required.

A graphics window for the curve plot will be opened. On the right margin of the curve plot window, the data file names of the currently shown curves are displayed. The axis titles of the plot will be set according to the individual content of the data files displayed. If data files containing different quantities on the same axis are displayed together, the corresponding axis title remains blank.

Actions taken by this program don't modify the original data files. Scaling of curves and masking of unwanted data points only affects the screen display, the print or graph file output, and the writing of edited files with new file names, and mainly serves as a tool for "beauty corrections" of this output for further processing or for publication.

On some computer types, the keyboard input remains permanently directed to the DECterm window where you typed the command line to start the program. You can enter commands even while a graphics window is highlighted, and you only have to highlight the DECterm window explicitly by a mouse click if the graphics window hides a part of the DECterm window that you want to see. In contrast, on some other computer types the input will be always directed to the currently highlighted window. Therefore, no keyboard input is recognized by the program when a graphics window is highlighted. To enter any keyboard input, the DECterm window must be highlighted first by a mouse click. Since after the start of the program the contour plot window is always highlighted automatically, on this computer type this has to be your first action before entering any command from the PC keyboard.

The main menu appears which lists all options provided by the program.

Read Delete X-axis Y-axis Masked Print Save mOde Vms Quit
Option? R/D/X/Y/M/P/S/O/V/Q:

Enter one of the following options (1) to (10):

Option (1): **Read**

Enter "r" for "Read" to read an isotropic data file "Dnnnnnnn.nnn" of "SANSDIso" type.

Data file <Run> [<Extension>] or Next:

Enter the run number and the extension number of the data file to be read, separated by a space. <Run> is a positive integer number between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". If <Extension> is missing the default value "1" is assumed. Or enter "n" to read the next existing run number with the same extension as before. "Next" is only available after an initial input of a correct data file specification setting the starting point for continuation. It does not require a continuous range of run numbers but increments the last run number loaded until a new data file has been found. To avoid an infinite loop in case no other data file follows, the maximum size of a gap allowed between two run numbers is limited to 100. If you do not wish to read a data file, simply press RETURN.

If the input file does not exist or is not a valid data file you will be prompted for a new input. If you entered the name of a valid data file, information on this file is written to the screen, the new data are added to the curve plot window, and the list of data file names in the curve plot window is updated.

The maximum number of data files to be loaded is limited to 12.

Option (2): **Delete**

Enter "d" for "Delete" to delete the current plot in the curve plot window, and to set the number of loaded curves to zero.

Option (3): **X-axis**

Enter "x" to format the horizontal "X"-axis of the curve plot. The current settings of the "X"-axis will be written to the screen. The default settings after the start of the program are "Logarithmic" and "Automatic scaling".

Axis type:

Choose an axis type from the menu list and enter the appropriate number. If you do not wish to change the current axis type, simply press RETURN.

Axis range <Minimum> <Maximum> or Auto:

Enter two real or integer numbers, separated by a space. Or enter "a" to set the axis range automatically according to the total "X"-range covered by all currently displayed curves. If you do not wish to change the current range settings, simply press RETURN.

If any of the settings for axis type or axis range have been changed, and at least one curve is displayed in the curve plot window, it will be redrawn with these new settings. The number of data points actually visible in the curve plot window will be written to the screen for each curve. If the axis has been defined in a way that some data points cannot be displayed because they are outside the axis limits or invalid for the current axis type (e.g. a negative value on a logarithmic axis), the numbers of these additional data points will be written to the screen, too. If no data points fit to the current axis settings, the curve plot window will only show the axis.

If the axis range is invalid for the current axis type (e.g. a negative minimum on a logarithmic axis), a message will be written to the screen, and you will be prompted for new axis settings. Please note that this error message may also appear when you only selected a new axis type, but did not enter a new axis range. In this case, a range setting from the last application of this sub-option incompatible with the current axis type may still be in effect.

The new settings will be used to display all following curves until they are modified again.

Option (4): **Y-axis**

Enter "y" to format the vertical "Y"-axis of the curve plot. The default settings after the start of the program are "Logarithmic" and "Automatic scaling". The terminal dialogue will be performed exactly in the same way as described for option (3) "X-axis".

Option (5): **Masked**

Enter "m" for "Masked" to hide or expose points that are implicitly masked in the data files. This option is only available when an implicit mask has been detected in at least one of the data files. When a data point is masked, this point is temporarily removed from the curve, without modifying the original data file.

This option works in a toggle mode: Entering "m" while implicit masking is disabled sets it to the enabled state, and vice versa. The default setting after the start of the program is "disabled".

When you delete the current curve plot using option (2) "Delete", this option is automatically reset to "disabled".

<u>Option (6):</u> **Print**

Enter "p" for "Print" to print the current curve plot (see Fig.1). This option is only available if at least one curve is displayed in the curve plot window.

Graphics layout type? (1)/2/3:

Enter "1" (or simply press RETURN) to print a large plot of the curves on a single page. A printed output similar to the picture currently shown in the curve plot window will be created. The page will only contain the data file names, but no additional data file information.

Enter "2" to print a small plot of the curves on a single page. A printed output similar to the picture currently shown in the curve plot window will be created. The page will contain the data file names, plus a set of selected data file information that still fits on the remaining space of the page.

Enter "3" to print a large plot of the curves on a first page as created with option "1", plus full data file information on a second page.

A menu appears which lists all available printers and their locations.

Printer number:

Enter the number of the printer to be used. To select the printer marked as "default", simply press RETURN. Depending on the load of the computer and the network and on the complexity of the picture, the printing may require up to a few minutes.
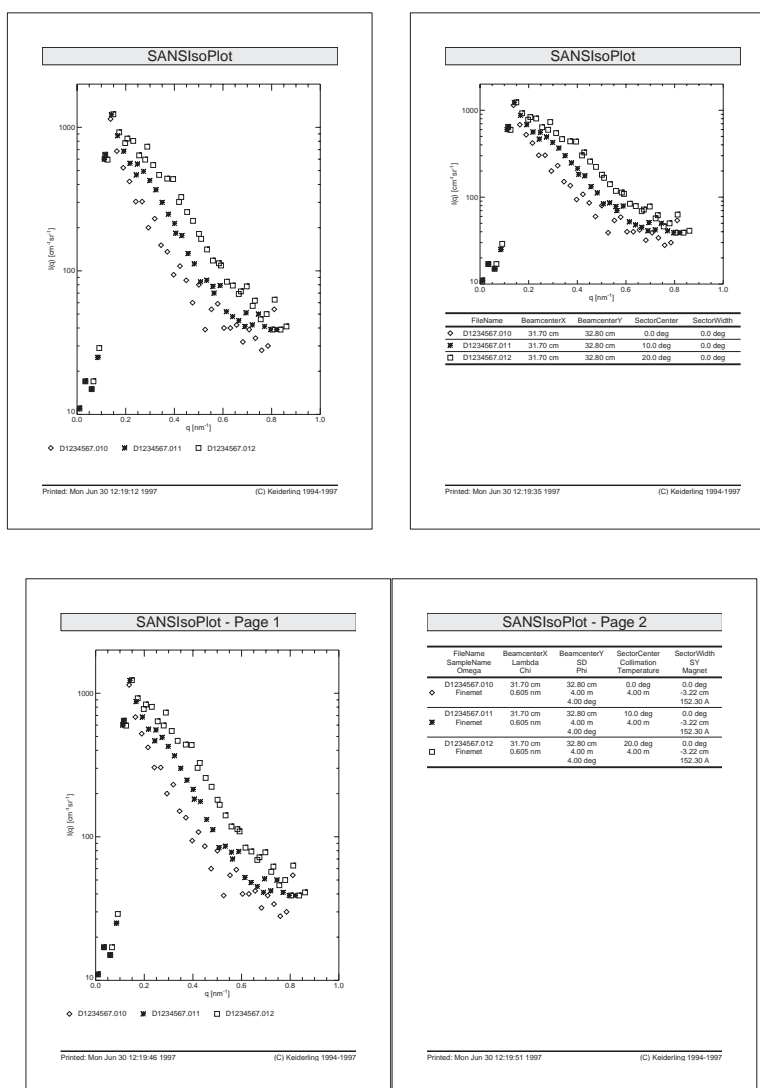
Fig.1: Printer output pages created using graphics layout types "1" to "2" (first line, left to right) and "3" (second line).

Option (7): **Save**

Enter "s" for "Save" to save the current curve plot as an "Encapsulated PostScript" graph file, ready for import into common text or graphics programs which support this file format, e.g. "Microsoft Word" or "CorelDraw!" (see Fig.2). This option is only available if at least one curve is displayed in the curve plot window.

Output file name (no extension):

Enter the name of the output file but do not type an extension. The standard extension "*.EPS" will be appended by the program. If you do not wish to save a graph file, simply press RETURN.

There is no check whether a graph file of the same name already exists in the current directory. If a file exists it will be overwritten without a warning.

Graphics layout type? (1)/2/3/4/5/6:

Enter "1" (or simply press RETURN), "2", or "3", to create a graph file in portrait, square, or landscape format, respectively, containing the plain diagram without data file names.

