
# S_U_P_E_R_S_A_X_S

## PROGRAM PACKAGE FOR DATA TREATMENT, ANALYSIS AND MODELING

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USER MANUAL v_1.0

## 1. INTRODUCTION

Data treatment for measured data is the crucial part for a well succeed data analysis. Particularly for Small Angle Scattering (SAS) a trustful data treatment is necessary for the correct interpretation of the data and posterior modeling. In this manual we present a package of home-build programs which were made using algorithms that have been largely used by Professor Jan Skov Pedersen in many years of his work. This is the beta version of the manual for the programs and many mistakes might be found.

## 2. GENERAL INFORMATION

The programs are made in FORTRAN™ and uses GNUPLOT™ graphical interface. At the actual stage of development the programs were made for Intel-PC machines with WINDOWS™ operating systems. The installation is simple and requires only the copy of the executable files to a folder inside of the machine and the configuration of the system path according to the following instructions:

```
Installation instructions:
       1- Create a folder where you want to store the files (ex: c:\SUPERSAXS)

IN WIN95,98 MACHINES
       2- Add these lines to autoexec.bat
                REM Sets to path
                SET PATH=%PATH%;C:\SUPERSAXS
In WIN2000
        2- Find the autoexec.nt file.
             Search this file, add the above lines and restart the machine.

In WINXP or later
       2- Click on START->CONTROL PANEL->SYSTEM
          In the window System Properties click on the tab Advanced
          Click on the button Environment Variables
          In System Variables find the variable Path
          Click on it and later in Edit
          In Variable value add the full path for the programs (ex: c:\SUPERSAXS), separating
            from the previous input using dot-comma ";"

       3- Copy the MS-DOS Prompt shortcut from the programs folder to the folder that you want to work
out.

       4- Run this shortcut and in the command window, call the program name to run it.

       6- For a list of available programs, type "progs (Enter)"
```

The available programs can be seen typing PROGS↵[1]. The following programs are in the package:

```
*****************************************
         S_U_P_E_R_S_A_X_S   PROGRAMS
*****************************************
List of Available Programs:
LIST.EXE    -> Creates file lists for other programs
WAVG.EXE    -> Averages RAD RDS RSR files giving chi2
WCOMP.EXE   -> Compares and rescales two input files
WCOMV.EXE   -> Converts any data file to JSP format files
WGNUPLOT.EXE-> Gnuplot Program  (www.gnuplot.info)
WGCNORM.EXE -> Creates a normalization file for beam stopper shadow correction
WPLOT.EXE   -> Plots JSP format files. Reads a list of files.
WREBINL.EXE -> Performs a logarithm rebinning of input files. Reads TORAD.FIL file.
WSXH2O.EXE  -> Data treatment for water files and zero intensity fit
WSXSUB.EXE  -> Data treatment for SAXS data files and normalization to absolute scale
WTORAD.EXE  -> Converts RAW files to RAD files. Reads TORAD.FIL file.
```

[1] The symbol ↵ will be uses to represent [ENTER] button.

## 3. FILE EXTENSIONS

In some cases the programs assume pre-defined file extensions. In this way, to work with the programs is easier to adopt the following extensions

```
RAW files-> Angular Integrated Data from the acquisition program
RAD files-> RAW data converted to JSP format
RDN files-> Beam stopper shadow correction file
RDS files-> Background subtracted Data
RSR files-> Rebinned data
SCA files-> Scaled Data
PAR files-> Water normalization values
LIS files-> List of files for many applications
```

## 4. CREATING LISTS

The programs use list direct procedures. In this working approach the file names are passed to the programs using lists of file names. The SUPERSAXS package has a program to create the list of files in a very fast way. In your working directory open the command window and type LIST↵. The following options will appear:

```
*****************************************
*                                       *
*      G E N E R A T E      L I S T     *
*                                       *
*supersaxs programs         crislpo 22/09/08*
*****************************************

Create list for :
 (1) CONVERT FILES TO RAD AND RSR
 (2) DATA TREATMENT LIST FILE
 (3) PLOT LIST FILE
 (4) AVERAGE LIST FILE
 (5) JOIN FILES INTO ONE MATRIX
 (6) DATA FITTING LIST
 (7) LARGE DATASETS TOOLS

Select Option :
```

In the next topics each option will be explained. The program LIST creates the necessary file lists for the other programs and can also call the other programs in the working procedure.

