SonoXYZ Application

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SonoXYZ

Welcome

Welcome to Sonometrics SonoXYZ Help pages. Please select a topic listed below.

Overview SonoXYZ Configuration Window SonoXYZ Input Files Overview SonoXYZ Output Files Overview Version History

Overview

SonoXYZ Overview

The 3-dimensional analysis software (SonoXYZ) converts a set of distance measurements into 3-D coordinates. A triangulation algorithm and iterative filtering converts these measurements into 3-D coordinates (with respect to some coordinate system) that can then be viewed using a 3-D viewing program.

Four crystals are selected to define the local coordinate system. One crystal is taken as the origin of the coordinate system, another defines the x-axis, a third helps to define the x-y plane, and a fourth is used to set the positive z direction. The x,y,z coordinates of all other crystals are referenced to this set of points that make up the coordinate system. Simple triangulation is used to obtain the first estimate of the crystal coordinates, which are then refined through iterative filtering using a "multidimensional scaling" algorithm.

Ideally, these calculated distances should be identical to the experimental distances, however, some measurement error does occur. The sum total of the differences between distance data collected during the experiment and computed distances is considered the "reconstruction error". Using minimization techniques, the x,y,z coordinates of the reconstructed data set are also adjusted. This serves to reduce the total reconstruction error value.

This software is often referred to as "x,y,z coordinate calculation software". Once the 3-dimensional coordinates have been computed, an image can be constructed using 3-D Viewing software, View3D.

SonoXYZ Analysis

SonoXYZ Configuration Window

The following is a sample of the primary window that appears after the splash screen when the SonoXYZ application is first executed:

SonoXYZ		×
Eile Applications Options Help		
Time Slice as Start Point	Time Slice as End Point	Select File(s) to Process
1 1~200 1136	1 1136 1136 J	i:
Maximum Number of Iterations	Minimum Error and Temperature 1E-20 1E-6 1E-1 C Small Medium Large 	103108 110608 111808 111908 ✓
User Defined Reference Crystals	File(s) to Process	09130702.ssb EsEdPVLoop.slb EsEdPVR.slb EsEdPVR.ssb EsEdPVRa.slb mousePV.slb OverLong.slb PRSW.slb PRSW.ssb
Crystal Size File		
I:\SonoSOFT\crystalsize.sxs		Edit
Fixed Distance File		Edit
Calculate View 3D Histogram	m Replace SonoTwist	<u>C</u> lose <u>H</u> elp
Calculation finished.		

Additional help can be obtained on the following sections:

- Time Slice as Start Point
- Time Slice as End Point
- Maximum Number of Iterations
- <u>Minimum Error and Temperature</u>
- <u>User Defined Reference Crystals</u>
- <u>Crystal Size File</u>
- <u>Fixed Distance File</u>
- Select File(s) to Process
- File(s) to Process
- Recommended Procedures
- · Additional Features (View3D, Histogram, Replace, SonoTwist)
- <u>SonoXYZ Input FilesOverview</u>

<u>SonoXYZ Output Files Overview</u>

Time Slice as Start Point

SonoXYZ uses a specific point in selected data file for coordinate processing. Ideally, this starting point (must be an integer number) should occur when the majority of data traces are clean.

The program has a built-in scanning mechanism that scans through the first 200 data points and determines best time point to start processing. It is recommended this feature be used if unsure of an appropriate start point. To activate this automatic point selection function, simply click on the Auto scan box and a check mark appears.

Time Slice as End Point

If entire file is to be processed, click on the Last Point box. Otherwise, the user may enter the number of the data point where the 3-D coordinate calculation software is to stop processing the file. For example, if there are 1000 points in the data file, using 500 as the argument will cause the 3-D program to process half of the data file (assuming, of course, that the time slice used as the starting point is 1).

Maximum Number of Iterations

The larger the number of iterations, the more accurate the data is and the longer the processing time.

The user may select one of three values, ("large", "medium" or "small") to control the number of iterations, or a specific number may be chosen. If the data is free of noise and consistent, a small number (i.e. 800) can be used. If the data is very noisy a larger value (i.e. 5000) should be used. There is a point, where a very large value (e.g. 100,000) will not give a more accurate result than a relatively large value like 5000. This will usually lengthen the processing time without offering any substantial difference in the accuracy of the result.

Minimum Error and Temperature

This argument determines the minimum sum square error of the final calculation for each (x, y, z) coordinate. Due to increased mathematical computations, processing time will be substantially longer if a smaller error is desired.

Three default settings large, medium, or small, can be used as the input argument. The word "large" corresponds to a numeric value of 1E-4, "medium" to a value of 1E-6, and "small" to a value of 1E-8. To have more control you can directly enter a number instead.

User Defined Reference Crystals

The 3-D program automatically determines the reference crystals used to define the x, y and z-axes. The program will select crystals to maximize computational accuracy. The user however may wish to remap the axes differently to help visualize the resulting 3-dimensional computations.

To enable this function, click on the "User Defined Mapping" check box so that the check appears in the box. Use the up/down controls to select the appropriate values for each of the fields: Origin, X-Axis, XY-Plane and Z-Axis.