Enter "4", "5", or "6", to create a graph file in portrait, square, or landscape format, respectively, containing the diagram enhanced with a list of the data file names.
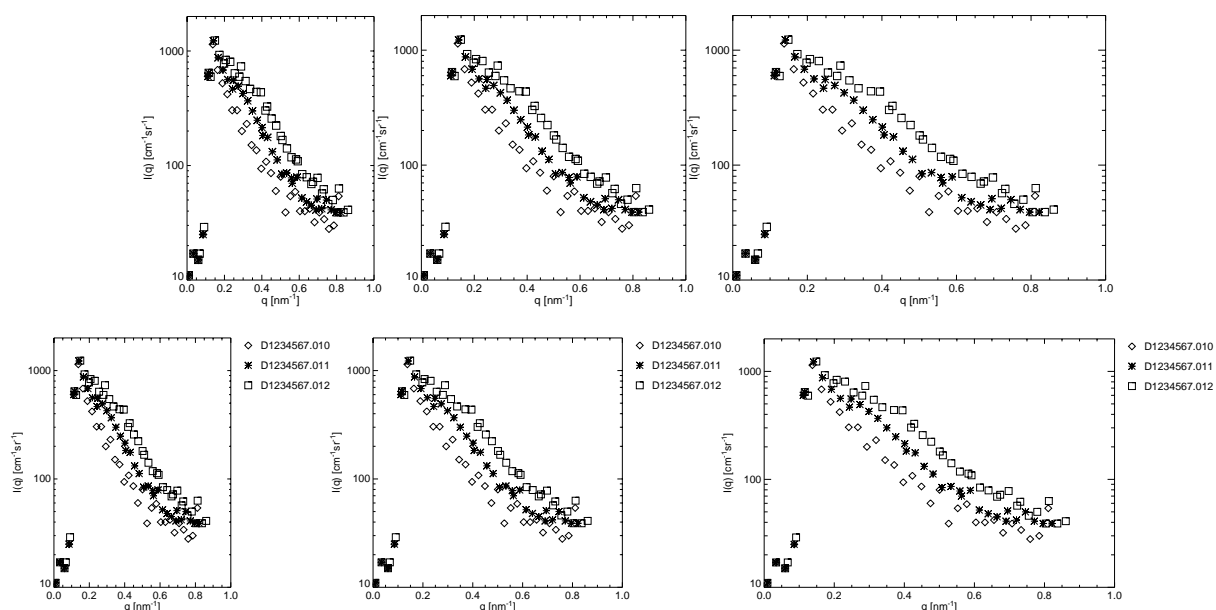
Fig.2: Graph files created using graphics layout types "1" to "3" (first line, left to right) and "4" to "6" (second line, left to right).

Option (8): `mOde`

(xxx) This option will soon be available.

Option (9): `Vms`

Enter "v" for "VMS" to obtain a temporary command prompt of the VMS operating system. From this prompt, any DCL command can be executed while the program "SANSIsoPlot" is still present in the background. To return to "SANSIsoPlot", type "logout". You will find the program exactly as you left it.

All commands will be executed in a spawned child process with it's own process environment. As a result of this, your actions will not affect the proper work of "SANSIsoPlot" as long as you do not delete or rename any files used by the program. Please note that due to this separate process environment, the DCL commands "SET DEFAULT" and "CD" cannot be used to change the default directory the program works in, since the result of this action is lost as soon as you leave the child process with "logout" and return to "SANSIsoPlot".

Option (10): `Quit`

Enter "q" for "Quit" to terminate the program.

Input requirements

None.

NOTE

If you want to run this program from a PC with "eXcursion" software or from a X Windows terminal for the first time, you may have to redirect the graphics output using command file "SANSDisplay" first before starting this program. If still a message "Unable to open X Windows display." appears please

consult the device responsible. If you run this program on a workstation with directly connected screen, execution of command file "SANSDisplay" is not necessary.

When a part of a graphics window that was previously hidden by another window is exposed, the damaged part will usually be restored by the window manager system automatically. Since this transfer of graphical bitmap data is a time-consuming process it may require up to a few seconds, depending on the load of the computer and the network. If this restoration fails or produces unusual colors, type "new" on the main menu prompt to redraw the graphics window from the program.

If a message "Internal error." appears please consult the device responsible.

SANSMask

Description

This program creates a mask file "*.MSK" for data reduction programs "SANSAni", "SANSAniDo", "SANSArea", "SANSTrans", "SANSTransDo" and for graphics program "SANSAniPlot". An anisotropic data file "Dnnnnnnn.nnn" of "SANSDRaw" or "SANSDAni" type can be used as a background picture for on-screen mask design. The graphics output can optionally be printed on paper or saved as a PostScript file.

"help" can be entered at any prompt to get on-line assistance if required.

Terminal dialogue

Type the command line

SANSMask

No command line parameters are required.

A graphics window for the contour plot will be opened displaying the square area, with the co-ordinates (0,0) in the lower left corner and the co-ordinates (<DetectorSize>-1,<DetectorSize>-1) in the upper right corner. All cells are set to "not masked" and displayed as black squares. When a cell is set to "masked" later in the program, it will be inverted to a grey square in the display. If a background data file contains information on a beam center, the position of this beam center is displayed as a cross "+". On the bottom line of the contour plot window, the current mask file name and the current background data file name are displayed.

Generally, the selection and unselection of mask cells works in a toggle mode: each unmasked cell in a selected mask area is set to the "masked" state, and vice versa, each masked cell is set to the "unmasked" state. You can experience this effect by selecting any rectangle in the mask, and then selecting another rectangle which partially overlaps with the first one.

On some computer types, the keyboard input remains permanently directed to the DECterm window where you typed the command line to start the program. You can enter commands even while a graphics window is highlighted, and you only have to highlight the DECterm window explicitly by a mouse click if the graphics window hides a part of the DECterm window that you want to see. In contrast, on some other computer types the input will be always directed to the currently highlighted window. Therefore, no keyboard input is recognized by the program when a graphics window is highlighted. To enter any keyboard input, the DECterm window must be highlighted first by a mouse click. Since after the start of the program the contour plot window is always highlighted automatically, on this computer type this has to be your first action before entering any command from the PC keyboard.

The main menu appears which lists all options provided by the program.

Read Add Write Edit Delete dataFile Levels Table Copy Print Save mOde Vms Quit
Option? R/A/W/E/D/F/L/T/C/P/S/O/V/Q:

Enter one of the following options (1) to (14):

Option (1): **Read**

Enter "r" for "Read" to read an existing mask from a file. The current mask will be lost and replaced with the new one. There is no check whether there have been any unsaved changes of the current mask.

Mask file name (no extension):

Enter the name of the mask file to be read but do not type an extension. The standard extension "*.MSK" will be appended by the program. If you do not wish to read a mask file, simply press RETURN.

If the input file does not exist or is not a valid mask file you will be prompted for a new input. If you entered the name of a valid mask file, information on this file is written to the screen, the new mask is displayed in the contour plot window, and the mask file name in the contour plot window is updated.

Option (2): **Add**

Enter "a" for "Add" to add an existing mask from a file to the current mask. The current mask will be combined with the new one by a logical "OR" operation: if a cell is masked in one or both of the two input masks it will be masked in the resulting mask, too.

Mask file name (no extension):

Enter the name of the mask file to be added but do not type an extension. The standard extension "*.MSK" will be appended by the program. If you do not wish to add a mask file, simply press RETURN.

If the input file does not exist or is not a valid mask file you will be prompted for a new input. If you entered the name of a valid mask file, information on this file is written to the screen, and the resulting mask is displayed in the contour plot window. The mask file name in the contour plot window remains unchanged.

Option (3): **Write**

Enter "w" for "Write" to write the mask to a file.

Mask file name (no extension):

Enter the name for the mask file to be written but do not type an extension. The standard extension "*.MSK" will be appended by the program.

If no mask file name exists yet, you must enter a name. If a mask file name already exists, this name will be offered as a default input. Simply press RETURN to accept this name, or enter a new name. If you entered a new name, the mask file name in the contour plot window will be updated with this new input name.

There is no check whether a mask file of the same name already exists in the current directory. If a file exists it will be overwritten without a warning.

Comment:

Enter any comment text to be saved with the mask file. For practical reasons, this input prompt limits the comment to a single line. If you feel any need to add more comment lines, you can edit the mask file with a text editor after it has been saved, and add as many comment lines as you want to. For a detailed description of comment syntax, please refer to chapter "File Formats". If you don't want to use a comment, simply press RETURN.

Please note that comments are never copied from the current mask to the new mask file written. Even if you pressed RETURN to accept the offered default file name, pressing RETURN again on the ' Comment: ' prompt will save the new mask file without a comment.

Option (4): **Edit**

Enter "e" for "Edit" to edit the current mask. Depending on the setting of option (12) "mOde", this can be done either using the mouse, or using the keyboard.

a) Editing the mask using the mouse:

Click with the mouse into the contour plot window. Three numbers in the lower right corner of the contour plot window display the current (X,Y) cursor position and the data intensity at this position. Move the mouse to the first corner of the rectangle you want to select, press the LEFT mouse button, and keep it pressed. Now, move the mouse to the second corner of the rectangle and release the LEFT mouse button again. Unmasked (black) cells within the rectangle between the two selected corners will be inverted to masked (grey) cells in the display, and vice versa. This inversion will not become visible while the mouse button is still pressed, even if you move the mouse. To select a single cell, simply click on it with the LEFT mouse button.

