MuMag2022 — Toolbox: User Guide

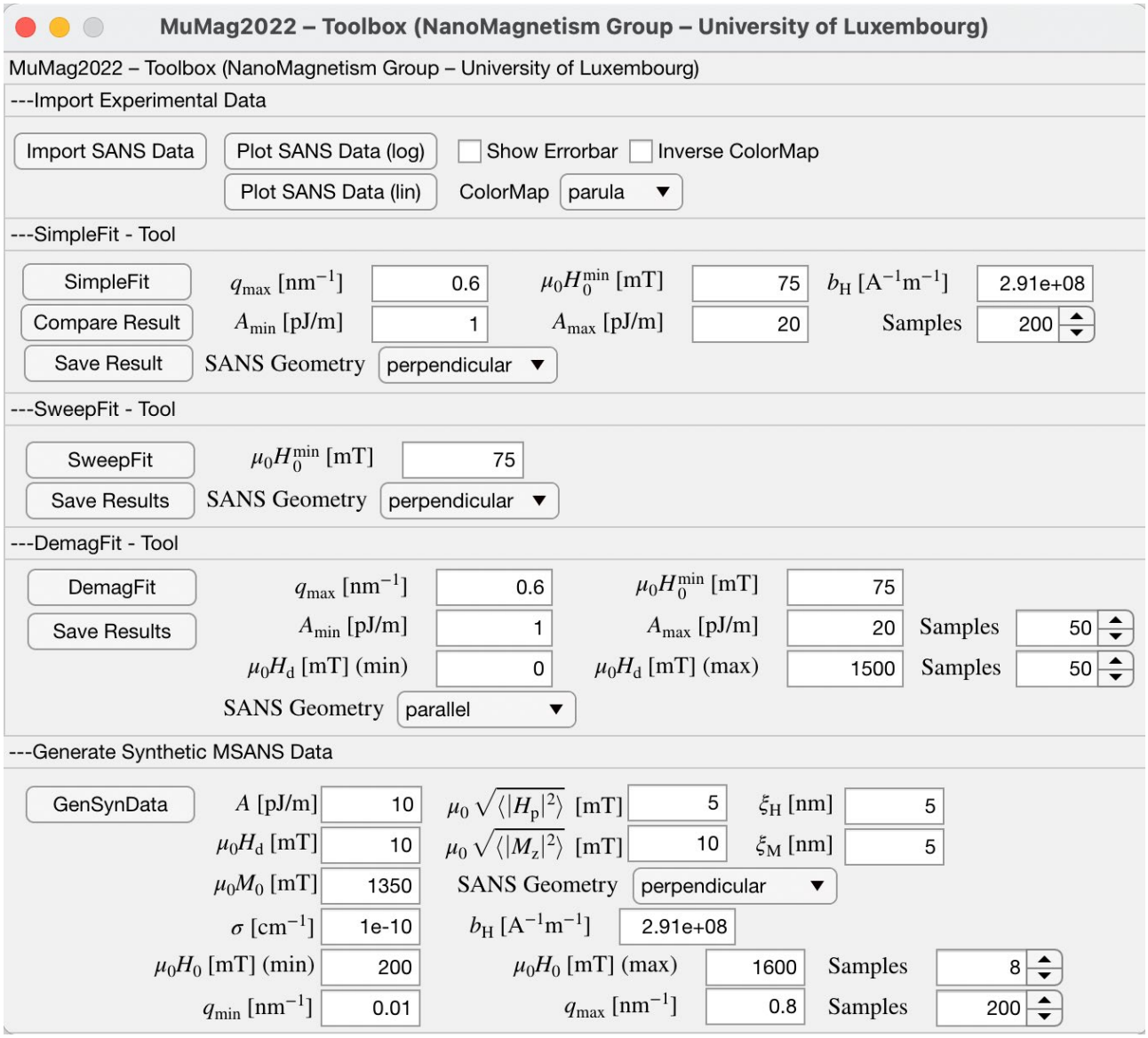

Fig. 1: User interface of the MuMag2022 software.