## 5. CONVERTING FILES RAW->RAD

The SUPERSAXS programs use files in JSP format (.RAD files). This format are represented below in the two possible cases:

*A. When using normal beam stopper*

In this case is necessary to transfer the information about incident intensity (relative), time and sample transmission to the data treatment procedure. This information will be stored in the file header:

```
 I_PE (cps)      TIME          TRANSM
 580.500        300.000       0.495000
      161
0.000000        1.04840        1.04840       0.000000
0.142200E-02    1.42578       0.417893       0.200000E-01
0.284500E-02    5.83120       0.597596       0.400000E-01
0.426700E-02    19.5603       0.893654       0.600000E-01
...
```

The next line is the number of points and the subsequent lines are the scattering data. The columns are the: “q” values, intensity, errors and a dummy column. In RAD format this column will be the 2θ values.

*B. When using semi transparent beam stopper*

The values of incident beam and sample transmission will be obtain directly form the scattering data. In this case is only necessary to store the exposition time:

```
    TIME
10800.0000
246
0.00000000E+00 12961.2031 207.106979 0.00000000E+00
1.42200000E-03 11353.3076 60.5847626 1.99999996E-02
2.84500001E-03 7266.95654 34.3846741 3.99999991E-02
4.26700013E-03 3280.74048 18.8632793 5.99999987E-02
...
```

Creating list of files to convert:

- In the command window type LIST↵.
- Select option number 1
- Type extension RAW↵
- A list of .RAW files will be shown
- Type the number of files to convert. If you want to convert all files, type -1.
- If you haven't selected all files, type the file indexes. Note that you have just to type the file indexes, not the file names.
- The list of files will be saved in file TORAD.FIL

Converting files:

- If you just created the list with program LIST you can select option 1 in the last line. This will call the program WTORAD.
- In the case that you have finished the program LIST, in the command window type WTORAD↵.
- Select normalization parameters. Option (1) for type all values to the files. Option (2) if you have used semi transparent beam stopper.
- If you selected option (2) you can choose to use the same value of time for all files. Type Y or N and ↵.
- Type the parameters. In case (1) you have to type I_PE, Time and Transmission. In case (2) just Time is needed.
- Repeat the procedure for all files.

## 6. CREATING SHADOW CORRECTION FILE

Creating shadow correction file:

- In the command window type WGCNORM↵. A list of .RAD files will be shown
- Select desired file index. Generally the Glassy Carbon file.
- The converted file will be saved with extension .RDN

## 7. DATA TREATMENT

The expression used for the data treatment is given by[2],

$$I_{Treated}(q)=\left[\left(\frac{I_{sample}(q)}{\Phi_s.T_s.t_s}-\frac{I_{back}(q)}{\Phi_b.T_b.t_b}-\frac{I_{noise}(q)}{t_{noise}\left(\Phi_s.T_s-\Phi_b.T_b\right)}\right)\frac{1}{I_{shadow}(q)}\right]\frac{d\Sigma/d\Omega_{water,20^oC}}{I(0)_{water,20^oC}}$$

And the error propagation is given by[3]

[2] For a description about SAXS data treatment check *chapter 2 on Neutrons, X-rays and Light: Scattering Methods Applied to Soft Condensed Matter, Lindner and Zemb (2002)*

[3] For a description about error calculation and propagation check *Bevington (1992), Data Reduction and Error Analysis for the Physical Sciences*

$$\sigma_{treated}(q) = \left( \frac{\sigma_1(q)^2}{I_{shadow}(q)^2} + \left( \frac{I_{sample}(q)}{\Phi_s.T_s.t_s} \right)^2 \frac{\sigma_{shadow}(q)^2}{I_{shadow}(q)^2} \right)^{1/2}$$

$$\sigma_1(q) = \sigma_{sample}(q)^2 + \sigma_{back}(q)^2 + \sigma_{noise}(q)^2 . \left( \frac{1}{\Phi_s.T_s} - \frac{1}{\Phi_b.T_b} \right)^2$$

Where,

- ***I(q)*** is the measured (integrated) scattering intensities
- ***Φ*** is the intensity incident beam
- ***T*** is the sample transmission
- ***t*** is the exposition time
- ***σ(q)*** is the statistical error of each point.
- ***$I_{shadow}$ (q) , $\sigma_{shadow}$ (q)*** are the normalized intensity and error for the beam stopper shadow correction
- ***(dΣ/dΩ)=0.01632 [$cm^{-1}$]*** is the theoretical scattering cross section for water at 20ºC.