If you are not satisfied with the result of your operation, click the RIGHT mouse button once. This will undo the operation and restore the state of the mask as it was before. Please note that there is no "trace-back" of all the editing done with the mask. Clicking the RIGHT mouse button repeatedly will always toggle between the two states before and after the last operation.

To end this option and return to the main menu, press the LEFT and RIGHT mouse buttons together at the same time until the menu appears. Now click on the DECterm window once again to redirect the keyboard input to that window.

b) Editing the mask using the keyboard:

A menu appears which lists all "Edit" sub-options provided by the program.

Rectangle Cell X-line Y-line Undo End
Option? R/C/X/Y/U/E:

Enter one of the following sub-options (4-1) to (4-6):

Sub-option (4-1): **Edit|Rectangle**

Enter "r" to select a rectangle. You will be prompted for the co-ordinates of the rectangle corners.

Co-ordinates <X-Min> <X-Max> <Y-Min> <Y-Max>:

Enter four integer numbers between "0" and "<DetectorSize>-1", all separated by spaces. If <X-Min> is greater than <X-Max> or <Y-Min> is greater than <Y-Max> both numbers are swapped. If you do not enter integer numbers the input values will be truncated.

This command is the most general one and allows to select all desired shapes in the mask. Three special sub-options (4-2) to (4-4) have been derived from this one to reduce input typing.

Sub-option (4-2): **Edit|Cell**

Enter "c" to select a single cell. You will be prompted for the co-ordinates of the cell.

Co-ordinates <X-Cell> <Y-Cell>:

Enter two integer numbers between "0" and "<DetectorSize>-1", separated by a space.

Sub-option (4-3): **Edit|X-line**

Enter "x" to select a complete X-line. You will be prompted for the number of the line.

Co-ordinate <X-Line>:

Enter one integer number between "0" and "<DetectorSize>-1".

Sub-option (4-4): **Edit|Y-line**

Enter "y" to select a complete Y-line. You will be prompted for the number of the line.

Co-ordinate <Y-Line>:

Enter one integer number between "0" and "<DetectorSize>-1".

Sub-option (4-5): **Edit|Undo**

Enter "u" if you are not satisfied with the result of your operation. This will undo the operation and restore the state of the mask as it was before. Please note that there is no "trace-back" of all the editing done with the mask. Entering "u" repeatedly will only toggle between the two states before and after the last operation.

Sub-option (4-6): **Edit|End**

Enter "e" to end option "Edit" and return to the main menu.

Option (5): **Delete**

Enter "d" for "Delete" to delete the current mask. All cells will be set to "not masked", and the mask file name in the contour plot window will be removed. There is no check whether there have been any unsaved changes of the current mask. This action only affects the mask contained in the program, without modifying the original mask file.

Option (6): **dataFile**

Enter "f" for "dataFile" to read an anisotropic data file "Dnnnnnnn.nnn" of "SANSDRaw" or "SANSDAni" type as a background picture for on-screen mask design. This option enables you to see the exact position of the beamstop and other anomalies in the measured data and to mask exactly the cells you want to exclude from data reduction, leaving a maximum of correct cells for better statistics.

Data file <Run> [<Extension>] or Next:

Enter the run number and the extension number of the data file to be read, separated by a space. <Run> is a positive integer number between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". If <Extension> is missing the default value "1" is assumed. Or enter "n" to read the next existing run number with the same extension as before. "Next" is only available after an initial input of a correct data file specification setting the starting point for continuation. It does not require a continuous range of run numbers but increments the last run number loaded until a new data file has been found. To avoid an infinite loop in case no other data file follows, the maximum size of a gap allowed between two run numbers is limited to 100. If you do not wish to read a data file, simply press RETURN.

If the input file does not exist or is not a valid data file you will be prompted for a new input. If you entered the name of a valid data file, information on this file is written to the screen, the new data are displayed in the contour plot window, and the data file name in the contour plot window is updated.

If the data file was read as "Next", the levels for the contour plot of the data remain unchanged. Otherwise, the levels are re-defined automatically in equidistant steps between the minimum and maximum intensities of the new data file.

Option (7): **Levels**

Enter "l" for "Levels" to change the contour plot levels for the background data file. Intensities within a data file may extend over many decades. You may find it necessary to experiment with different level values to reveal all anomalies in the measured data that have to be masked.

An information on the intensity range covered by the current data, and on the contour plot levels currently defined is written to the screen.

Up to 6 levels or Auto:

Enter up to 6 real or integer numbers, all separated by spaces. The numbers must be in the range between "Minimum" and "Maximum" values of the data intensity. The input values will be sorted in

ascending order, and redundant inputs of the same value will be removed. Or enter "a" to set the contour plot levels automatically. The data are displayed in the contour plot window with the new contour plot levels. If you do not wish to change the current levels, simply press RETURN.

Option (8): **Table**

Enter "t" for "Table" to display a sub-area of the data file as a table. After selecting the center point of the desired sub-area, a table is written to the screen displaying a square sub-area of 11 by 11 cells, centered symmetrically around the selected center point. The numbers in the top line and in the left column of the table represent the X and Y co-ordinates of the displayed cells, respectively. If the center point has been selected very close to the edge of the detector area, it is shifted automatically to a distance of 5 cells from the edge in order to obtain a fixed table size.

The numbers in the table usually represent the original content of the detector cells. Optionally, these numbers can also be normalized to an integer range of "0".."10000", where "0" corresponds to the minimum intensity in the selected sub-area, and "10000" corresponds to the maximum intensity in the selected sub-area. This may be useful for some applications. The minimum, maximum and average intensities of the data file sub-area displayed in the table are always given in absolute values.

For original intensities from data files of "SANSDRaw" type and for normalized intensities from all data file types, the output format of the numbers is "I6". For original intensities from data files of "SANSDAni" type, the output format is "F6.2". All numbers which are too large for these output formats are displayed as "******".

Depending on the setting of option (12) "mOde", the selection of the center point can be done either using the mouse, or using the keyboard.

a) Selecting the center point using the mouse:

Click with the mouse into the contour plot window. Three numbers in the lower right corner of the contour plot window display the current (X,Y) cursor position and the data intensity at this position. Move the mouse to the cell you want to select as the center point for the table. Click the LEFT mouse button once to create a table of original intensities. Click the RIGHT mouse button once to create a table of normalized intensities.

To end this option and return to the main menu, press the LEFT and RIGHT mouse buttons together at the same time until the menu appears. Now click on the DECterm window once again to redirect the keyboard input to that window.

b) Selecting the center point using the keyboard:

You will be prompted for the co-ordinates of the center point.

Sub-area co-ordinates <X-Mid> <Y-Mid> [Normalized]:

Enter two integer numbers between "0" and "<DetectorSize>-1", separated by a space. Enter an additional "n" on the same input line to display normalized intensities instead of the original ones. To end this option and return to the main menu, simply press RETURN.

Option (9): **Copy**

Enter "c" for "Copy" to copy the implicit masking of the data file to the current mask. The current mask will be combined with the new one by a logical "OR" operation: if a cell is masked in one or both of the two input masks it will be masked in the resulting mask, too. The resulting mask is displayed in the contour plot window. The mask file name in the contour plot window remains unchanged.

Option (10): **Print**

Enter "p" for "Print" to print the current mask (see Fig.1). This option is only available if at least one file (a mask file or a data file) has been read in before, or if any editing of the current mask has been performed.

A menu appears which lists all available printers and their locations.

Printer number:

Enter the number of the printer to be used. To select the printer marked as "default", simply press RETURN. A printed output similar to the picture currently shown in the contour plot window will be created. In contrast to the screen picture, in the print the masked cells are transparent so the contour lines and the beam center (if any) remain visible in the masked areas, too. Depending on the load of the computer and the network and on the complexity of the picture, the printing may require up to a few minutes.

If the current mask has been read from a file, the printed page contains information on this mask file. If the mask has been modified since the file was read by the program, the printed page contains a note "State: MODIFIED" to remind you that the current state of the mask shown in the picture might be different from the original content of the file. If the mask file contains a comment, the number of comment lines printed depends on the space available at the bottom of the page.

If a background data file has been read by the program, the printed page contains the data file name and some selected information on this file.
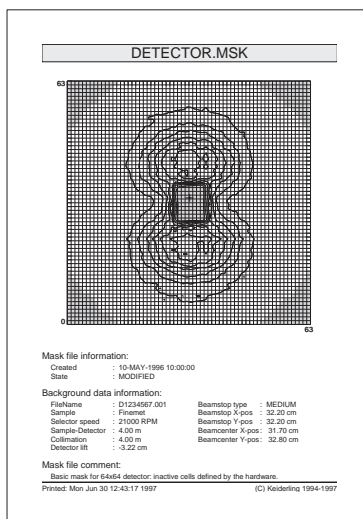
Fig.1: Printer output page.