Table of Contents

UNIVERSITÉ DU LUXEMBOURG

1. Expected file format of the experimental SANS data

The experimental unpolarized total (nuclear + magnetic) SANS data are expected to be stored in a separate folder, e.g., named as *ExperimentalSANSData*. The following information on the experimental data must be specified through the file names stored in the folder *ExperimentalSANSData*.

filenames:

1_0_1340_10.csv
2_20_1340_10.csv
3_35_1340_10.csv
4_50_1340_10.csv
⋮

1. Value: Index of the files (e.g., 1, 2, 3, 4, …)
2. Value: Externally applied magnetic field $\mu_0 H_0$ in mT (e.g., 0, 20, 25, 50, …)
3. Value: Saturation magnetization $\mu_0 M_0$ in mT (e.g., 1340, 1340, 1340, 1340, …)
4. Value: Demagnetization field $\mu_0 H_d$ in mT (e.g., 10, 8, 7, 6, 5, …)

All these values (points 2-4) can also be written as a float number with a dot separator, e.g., 10.4345

For unknown demagnetizing field H_d, the *DemagFit* tool (see section 4) allows one to estimate this quantity. In this case, use a default value for H_d in the file name (for example '0'). In each of the files the scattering vector data, the azimuthally-averaged magnetic SANS data, and the corresponding standard deviation are stored. In the case that the standard deviation is unknown, it must be set to one. In the following, the data format is shown:

q [1/nm]	$\frac{d\Sigma}{d\Omega}(q)$ [cm^{-1} or arb. units]	std [cm^{-1} or arb. units]
3.62523e-02	2.85917e+03	2.28223e+01
4.07000e-02	1.03769e+03	1.39076e+01
4.51118e-02	4.61741e+02	9.64427e+00
4.95924e-02	2.83047e+02	7.65175e+00
⋮		

Each of the data files must have the same length and must be sorted from the smallest (first value) to the largest (last value) q-value. In the files, only the numerical data must be stored, no headers please.

2. Import and plot of experimental SANS data

Fig. 2: Panel for the import of experimental SANS data.

1. Click the button *Import SANS Data*.
2. A new window will open up, where you have to select the folder in which your data are stored.
3. Click the *open* button and your data are loaded.
4. To check that your data are correctly loaded, click the button *Plot SANS Data (log)* or *Plot SANS Data (lin)*. This plots your data on a logarithmic or linear scale. Use the check boxes *Show Errorbar* and *Inverse ColorMap* and the dropdown menu *Colormap* to modify the plot (see Fig. 3).

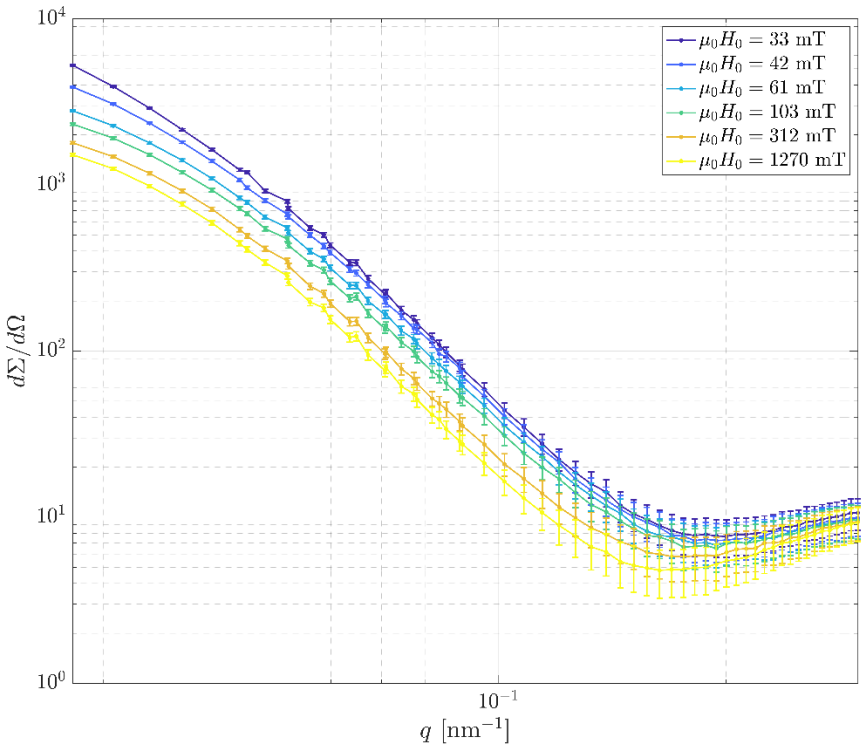

Fig. 3: Example of the *Plot SANS data (log)* feature with experimental SANS data. In this case, the *Show Errorbar* checkbox is enabled. Data taken from D. Honecker et al., PHYSICAL REVIEW B 88, 094428 (2013).