Crystal Size File

The crystal size file defaults to the default given in the root SonoSOFT directory. It provides information on the crystal sizes.

A detail discussion can be found here: Crystal Size File (.SXS).

Fixed Distance File

The Fixed Distance File is an optional file which specifies certain TRx channels as being a fixed constant value for the purposes of the x,y,z calculations.

A detail discussion can be found here: Fixed Distance File (.FDF)

Select File(s) to Process

The Select File(s) to Process area contains two list boxes. The upper list box allows the user to select the directory containing the .SLB and/or .SSB files for processing into x,y,z data. The lower list box contains the files in the directory specified by the upper list box. The user is able to select one or more files in the lower list box. Selection will result in the file names appearing in the "File(s) to Process" area's list box.

File(s) to Process

The File(s) to Process list box will contain one or more file names. These are the files which will be processed by SonoXYZ when the user activates the OK button.

Recommended Procedures

The process of generating x,y,z coordinates from the distances given in an .SLB or .SSB file is a relatively complex procedure. The recommended procedure is as follows:

- 1. Examine each trace and trace pair. Apply filtering where necessary and mark them as good or bad. Some notes:
 - Traces that appear to be reasonably clean should be marked good. The SonoXYZ algorithms will handle small amounts of noise. Remember, the crystal distances are usually generated in pairs (i.e. TRX01:02 and TRX02:01), if the pairs' distance values do not agree within reasonable limits, one or both of the traces should be marked bad.
 - · If a trace contains a small number of outliers, perform some filtering to see if these artifacts can be removed.
 - · If the trace contains level shifts, these also can be corrected, but this may require a significant amount of manual processing.
- 2. Process the .SLB or .SSB file (filtering an .SLB file will usually result in an .SSB file) through SonoXYZ. If there is a particular orientation of crystals, be sure to specify them in the "User Defined Reference Crystals" area. **Note**: the SonoXYZ will always determine the best reference crystals to be used in the calculation phase according to the discussions given in the section <u>Version 1.0.20.1</u>. The x,y,z results are then remapped to the user defined coordinates.
 - NOTE: If the user does not specify the reference crystals, the solution may not appear as expected. There are several correct solutions and the user should set the reference crystals for the desired orientation.
- 3. Examine the generated .SXA, .SXD, .SXE and .SXH files. Some notes:
 - The positioning and orientation of the resulting x,y,z may not be as expected as multiple equally valid solutions are possible. You may have to manually transform the data in order to obtain the desired orientation (i.e. flipping the sign of on some x, y, or z crystal values).
 - Examine the header of the <u>.SXA File</u>. If any of the crystals are given a value of -1 in the "CRYSTALSPEC:", it indicates that the crystal has fewer than three valid distances between itself and other crystals. Reexamine the traces for that particular crystal and see if it is possible to apply some filtering so as to be able to mark some additional traces as good. If a known distance value is available, the use of the .FDF file specifying the fixed distance value might be appropriate.
 - Examine the <u>.SXE File</u> and see if there are particular time points that have an unusually high high error values in comparison to the other time points. If such time points exist, reexamine the corresponding trace data to see if filtering might improve the results.
 - Examine the <u>.SXH File</u>, looking for pairs of distance difference anomalies. For such anomalies, reexamine the associated trace data and attempt to filter these traces to remove these animalies.

- 4. View the <u>.SXA File</u> in either the DOS based View3D program or the windows View3D program. If the results are not as expected, reexamine your .SLB/.SSB files for more filtering or marking of traces. If repeated attempts have not resulted in reasonable x,y,z values proceed to the next step.
- 5. Contact Sonometrics for assistance.

Additional Features

SonoXYZ has several additional features that can be accessed by activating the buttons labeled "View3D", "Histogram", "Replace" and "SonoTwist" (c.f. <u>SonoXYZ Configuration Window</u>). The result of activating each button is as follows:

- "View3D" will display the contents of the last calculated x,y,z data set (.SXA file) in the windows based viewer.
- "Histogram" will display the contents of the last calculated file's .SXH file in Note Pad.
- "Replace" will bring up the "Replace" dialog window. The Replace dialog will permit the user to integrate the results of the x,y,z calculation back into the originating .SLB/.SSB file by using the values contained in the .SXC distances file. The Replace dialog window should be similar to:

🛱 Replace Bad TRx Chai	nnels	
Target Binary File (.SLB or .SS I:\SonoSOFT\Data\0913070	B) 2.ssb	
Source Distance File (.SXC) I:\SonoSOFT\Data\0913070	2.sxc	
Select TRx Channel(s) to repla TRx 04 : 01 TRx 05 : 07	ace	
▼ TRx 08 : 09	Mark Channel(s) as Good	
		Close

The list box contains all of the channels in the originating .SLB/.SSB file that have been marked as Bad and were not included in the calculation. By activating the "Replace Checked" button, SonoXYZ will take the data from the given .SXC file and replace the data of the Bad TRx channels provided that their associated check box is checked.

