SASCollOpt.py – User's Manual

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1 Introduction

`SASCollOpt.py` is a stand-alone Python script for calculating the parameters of the three-pinhole collimation scheme in small-angle scattering experiments, as well as for exploring the corresponding configuration space.

2 Installation

The script does not need special installation: should work by just executing the script with a recent version of the Python interpreter (version 3 is preferred). It does depend however on the following libraries:

- the Tk toolkit (tkinter, as well as its submodules ttk, font and messagebox in Python v3; Tkinter, ttk, tkFont and tkMessageBox in Python v2) for the graphical user interface,

- numpy for numeric computations and

- matplotlib for plotting.

In order to install these dependencies, kindly refer to the documentation of your Python distribution.

3 Usage

The user interface of the program is laid out in a notebook scheme. Each page of the notebook is accessible by a corresponding tab at the top, and corresponds to a different optimization scheme, detailed in the main article. The button bar at the bottom contains common operations: quit the program, execute the currently visible notebook page, store the found optimum geometry into the memory and retrieve the parameters of the stored geometry into the current page.
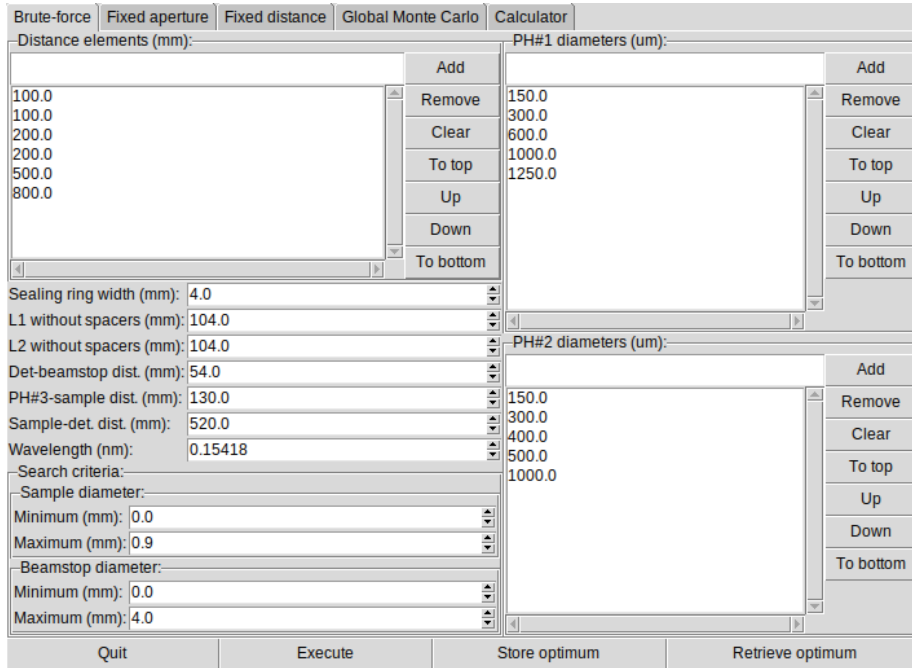
Figure 1: The brute-force optimization tool

3.1 Brute-force optimization

The program starts with the tool for brute-force optimization as shown in Fig. 1.

The top left listbox contains the lengths (given in millimetres) of the available spacers between two pinhole stages. If more than one pieces exist from the same length, the corresponding number has to be repeated that many times. The list can be cleared by the "Clear" button. Elements can also be removed one-by-one by selecting one and pressing the "Remove" button. A new element can be added by writing its length into the entry field just above the listbox and pressing the "Add" button on the right. Re-organization of the list elements is provided for aesthetical reasons. The buttons "To top", "Up", "Down" and "To bottom" can be used to move the selected element accordingly.

The other two listboxes correspond to the available pinhole sizes in the first and the second stage, respectively.

Given the elements $d_{1..n}$ between pinhole #1-#2 or #2-#3, spacings are calculated as $< L1 with out spacers > + \sum_{i=1}^{n} d_i + (n+1) < Sealing ring width >$ or $< L2 with out spacers > + \sum_{i=1}^{n} d_i + (n+1) < Sealing ring width >$, respectively.

Other parameters, such as the distance of the upstream front of the beamstop from the detector surface, the distance between pinhole #3 and the sample, the sample-to-detector distance and the wavelength of the radiation can also be

given in this column.

Lower and upper bounds for the beam size at the sample and the beamstop can be given in the lower left portion of the window.

After the parameters have been entered, pressing the "Execute" button at the bottom of the window starts the procedure of enumerating all possible configurations and selecting just those which satisfy the beam size criteria.

The results are enumerated in a tabular format in another window. The table can be sorted by clicking on the columns. The selected configurations (rows) can be exported in HTML format by pressing the appropriate button.