Option (11): **Save**

Enter "s" for "Save" to save the contour plot as an "Encapsulated PostScript" graph file, ready for import into common text or graphics programs which support this file format, e.g. "Microsoft Word" or "CorelDraw!" (see Fig.2). This option is only available if at least one file (a mask file or a data file) has been read in before, or if any editing of the current mask has been performed.

Output file name (no extension):

Enter the name of the output file but do not type an extension. The standard extension "*.EPS" will be appended by the program. If you do not wish to save a graph file, simply press RETURN.

There is no check whether a graph file of the same name already exists in the current directory. If a file exists it will be overwritten without a warning.
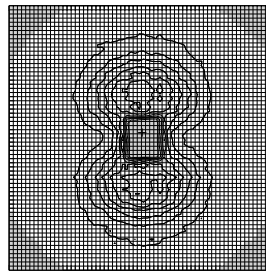
Fig.2: Graph file.

Option (12): `mOde`

Enter "o" for "mOde" to toggle the input mode for options (4) "Edit" and (8) "Table" between mouse input and keyboard input. The default setting after the start of the program is "mouse". Choosing option "keyboard" instead of "mouse" is recommended especially for morning work after heavy consumption of German beer.

Option (13): `Vms`

Enter "v" for "VMS" to obtain a temporary command prompt of the VMS operating system. From this prompt, any DCL command can be executed while the program "SANSMask" is still present in the background. To return to "SANSMask", type "logout". You will find the program exactly as you left it.

All commands will be executed in a spawned child process with it's own process environment. As a result of this, your actions will not affect the proper work of "SANSMask" as long as you do not delete or rename any files used by the program. Please note that due to this separate process environment, the DCL commands "SET DEFAULT" and "CD" cannot be used to change the default directory the program works in, since the result of this action is lost as soon as you leave the child process with "logout" and return to "SANSMask".

Option (14): `Quit`

Enter "q" for "Quit" to terminate the program. If the program detects any unsaved modifications of the current mask since the last read or write operation, a warning will be written to the screen.

`Save changes before quit? (Y)/N:`

If you want to keep these modifications, enter "y" (or simply press RETURN) to write the current mask to a file. You will first go through complete option (3) "Write", and then terminate the program automatically. If you don't want to keep these modifications, enter "n" to terminate the program immediately.

Input requirements

If you intend to use an existing mask file "*.MSK" as a template or add-on for your own creation, the file name of that mask file must be known.

NOTE

If you want to run this program from a PC with "eXcursion" software or from a X Windows terminal for the first time, you may have to redirect the graphics output using command file "SANSDisplay" first before starting this program. If still a message "Unable to open X Windows display." appears please consult the device responsible. If you run this program on a workstation with directly connected screen, execution of command file "SANSDisplay" is not necessary.

When a part of a graphics window that was previously hidden by another window is exposed, the damaged part will usually be restored by the window manager system automatically. Since this

transfer of graphical bitmap data is a time-consuming process it may require up to a few seconds, depending on the load of the computer and the network. If this restoration fails or produces unusual colors, type "new" on the main menu prompt to redraw the graphics window from the program.

If a message "Internal error." appears please consult the device responsible.

SANSNews

Description

This command file displays the latest news about the "BerSANS" program package that may not yet be included in this manual. All information is written to the screen in reverse order of date, i.e. the last news first.

Terminal dialogue

Type the command line

SANSNews

No command line parameters are required.

Input requirements

None.

SANSTrans

Description

This program pre-processes anisotropic data files "Dnnnnnnn.nnn" of "SANSDRaw" and "SANSDAni" types from the current directory interactively and creates a command file "*.SCT" for actual transmission calculation by the program "SANSTransDo". The created command file can be edited before execution and can also be printed to obtain a complete listing of data and parameters used in transmission calculation.

"help" can be entered at any prompt to get on-line assistance if required.

Terminal dialogue

Type the command line

SANSTrans

No command line parameters are required.

Command file name (no extension):

Enter the name of the command file to be created. Choose any name that is suitable for your own purposes but do not type an extension. The standard extension "*.SCT" will be appended by the program. If you want to copy the file to a DOS or Windows 3.x PC later use a name not longer than 8 characters. You must enter a name.

Limit detector area for transmission calculation? Y/(N):

If you only want to use the counts from a limited part of the detector area for the transmission calculation, enter "y". If you want to use the counts from the entire detector area, enter "n" (or simply press RETURN).

If you choose a limitation, you will be prompted for a description of it.

Enter <X-Min> <X-Max> <Y-Min> <Y-Max> or Mask:

To proceed the calculations for a plain rectangular area, enter the co-ordinates of the rectangle corners. Enter four integer numbers between "0" and "<DetectorSize>-1", all separated by spaces. <X-Max> must be greater or equal <X-Min>, and <Y-Max> must be greater or equal <Y-Min>. For all samples, only the counts within this rectangle will be used for the calculation.

Instead of this rectangular area, you can also use a mask file created with program "SANSMask". In this case, all cells within the detector area that are not masked will be used for the calculation, while masked cells are considered as "zero intensity". There are no limitations for the arrangement of masked and unmasked cells in the mask file. To choose this option, enter "m" instead of the four numbers. You will be prompted for the name of the mask file.

Mask file name (no extension):

Enter the name of the mask file to be used but do not type an extension. The standard extension "*.MSK" will be appended by the program. If you do not wish to use a mask file, simply press RETURN. If the input file does not exist or is not a valid mask file you will be prompted for a new input.

Accept this mask file? (Y)/N:

If you entered the name of a valid mask file information on this file is written to the screen. If you agree that this is the file you intended to use, enter "y" (or simply press RETURN) to confirm. If you don't want to use this mask file, enter "n" to choose a new one.

Use implicit masks of data files? Y/(N):

This option defines whether an implicit mask (coded as "Error < 0") that may be present in some of the anisotropic input data files of "SANSDAni" type should be considered for the transmission calculation. Invalid cells in data files of "SANSDAni" type (coded as "Error = 0") are never used.

Enter "y" to use existing implicit masks. The limitations entered above (plain area or mask file) will then be combined with the implicit masks by a logical "OR" operation: if a cell is excluded from processing by the above limitations, or implicitly masked, it will not be used for transmission calculation. If the implicit mask is contained in an input data file for "Cadmium", it will affect the calculations for all samples. If the implicit mask is contained in an input data file for "EmptyHole", it will only affect the calculations for the set of samples referring to this particular empty hole. If the implicit mask is contained in an input data file for a particular "SampleN", it will only affect the calculation for this particular sample. The setting of this item will have no effect on processing raw data files of "SANSDRaw" type since these files never contain an implicit mask.

Enter "n" (or simply press RETURN) to omit all implicit masks that may be present within the input data files.

Use "<DataType>"? Range/Search/Continue/(No):

The program now prompts for input data types "Cadmium", "EmptyHole" and "SampleN" (N = 1..50), respectively.

To select the input mode of data files for the particular data type, enter one of the following options (1) to (4):

Option (1): **Range**

Enter "r" for "Range" if the data files you want to use form a continuous range of run numbers, and if you already know the first and the last run number of this range. Within the range, all files will be selected that pass the test for a valid data file. This option often provides a faster operation than "Search", and it requires less input typing.

Range limits <FirstRun> <LastRun> [<Extension>]:

Enter the first run number, the last run number, and the extension number of the data file range to be processed, all separated by spaces. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". <LastRun> must be greater or equal <FirstRun>. If <Extension> is missing the default value "1" is assumed. All data files must have the same extension number.

Files will now be processed. For each individual data file, the file name is listed together with the sample name. If an input file does not exist or is not a valid data file the run number is skipped. The numbers of files expected in the entered range and of files actually found are compared.

Accept this selection? (Y)/N:

If you agree that these are the files you intended to use, enter "y" (or simply press RETURN) to confirm. If you don't want to use these data files, enter "n" to choose a new range.

The number of files found will usually be equal to the number of files expected. If it is smaller then some data files have not been found or have not passed the test for a valid file type.

A set of input data files may contain no files at all, may consist of one or more data files of "SANSDRaw" type, or may consist of exactly one data file of "SANSDAni" type. No mixing of "SANSDRaw" and "SANSDAni" data files and no adding of "SANSDAni" data files is permitted.

Add another set of files? Y/(N):

Enter "y" to select another set of files for the current data type. This returns you to the ' Range limits <FirstRun> <LastRun> [<Extension>]: ' prompt.

Enter "n" (or simply press RETURN) if you don't want to use this option. This ends option (1) "Range" and returns you to the ' Use "<DataType>"? ' prompt.

Option (2): **Search**

Enter "s" for "Search" if the data files you want to use do not form a continuous range of run numbers, or if you are not certain about the limits of the range. With this option, you can select the files used for data reduction by scanning a run number range for certain item values. Only those files within the range are selected that match all conditions. This option provides a slower operation than "Range" if the run number range to be scanned is large, and it requires more input typing.