Some things to note:

- 1. If the Target Binary File has the .SLB extension, a new file with the extension .SSB will be created; otherwise the contents of the current target file are updated.
- 2. The check box "Mark Channel(s) as Good" is unchecked by default. If the desire is to have the replaced Bad TRx channels marked as good in the target file, then the user should make sure that this check box is checked.
- "SonoTwist" will pass the last calculated x,y,z data set (.SXA file) to the SonoTwist application. SonoTwist is a licensed product which can be used to provide angular analysis and visualizations. More information is contained in the SonoTwist help file.

SonoXYZ Input Files

SonoXYZ Input Files Overview

SonoXYZ Input Files

SonoXYZ requires one or more .SLB and/or .SSB files as well as a <u>Crystal Size File (.SXS)</u> as input. Optionally the user can specify a <u>Fixed Distance File (.FDF)</u> and/or a <u>Center Of Mass File (CenterOfMass.txt)</u>.and/or <u>Crystal Ignore File (CrystalsToIgnore.txt)</u> and /or <u>TRx Level Shift File (TRxLevelShift.txt)</u>. Details of these are given in these sections:

- <u>Center Of Mass File (CenterOfMass.txt)</u>
- Crystal Size File (.SXS)
- Fixed Distance File (.FDF)
- <u>Crystal Ignore File (CrystalsToIgnore.txt)</u>
- <u>TRx Level Shift File (TRxLevelShift.txt)</u>

Crystal Size File (.SXS)

The Crystal Size File (extension .SXS) contains a list of floating point numbers, one number per line, representing the size of the crystal. There should be a maximum of 32 lines, with each line containing one of the following values: (3.0 (for TAC), 2.3 (for LRG), and 1.0 (for SML), and 0.75 (for MIC)).

NOTE: There is no allowance for blank or comment lines.

The contents of the default crystal size file ("crystalsize.sxs") is as follows:

2.3 2.3

2.3 2.3 2.3 2.3 2.3 2.3 2.3

In version 1.0.20.12, an editor is provided for the crystal size files. The typical appearance of this editor is as shown:

🐃 Edit Crystal Size File - Existing File 📃 🚬									
File: C:\SonoSOFT\Data\crystalsize.sxs									
. E			_				_		
1 2	2 mm 💌	9 2 mm	_	17	2 mm ▼	25 2 mm	-		
2 2	2 mm 💌	10 2 mm	•	18	2 mm 💌	26 2 mm	•		
3 2	2 mm 💌	11 2 mm	-	19	2 mm 💌	27 2 mm	•		
4 2	2 mm 💌	12 2 mm	-	20	2 mm 💌	28 2 mm	•		
5 2	2 mm 💌	13 2 mm	•	21	2 mm 💌	29 2 mm	•		
6 2	2 mm 💌	14 2 mm	•	22	2 mm 💌	30 2 mm	•		
7 2	2 mm 💌	15 2 mm	•	23	2 mm 💌	31 2 mm	•		
8 2	2 mm 💌	16 2 mm	•	24	2 mm 💌	32 2 mm	•		
All Crystals									
L									

Fixed Distance File (.FDF)

The Fixed Distance File (extension .FDF) contains of a list of fixed distance descriptors, one per line. The descriptors will force SonoXYZ to use the defined distance for a given crystal transmitter/receiver pair. Each line should contain the following information: the transmitter number (1..32), the receiver number (1..32), and the fixed distance value (1.0..300.0). Note: the fixed distance values are centre to centre. These numbers should be separated by white space characters (space or tab). Lines that begin with non-numeric characters ((0..9) ignoring white space) are skipped and thus can be used for embedding comments. A typical FDF file might appear as follows:

```
; Fixed Distance file for test.slb
; Format is: Tx Rx distance
1 2 3.0
2 1 3.0
```

In this example, specifying the FDF file will force SonoXYZ to use the value of 3.0 for the distance values between crystals 1 and 2. Note, if the user had marked these crystal distances as bad (that is TR01:02 and TR02:01) in the .SLB file, their definition in the FDF will override the marked setting and thus allow their usage in the calculations.

In Version 1.0.20.12, an editor is provided for the fixed distance files. The fdf editor has the following appearance:

🖷, Edit Fixed Distance File	e - New File		×
File: C:\SonoSOFT\Data\T	est.fdf		
Fixed Distance Tx: 1 2	Rx: ▼	Distance	Add
Comment			
; Version 1.0.20.12			Add
; Fixed D ; Formati ; i.e.: Remove <<	istance file is: Tx Rx Distar 1 2 3.0	ice	
	Save		Cancel

Center Of Mass File (CenterOfMass.txt)

The Center of Mass file (CenterOfMass.txt" contains the information needed by SonoXYZ to calculate the Center(s) of Mass for the given sequences of crystals. This file should be placed in the working directory of the files being analyzed if the Center of Mass calculations are desired. Currently only one CenterofMass.txt file per working directory is supported. An example of a CenterOfMass.txt file for a seven crystal slb/ssb file follows:

1237 456

This file can contain from 1 to five lines of Crystal sequences. This example would calculate two additional x,y,z triplets in the sxa, one giving the center of mass for Crystals 1, 2, 3 and 7. The other x,y,z triplets would be for Crystals 4, 5 and 6. SonoXYZ will process up to the first five lines in the CenterOfMass.txt file. The output in the .sxa file would appear as follows:

TITLE: Crystals 3D coordinate VERSION: 4.00 PARENT FILE: e:\Temp\SonoTwistTest\3D_TW506.slb INPUT FILE: e:\Temp\SonoTwistTest\3D_TW506.slb CRYSTALS: 7 A/D: 8 CofM: 2 CofM(1): 1 2 3 7 CofM(2): 456 TIME: 1 INDEX COLUMN #: 1 # of COLUMNS: 36 # of A/D: 8 # of AUX: 0 Explanation for CrystalSpec: CrystalSpec is an integer array with 32 entries. 1 = Good, -1 = Bad, 0 = Not use. ORG-REF: 3 (Calculations used:3) X-REF: 4 (Calculations used:4) XY-REF: 7 (Calculations used:7) Z-REF: 5 (Calculations used:5)

DATA DESCRIPTION: Column 1: Time Column 2: X coordinate of the 1st crystal Column 3: Y Coordinate of the 1st crystal Column 4: Z Coordinate of the 1st crystal Column 5 - 3N+1 Repeat the (X,Y,Z) triplets of N crystals Column 3N+2 - 3N+8 Center of Mass (X,Y,Z) triplets Column 3N+9 - Last Column: A/D and Aux data DATA NAME/UNITS: Time X Y Z (01) ... CofM: X Y Z (01) ... Seconds mm mm mm ... BEGIN DATA: 0.000000 20.786 -1.281 -9.235 29.560 1.171 14.729 ...

END DATA

Note that the .sxa files contains the additional information:

- 1. The number of CofM
- 2. The Crystal sequences for each CofM (CofM(#):
- 3. The x,y,z triplet data for each CofM with the heading "CofM: X Y Z (0#)"

NOTE: Version 1.0.0.26 and above of the View3D program can properly display the center of mass x,y,z triplets if defined in the .sxa file.

Crystal Ignore File (CrystalsToIgnore.txt)

The CrystalsToIgnore File (CrystalsToIgnore.txt) contains of a list of crystal numbers (1..32), one per line. This data will be used by SonoXYZ to effectively mark the traces associated with the specified crystals as being bad during the xyz calculation. Lines that begin with a ';' are skipped and are used for embedding comments. A typical CrystalsToIgnore file might appear as follows:

```
; List of crystals to ignore
; Created on:10/26/2016 - 12:20:16 PM
14
15
16
```

SonoXYZ, in this instance, effectively marks the traces associated with crystals 14, 15 and 16 as bad, thus eliminating them from the xyz calculation. This does not effect the ssb/slb binary files. If this file is required, it should reside in the current working data directory of SonoXYZ and will only be used on all xyz calculations based in that directory (the file would have to be renamed or deleted if its inclusion is not desired).

And editor has been provided to modify the Crystal Ignore File. The user must have a file in the "File(s) to Process" in order to have proper crystal information for the dialog to work properly. It can be accessed from the Options ==> Crystals To Ignore menu item:

🗶 s	ionoXYZ			
File	Applications	Options	Help	
Tir #	me Slice as S	Crysta Trace	als To Ignore Level Shift Offsets	Slice as End Point

Doing so brings up the Crystals to Ignore dialog:

Crystal	s to Ig	nore in XYZ calculations 🛛 🔀
Cutput File		
C:\Support	rt\Test2	20161019\CrystalsTolgnore.txt
- Select Cru	atala ta	
Jelecticity	stais tu	Ignore.
	1	F 17
	2	F 18
Г	3	F 19
	4	F 20
Г	5	Г 21
	6	F 22
Г	7	F 23
Г	8	F 24
Г	9	F 25
Г	10	F 26
Г	11	1 27
Г	12	F 28
Г	13	F 29
	14	I 30
	15	F 31
	16	F 32
		OK Cancel

Activating the OK button will force the CrystalsToIgnore.txt file to be updated or created.

TRx Level Shift File (TRxLevelShift.txt)

The TRx Level Shift File (TRxLevelShift.txt) contains of a list of offset distances, one per line. The data will be used by SonoXYZ to adjust the distance for the given crystal transmitter/receiver pair (TRx##:##). Each line should contain the following information: the transmitter number (1..32), the receiver number (1..32), and the offset distance value (-10.0 to 10.0 mm). These numbers should be separated by white space characters (space or tab). Lines that begin with a ';' are skipped and are used for embedding comments. A typical TRxLevelShift file might appear as follows:

```
; TRx trace Level Shift / Offset File
; Created On: 11/1/2016 - 12:06:33 PM
; Tx Rx Distance
1 13 -1.4
```

SonoXYZ, in this instance, would add -1.4 to every value of the trace labeled TRx01:13 for the xyz calculation. This does not effect the ssb/slb binary files. If this file is required, it should reside in the current working data directory of SonoXYZ and will only be used on all xyz calculations based in that directory (the file would have to be renamed or deleted if its inclusion is not desired).