3. SimpleFit tool

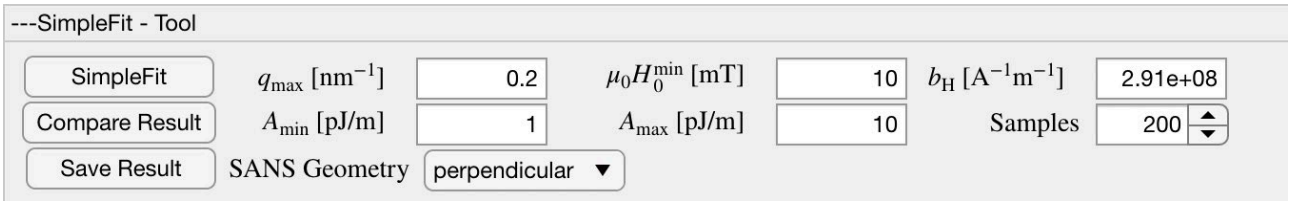

Fig. 4: Panel of the SimpleFit tool.

Once you have loaded your data, as explained in section 2, you can use the *SimpleFit* tool to estimate the exchange-stiffness constant A. Follow these steps:

1. Select the scattering geometry (external field perpendicular or parallel to the neutron beam).
2. Choose the expected range of values for the exchange-stiffness constant A in pJ/m.
   i. Enter the smallest value for A in the *min* edit field.
   ii. Enter the largest value for A in the *max* edit field.
   iii. Enter the number of sampling points in the range of min and max in the *Samples* edit field.
3. Remember that the micromagnetic SANS theory is valid for applied magnetic fields within the approach-to-saturation regime of the macroscopic magnetization. Enter the smallest externally applied field value in the $\mu_0 H_0^{min}$ [mT] edit field that lies within this regime. Here, the user must decide what is reasonable!
4. Beyond a certain maximum momentum-transfer value, the SANS cross section becomes field-independent and the fitting procedure does not work anymore. Enter this cut-off value in the q_{max} [nm^{-1}] edit field. Here, the user must decide what is reasonable!
5. Once you have fixed the settings, click the *SimpleFit* button, which yields the output that is shown in Fig. 5. The χ^2(A) error function and its minimum (best fit for A) are displayed on the top left (a). The data sets for $\frac{d\Sigma_{res}}{d\Omega}$ (b), S_H (c), and S_M (d) are displayed on a log-log scale.
6. After the fitting procedure is finished, you may want to compare the output from the fit model with the experimental data. To do this, press the *Compare Result* button, which gives an output as shown in Fig. 6.
7. Once you have obtained an estimation for the value of A, the fitting can be improved by choosing a larger number of sampling points (e.g., changing the setting from 50 to 200), so that the result will have a finer resolution. A recommendation is to change the value of A_{min} and A_{max} to make the interval narrower; for instance, if the result is $A = 12pJ/m$, then choose $A_{min} = 8pJ/m$ and $A_{max} = 16pJ/m$.
8. You can also export the fit results by clicking on the *Save Result* button. The output of the fit is stored in the same data format as the experimental input data. The data are stored in a folder with a time stamp and a structure like the one shown in Fig. 7.

For the demonstration of the previous points, we used the experimental SANS data from D. Honecker et al., PHYSICAL REVIEW B 88, 094428 (2013).