Range limits <FirstRun> <LastRun> [<Extension>]:

Enter the first run number, the last run number, and the extension number of the data file range to be scanned, all separated by spaces. <FirstRun> and <LastRun> are two positive integer numbers between "1" and "9999999". <Extension> is a positive integer number between "1" and "999". <LastRun> must be greater or equal <FirstRun>. If <Extension> is missing the default value "1" is assumed. All data files must have the same extension number.

A menu appears which lists all items that may be present in a data file. For a detailed description of this menu, please refer to "File Item Search Menu" in chapter "Standard Menus".

Files will now be processed. For each individual data file that matches all conditions, the file name is listed together with the sample name. If an input file does not exist or is not a valid data file the run number is skipped. If you choose an item that is not present in a particular data file it will be treated as "no matching". The numbers of files expected in the entered range and of files actually found are compared.

Accept this selection? (Y)/N:

If you agree that these are the files you intended to use, enter "y" (or simply press RETURN) to confirm. If you don't want to use these data files, enter "n" to choose a new range.

The number of files found and the number of files expected may differ considerably, depending on the size of the scan range entered.

A set of input data files may contain no files at all, may consist of one or more data files of "SANSDRaw" type, or may consist of exactly one data file of "SANSDAni" type. No mixing of "SANSDRaw" and "SANSDAni" data files and no adding of "SANSDAni" data files is permitted.

Add another set of files? Y/(N):

Enter "y" to select another set of files for the current data type. This returns you to the ' Range limits <FirstRun> <LastRun> [<Extension>]: ' prompt.

Enter "n" (or simply press RETURN) if you don't want to use this option. This ends option (2) "Search" and returns you to the ' Use "<DataType>"? ' prompt.

Option (3): **Continue**

Enter "c" for "Continue" to use a special option that has been designed for quickly processing data from transmission measurements organized in a way that there is always the same number of data files for each sample.

After typing "c", for the current "SampleN" data type the same number of runs and the same extension number like for the preceding "SampleN-1" data type will be used. The run number range for "SampleN" starts with the run following the last run of the preceding "SampleN-1" data type. Example: "Sample2" covered runs 17 to 19 with extension number 1. Choosing option "Continue" for "Sample3" selects runs 20 to 22 with extension number 1.

This option is only available for a "SampleN" data type and after an initial "Range" command setting the starting point, the step width for continuation and the default extension number.

Files will now be processed. For each individual data file, the file name is listed together with the sample name. If an input file does not exist or is not a valid data file the run number is skipped. The numbers of files expected in the entered range and of files actually found are compared.

Accept this selection? (Y)/N:

If you agree that these are the files you intended to use, enter "y" (or simply press RETURN) to confirm. If you don't want to use these data files, enter "n" to choose a new range. In this case, you will be prompted for limits and extension number of the run number range like in option (1) above. Please note that this action sets new initial values for the starting point, the step width for continuation and the default extension number for option "Continue".

The number of files found will usually be equal to the number of files expected. If it is smaller then some data files have not been found or have not passed the test for a valid file type.

A set of input data files may contain no files at all, may consist of one or more data files of "SANSDRaw" type, or may consist of exactly one data file of "SANSDAni" type. No mixing of "SANSDRaw" and "SANSDAni" data files and no adding of "SANSDAni" data files is permitted.

This ends option (3) "Continue" and returns you to the ' Use "<DataType>"? ' prompt for the next sample directly. Please note that unlike options (1) "Range" and (2) "Search", no addition of another set of data files for the same sample is supported.

Option (4): **No**

Enter "n" for "No" (or simply press RETURN) if you don't want to use the specified data type.

Choosing this option for "Cadmium" returns you to the ' Use "<DataType>"? ' prompt directly.

If the current data type is "SampleN", option "No" terminates the input sequence for a set of samples "Sample1" to "SampleN-1" for which the empty hole selected before will be used. Please note that this option is not available for "EmptyHole" and "Sample1" because at least one empty hole and one sample are required for a useful operation.

Another empty hole? Y/(N):

Enter "y" to choose another empty hole which will be valid for the following set of samples until you change the empty hole again. Use this option if you measured your samples with different slit sizes but with the same "Cadmium" files. In this case, you won't have to type in all these files again. Typing "y" ends option "No" and returns you to the ' Use "EmptyHole"? ' prompt.

If you want to change the data files used for "Cadmium" you must execute this program again.

Enter "n" (or simply press RETURN) if you don't want to use another empty hole. The output command file "*.SCT" will now be written, including all data required to proceed the actual transmission calculation, and must be executed using the program "SANSTransDo".

Execute the command file now? Y/(N):

Enter "y" to start this execution now.

Enter "n" (or simply press RETURN) to run the program "SANSTransDo" later. You may then print or edit the command file first to verify and possibly to correct it's content before execution.

Input requirements

Run numbers of the data files to be processed for each data type must be known, or the item values in the data files must be set in a way that the files corresponding to one particular data type can be identified by a unique combination of these item values.

If you intend to mask data explicitly the mask file "*.MSK" must be created first using the program "SANSMask", or an appropriate pre-defined mask file must be chosen.

<u>**NOTE**</u>

The calculation of transmissions is only useful for uncorrected raw data, which are normally contained in raw data files "Dnnnnnnn.001" of "SANSDRaw" type. For compatibility with rare special requirements of skilled users, this program also accepts anisotropic input data files of "SANSDAni"

type produced by the programs "SANSAni" and "SANSAniDo", but in most cases these files will not contain data suitable for transmission calculation. Therefore, you should only input raw data files, unless you really know what you are doing.

If a message "This program can only handle up to ... data files." appears please consult the device responsible.

SANSTransDo

Description

This program processes anisotropic data files "Dnnnnnnn.nnn" of "SANSDRaw" and "SANSDAni" types from the current directory by executing a transmission command file "*.SCT" of "SANSCTrans" type created interactively with the program "SANSTrans". All required information is included in the command file and in the data files themselves.

Data pre-processing is done for each detector cell (i,j) individually. Raw data intensities $I_{ij\text{-Measured}}$ coming from input files of "SANSDRaw" type are first corrected by the program for detector deadtime τ according to the formula

$$I_{ij-Corrected} = \frac{I_{ij-Measured}}{1 - \frac{\tau}{t}\sum_{i,j} I_{ij-Measured}} \tag{1}$$

In this equation, I represents each of the input data types "Cadmium", "EmptyHole", and "Sample", respectively, and t is the total measurement time used for the appropriate input data type. The detector deadtime τ has been experimentally determined, and is written into the "Deadtime" item in block "%Default" of the command file by the program "SANSAni" automatically. This value can be modified before execution of the command file. However, it is strongly recommended to use the pre-defined value only, unless you really know what you are doing.

After this correction, intensities are normalized to the individual monitor values recorded in the data files. Anisotropic data coming from input data files of "SANSDAni" type are considered as already being corrected for deadtime and normalized. For the transmission calculation, only those cells are used which are located within the selected rectangular area, and which are not masked by an explicit mask file or by implicit masking.

The program calculates the transmission T from the total sums of the corrected and normalized intensities of all unmasked detector cells of the input data types "Cadmium" (Cd), "EmptyHole" (EH), and "Sample" (S) according to the formula

$$T = \frac{S - Cd}{EH - Cd} \tag{2}$$

The absolute transmission error ΔT is calculated from the errors of the total sums of the input data types "Cadmium" (ΔCd), "EmptyHole" (ΔEH), and "Sample" (ΔS) according to the formula

$$\Delta T = \sqrt{\left(\frac{\partial T}{\partial Cd}\Delta Cd\right)^2 + \left(\frac{\partial T}{\partial EH}\Delta EH\right)^2 + \left(\frac{\partial T}{\partial S}\Delta S\right)^2} \tag{3}$$

using the partial derivatives of equation (2).

Terminal dialogue

Type the command line

SANSTransDo <CommandFileName>

Parameter is the name of the command file to be executed. <CommandFileName> is a string compatible to the requirements of the operating system, without extension. The standard extension "*.SCT" will be appended by the program. Only a proper command line is accepted.

Information on the command file and the mask file used by the program is written to the screen. If an input file does not exist or is not a valid command file or mask file the program aborts.

The following screen listing of data files processed is grouped into separate blocks. The first block always contains one set of files for data type "Cadmium", which are valid for all samples. This block is followed by one or more blocks that all start with a set of files for data type "EmptyHole" and only contain those data types "SampleN" that refer to these particular empty hole data.

For each individual data file, the file name is listed together with the sample name during processing. Please note that this sample name is taken from the data file directly. The sample name included in the corresponding line of the command file is only a comment, so editing the name in the command file will have no effect on the screen output. If you use the original command file as created by the program "SANSTrans" without subsequent editing this fact is not important for you.

If an input file does not exist or is not a valid data file the program aborts.

After a set of input data files for a data type "SampleN" has been processed the calculated transmission and transmission error values are written to the screen. If any anisotropic data files of "SANSDAni" type have been used for the transmission calculation of a particular sample, no transmission error will be calculated for this sample.

A set of input data files may contain no files at all, may consist of one or more data files of "SANSDRaw" type, or may consist of exactly one data file of "SANSDAni" type. No mixing of "SANSDRaw" and "SANSDAni" data files and no adding of "SANSDAni" data files is permitted. The program "SANSTrans" automatically verifies this upon creation of the command file but if you edit the command file before execution you have to respect this condition, otherwise the program aborts.