The data treatment assumes that you have converted all RAW files to RAD format and also that you have the Shadow correction file. It is also necessary to have a noise file (measurement with the beam blocked by a piece of lead) and the normalization water files. For option (1) the program assumes that you have the file WATER.PAR in the working directory. For option (2) the file WATERNM.PAR will be used. To create the files see the topic CREATING WATER FILES. The format of the water files is shown below:

```
WATER.PAR: PE_INT, TIME, TRANSMISSION, I(0)
561.1, 14400, 0.1357, 1.0424
561.1, 14400, 0.1357, 1.0424
…

WATERNM.PAR: TIME, I(0)
1800,136.22
1800,129.85
…
```

The number of lines corresponds to the number of capillaries that you have used in your experiment. Note that just the numbers have to be present in the water files.

For the data treatment the intensity files, background files, shadow correction file, noise and water file has to be in the same directory.

Creating list of files to treat:

- In the command window type LIST↵.
- Select option number 2
- Select Creation Mode. In mode (1) all parameters (capillary number, intensity file and background file) will be asked every time. In mode (2) the capillary number and background file is asked once and used for the rest of the list.
- Type list file name. Use extension .LIS
- A list of .RAD files will be shown. Type the number of files that you want to treat. Note that this is the number of intensity files that you want to workout, not the number of intensity + number of background files.
- Select noise file. Generally the “lead” file.
- Select shadow correction file.
- Type first capillary number.
- Select first Intensity File
- Select first Backgound File
- Type scale of transmission. Press ↵ for the default 1.0
- Type second capillary number.

- Select second Intensity File
- Proceed until reach the number of files
- List Saved!

If you have made some mistake in the list creation, you can correct it opening the list in any text editor, or running LIST again.

Performing Data Treatment:

- If you just created the list with program LIST you can select option 1 in the last line. This will call the program WSXSUB.
- In the case that you have finished the program LIST, in the command window type WSXSUB↵.
- Select BATCH MODE (1) or INTERACTIVE MODE (2). In batch mode the program performs the data treatment without interaction with user and without showing any graph. In interactive mode the program show the data treatment for each file and the user can correct/change it.
- Select Machine Setup. High Resolution (H : long distance), Standard (S), Low Resolution (L : short distance) or Custom (C : Custom). If you select "Custom" the number of points to be integrated behind the beam stop will be asked.
- Select normalization parameters. Option (1) for type all values to the files. Option (2) if you have used semi transparent beam stopper.
- A list of .LIS files will be shown.
- Select the data treatment list file.
- In Batch mode the program will perform the data treatment until the last file. The output files are save with the same file name as the input files but with extension .RDS
- In Interactive mode a list of treatment values is shown in the command window and a graphic window with plots for the Intensity file, background file and treated file.
- Close the graphic window pressing ↵ or clicking on OK button in *gnuplot pause window*.
- Now you can change the scale of transmission. This will change the amount of background that is subtracted from the intensity file. As a default, 1.0 (100%) is subtracted. If you are satisfied with the treatment result it is not necessary to change this number. Press N↵ and proceed to the other file. If you want to correct the data treatment, press Y↵, type the new value, and check in the graphic window if the results are acceptable. If you are satisfied press N↵ in scale of transmission and proceed to other file.
- Treat the files until the end of the list. The output files are save with the same file name as the input files but with extension .RDS
- The program creates a file called OUTPUT.DAT where a short summary of the data treatment is stored.

## *8. REBINNING DATA*

Having the treated RDS files it is possible to perform a logarithm rebinning of the data, which will decrease the number of points by an average of the data, spacing the points logarithmically in the "X" scale.

Creating list of files to rebin:

- In the command window type LIST↵.
- Select option number 1
- Type extension RDS↵
- A list of .RDS files will be shown
- Type the number of files to convert. If you want to convert all files, type -1.

- If you haven't selected all files, type the file indexes. Note that you have just to type the file indexes, not the file names.
- The list of files will be saved in file TORAD.FIL

Rebinning files:

- If you just created the list with program LIST you can select option 2 in the last line. This will call the program WREBIN.
- In the case that you have finished the program LIST, in the command window type WREBIN↵.
- The program will perform the logarithm rebinning until the last file name.

## 9. SCALING AND COMPARING DATASETS

Files comparison and scale is very useful when dealing with a series of concentrations. Changes on the concentration of a sample can, besides of many other possible effects, promote the formation of aggregates or increase the particle interaction. In both cases the initial part of the scattering profile will be affected.

Because of these possible effects, to comparing curves a decremental comparison is applied. In this procedure initially the full curve (N points) are compared and scaled ($\chi^2$ value, scale factor and background factor for the N points). In the next step the first point is skipped and the remaining (N-1) points are scaled ($\chi^2$ value, scale factor and background factor for the N-1 points). Next the two first points are skipped and the process continues until the end of file.