UNIVERSITÉ DU LUXEMBOURG

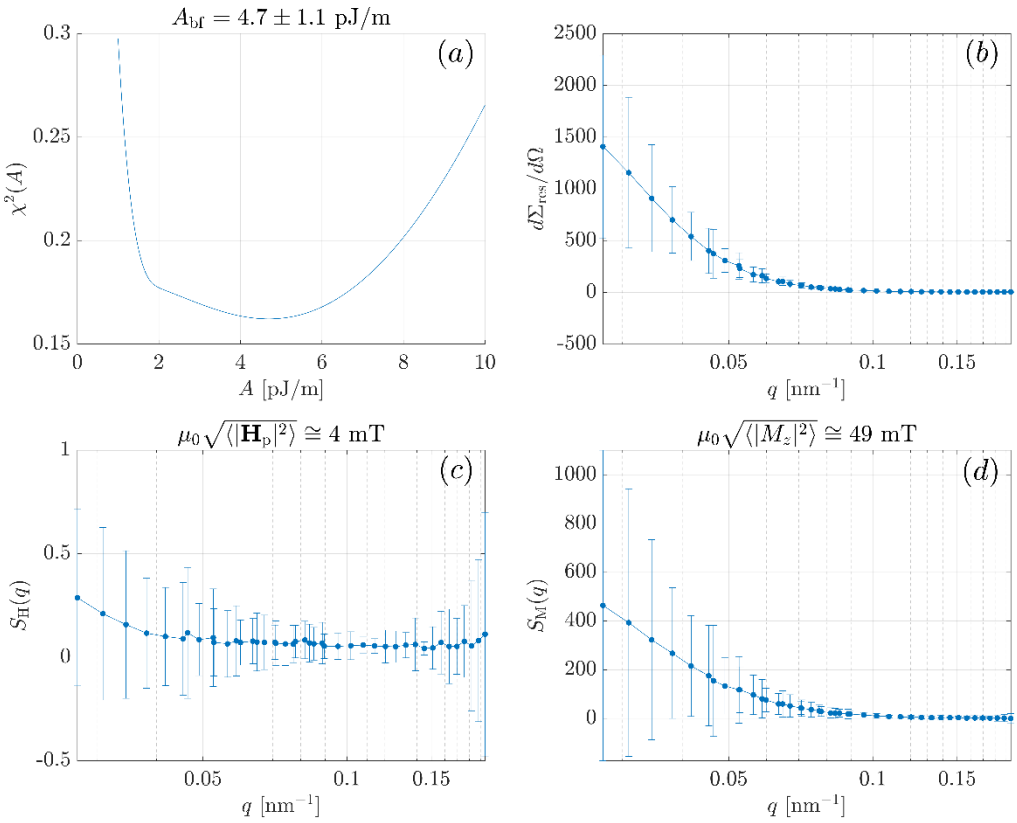

Fig. 5: Example output from the *SimpleFit* tool. Settings taken from Fig. 4.

