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MUSCAT

A Monte Carlo program for multiple scattering simulations dedicated for Compton scattering experiments.

Instruction manual

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1 Introduction

MUSCAT is the program for numerical Monte Carlo simulations of photon transport in the sample. It was designed to determine the multiple scattering spectrum for Compton scattering experiments. MUSCAT was originally written in Scilab, but later rewritten in Octave because of the much better simulation efficiency (shorter simulation time).

Program package contains three versions of MUSCAT:

- ver. 1.0 – for unpolarized beam,
- ver. 2.0 – for polarized beam including the geometrical consideration of electric vector rotation after the scattering,
- ver. 3.0 – for polarized beam including the Stokes parameters.

Program automatically chooses the calculation method after choosing the adequate version

Although the different versions use different equations for scattering cross-sections calculations the simulation algorithm is exactly the same. For the moment only ver. 2.0 was experimentally tested and described. That's why it is strongly suggested to use this version for your calculations. Physical basics and the details of calculation procedure of MUSCAT program can be found in: [M. Brancewicz, M. Itou, and Y. Sakurai, J. Synchrotron Rad. **23**, 244 \(2016\)](#). As a courtesy to the author please cite this article when you publish your results obtained with the use of MUSCAT program.

This manual will only present the necessary operations with no physical basis to run MUSCAT simulation procedure and get the simulation results.

2 Installation

Download and install Octave 4.2.1 (<https://www.gnu.org/software/octave/>). MUSCAT program have been tested on Octave 4.2.1 (64 bit) Windows versions. Octave is available for Windows, Linux and MacOS and there shouldn't be any problems with using MUSCAT on that operation systems.

Download and unpack the MUSCAT program. The most current version of program can be downloaded from the official MUSCAT website: <http://physics.uwb.edu.pl/wf/brancew/muscat/>. Here you can also find all necessary links and this manual. The history of changes will be also published here.

Copy MUSCAT folder with entire content to desired location on your hard drive (with appropriate changes of the path later). The default working directory for MUSCAT will be: **MUSCAT/** in your desired location.

Run Octave. Change working directory in the File Browser window (on the left) or use command: **chdir ('.../MUSCAT')** (where ... is your desired location). The structure of MUSCAT folder should now appear on the left window. Using command **pwd** in Octave command line will display the current path.

2.1 Structure of MUSCAT folder

MUSCAT folder contains main program Octave executable text file **MUSCAT.m** and 6 subfolders:

- **MUSCAT/crosssections/** containing text files with information about the sample material (mass attenuation coefficients, atomic form factors, incoherent scattering functions, Compton profile, tables for binding corrections and anomalous scattering corrections).
- **MUSCAT/geometries/** containing executable Octave text files with information about the experimental setup (source and detector).
- **MUSCAT/samples/** containing executable Octave text files with information about the samples (material, size, position).
- **MUSCAT/functions/** containing all Octave functions and procedures for MUSCAT program.
- **MUSCAT/results/** containing three subfolders (**v.1.0**, **v.2.0**, **v.3.0**) for the final results storage depends of the used MUSCAT version.

- **MUSCAT/XCOM/** containing an XCOM program (from NIST) for mass attenuation coefficients calculations.

3 Preparation of data and input files

Before starting the calculation procedure user must prepare some data and input text files.

3.1 Compton profile

Make a 2-column text file containing Compton profile of studied material. First column contains the values of p_z [a.u.], second one – $J(p_z)$ [el./a.u.] values. Provide both sides (- and +) Compton profile on any grid, but the wider is better. Name the file with following scheme: **material.cp**. Remember that *material* name is a variable used in program. Move or copy the file into the **MUSCAT/crosssections/** folder. See the **Al.cp** file containing theoretical Al Compton profile as an example.

3.2 Mass attenuation coefficients

In order to create a text file containing mass attenuation coefficients use XCOM program from NIST. A copy of program is included in MUSCAT folder.

Go to **MUSCAT/XCOM/**. A file named **muscat.ene** contains a standard 1000-elements uniform energy grid for the mass attenuation coefficients calculation from 0.001 to 1.000 [MeV], which should be enough for all Compton scattering experiments. It is possible to provide the different energy grid if needed. Please make sure that it will cover possible photon energy range in your experiment.

Run **XCOM.exe**. Follow the instructions providing the data for considered material. In case of the “Options for output quantities:” appears, choose 3 - “Partial interaction coefficients and attenuation coefficients in cm²/g”. For the next option “Options for energy list for output data:”, choose 3 - “Additional energies only”. For “Modes of entering additional energies:” choose 2 - “Entry from prepared input file”. “Specify file that contains input energy list”, enter **muscat.ene** (no additional path is needed if the energy file is in the same location). “Specify file on which output (cross section table) is to be stored”, enter the file name with following scheme: **material.mac**, where *material* is a text variable that will be used inside the program (the same as before). Finally enter 1 for no more output. A

text file **material.mac** should appear in the XCOM folder. Edit **material.mac** (e.g. using Notepad++) and delete all comment lines (except the first 13) that divide the table of numerical data. Save file in **MUSCAT/crossections/** folder. Example file for Aluminum (**Al.mac**) is included.