A plot of the $\chi^2$ values vs. initial point is shown and the user has to choose one value for the initial point. In general a value where the $\chi^2$ is in a plateau is the right value. However if the curves are different in the whole comparison it will never be shown a plateau and the $\chi^2$ values will be close to 1. Just in the end of the curve which means that just a few points are compared.

To compare and scale curves follow:

- In the command window type WCOMP↵.
- Type the desired extension or -1 to write the file names
- In the case where you typed the extension a list of files will be shown.
- Select the first file index or type the first file name.
- Select the second file index or type the second file name
- A plot of $\chi^2$ values vs. point number will be shown. Look for the best point number.
- Close the graphic window pressing ↵ or clicking on OK button in *gnuplot pause window*.
- Type selected point number.
- Type the output file name.
- Do you want to plot? (Y/N)
- If YES follow the instructions on the screen and check the comparison (see the topic PLOTING CURVES).
- The scaled file is saved with the desired filename.

## 10. PLOTTING CURVES

Given a list of files plot them with specified X- Y- axis.

Creating list of files to plot:

- In the command window type LIST↵.
- Select option number 3
- Type list file name.
- Type desired extension.
- A list of files will be shown.

- Type the number of files to plot.
- Type the file indexes. Note that you have just to type the file indexes, not the file names.
- Type scale factor and background factor for each file. The default values are 1.0 and 0.0
- Add more file extensions to plot? If "Y" you type the new file extension and choose the other files.
- The list is saved. If you have made some mistake you can edit the list of files manually or create it again.
- Plot Results? If press "N" the program is finished.

Plotting curves

- If you just created the list with program LIST you can select "Y" in the last line. This will call the program WPLOT.
- If you call program WPLOT you have to write the list file name. In this case the file names will be listed and you select the number of files you want to plot.
- Input background factor to be subtracted from all files. As default this value is 0.0
- Choose between symbols or curves (default) to plot the files.
- Choose the Y-axis. Eleven options are available.
- Choose X-axis. Four options are available.
- A graphic window with the plots for the input files will be shown.
- Close the graphic window pressing ↵ or clicking on OK button in *gnuplot pause window*.
- Plot again (Y,N=def)? If you select "Y" you can select again the number of files to be plotted and change the X- Y- axis. Selecting "N" the program is finished.

## *11. AVERAGING FILES*

Given a series of files the program average them, calculating the correct resulting error value and showing the $\chi^2$ value of the files when compared with the first file of the list.

Creating list of files to average:

- In the command window type LIST↵.
- Select option number 4
- Type desired extension.
- A list of files will be shown.
- Type the number of files to average. If you want to convert all files, type -1.
- If you haven't selected all files, type the file indexes. Note that you have just to type the file indexes, not the file names.
- Type the list file name.
- The list is saved.

Averaging Files:

- If you just created the list with program LIST you can select "Y" in the last line. This will call the program WAVG.
- In the case that you have finished the program LIST, in the command window type WAVG↵.
- A list of .LIS files will be shown.
- Select corresponding average list file.
- The filenames of list file will be shown
- Type the number of files to average (-1 for all files).
- Type the output file name (without extension).

- The files are averaged and the values of $\chi^2$ of the files corresponding to the first file are shown on the screen.
- The average is saved with the desired file name and extension .AVG

## 12. JOINING FILES IN ONE MATRIX

Given a series of files the program joins all them in one file, using only one X-axis column. The intensity columns of each file are stored in sequence without error values.

Joining files in one matrix:

- In the command window type LIST↵.
- Select option number 5
- Type desired extension.
- A list of files will be shown.
- Type the number of files to add.
- Type the file indexes. Note that you have just to type the file indexes, not the file names.
- The joined files are saved in file FILEOUT.DAT

## 13. CREATING WATER FILES

The procedure is similar to the normal data treatment of scattering data. It is necessary to have scattering data for the water samples and also for the empty capillaries. These empty capillaries intensities will be used as background for the water files.

Creating list of WATER files to treat:

- In the command window type LIST↵.
- Select option number 2
- Select Creation Mode. In mode (1) all parameters (capillary number, intensity file and background file) will be asked every time. In mode (2) the capillary number and background file is asked once and used for the rest of the list.
- Type list file name. Use extension .LIS
- A list of .RAD files will be shown. Type the number of files that you want to treat. Note that this is the number of intensity files that you want to workout, not the number of intensity + number of background files.
- Select noise file. Generally the “lead” file.
- Select shadow correction file.
- Type first capillary number.
- Select first WATER File
- Select first EMTPY CAPILLARY File
- Type scale of transmission. Press ↵ for the default 1.0
- Type second capillary number.
- Select second Intensity File
- Proceed until reach the number of files
- List Saved!