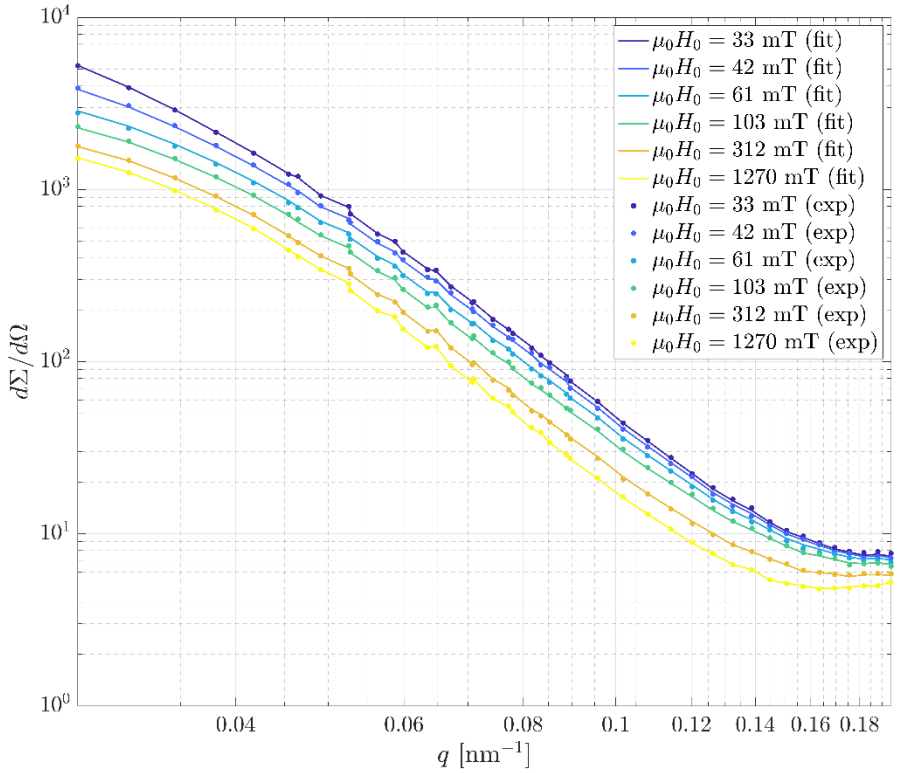

Fig. 6: Comparison of the fit results (solid lines) and the experimental data (•). Settings taken from Fig. 4.

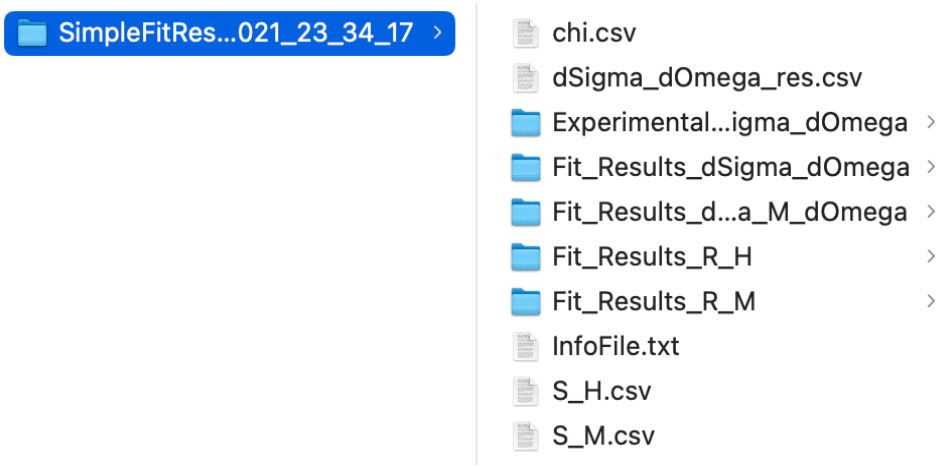

Fig. 7: Folder structure of the saved fit results.

4. SweepFit tool

Fig. 8: Panel of the *SweepFit* tool.

Using the *SweepFit* tool you have the possibility to analyze how the best-fit value A_{bf} for the exchange-stiffness constant varies in dependency of different cut-off values for the scattering vector (q_{max}) and the externally applied field (H_0^{min}). To use this tool, load your SANS data as explained in section 2. If this is done, follow the next steps:

1. Enter the smallest externally applied field value in the $\mu_0 H_0^{min}$ [mT] edit field that lies within the approach-to-saturation regime. Here, the user must decide what is reasonable!
2. Click the *Sweep Fit* button to start the fitting procedure. During the fitting procedure the progress bar shows you the current state of the process.
3. Once the fitting procedure has finished, a new figure like the one shown in Fig. 9 appears. This plot gives you information about the convergence of the fitting procedure depending on the chosen cut-off values. In the case that relatively large fluctuations or oscillations become visible in this plot, the experimental data might not be well behaved for precise predictions of the exchange-stiffness constant. In the case that some configurations do not work, an information window pops up, which tells you that these values are set to zero by default.
4. You can export the results by clicking the *Save Results* button.