3.2 Fixed-aperture optimization

The page for the fixed-aperture optimization is shown in Fig. 3. In this window the diameters of the first two apertures can be given, as well as the size criteria and other parameters already detailed at the brute-force optimization method. Upon clicking "Execute", the geometry is calculated and a graphical representation of the solution is plotted in the l_1-l_2 plane. The beam size at the beamstop is at its upper limit for points on the red line, and is below it in the area shaded with red. The same applies for the sample size and the blue line and shaded area. The grayscale shading is the intensity factor $\mathcal{I}$ defined in the main article. The optimum point is given by the intersection of the red and blue lines. The corresponding pinhole spacings l_1 and l_2, the total collimation length $l_1 + l_2$, the calculated intensity $\mathcal{I}$, the suggested size of the 3rd pinhole, as well as the lowest value of q and the corresponding Bragg spacing are displayed in the textbox at the top left corner of the graph.

3.3 Fixed-distance optimization

The user interface for the fixed-distance optimization is very similar to the previously discussed fixed-aperture optimization (cf. Fig. 4).

3.4 Monte-Carlo optimization

The fourth page of the notebook corresponds for the global optimization. Initial data can be entered in three different frames: geometrical parameters (sample-to-detector distance, wavelength, beamstop and sample shift), constraints (maximum beam size at the sample and the beamstop, largest allowed pinhole apertures, largest allowed collimation length) and the driving parameters for the Monte Carlo procedure.

The Monte Carlo optimization loop is executed several times, each execution is termed a "run". The first run starts with a completely random state sastisfying all the above given constraints. In each step of the run a change is introduced into one of the parameters (l_1, l_2, r_1 or r_2). If the change does not results in the violation of any of the criteria, the move is accepted according to the Metropolis prescription, i.e. with a probability of $min(1, e^{\frac{\mathcal{I}_{new} - \mathcal{I}_{old}}{T}}$, where T is the equivalent of the Boltzmann energy. If any of the criteria is violated,

L1 (mm)	L2 (mm)	L1 parts	L2 parts	S-D dist (mm)	PHI1 (um)	PHI2 (um)	alpha (rad)	Sample diam. (mm)	BS diam. (mm)	qmin (1/nm)	dmax (nm)	Dspheremax (nm)	PHI3 (um)	Intensity factor (um^4/mm^2)	Hotspot diameter (nm)	Hotspot distance mismatch (nm)	Limiting mode
1220	212	100 + 200 + 800	100	520.00	1250	400	0.00068	0.863	3.742	0.16361	38.4	15.8	687	8244.99	0.52	-287.88	sample
1016	212	100 + 800	100	520.00	1000	400	0.00069	0.871	3.762	0.16451	38.2	15.7	692	7608.56	0.51	-184.67	sample
1020	212	200 + 200 + 500	100	520.00	1000	400	0.00069	0.869	3.758	0.16432	38.2	15.7	691	7549.00	0.51	-182.00	sample
716	212	100 + 500	100	520.00	600	400	0.00070	0.878	3.778	0.16517	38.0	15.6	696	5515.26	0.49	570.00	sample
516	212	200 + 200	100	520.00	300	400	0.00068	0.864	3.745	0.16376	38.4	15.8	688	2654.81	0.42	-2926.00	sample

Select all | Deselect all | Copy as HTML | Store selected as optimum | Close window