If you have made some mistake in the list creation, you can open the list in any text editor and correct it.

Performing Data Treatment:

- If you just created the list with program LIST you can select option 1 in the last line. This will call the program WSXH2O.
- In the case that you have finished the program LIST, in the command window type WSXH2O↵.

- Select normalizatio0n parameters. Option (1) for type all values to the files. Option (2) if you have used semi transparent beam stopper.
- A list of .LIS files will be shown.
- Select the data treatment list file.
- A graphic window with plots for the Intensity file, background file and treated file will be shown.
- Close the graphic window pressing ↵ or clicking on OK button in *gnuplot pause window*.
- You can change the scale of transmission as mention before for the Data Treatment process.
- Select fitting interval for the linear fit. Type Qmin and Qmax values.
- A plot with the linear fit of the intensity will be shown.
- Close the graphic window pressing ↵ or clicking on OK button in *gnuplot pause window*.
- Change Q fitting range(Y/N)? Selecting "Y" you can change the Qmin and Qmax values and check again the fitting in the graphic window. Selecting "N" the program proceeds to the next file.
- Treat the files and fit the linear water curves until the end of the list. The output files are save with the same file name as the input files but with extension .RDS
- The program creates a file called OUTPUT.DAT where a short summary of the data treatment is stored, including the fitting results values necessary for the water files.

The format of the water files is shown below:

```
WATER.PAR: PE_INT, TIME, TRANSMISSION, I(0)
561.1, 14400, 0.1357, 1.0424
561.1, 14400, 0.1357, 1.0424
...

WATERNM.PAR: TIME, I(0)
1800,136.22
1800,129.85
...
```

The number of lines corresponds to the number of capillaries that you have used in your experiment. Note that just the numbers have to be present in the water files.

## *14. LARGE DATASETS TOOLS*

The procedures presented above are mostly applied for a low number of datasets where each file can be selected individually from a list. When dealing with a large number of files, for example, from a time resolved experiment, etc, it is very time consuming to work out the files using the presented tools. In this way a special option for the SUPERSAXS programs as created in order to deal with large number of datasets in a simple way.

In your working directory open the command window and type LIST↵. The following options will appear:

```
C:\crislpo\DOS-Prog>list
*****************************************
*                                       *
*     G E N E R A T E     L I S T       *
*                                       *
*supersaxs programs         crislpo 22/09/08*
*****************************************

Create list for :
 (1) CONVERT FILES TO RAD AND RSR
 (2) DATA TREATMENT LIST FILE
 (3) PLOT LIST FILE
 (4) AVERAGE LIST FILE
 (5) JOIN FILES INTO ONE MATRIX
 (6) DATA FITTING LIST
 (7) LARGE DATASETS TOOLS
```

Selecting option 7 a new set of options appear:

```
Select Option : 7

Create list for :
 (1) CONVERT MANY RAW TO RAD FILES
 (2) CONVERT MANY RDS TO RSR FILES
 (3) TREAT MANY DATA SETS
 (4) PLOT MANY FILES
 (5) EXTRACT DATA FROM GFRM FILES
 (6) EXTRACT CREATION TIMES FROM FILES

Select Option :
```

The first and second options are for converting files from RAW (integrated PLOTSO data from Brucker software) to RAD format and from RDS (treated files) to RSR (rebinned data).

## A) Converting many RAW to RAD format

- In the command window type LIST↵.
- Select option number 7.
- Select option 1.
- Type the desired file extension.
- The program will write the number of files with this extension that are in the working directory. Press ↵ to show the files.
- The files names will be shown in a single indexed list column.
- Select if you want (Y) or not (N) to apply time rules for the list of files. This is needed since the RAD files must have the exposition time in seconds in the file header. If you press "N" no time rule will be assumed and the user will have to write individually each time value. Pressing "Y" it will be possible to use a time rule.
- If you pressed "Y": The program will ask the number of different times you want to add. For example, in a experiment the first frames were measured in 30 seconds, others 600 seconds and the last ones 1000 seconds. In this case the number of different times would be 3.
- The program will ask the breaking point and the exposition time. Starting on the first file, type the file index (as shown in the list) where the first time rule finishes with the exposition time. Next write the index where the second tune rule finishes with the second exposition time and successively until the end of different exposition times. Note that the last break point must be the last file index.
- The list of times that will be used for each file is saved in the file TIMES.FIL
- The list of files to be converted will be saved in file TORAD.FIL