After each execution of a command file, a listing of input data file names and calculation parameters actually used and of transmissions and transmission errors calculated is appended to the end of the command file. This automatic recording of log information increases the size of the command file by adding comment lines which do not affect later executions. If you do not wish to add this log information to the command file you can disable this feature by editing the file and changing entry "Logging=YES" in block "%File" to "Logging=NO". However, it is strongly recommended to leave this feature enabled since it provides you with a complete printer-ready recording of the work you've done.

Input requirements

The command file "*.SCT" must be created first using the program "SANSTrans". The mask file and the data files that were used during this creation must be present.

NOTE

If a message "Command file is too long." appears please consult the device responsible.

FILE FORMATS

1. General overview

This chapter contains detailed descriptions of all file types used within the "BerSANS" program package. The file types are listed in alphabetical order. The standard format is:

A) File type name

B) Filename

This part contains the standard convention for creating the file name, which is independent from the operating system.

C) Block "%BlockName"

These parts contain a very detailed description of all standard blocks that may appear within a file, and of all standard items that may appear within each standard block. Standard blocks and standard items are recognized by some or by all programs from the "BerSANS" program package. Additional blocks or items can be added by the user without affecting the proper operation of the "BerSANS" program package but these new blocks or items cannot be accessed by the standard programs provided and will require user-written software for being processed.

Blank lines are allowed everywhere within a file except in blocks "%Counts" and "%Errors". They are skipped when read in by programs.

Comment lines are allowed everywhere within a file. The first character of a comment line is an asterisk "*". Beginning from column two, all characters are allowed. Comment lines are intended to add notes to individual items in the file, or to prevent individual lines in the file from being read in by a program without deleting them completely. Rather than lines in the "%Comment" block which are processed by some programs, comment lines are always skipped.

Each item occupies a single line in the data file, and has the general structure "Item=<value>". If one item should appear more than once in the same data file, in all cases only the last appearing value will be used, i.e. the one with the line position closest to the end of the file. The number of items appearing within a block is virtually unlimited. There are no preliminary conditions concerning the sequence of the items within a block.

When an item of the experimental set-up was permanently disabled the corresponding line "Item=<value>" is not included in the files. When the item was temporarily disabled (e.g. switched to manual operation) the value is set to "*Disabled". When the item was enabled but for some reason the measurement control program was unable to determine the value it is set to "*Undefined". The strings "*Disabled" and "*Undefined" are used for both string type and numeric type values.

The type of an item determines the way it is handled by a program during input, output, search, or compare operations. Whenever it is important for you to distinguish between different item types there will be a note in the description of the particular program. In the file format descriptions, the item types are coded according to the following scheme:

{ w } - word format (string without spaces, compared for "equal")

{ t } - text format (string, spaces allowed, compared for "equal")

{ i } - integer format (number, compared for "greater or equal" / "less or equal")

{ r } - real format (number, compared for "greater or equal" / "less or equal")

{ d } - date/time format (date/time string, without spaces, compared for "substring")

All blocks "%Comment" are of comment format (string, spaces allowed, compared for "substring").

Anisotropic command file "SANSCAni"

Filename

xxxxxx.SCA   xxxxxx - any set of characters compatible with the operating system

Block "%File"

FileName=xxxxxx.SCA	{ w }	file name
FileDate=<string>	{ d }	date of file creation, in the operating system format
FileTime=<string>	{ d }	time of file creation, in the operating system format
Type=SANSCAni	{ w }	file type identifier
Logging=<string>	{ w }	append log information generated during execution to the command file; <string> = [YES	NO]

Block "%Default"

Deadtime=<real>	{ r }	electronical deadtime of the detector [sec]
MaskFile=<string>	{ w }	name of mask file used for implicit masking

Block "%Commands"

List of raw or anisotropic input data files to be used in data reduction. Each data type block is terminated by the reserved word "End". All blocks except "Cadmium" contain a transmission value. The blocks for "Water" and "SampleN" contain an additional scaling factor value. The blocks for "SampleN" contain additional attenuation factor and scattering probability values. The block "SampleBg" contains a minimum value for the extension of all output data files to be created using this background. The sequence of the input data types given below must not be changed but all data types except "Sample1" can be omitted. After the "SampleN" block another "SampleBg" may appear again followed by "Sample1" etc. for which this new "SampleBg" will be valid. The "SampleName" read from the data file is appended to each line as a comment only and will not be processed. Several additional blank or comment lines may appear in the file. General structure is:

```
Cadmium                 <Run>   <Extension>     -       <SampleName>
   "                       "        "           "           "
Cadmium                 <Run>   <Extension>     -       <SampleName>
End

Water                   <Run>   <Extension>     -       <SampleName>
   "                       "        "           "           "
Water                   <Run>   <Extension>     -       <SampleName>
<Transmission - real>
<Scaling factor - real>
End

WaterBg                 <Run>   <Extension>     -       <SampleName>
   "                       "        "           "           "
WaterBg                 <Run>   <Extension>     -       <SampleName>
<Transmission - real>
End

SampleBg                <Run>   <Extension>     -       <SampleName>
   "                       "        "           "           "
SampleBg                <Run>   <Extension>     -       <SampleName>
<Transmission - real>
<Minimum output extension - integer>
End
```

```
Sample1                    <Run>   <Extension>    -      <SampleName>
      "                       "        "          "          "
Sample1                    <Run>   <Extension>    -      <SampleName>
<Transmission - real>
<Scaling factor - real>
<Attenuation factor - real>
<Scattering probability - real>
End

…

SampleN                    <Run>   <Extension>    -      <SampleName>
      "                       "        "          "          "
SampleN                    <Run>   <Extension>    -      <SampleName>
<Transmission - real>
<Scaling factor - real>
<Attenuation factor - real>
<Scattering probability - real>
End

etc.
```

NOTE:

At the end of the file, a large number of comment lines containing log information generated during the execution of the command file may appear.

Isotropic command file "SANSCIso"

Filename

xxxxxx.SCI   xxxxxx - any set of characters compatible with the operating system

Block "%File"

FileName=xxxxxx.SCI	{ w }	file name
FileDate=<string>	{ d }	date of file creation, in the operating system format
FileTime=<string>	{ d }	time of file creation, in the operating system format
Type=SANSCIso	{ w }	file type identifier
Logging=<string>	{ w }	append log information generated during execution to the command file; <string> = [YES	NO]

Block "%Default"

Lambda=<real>	{ r }	wavelength [nm]
SD=<real>	{ r }	sample-detector distance [m]
BeamcenterX=<real>	{ r }	"X" co-ordinate of the beam center [cells]
BeamcenterY=<real>	{ r }	"Y" co-ordinate of the beam center [cells]
UseDefault=<string>	{ w }	use some values in "%Default" instead of values in "%Commands"; <string> = [YES	NO]
RadialSteps=<real>	{ r }	step width for radial averaging [cells]
Sectors=<integer>	{ i }	number of sectors for radial averaging; for each sector, a separate output file is created
SectorStart=<real>	{ r }	center angle of first sector in the set of output files [deg]
SectorInc=<real>	{ r }	increment for center angles of sectors for radial averaging [deg]
SectorWidth=<real>	{ r }	width of a sector for radial averaging [deg]
MaskFile=<string>	{ w }	name of explicit mask file for radial averaging
ImplicitMask=<string>	{ w }	use implicit mask of anisotropic data files for radial averaging; <string> = [YES	NO]
CalcMode=<string>	{ w }	calculate intensity as a function of different parameters <string> = [INT(Q)	INT(2THETA)	INT(R)]
MagFit=<string>	{ w }	type of additional splitting into nuclear and magnetic component; <string> = [NO	HORIZONTAL	VERTICAL]

Block "%Commands"

List of anisotropic data files to be radially averaged, and of individual values for items Lambda, SD, BeamcenterX and BeamcenterY for each data file. If no individual value is available for a data file it is replaced with an asterisk "*" serving as a dummy character to have a constant number of entries in each line. The "SampleName" read from the data file is appended to each line as a comment only and will not be processed. Several additional blank or comment lines may appear in the file. General structure is:

```
 <Run>  <Ext-In>  <Ext-Out>  <Lambda>  <SD>  <BC-X>  <BC-Y>    -  <SampleName>
   "        "          "          "        "      "        "        "      "

End
```

NOTE

Block "%Default" contains default values of items "Lambda", "SD", "BeamcenterX" and "BeamcenterY" for all data files processed with the command file. If "UseDefault=NO", the defaults for these four items are only used as a substitute for those data files which have no individual values entered in block "%Commands". You can force the program "SANSIsoDo" to override all individual values existing for these four items with the defaults by setting "UseDefault=YES". For all other items in block "%Default", the defaults are always used and no individual settings are allowed.

At the end of the file, a large number of comment lines containing log information generated during the execution of the command file may appear.