3.3 Atomic form factor

Prepare 2-column text file with a table of atomic form factor function $F(x,Z)$ values. First column: $x=\sin(\theta/2)/\lambda$ [\AA^{-1}], second column: $F(x,Z)$. For single elements use the atomic form factors table from: J. H. Hubbell and I. Overbo, J. Phys. Chem. Ref. Data 8, 69 (1979). For compounds or mixtures use the weighted values. Weight fractions for elements can be found in 4th line of a **material.mac** file (output file from XCOM). Name the file with the following scheme: **material.aff**. Save the file in **MUSCAT/crossections/** folder. It is possible to provide different table of x and $F(x,Z)$. Please make sure that x will cover the possible range. Example file for Aluminum (**Al.aff**) is included.

3.4 Incoherent scattering function

Prepare 2-column text file with a table of incoherent scattering function $S(x,Z)$ values. First column: $x=\sin(\theta/2)/\lambda$ [\AA^{-1}], second column: $S(x,Z)$. For single elements use the incoherent scattering function table from: J. H. Hubbell, W. J. Veigele, E. A. Briggs, R. T. Brown, D. T. Cromer, and R. J. Howerton, J. Phys. Chem. Ref. Data 4, 471 (1975). For compounds or mixtures use the weighted values. Weight fractions for elements can be found in 4th line of a **material.mac** file (output file from XCOM). Name the file with following scheme: **material.isf**. Save the file in **MUSCAT/crossections/** folder. It is possible to provide different table of x and $S(x,Z)$. Please make sure that x will cover the possible range. Example file for Aluminum (**Al.isf**) is included.

3.5 Binding correction and anomalous scattering

Although the functions for binding correction and anomalous scattering exists, those features have not been finally developed and tested yet and they have a negligible influence to the final Compton scattering spectra, which is usually measured with the use of high energy X-rays.

3.6 Sample file

A file describing sample is an Octave executable text file (*.m). It is possible to create it in a

standard text editor or by using Octave text editor. Open Octave and using file browser in left window go to **MUSCAT/samples/** folder (to store sample data files). Double click on **test_sample.m** file to open. Please make sure to save as a new file before any changes. It is possible to use any name for the sample file but it is suggested to leave the ***.m** extension for convenience. Sample file contains the variable names, values and simple description. Please don't change any variable name. Change only values accordingly to your sample material, shape and position (in lines 2-12). It is only possible to define three types of sample shapes: cuboid, roller and ball. Default translation vector (tx,ty,tz) of a sample is (0,0,0) and sets the sample center into a (0,0,0) position in Cartesian coordinate system.

3.7 Geometry file

Geometry file is also Scilab executable text file (***.m**) and can be edited the same way like the sample file. In Octave browser go to **MUSCAT/geometries/** folder (to store geometry data files). Double click on example file **test_geometry.m** to open. It contains information about the X-ray source and detector: variable names, values and their simple description. It is suggested to save it as a new file before making any changes. It is possible to use any name for the geometry file but it is suggested to leave the ***.m** extension for convenience. Please don't change any variable name. Change only values, accordingly to the experimental setup that needs to be defined (lines 2-16 and 23-31). Some necessary explanation about editing the geometry file will be given below.

The source and detector positions are defined in the Cartesian coordinate system. Initial positions of the source and slit are on the Y axis. Initial positions of the detector and collimator are on the Z axis.

The incident beam can be rectangular or circular depend on the **typ** parameter. It is defined by the size of the source (**wx, hx**), initial position of the source on Y axis (**yx**) and similar parameters of a slit (**ws, hs, ys**). Then the primary beam can be rotated around 3 axes (**ax, bx, cx** angles in degrees). See for more details in the comments in geometry file (e.g. polarization).

The initial position of detector is on Z axis (**zd**). It is also possible to define the detector collimator that is placed just in front of detector. Collimator can be circular or rectangular depend on the **typ** parameter. Parameters **lc, xc** and **yc** define the collimator size. Position of detector can be

changed also by additional rotations (**ad**, **bd**, **cd** angles in degrees) around X, Y and Z axes. Energetic resolution of detector can be given in **res** parameter. In case **res** is different than 0 the final spectra will be convoluted with a Gaussian of FWHM=**res**.

For the visual test of geometry; beam, detection area, sample, please change the second parameter in **showgeometry** function (25th line of a main program) to '**f**' (figure) or leave '**n**' (no figure) if you don't want to see the geometry plot. The first parameter is a range of geometry plot in meters from the beginning of coordinate system. If you want to do some more geometry tests before the simulations you can add **return** command after. Don't forget to delete or comment it before the simulations.