Converting files:

- If you just created the list with program LIST you can select option 1 in the last line. This will call the program WTORAD.
- In the case that you have finished the program LIST, in the command window type WTORAD↵.
- Select normalization parameters. Option (1) for type all values to the files. Option (2) if you have used semi transparent beam stopper.
- If you selected option (2) you can choose to use the same value of time for all files or use the function for large datasets. Type Y, N or L and ↵.
- If you had selected time rules in the previous options, just type L and all files will be automatically converted and saved with the correct times.

- Typing Y the program will ask a single time that will be used for all files.
- Typing N the program will ask the time for each file.
- If you have not used a semi-transparent beamstop you have to write all the needed parameters for each file.

## B) Converting many RDS to RSR format

- In the command window type LIST↵.
- Select option number 7.
- Select option 2.
- Type extension RDS↵
- All RDS files in the directory will be selected and their filenames will be saved in the file TORAD.FIL. The program WREBINL will be called and all the files will be converted automatically to RSR format.

## C) TREAT MANY DATA SETS

This procedure assumes that all scattering data will use the same background file and capillary position.

- In the command window type LIST↵.
- Select option number 7.
- Select option 1.
- Type the file name for the data treatment list. Use extension ".LIS"
- Type capillary number to be used in the WATER.PAR or WATERNM.PAR file.
- Select shadow correction file (glassy carbon). To be able to select the proper file write part of the name or the full name of the RDN file. For example, if the filename is GCFILE.RDN it is sufficient to type GCFI and the program will show all the GCFI* files that are in the directory.
- Type the file index. Note that you have just to type the file index, not the file name. If the list that the program shows does not contain the desired file, type -1 and select the file again.
- Select noise file. Type part of the file and the press ↵.
- Type the file index. Note that you have just to type the file index, not the file name. If the list that the program shows does not contain the desired file, type -1 and select the file again.
- Select background (buffer) file. Type part of the file and the press ↵. Note that this background file will be used for the data treatment of all files.
- Type the file index. Note that you have just to type the file index, not the file name. If the list that the program shows does not contain the desired file, type -1 and select the file again.
- Select intensity files. In a sequential acquisition of data is a common practice to name the files with a ordinal numbering (FILE001.RAD, FILE002.RAD, …, FILEN.RAD). In order to show the right sequence of files is type part of the file name followed by "*.RAD", for example, FILE*.RAD. The program will show all the files with this part of filename and extension[4].
- Select the file interval. You have to type the first and last file index that you want to treat with the selected background file. Note that you have just to type the file indexes, not the file names. If the list that the program shows does not contain the desired files, type -1 -1 and select the interval again.

[4] DOS users, sorry for this amount of details. But some young students do not know that "DIR" means.

- Apply transmission rules? If you know a priori that a some files might have a lower transmission than the background you can explicitly write these values here. Selecting Y the program will ask the number of different transmissions and later the break indexes and transmissions values in a similar way to the time selection present in option (A) above. Selecting N the transmissions will be assumed to be 1.0. Remember that you can always play around with the transmission values later in the data treatment procedure.
- List Saved!

If you have made some mistake in the list creation, you can correct it opening the list in any text editor, or running program LIST again.

Performing Data Treatment:

- If you just created the list with program LIST you can select option 1 in the last line. This will call the program WSXSUB.
- In the case that you have finished the program LIST, in the command window type WSXSUB↵.
- Select BATCH MODE (1) or INTERACTIVE MODE (2). In batch mode the program performs the data treatment without interaction with user and without showing any graph. In interactive mode the program show the data treatment for each file and the user can correct/change it.
- Select Machine Setup. High Resolution (H : long distance), Standard (S), Low Resolution (L : short distance) or Custom (C : Custom). If you select "Custom" the number of points to be integrated behind the beam stop will be asked.
- Select normalization parameters. Option (1) for type all values to the files. Option (2) if you have used semi transparent beam stopper.
- A list of .LIS files will be shown.
- Select the data treatment list file.
- In Batch mode the program will perform the data treatment until the last file. The output files are save with the same file name as the input files but with extension .RDS
- In Interactive mode a list of treatment values is shown in the command window and a graphic window with plots for the Intensity file, background file and treated file.
- Close the graphic window pressing ↵ or clicking on OK button in *gnuplot pause window*.
- Now you can change the scale of transmission. This will change the amount of background that is subtracted from the intensity file. As a default, 1.0 (100%) is subtracted. If you are satisfied with the treatment result it is not necessary to change this number. Press N↵ and proceed to the other file. If you want to correct the data treatment, press Y↵, type the new value, and check in the graphic window if the results are acceptable. If you are satisfied press N↵ in scale of transmission and proceed to other file.
- Treat the files until the end of the list. The output files are save with the same file name as the input files but with extension .RDS
- The program creates a file called OUTPUT.DAT where a short summary of the data treatment is stored. When treating a large dataset in batch mode is a good practice to open this file and check the transmission values.