Transmission command file "SANSCTrans"

Filename

xxxxxx.SCT	xxxxxx - any set of characters compatible with the operating system

Block "%File"

FileName=xxxxxx.SCT	{ w }	file name
FileDate=<string>	{ d }	date of file creation, in the operating system format
FileTime=<string>	{ d }	time of file creation, in the operating system format
Type=SANSCTrans	{ w }	file type identifier
Logging=<string>	{ w }	append log information generated during execution to the command file; <string> = [YES | NO]

Block "%Default"

Deadtime=<real>	{ r }	electronical deadtime of the detector [sec]
AreaLimits=<string>	{ t }	limits (Xmin Xmax Ymin YMax) of the rectangular detector area used for transmission calculation, separated by spaces
MaskFile=<string>	{ w }	name of mask file used for additional limitation of detector area
ImplicitMask=<string>	{ w }	use implicit mask of input data files for transmission calculation; <string> = [YES | NO]

Block "%Commands"

List of raw or anisotropic input data files to be used for transmission calculation. Each data type block is terminated by the reserved word "End". The sequence of the input data types given below must not be changed but all data types except "EmptyHole" and "Sample1" can be omitted. After the "SampleN" block another "EmptyHole" may appear again followed by "Sample1" etc. for which this new "EmptyHole" will be valid. The "SampleName" read from the data file is appended to each line as a comment only and will not be processed. Several additional blank or comment lines may appear in the file. General structure is:

```
Cadmium            <Run>   <Extension>    -      <SampleName>
   "                 "          "         "           "
Cadmium            <Run>   <Extension>    -      <SampleName>
End

EmptyHole          <Run>   <Extension>    -      <SampleName>
   "                 "          "         "           "
EmptyHole          <Run>   <Extension>    -      <SampleName>
End

Sample1            <Run>   <Extension>    -      <SampleName>
   "                 "          "         "           "
Sample1            <Run>   <Extension>    -      <SampleName>
End

…

SampleN            <Run>   <Extension>    -      <SampleName>
   "                 "          "         "           "
SampleN            <Run>   <Extension>    -      <SampleName>
End

etc.
```

NOTE:

At the end of the file, a large number of comment lines containing log information generated during the execution of the command file may appear.

Anisotropic data file "SANSDAni"

Filename

Dnnnnnnn.eee   nnnnnn - 7-digit number; eee - 3-digit number

Block "%File"

FileName=Dnnnnnnn.eee	{ w }	file name
FileDate=<string>	{ d }	date of file creation, in the operating system format
FileTime=<string>	{ d }	time of file creation, in the operating system format
Type=SANSDAni	{ w }	file type identifier
DataSize=4096	{ i }	number of detector cells
Title=<string>	{ t }	measurement title (1)
User=<string>	{ t }	user name (1)

Block "%Sample"

SampleName=<string>	{ t }	sample name (1)
Environment=<string>	{ t }	sample environment string set in measurement program (1)
Omega=<real>	{ r }	"Omega" co-ordinate of turntable position [deg] (1)
Phi=<real>	{ r }	"Phi" co-ordinate of turntable position [deg] (1)
Chi=<real>	{ r }	"Chi" co-ordinate of turntable position [deg] (1)
Temperature=<real>	{ r }	mean value of control temperature [°C or K] (1)
TempDev=<real>	{ r }	maximum deviation of a momentary control temperature from the mean value [°C or K] (1)
Magnet=<real>	{ r }	current of electromagnet [A] (1)
Pressure=<real>	{ r }	sample pressure [a.u., setup-specific] (1)
Fl1Pickup=<real>	{ r }	pickup voltage of Flipper 1 [V] (1)

Block "%Setup"

Lambda=<real>	{ r }	wavelength [nm] (1)
LambdaC=<integer>	{ i }	selector speed [rpm] (1)
Tilting=<real>	{ r }	selector tilting angle [deg] (1)
Attenuator=<string>	{ w }	attenuator type; <string> = [NONE | ONE | TWO | THREE] (1)
Collimation=<integer>	{ i }	collimation length [m] (1)
SD=<real>	{ r }	sample-detector distance [m] (1)
SY=<real>	{ r }	detector lift [cm] (1)
Beamstop=<string>	{ w }	beamstop type; <string> = [SMALL | MEDIUM | LARGE] (1)
BeamstopX=<real>	{ r }	"X" co-ordinate of beamstop center [cells] (1)
BeamstopY=<real>	{ r }	"Y" co-ordinate of beamstop center [cells] (1)

Block "%History"

TotalTime=<real>	{ r }	sum of counters "TIME" in all sample data files [sec]
Transmission=<real>	{ r }	sample transmission to be used in next step of data reduction
Scaling=<real>	{ r }	sample scaling factor to be used in next step of data reduction
Attenuation=<real>	{ r }	sample attenuation factor to be used in next step of data reduction
Probability=<real>	{ r }	sample scattering probability to be used in next step of data reduction
BeamcenterX=<real>	{ r }	"X" co-ordinate of the beam center [cells] (1)
BeamcenterY=<real>	{ r }	"Y" co-ordinate of the beam center [cells] (1)
MaskFile=<string>	{ w }	name of last mask file used for implicit masking (2)

Block "%Comment"

Any number of text lines containing more or less useful information. All characters are allowed except "%", "*" or " " as the first character in a line.

Block "%Counts"

512 lines of 8 real numbers each, formatted "1PE10.3", without separators. Contain counts from 4096 detector cells. Format is +0.000E+00 (= 10 characters per number). Values are normalized to the monitor.

Block "%Errors"

512 lines of 8 real numbers each, formatted "1PE10.3", without separators. Contain errors from 4096 detector cells. Format is +0.000E+00 (= 10 characters per number). A negative value denotes a masked cell, a zero value denotes an invalid cell. Values are normalized to the monitor.

NOTE

The program "SANSAniDo" always uses the last run number of the input data files for a particular sample as the run number for the output data file. The item values marked (1) are taken from this last input file only. The item values marked (2) are taken from the command file "*.SCA" that produced the output data file. There is no check if these values are the same in all input files. All other unmarked item values are newly defined by the program "SANSAniDo".

Isotropic data file "SANSDIso"

Filename

Dnnnnnnn.eee   nnnnnn - 7-digit number; eee - 3-digit number

Block "%File"

FileName=Dnnnnnnn.eee	{ w }	file name
FileDate=<string>	{ d }	date of file creation, in the operating system format
FileTime=<string>	{ d }	time of file creation, in the operating system format
Type=SANSDIso	{ w }	file type identifier
Title=<string>	{ t }	measurement title (1)(4)(6)
User=<string>	{ t }	user name (1)(4)(6)
ContentX=<string>	{ w }	content of 1st column of block "%Counts"; <string> = [Q	2Theta	Cell]
ContentY=<string>	{ w }	content of 2nd and 3rd column of block "%Counts"; <string> = [Cut	AvgSector	AvgFull	FitNuc	FitMag	FitAdd]

Block "%Sample"

SampleName=<string>	{ t }	sample name (1)(4)(6)
Environment=<string>	{ t }	sample environment string set in measurement program (1)(4)(6)
Omega=<real>	{ r }	"Omega" co-ordinate of turntable position [deg] (1)(4)(6)
Phi=<real>	{ r }	"Phi" co-ordinate of turntable position [deg] (1)(4)(6)
Chi=<real>	{ r }	"Chi" co-ordinate of turntable position [deg] (1)(4)(6)
Temperature=<real>	{ r }	mean value of control temperature [°C or K] (1)(4)(6)
TempDev=<real>	{ r }	maximum deviation of a momentary control temperature from the mean value [°C or K] (1)(4)(6)
Magnet=<real>	{ r }	current of electromagnet [A] (1)(4)(6)
Pressure=<real>	{ r }	sample pressure [a.u., setup-specific] (1)(4)(6)
Fl1Pickup=<real>	{ r }	pickup voltage of Flipper 1 [V] (1)(4)(6)

Block "%Setup"

Lambda=<real>	{ r }	wavelength [nm] (1)(5)(6)
Tilting=<real>	{ r }	selector tilting angle [deg] (1)(4)(6)
Attenuator=<string>	{ w }	attenuator type; <string> = [NONE	ONE	TWO	THREE] (1)(4)(7)
Collimation=<integer>	{ i }	collimation length [m] (1)(4)(7)
SD=<real>	{ r }	sample-detector distance [m] (1)(5)(7)
SY=<real>	{ r }	detector lift [cm] (1)(4)(7)
Beamstop=<string>	{ w }	beamstop type; <string> = [SMALL	MEDIUM	LARGE] (1)(4)(7)
BeamstopX=<real>	{ r }	"X" co-ordinate of beamstop center [cells] (1)(4)(7)
BeamstopY=<real>	{ r }	"Y" co-ordinate of beamstop center [cells] (1)(4)(7)

Block "%History"

TotalTime=<real>	{ r }	sum of counters "TIME" in all sample data files [sec] (1)(4)(7)
BeamcenterX=<real>	{ r }	"X" co-ordinate of the beam center [cells] (1)(5)(7)
BeamcenterY=<real>	{ r }	"Y" co-ordinate of the beam center [cells] (1)(5)(7)
RadialSteps=<real>	{ r }	step width used for radial averaging [cells] (3)(5)(7)
SectorCenter=<real>	{ r }	center angle of sector used for radial averaging [deg] (2)(5)(6)
SectorWidth=<real>	{ r }	width of sector used for radial averaging [deg] (2)(5)(6)
MaskFile=<string>	{ w }	name of explicit mask file used for radial averaging (2)(5)(7)

ImplicitMask=<string>   { w }   implicit mask of anisotropic data file used for radial averaging;
                                            <string> = [YES | NO] (2)(5)(7)

Block "%Comment"

Any number of text lines containing more or less useful information. All characters are allowed except "%", "*" or " " as the first character in a line.