Figure 2: Results of the brute-force optimization
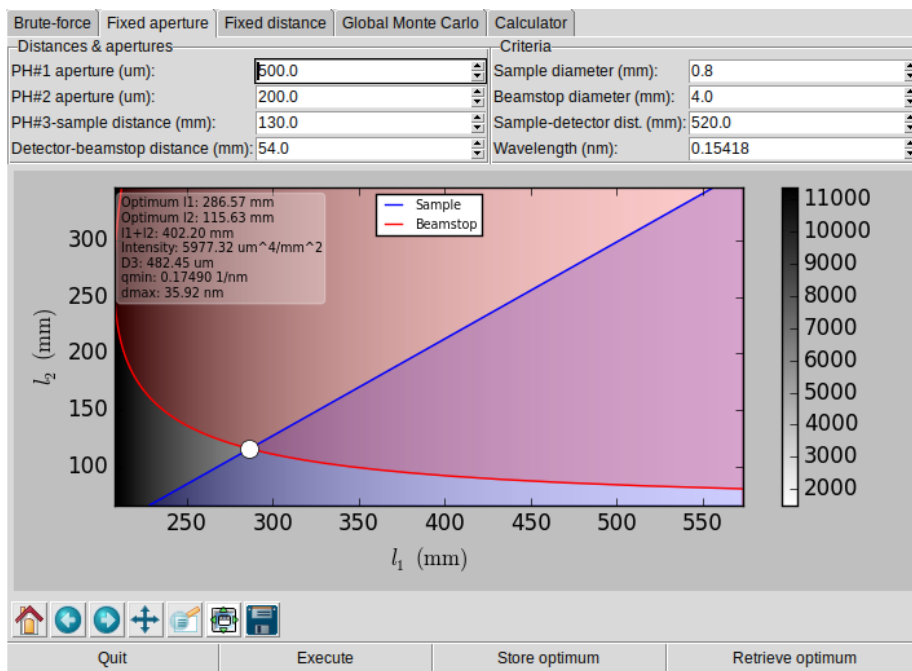
Figure 3: Fixed-aperture optimization
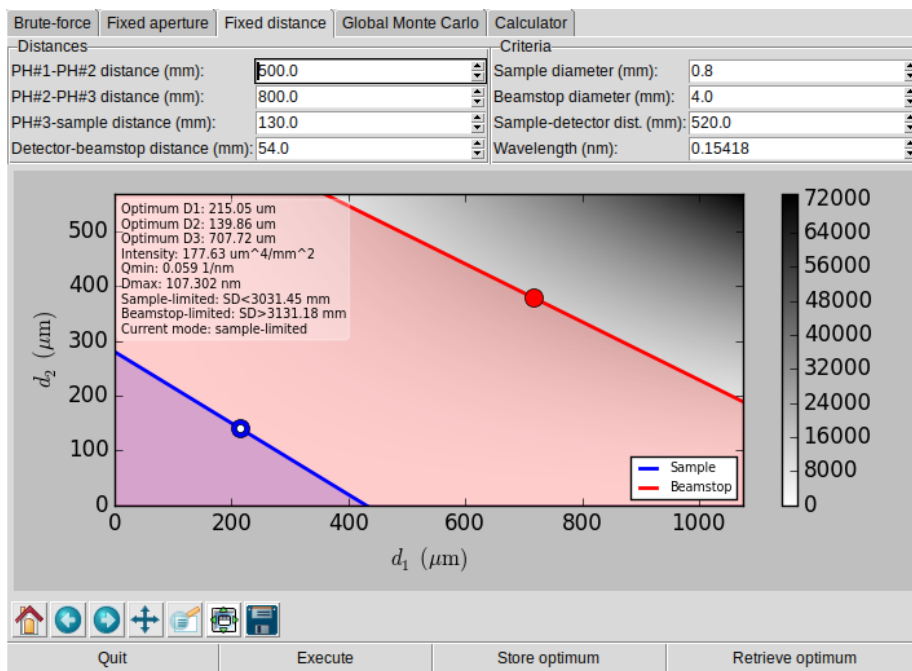
Figure 4: Fixed-distance optimization

Figure 5: Monte-Carlo optimization

Brute-force	Fixed aperture	Fixed distance	Global Monte Carlo	Calculator	
PH#1 aperture (d1, um):			500.0		
PH#2 aperture (d2, um):			200.0		
PH#1-PH#2 distance (l1, mm):			500.0		
Intensity factor (intensity, um^4/mm^2):			1963.4954084936207		
PH#2-PH#3 distance (l2, mm):			800.0		
PH#3 aperture (d3, um):			1320.0		
PH#3-Sample distance (ls, um):			130.0		
Beam size at sample (dsprime, mm):			1.502		
Extent of parasitic scattering at sample (ds, mm):			1.5670000000000002		
Sample-to-detector distance (d, mm):			520.0		
PH#3-Detector distance (l3, mm):			650.0		
Beam size at detector (ddetprime, mm):			2.23		
Extent of parasitic scattering at detector (ddet, mm):			2.5549999999999997		
Wavelength (wavelength, nm):			0.15418		
Lowest attainable q (qmin, 1/mm):			0.10723241687101454		
Maximum lattice spacing (dmax, mm):			58.594084610975166		
Detector-Beamstop distance (lbs, mm):			54.0		
Beam size at beamstop (dbsprime, mm):			2.1544		
Extent of parasitic scattering at beamstop (dbs, mm):			2.4524		
Quit		Execute	Store optimum		Retrieve optimum

Figure 6: Step-by-step pinhole geometry calculator

another change tried *in the same Monte Carlo step*. If the criteria cannot be fulfilled after several subsequent trials, the situation is considered a deadlock and the current run is terminated.

At the end of each run the acceptance ratio is evaluated. If it is higher or lower than the desired value given in the user interface, the temperature parameter is decreased or increased, respectively.

The set-up with the highest intensity is kept across runs, and returned at the end.

3.5   Step-by-step calculator

The last tab is a calculator for various parameters pertaining the collimation geometry. It is organized in a top-to-down fashion, based on the dependencies of the quantities. In each row, either a value can be entered into the spin box or the corresponding quantity can be calculated from those above it by pressing the label button. The whole calculation can be executed at once by pressing "Execute".

4   Reporting bugs and submitting feature requests

Programming errors can be reported directly to the author via e-mail (wacha.andras@ttk.mta.hu). Newer versions of the software are also available on request.