## D) PLOT MANY DATA FILES

- In the command window type LIST↵.
- Select option number 7.
- Select option 4.

- Type the file name for the plotting list. Use file ".LIS"
- Type desired extension.
- The number of files with the desired extension will be shown. Press ↵ to show the files.
- The files names will be shown in a single indexed list column.
- Type the file interval that you want to plot.
- If wanted different extensions can be added. Type Y and repeat the selection process. If not, press N.
- List saved! Plot Results? (Y/N). If you know that you did any mistake in the file selection, open the list file and edit it manually. Pressing Y the program WPLOT will be called and the selected list of files will be plotted.

Plotting curves

- If you just created the list with program LIST you can select "Y" in the last line. This will call the program WPLOT.
- If you call program WPLOT you have to write the list file name. In this case the file names will be listed and you select the number of files you want to plot.
- Input background factor to be subtracted from all files. As default this value is 0.0
- Choose between symbols or curves (default) to plot the files.
- Choose the Y-axis. Eleven options are available.
- Choose X-axis. Four options are available.
- A graphic window with the plots for the input files will be shown.
- Close the graphic window pressing ↵ or clicking on OK button in *gnuplot pause window*.
- Plot again (Y,N=def)? If you select "Y" you can select again the number of files to be plotted and change the X- Y- axis. Selecting "N" the program is finished.

## E) EXTRACT DATA FROM GFRM FILES

Before all the processes presented above it is necessary to integrate the 2D measured data into a 1D curve. This of course depends on the instrumental facility and acquisition system that is used. In this section it will be assumed two dimensional GFRM files obtained with Brucker systems. After the data acquisition the program enables the integration of the 2D data into a 1D curve using a dialog menu or a command mode, where a list of instructions is red. When dealing with a large amount of files the integration process is, by itself, very time consuming and cumbersome if needed to be done manually. There is also an additional problem. The integrated files might be in format PLOTSO and this file does not contain information about the acquisition time. Because of this it is needed to provide the acquisition times when converting files from RAW to RAD format. All this process, from integration to conversion to RAD format is made easier with this especial option in the SUPERSAXS package.

- In the command window type LIST↵.
- Select option number 7.
- Select option 5.
- The number of files with the desired extension will be shown. Press ↵ to show the files.
- The files names will be shown in a single indexed list column.
- Type the file interval that you want to convert (first, last) and press ↵. The program will now ask information about the integration parameters needed to integrate the 2D spectra.
- 2θ (scattering) angle: Type initial value (in degrees).
- 2θ (scattering) angle: Type final value (in degrees).
- Chi (circle) angle: Type initial value (in degrees).

- Chi (circle) angle: Type final value (in degrees). For full circle type, for example, zero as initial value and 360 for the final value.
- Type the desired step in Chi (circle) angular. In general this value must be 0.02 or 0.05 depending on the machine setup.
- Pressing ↵ a multistep process will be performed. First each 2D GFRM file will be opened and the acquisition time will be read. The files TORAD.FIL and TIMES.FIL needed later to convert to RAD format using the program WTORAD.EXE will also be created. Finally, the file RUN.SLM is also created. This file contains the commands recognized by Brucker systems to perform the 2D integration and saving of each gfrm file. The output integrated files will have the same filename but extension RAW.
- In the command mode interface of your Brucker system program, call the file RUN.SLM created above. The integration of each file will be performed. This can take several minutes, depending on the number of frames that you collected.
- After the integration of all frames in the command window call the program WTORAD.EXE.
- The file TIMES.FIL created above is only useful if the semi transparent beamstop is used.
- Select normalization parameters. Option (1) for type all values to the files. Option (2) if you have used semi transparent beam stopper.
- If you selected option (2), type L and all files will be converted with the correct acquisition times red from the GFRM files.
- If you have not used a semi-transparent beamstop you have to write all the needed parameters for each file.