And editor has been provided to modify the TRxLevelShift.txt File. The user must have a file in the "File(s) to Process" in order to have proper crystal information for the dialog to work properly. It can be accessed from the Options ==>Trace Level Shift Offsets menu item:

SonoX\	/Z			
File Applica	ations	Options	Help	
\int_{+}^{+}	e as S	Crysta Trace	als To Ignore Level Shift Offsets	Slice as End Point
#		maco	Loror Shine of ISOCS	#

Doing so brings up the TRx Offset File editing dialog:

🖻 Edit TRx Offs	et File - Existing File	×
File: C:\Support\	Fest20161019\TRxLevelShift.txt	
Fixed Distance Tx:	Rx: Distance	
Comment	Add	
Remove <<	; TRx trace Level Shift / Offset File ; Created On: 11/1/2016 - 12:06:33 PM ; Tx Rx Distance 1 13 -1.4	
	Cance	

Activating the OK button will force the TRxLevelShift.txt file to be updated or created.

SonoXYZ Output Files

SonoXYZ Output Files Overview

SonoXYZ generates four output files. These are text based files with tab delineation and are typically named with same primary filename as the file(s) processed, having extensions: .SXA, .SXD. .SXE, .SXH. Details of each of the file contents can be found at:

- <u>.SXA File</u>
- <u>.SXC File</u>
- <u>.SXD File</u>
- .SXE File
- <u>.SXH File</u>

.SXA File

The .SXA file contains the x,y,z coordinates generated by the reconstruction algorithms. The file consists of two parts, the header and the x,y,z data. The header provides specific details about the source file, crystals and the x,y,z data structures. The x,y,z data follows the header (between "BEGIN DATA:" and "END DATA").

In <u>Version 1.0.20.17</u> a new version (VERSION: 3.00) was introduced. It does not include the distance data for crystals that have been "removed" from the calculation (c.f. <u>SXE File</u>).

The typical SXA file will contain information similar to the following:

```
TITLE: Crystals 3D coordinate
VERSION: 2.00
PARENT FILE: C:\SonoSOFT\Data\Samples\PRSW.slb
INPUT FILE: C:\SonoSOFT\Data\Samples\PRSW.slb
CRYSTALS: 4
A/D: 9
TIME: 1
INDEX COLUMN #: 1
# of COLUMNS: 22
# of A/D: 3
# of AUX: 6
Explanation for CrystalSpec: CrystalSpec is an integer array with 32 entries. 1 = Good, -1 =
Bad, 0 = Not use.
ORG-REF: 1 (Calculations used:1)
X-REF: 4 (Calculations used:4)
XY-REF: 2 (Calculations used:2)
Z-REF: 3 (Calculations used:3)
DATA DESCRIPTION:
Column 1: Time
Column 2: X coordinate of the 1st crystal
Column 3: Y Coordinate of the 1st crystal
Column 4: Z Coordinate of the 1st crystal
Column 5 - 3N: Repeat the (X,Y,Z) triplets of N crystals
Column 3N+1 - Last Column: A/D and Aux data
DATA NAME/UNITS:
Time X Y Z (01) X Y ...
Seconds
       mm
           mm mm mm ...
BEGIN DATA:
0.019440
       0.000
               0.000
                     0.000
                            16.588
                                   26.163 ...
18.296928
         0.000
               0.000
                      0.000
                            16.588
                                    26.163 ...
END DATA
```

In<u>Version 1.0.20.27</u> a new format (VERSION: 4.00) of .SXA file was introduced to accommodate the Center of Mass calculations. More information on this format can be found in <u>Center Of Mass File (CenterOfMass.txt)</u>.

.SXC File

The .SXC file is similar to the <u>.SXD File</u> except that redundant data has been removed. Distance data for channels such as TRx01:01, TRx02:02 are absent. Also, since the calculated data is symmetric, only one channel per pair is reported (i.e. given TRx01:02 and TRx02:01, only TRx01:02 is in the file).

NOTE: With <u>Version 1.0.20.17</u> the .SXC file no longer will include the distance data for crystals that have been "removed" from the calculation (c.f. <u>.SXE File</u>).

A typical .SXC file might appear as follows:

Sampling Period: 0.003888 Time TRx01:02 TRx01:03 TRx01:04 TRx02:03 ... 0.019440 30.979 31.900 47.763 36.258 ...

.SXD File

The .SXD file contains the calculated distances between each of the crystals defined in the original .SLB or .SSB file. A typical .SXD file would appear as follows:

Sampling Period: 0.003888 Time TRx01:01 TRx01:02 TRx01:03 TRx01:04 TRx02:01 ... 0.019440 0.000 30.979 31.900 47.763 30.979 ...

.SXE File

The .SXE provides four sections of error information:

- 1. The first is a listing of useable distances for each crystal listed as a Transmitter and as a Receiver.
- 2. The second will list any Crystals that have been removed from the x,y,z calculations. If no crystals were removed, this section will not appear in the file.
- 3. The third lists the crystal pair distance variances that have the largest difference between calculated and actual values.
- 4. The last section presents the overall error at each time point processed. The error value is the sum of the squares of the differences between the calculated distance and the actual experimental distance divided by the number of differences. Error values larger than 0.5 mm indicates that there are some difficulties with the input data, requiring user filtering or marking. Note that the error is limited to three significant digits after the decimal.