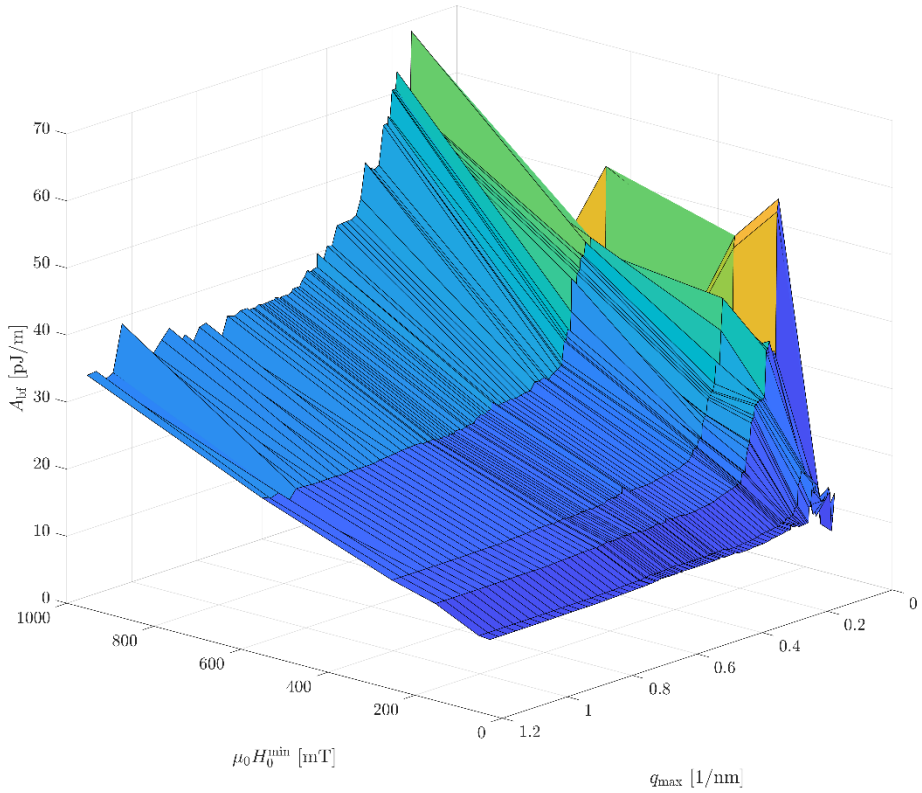

Fig. 9: Result of the *SweepFit* tool. Data taken from M. Bersweiler et al., IUCrJ 9, 65-72 (2022).

5. DemagFit tool

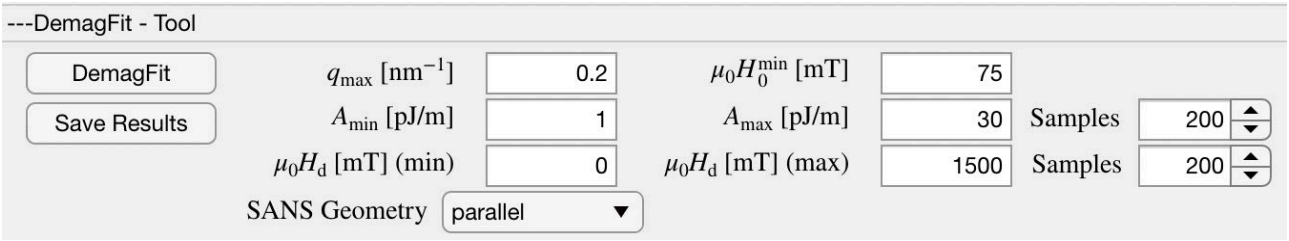

Fig. 10: Panel of the DemagFit tool.

In the case that the demagnetizing field H_d of the sample is unknown, the *DemagFit* tool provides the opportunity to search for the best-fit value of H_d (in addition to the exchange-stiffness constant A). In the *DemagFit* tool, it is assumed that H_d does not depend on the applied magnetic field H_0, and, therefore, the fit result provides a single value for the demagnetizing field H_d. This behavior corresponds to the fully saturated magnetization state. Note that the *DemagFit* tool does not provide a data export option like the *SimpleFit* tool. Therefore, the strategy is to first find the best-fit demagnetizing field from the *DemagFit* tool (e.g., $\mu_0 H_d$ = 1061 mT) and then include this value in the file name (e.g., change "1_8000_1600_1.csv" to "1_8000_1600_1061.csv"). Then, the process has to be repeated from the beginning, meaning that the user has to repeat the steps explained in sections 2, 3, and 4, i.e., reimport the data (section 2) and then perform the *SimpleFit* (section 3) and *SweepFit* (section 4) procedures. The steps of how to use both the *DemagFit* and *SimpleFit* tools are equivalent (see description on how to use the *SimpleFit* tool in section 3). In Fig. 11 below, we display the output from the *DemagFit* tool.