Block "%Counts"

Varying number of lines containing 3 real numbers each, formatted "1PE10.3", separated by commas. Format is +0.000E+00 (= 10 characters per number).

Each line represents the following information for one data point:

- 1st number: Q [nm^{-1}], 2θ [deg] or R [cells], depending on item "ContentX"
- 2nd number: Intensity [cm^{-1}*sr^{-1}], calculated with the method denoted in "ContentY".
- 3rd number: Error [cm^{-1}*sr^{-1}], calculated with the method denoted in "ContentY".

NOTE

If the file has been created as a cut through an anisotropic input data file with the program "SANSAniPlot", item values marked (1) are normally taken from this input file. Only if one of these items is not present in the input file, but required for the calculation of the cut, the program "SANSAniPlot" prompts for this item and writes the item value entered to the isotropic output data file. Item values marked (2) are set during the interactive dialogues in program "SANSAniPlot". Any values for these items that may be present in the input file will be ignored. Item values marked (3) are not present in the output data file since they do not have a relation to the creation method applied.

If the file has been created by radial averaging or sin^2(ψ)-fitting of an anisotropic input data file with the program "SANSIsoDo", item values marked (4) are taken from this input file. Item values marked (5) are always taken from the command file "*.SCI" that produced the isotropic output data file. Any values for these items that may be present in the input file will be ignored.

When the program "SANSIsoPlot" is used to combine isotropic data files measured for the same sample in different Q-ranges, this program always uses the run number of the input data file containing the largest Q-values as the run number for the output data file. Item values marked (6) are taken from this input file only. There is no check if these values are the same in all input files. Item values marked (7) contain Q-range-related information. After a combination of different Q-ranges, these items become obsolete, and are therefore omitted from the isotropic output data file.

All other unmarked item values are newly defined by the programs "SANSIsoDo", "SANSAniPlot" or "SANSIsoPlot", respectively.

Raw data file "SANSDRaw"

Filename

Dnnnnnn.eee   nnnnn = 7-digit number; eee = 3-digit number

Block "%File"

FileName=Dnnnnnn.eee	{ w }	file name
FileDate=<string>	{ d }	date of file creation, in the operating system format
FileTime=<string>	{ d }	time of file creation, in the operating system format
Type=SANSDRaw	{ w }	file type identifier
DataSize=4096	{ i }	number of detector cells
FromDate=<string>	{ d }	start date of measurement, in the operating system format
FromTime=<string>	{ d }	start time of measurement, in the operating system format
ToDate=<string>	{ d }	end date of measurement, in the operating system format
ToTime=<string>	{ d }	end time of measurement, in the operating system format
Title=<string>	{ t }	measurement title
User=<string>	{ t }	user name

Block "%Sample"

SampleName=<string>	{ t }	sample name
Environment=<string>	{ t }	sample environment string set in measurement program
Position=<integer>	{ i }	sample position number on sample holder
Omega=<real>	{ r }	"Omega" co-ordinate of turntable position [deg]
OmegaC=<integer>	{ i }	"Omega" co-ordinate of turntable position [codersteps]
Phi=<real>	{ r }	"Phi" co-ordinate of turntable position [deg]
PhiC=<integer>	{ i }	"Phi" co-ordinate of turntable position [codersteps]
Chi=<real>	{ r }	"Chi" co-ordinate of turntable position [deg]
ChiC=<integer>	{ i }	"Chi" co-ordinate of turntable position [codersteps]
Temperature=<real>	{ r }	mean value of control temperature [°C or K]
TempDev=<real>	{ r }	maximum deviation of a momentary control temperature from the mean value [°C or K]
Temp1=<real>	{ r }	additional temperature [°C or K]
Temp2=<real>	{ r }	additional temperature [°C or K]
Temp3=<real>	{ r }	additional temperature [°C or K]
Temp4=<real>	{ r }	additional temperature [°C or K]
Magnet=<real>	{ r }	current of electromagnet [A]
Pressure=<real>	{ r }	sample pressure [a.u. setup-specific]
Fl1Frequency=<real>	{ r }	rf frequency of Flipper 1 [kHz]
Fl1Amplitude=<real>	{ r }	rf amplitude of Flipper 1 [V]
Fl1Pickup=<real>	{ r }	pickup voltage of Flipper 1 [V]

Block "%Setup"

Lambda=<real>	{ r }	wavelength [nm]
LambdaC=<integer>	{ i }	selector speed [rpm]
Tilting=<real>	{ r }	selector tilting angle [deg]
TiltingC=<integer>	{ i }	selector tilting angle [codersteps]
Attenuator=<string>	{ w }	attenuator type; <string> = [NONE | ONE | TWO | THREE]
Collimation=<integer>	{ i }	collimation length [m]
SD=<real>	{ r }	sample-detector distance [m]
SDC=<integer>	{ i }	sample-detector-distance [codersteps]
SY=<real>	{ r }	detector lift [cm]
SYC=<integer>	{ i }	detector lift [codersteps]
Beamstop=<string>	{ w }	beamstop type; <string> = [SMALL | MEDIUM | LARGE]

BeamstopX=<real>	{ r }	"X" co-ordinate of beamstop center [cells]
BeamstopXC=<integer>	{ i }	"X" co-ordinate of beamstop center [codersteps]
BeamstopY=<real>	{ r }	"Y" co-ordinate of beamstop center [cells]
BeamstopYC=<integer>	{ i }	"Y" co-ordinate of beamstop center [codersteps]

Block "%Counter"

Sum=<integer>	{ i }	total number of counts in block "%Counts"
Time=<real>	{ r }	value of counter "TIME" [sec]
Moni1=<integer>	{ i }	value of counter "MONI1"
Moni2=<integer>	{ i }	value of counter "MONI2"
Moni3=<integer>	{ i }	value of counter "MONI3"
Sum/Time=<real>	{ r }	calculated value [sec^{-1}]
Sum/Moni1=<real>	{ r }	calculated value
Sum/Moni2=<real>	{ r }	calculated value
Sum/Moni3=<real>	{ r }	calculated value

Block "%History"

Transmission=<real>	{ r }	sample transmission to be used in next step of data reduction
Scaling=<real>	{ r }	sample scaling factor to be used in next step of data reduction
Attenuation=<real>	{ r }	sample attenuation factor to be used in next step of data reduction
Probability=<real>	{ r }	sample scattering probability to be used in next step of data reduction
BeamcenterX=<real>	{ r }	"X" co-ordinate of the beam center [cells]
BeamcenterY=<real>	{ r }	"Y" co-ordinate of the beam center [cells]

Block "%Comment"

Any number of text lines containing more or less useful information. All characters are allowed except "%", "*" or " " as the first character in a line.

Block "%Counts"

512 lines of 8 integer numbers each, separated by commas. Contain counts from 4096 detector cells. Valid range is 0…2 147 483 647 (= max. 10 characters plus one separator per number). Values are not normalized to the monitor.

Mask file "SANSM"

Filename

xxxxxx.MSK   xxxxxx - any set of characters compatible with the operating system

Block "%File"

FileName=xxxxxx.MSK   { w }   file name
FileDate=<string>   { d }   date of file creation, in the operating system format
FileTime=<string>   { d }   time of file creation, in the operating system format
Type=SANSM   { w }   file type identifier
DataSize=4096   { i }   number of detector cells

Block "%Comment"

Any number of text lines containing more or less useful information. All characters are allowed except "%", "*" or " " as the first character in a line.

Block "%Mask"

<DetectorSize> lines of <DetectorSize> characters each. "-" represents a detector cell that is used for data reduction. "#" represents a detector cell that is hidden.

Initialization file "BerSANS.INI"

Filename

BerSANS.INI   pre-defined name

Block "%File"

FileName=BerSANS.INI   { w }   file name
Type=SANSIni   { w }   file type identifier

Block "%Printer"

Text lines containing a desription of the local printers available. All characters are allowed except "%", "*" or " " as the first character in a line.

NOTE

The purpose of this initialization file is to define miscellaneous permanent settings of the "BerSANS" program package outside the source code, but hidden from the normal program interfaces. This enables experienced users to customize their local software copies without re-compilation of the programs. The initialization file is read by each program which uses at least a part of its content, but a particular program may not use all of it. The initialization file is only read once when the programs start. Thus, modifications will only become effective after program termination and restart.

Editing of the file should be done carefully, in order to avoid "unusual" program responses. All entries are expected to be correct. If a severe error occurs in the file structure, the programs abort during startup. A detailed description of the file structure is contained as comment lines within the file itself. There are no specific programs for creation or modification of this file within the "BerSANS" program package.