4 Setting parameters

The current version of script that runs the simulation program is located inside the **MUSCAT/** folder. The script file name is: **MUSCAT_test.m**. Open file with Octave editor. The file contains some comments (lines started from #) that should appear in green when opened with Octave editor. Please don't edit anything that is not suggested here until you know what you are doing.

4.1 Initial operations

Dont' edit this part.

4.2 Paths (global variables)

Choose the MUSCAT version by typing it into a text variable **ver** ('1.0', '2.0' or '3.0'). It is recommended to use 2.0 version (it was tested).

Set your MUSCAT folder path (text variable **muscatdir**) depend on your system (Windows = ispc, Linux = isunix).

4.3 Loading functions and parameters

Enter the name of geometry file that needs to be used inside the function **source** (for example: '**test_geometry.m**'). Enter the name of sample file inside the function **source** (for example:

'test_sample.m'). In order to check the geometry and sample use **showgeometry** function by setting the second parameter to 'f' (figure). Save file and run the program using menu button on the top of editor window. It is possible to change the maximum range of a geometry plot by changing the value of first parameter in **showgeometry** function. This is the value of maximum (+ and -) X, Y, and Z given in meters. Check if geometry plot corresponds to your assumptions.

4.4 Initial parameters

nsc is the number of simulated scatterings (scattering depth). Please choose integer bigger or equal 1. Usually **nsc** parameter is set to 3, because the triple scattering intensity is negligible in the classic Compton scattering experiments, but there is no limitation for maximum value of this parameter and it should be increased in case of thick samples. **nof** is the number of photons for single simulation loop. In case of 8GB RAM memory and 64 bit OS is usually set to 1 000 000. If there will be problems with the stack size you can change this number to smaller one (for example 100 000). In case of the need for simulations with the larger number of photons change the number of loops (**nloops**). Example: for the simulations with 100 000 000 incident photons set: **nof** = 1 000 000 and **nloops** = 100 or **nof** = 1 00 000 and **nloops** = 1000. Do not edit lines commented as: "# inc. photons at sample" and "# detected events, photons", those are the starting values for photon counting procedure.

4.5 MCA parameters

In order to choose the energy range for the registered photons (final spectra) it is possible to choose two options. First one is automatic. In this case please uncomment line "automatic MCA scale" and comment line "manual MCA scale" by using "#". For manual input of minimum and maximum energy please do opposite and change **emin** and **emax** parameter values (energies in keV). Do not edit line "# energy scale for spectra", here the energy scale is calculated for MCA procedure. Do not edit lines "# spectra" and "# errors", those are the initial empty spectra and errors.

4.6 Main program

Do not edit this part until you know what you are doing.

4.7 Results: Display, save and plot

You can edit argument in function **plotresults** only (“**lin**” or “**log**”) if you want the final spectra image to be shown in linear or logarithmic intensity scale.

5 Starting simulations

Start simulations by clicking save and run button. During the simulations MUSCAT program will display some information about the work progress. After the successful completion a final spectra figure will be displayed and some final information either.

6 Results

As a first result after simulation finished, a figure with final spectra appears. The same figure is saved in results folder (**/MUSCAT/results/**) in appropriate subdirectory depend on the MUSCAT version was used. Some informations about the simulation results are displayed on the screen. The same and more information are saved in results directory. Every simulation result is saved in a different subdirectory with a name from the time (form: **YYYYMMDD_HHMMSS**). There are three result files inside. One is a figure (**spectra.pdf**) showing quick preview of the simulated spectra. Two others are the parameter and spectra ***.txt** files in the easy to impotr format. The information about the path and names of the saved results files will be displayed at the end of the calculation.

Parameter file contains all parameters used in program and some simulation results at the end of file. First is a scattering angle calculated based on the geometry of defined setup. Effective scattering angle is calculated based on the incident energy and the central position of a Compton peak. Finally, the partial spectra intensity ratios to the total intensity as a reference are given.

Spectra file contains numerical values for all simulated spectra. First column – energy in keV, second – momentum scale in a.u. Next columns contains intensity (number of photons registered by detector) after the first scattering (**S1**), second scattering (**S2**), third (**S3**) up to the defined earlier **nsc** (number of simulated scatterings). The columns after contains the errors for each partial spectrum respectively (**dS1, dS2, dS3...**).

7 Unresolved issues and how to avoid them

7.1 Complex numbers in results

It was observed that in case of 64 bit systems and roller sample sometimes complex numbers in the results appear when the number of incident photons (**nof**) is set to 1 000 000. The problem appears in 5th loop inside the function **dist_infroller** (for roller sample). It is suggested to decrease the number of photons **nof** (e.g. 10 times) and increase the number of loops **nloops** (e.g. 10 times) to get the same statistics. The problem disappears when the number of incident photons (**nof**) is set to 100 000 and even for 1000 loops (**nloops**) does not appear.

8 Bug report and technical support

In case of any problems or needed assistance with using MUSCAT please do not hesitate to contact author by e-mail: m.brancewicz@uwb.edu.pl. I will be grateful for any comments and bug reports.