The typical contents of an .SXE file might appear as follows:

.SXH File

...

The .SXH presents a columnar histogram of the frequency of differences between the calculated and actual (experimental) distances. An isolated frequency grouping not near 0.0 tends to indicate that the experimental trace data contains some spurious noise which may be eliminated by performing some filter operations on the corresponding traces.

Additional information may appear at the beginning of the .SXH file which will indicate that the crystal pair data has significant errors. That is, if the distance at time t for TRx01:02 is significantly greater or smaller than TRx02:01, an error message will be catalogued in the .SXH file. This should indicate that additional filtering or marking of traces is required.

The typical contents of an .SXH file might appear as follows:

References used										
org=2 x-axis=5 xy-plane=4 +ve Z=7										
rrx01:04/	/04:01 (p	t=153):	Trace da	ta quest	ionable,	not used	£			
TRX04:01/	/01:04 (p	t=153):	Trace da	ta quest	ionable,	not used	1			
TRX02:03/	/03:02 (p	t=1057):	Trace d	ata ques	tionable	e, not use	ed			
TRX03:02/	(02:03 (p	t=1057):	Trace d	ata ques	tionable	, not use	ed			
diff(mm)	c01	c02	c03	c04	c05	c06	c07	c08	c09	c10
c11										
0.000	4470	9348	3232	7456	8894	2758	6448	6526	16036	6402
194										
0.100	1674	4778	3090	4400	9158	5180	9274	7712	6778	5016
688										
0.200	4044	6032	1584	5290	8284	10550	8112	4482	1336	3622
2744										
0 300	4658	3624	1884	6044	6110	6008	6024	1042	316	6710
2696	1050	5021	1001	0011	0110	0000	0021	1012	510	0710
0 400	10206	1060	100	3456	1440	3118	4560	654	140	2310
5040	10200	1000	100	5150	1110	5110	1500	051	110	2310
0 500	3833	2176	646	4170	2458	5508	3718	5236	64	2992
2506	5022	21/0	040	4170	2450	5500	5710	5250	04	2992
2500	2170	1120	1 2 7 9	2016	2224	1424	156	2000	24	000
744	2170	4430	1270	2910	3334	1424	450	3222	54	908
0 700	2004	2474	2210	2600	1260	2226	1 5 0	700	2.2	740
0.700	3094	24/4	2210	2090	4300	2320	120	122	22	/40
204	2100	4000	1440	2040	F 0 0	2662	110	0.4	24	220
0.800	3180	4098	1448	2840	502	2002		84	24	230
100	1224	1440	B1 C	450	FC	70	F 0 0	20	1.4	coc
0.900	1334	1448	716	456	56	78	598	32	14	606
254	104		2040	0000	62.4	0.0	C 1	1.0		60
1.000	134	778	3842	2778	634	20	64	12	4	62
1120	4.0									~ ^ ^
1.100	42	138	2210	1344	$\perp \perp 4$	8	26	2	4	34
1474										
1.200	10	390	964	1306	382	6	34	-	-	34
2122										
1.300	б	3710	1088	1698	3718	2	24	8	-	24
2750										
1.400	2	96	332	850	94	-	2	-	-	2
1166										
1.500	-	8	102	544	б	-	8	-	2	10
628										
1.600	-	4	14	200	4	-	10	-	-	10
206										
1.700	2	2	6	40	-	-	4	-	2	4
44										
1.800	-	2	4	18	4	-	б	2	2	4
22										
1.900	-	-	4	24	-	-	б	-	-	б
28										
2.000	-	-	6	8	-	-	-	-	-	-
14										
2.100	-	-	4	4	-	-	-	-	-	-
8										

2.200	-	-	-	4	-	-	2	-	2	-	
4 2.300	_	_	4	4	_	_	_	_	_	_	
8											
2.400 2	-	-	-	2	-	-	-	-	-	-	
2.500	-	-	-	4	-	-	-	-	-	-	
2.600	-	-	2	2	-	-	-	_	_	_	
2.700	-	-	2	-	-	-	-	-	-	-	
2.800	-	-	-	2	-	-	-	-	-	-	
3.100	-	_	-	2	-	-	2	-	-	2	
2 diff(mm)	c01	c02	c03	c04	c05	c06	c07	c08	c09	c10)
cll mean	-0.0628	-0.0391 -	0.0813 -	-0.1277	-0.0304	-0.0322	-0.0241	-0.2428	-0.0117	-0.0410	-
0.1586 STD	0.4779	0.5965	0.7550	0.6293	0.5182	0.3990	0.3058	0.2348	0.1043	0.3435	
0.8333 Average	StdDev:	0.472496	(N = 11))							
Average	TRx-XYZ	differenc	e in mm	(2478 s	amples)						
Negativ	e values	==> TRx	traces r	marked a	s bad	-	_				
TX\RX 1	T	2	3	4	5	6 0 2 2	0 47	8	-2 5/	0 20 TU	11
2	0.87	-	0 74	0.31	1 29	0.23	0.47	0.05	0 08	0.39	-5 88
3	-x	0.74	_	1.03	0.12	-x	-x	-x	-x	0.23	1.21
4	0.51	0.32	1.03	_	0.61	0.80	0.33	0.19	0.06	0.17	1.37
5	0.75	1.29	0.12	0.61	_	0.34	0.15	0.16	0.08	0.34	0.28
6	0.23	0.25	-x -	-5.09	0.34	_	0.25	0.55	0.11	-7.39	0.51
7	0.47	0.10	-x	0.33	0.15	0.25	_	0.20	0.15	0.61	-6.14
Largest	Ava Diff	erences -	Good Ti	races							
4 11	1.371										
2 5	1.285										
5 2	1.285										
3 11	1,208										
3 4	1.032										
4 3	1 032										
2 1	0 867										
1 2	0.867										
4 6	0 796										
5 1	0.752										
Smallest	Avg Dif	ferences	- Bad Ti	races							
1 9	-3.542										
64	-5.087	(TR04:06	marked g	good)							
2 11	-5.881										