One additional, and very important, information is retrieved from the GFRM files. The file names, acquisition date, time and time spam of each file related to the oldest one is saved in the file GFRM_TIMES.DAT. This is better explained in the next section, but a typical file is shown below:

| FILENAMES | FILE DATE | FIL TIME | DIF IN SEC |
|---|---|---|---|
| S7_001.gfrm | 05/11/2008 | 11:32:26 | 0 |
| S7_002.gfrm | 05/11/2008 | 11:52:40 | 1214 |
| S7_003.gfrm | 05/11/2008 | 12:12:54 | 2428 |
| S7_004.gfrm | 05/11/2008 | 12:33:06 | 3640 |
| S7_005.gfrm | 05/11/2008 | 12:53:20 | 4854 |
| S7_006.gfrm | 05/11/2008 | 13:13:34 | 6068 |
| S7_101.gfrm | 05/11/2008 | 20:45:46 | 33200 |
| S7_102.gfrm | 05/11/2008 | 22:17:18 | 38692 |
| S7_103.gfrm | 05/11/2008 | 23:48:50 | 44184 |
| S7_104.gfrm | 06/11/2008 | 01:20:22 | 49676 |
| S7_105.gfrm | 06/11/2008 | 02:51:52 | 55166 |
| S7_106.gfrm | 06/11/2008 | 04:23:24 | 60658 |
| S7_107.gfrm | 06/11/2008 | 05:54:56 | 66150 |
| S7_108.gfrm | 06/11/2008 | 07:26:28 | 71642 |

## F) EXTRACT CREATION TIMES FROM FILES

Imagine that you are collecting a number of frames following a time resolved experiment. Maybe each frame has a different exposition time and you might also be measuring different samples, at different times. In the end of hours (or days) of measurement you perform all the data treatment and face dozens or hundreds of files that you want to plot as a function of the time of the starting of the process. Maybe you were careful and had written carefully all the time intervals between each frame and different samples and also the interval between one measurement and another. However, if you are like me, and will think about these numbers just after the end of measurements you will have to follow the creation time of each 2D spectrum (GFRM files) in order to be able to build this time dependent graph. The SUPERSAXS package can build this time span list in a very easy way using the time and date that each file was created. This procedure is done automatically when data is extracted from the GFRM files (see item “E” above) but by it obvious utility, can be applied to any desired extension.

- In the command window type LIST↵.

- Select option number 7.
- Select option 6.
- Type the desired file extension

The program will search the directory, find all files with the desired extension, sort them according to time and extract the time spans between the first (oldest) and subsequent files. As a result a file called EXT_TIMES.DAT (where EXT is the selected extension) is saved in the directory. This file contains the file names, date when the file was saved, time when the file was saved and the time span in seconds referred to the first (oldest) file. The program takes into account the full data and time, which enables the sorting in different times, days, months or even years:

| FILENAMES | FILE DATE | FIL TIME | DIF IN SEC |
|---|---|---|---|
| Wlsqsaxs2.exe | 21/11/2006 | 17:10:38 | 0 |
| WLSQ.exe | 27/11/2006 | 12:41:46 | 502268 |
| WLSQVASS.exe | 07/12/2006 | 15:14:32 | 2412234 |
| Wsubnonoise.exe | 05/03/2007 | 14:45:34 | 9236096 |
| WComp2.exe | 29/03/2007 | 08:03:00 | 11285542 |
| lorentz.exe | 06/07/2007 | 10:54:42 | 20022244 |
| WlsqFIBER.exe | 12/09/2007 | 14:48:08 | 25133850 |
| WCONV.exe | 13/09/2007 | 16:29:44 | 25226346 |
| Rho_SDS.exe | 30/10/2007 | 09:37:32 | 30126414 |
| test.exe | 16/11/2007 | 12:48:06 | 30656248 |
| WlsqBLANK.exe | 23/11/2007 | 15:26:44 | 31270566 |
| PDBCALC.exe | 28/01/2008 | 14:53:40 | 36970982 |
| Rho_SDSx.exe | 12/11/2008 | 15:25:30 | 61424092 |
| times.exe | 13/11/2008 | 13:15:08 | 61502670 |
| timesD.exe | 13/11/2008 | 14:45:42 | 61508104 |
| list_TEMP.exe | 14/11/2008 | 10:22:12 | 61578694 |

## 15. BUG REPORT!!!

This package is in constant development and many bugs might be found. If you want to report a bug, give a suggestion or send any comment about the SUPERSAXS package, please send an email to crislpo@chem.au.dk with the subject SUPERSAXS PROGRAMS.