7 11 -6.137 6 10 -7.389

This data indicates that there is a fair fit. There does appear to be some noise associated with the peak at 3.100 between crystals 4 and 11. Filtering may remove this artifact.

Three additional sections have been added to the Histogram file which presents information about the differences between the XYZ solution's data and the original data:

- 1) is a difference matrix showing the average differences between the XYZ solution and the original data. Negative values indicate differences for traces which were marked as bad in the source data file (a -x indicates that the difference was greater than 10 mm).
- 2) shows the sorted top 10 largest average differences for the good traces. In this instance, the largest difference is in agreement with the Histogram, with TRx04:11 being the primary trace at issue.

3) shows the top 10 smallest average differences for traces that were marked bad.

SonoXYZ History

Version History

SonoXYZ has gone through several revisions. These revisions are related to the file version of the 3dXYZComponent.dll file. Additional information concerning these revisions are available here:

- Version 1.0.20.42
- Version 1.0.20.27
- <u>Version 1.0.20.21</u>
- <u>Version 1.0.20.20</u>
- <u>Version 1.0.20.17</u>
- <u>Version 1.0.20.16</u>
- <u>Version 1.0.20.14</u>
- <u>Version 1.0.20.12</u>
- <u>Version 1.0.20.6</u>
- <u>Version 1.0.20.5</u>
- Version 1.0.20.1

Version 1.0.20.1

This version of SonoXYZ has several modifications and enhancements, namely:

- · the algorithm used to determine the best basis set of four reference crystals has been improved
- \cdot the algorithm used to determine the best starting point has been improved.
- · Fields for the input of the crystal size file and the fixed distance file have been added to the main user interface

The determination of the basis set of four crystals used in the calculation of the x,y,z coordinates is processed as follows:

- 1. a list containing the areas of all possible triangles formed by all valid combinations of three crystals is generated
- 2. this list is sorted, and the ten (or less for smaller data sets) largest triangles are selected. The largest triangles should provide the best basis from which to calculate the other crystals' spatial coordinates.
- 3. for each of ten largest triangles, the count of valid distances to other crystals is determined.
- 4. From the group of ten, the triangle having the most valid distances is used as the basis triangle. The longest side of this triangle is used to define the origin and x-plane, the remaining crystal defines the xy-plane.
- 5. using this basis triangle, the distances from the triangle's plane to each of the remaining crystals is determined. The crystal having the furthest distance from this plane is selected as crystal to define the positive z-axis direction.

The automated scan for the best starting point proceeds as follows:

- 1. using the basis set of four crystals determined above, the x,y,z coordinates of all the crystals are determined at each of the time points starting at 5 through 200. The first four time points are skipped so as to miss any anomalies typically present at the start of trace data.
- 2. At each time point, the differences between the actual and calculated crystals distances are summed into a per time point list.
- 3. the list is sorted and the ten lowest difference values are selected. Of these ten, the time point closest to the beginning of the trace is selected as the best starting point for the subsequent analysis.

Version 1.0.20.5

Several problems were corrected in this release of SonoXYZ:

• under certain conditions, the orientation of the data was incorrect (i.e. the results were mirrored through one of the reference axis) This has been corrected in this release.

A new method has been implemented for the first calculated solution of the crystal coordinates. This is a significant change to the procedure described in <u>Version 1.0.20.1</u>. The new procedure is as follows:

- 1. Statistics (average, standard deviations, etc) are gathered on every trace in the specified data file (.SLB or .SSB).
- 2. The average values from these statistics along with the user's marking of good/bad traces are used to form the first distance matrix.
- 3. This matrix is feed into the Multidimensional Scaling algorithm.
- 4. The results are further refined utilizing a conjugate gradient algorithm.
- 5. This result is used as the basis for all of the subsequent x,y,z calculations at each time point in the source file.

Version 1.0.20.6

An additional pre-calculation check has been added. This check will report up to the first fifteen TRX channels pairs (i.e TRX1:2 and TRX2:1) whose values differ by more than 2.0 mm. If the report popup dialog is shown, the user has the option of canceling the calculation. Samples of this popup dialog window are shown below:

SonoXYZ Message			×
File:C:\SonoSOFT\ TRX Pair Inconsiste	Data\Sam encies	ples\PRSW.slb)
TRX	Avg Diff	#/4703	
1: 4/ 4: 1	2.0	1	
Abort Calculation?			
Yes	<u>N</u> o	Help	

This indicates that there is a difference of 2.0 between TRX1:4 and TRX4:1 at one time point out of 4703 time points. These types of errors tend to suggest some sort of an outlier and in this instance the calculation could continue without the user having to filter the traces. The significance of the error increases with the number of time points showing inconsistencies.

SonoXYZ Messa	ge	×		
File:C:\SonoSO	=T\Data\Sam	ples\OverLong.slb		
TRX Pair Incons	istencies			
TRX	Avg Diff	#/65933		
1:3/3:1	2.0	2		
2:3/3:2	3.6	3839		
2:6/6:2	9.5	62		
3: 5/ 5: 3	2.0	2		
3: 6/ 6: 3	4.3	26		
4: 5/ 5: 4	2.0	1		
NOTE:				
Calculation reults will be guestionable,				
Filter or Mark as Bad some of				
the above mentioned channels				
Abort Calculatio	n?			
Vec	No	Help		
<u> </u>	140	, icih		

This instance has several problems. The user should abort the calculation and open the file in SonoSOFT. Since the number of time points for the TRX pair 2:3/3:2 is relatively large, it is recommended that the user first filter the traces. If the upon subsequently running SonoXYZ this trace pair is still showing a large number of inconsistent time points, it might be best to mark one of both of the traces as bad.

Version 1.0.20.12

Two editing interfaces have been added and can be activated from the "Edit" buttons on the SonoXYZ configuration window. These editing windows are shown in <u>Crystal Size File (.SXS)</u> and <u>Fixed Distance File (.FDF)</u> topics.

Version 1.0.20.14

Fixed some issues with handling of the trxspec structure within .SLB and .SSB files. Corrected the calculation of statistics reported in the histogram file (<u>.SXH</u>).

Version 1.0.20.16

A new output file <u>.SXC File</u> was introduced. This is similar to the <u>.SXD File</u> except that the redundant data has been removed. Several corrections were made to the histogram support routines (c.f. <u>.SXH File</u>).

Version 1.0.20.17

"View3D" and "Histogram" buttons have been added to the SonoXYZ main configuration window. These become enabled after a calculation has been completed. Clicking on the View3D button will bring up the Windows View3D program using the <u>.SXA File</u> of the last calculated file. Similarly, clicking on the "Histogram" button will bring up Note Pad containing the <u>.SXH File</u> of the last calculated file.

The output of the <u>.SXA File</u> and <u>.SXC File</u> has been modified so that the distances associated with crystals that were removed from the calculation no longer appear in the files. Previously, the removed crystals were assigned to the origin and as such the distances associated with these crystals were calculated from that point.

Version 1.0.20.20

Version 1.0.20.20 has the ability to reintegrate the SonoXYZ distance data from the <u>.SXC File</u> back into the originating binary distance file (file extension .SLB or .SSB). This is accomplished by activating the "Replace" button on the main <u>SonoXYZ Configuration Window</u>. Additional integration with other Sonometrics' applications (SonoTwist) has also been added (see <u>Additional Features</u> for more details).

Version 1.0.20.21

SonoXYZ will now provide a report indicating the quality of the x,y,z fit just calculated. The quality is determined by the average standard deviation between the actual and calculated distances. The report window is similar to:

Calculation Report		
File: I:\SonoSOFT\Data\EsEdPVR.ssb		
Confidence Level of 3D Solution: Good		
Average Standard Deviation: 0.0007 mm		
OK		

Version 1.0.20.27

SonoXYZ will now add additional x,y,z triplets into the .sxa file which are the calculated Centers of Mass for up to five given sets of crystals. These calculations and data are only performed if the file "CenterOfMass.txt" exists in the working directory of the files being analyzed. The format of the "CenterOfMass.txt" file consists of one to five lines containing space delimited sequences of crystal numbers. Each set will result in a triplet of x,y,z columns being added to the .sxa file.

NOTE: Version 1.0.0.26 and above of the View3D program can properly display the center of mass x,y,z triplets if defined in the .sxa file.

More information can be found in the Center Of Mass File (CenterOfMass.txt) section.

Version 1.0.20.42

Two new optional input files were introduced with this release:

- A text file named: "CrystalToIgnore.txt". This file contains a list of crystals which are excluded from the XYZ calculation. It resides in the SonoXYZ's current data directory. This was introduced to provide a quick method of effectively marking all the traces associated with a crystal as bad for the XYZ calculation purposes only. More information can be found at: <u>Crystal Ignore File (CrystalsToIgnore.txt)</u>
- 2) A test file named: "TRxLevelShift.txt". This file contains a list of Tx, Rx and distance (in mm) values. In the XYZ calculation, if this file is found in the SonoXYZ's current data directory, the specified distance values are added to the specified TRx##:## trace as specified by the Tx and Rx values. More information can be found at: TRx Level Shift File (TRxLevelShift.txt)

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