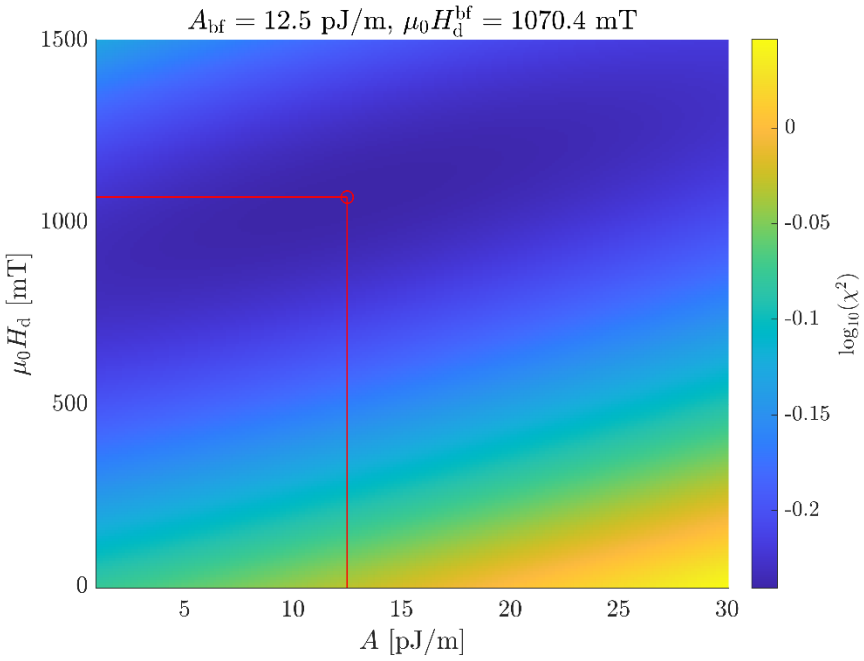

Fig. 11: Output of the *DemagFit* tool. Settings taken from Fig. 10. Data taken from J.-P. Bick et al., APPLIED PHYSICS LETTERS 102, 022415 (2013).

6. Generation of synthetic test data

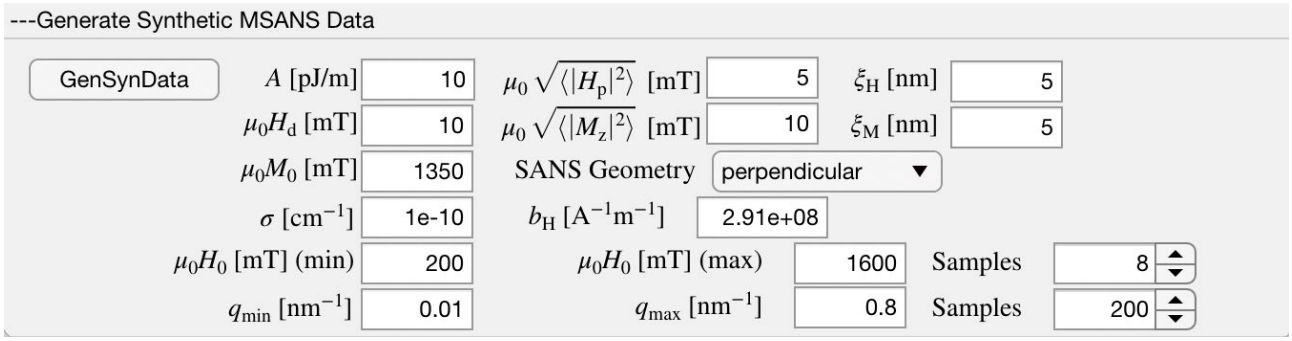

Fig. 12: Panel for the generation of synthetic test data.

With the *Generate Synthetic MSANS Data* tool you can generate test data for the perpendicular and parallel SANS scattering geometry and save it by clicking on the *GenSynData* button. This synthetic data can be used for further analysis and can also be read in through the *Import Experimental Data* panel, as described in section 2. Since the used model is free of statistical noise, the standard deviation σ has to chosen as a constant value for each generated data point.

The following equations for the micromagnetic SANS cross section are used to generate the synthetic data:

$$
\begin{aligned}
H_i &= H_0 - H_d > 0 \\
H_{eff}(q) &= H_i\left(1 + l_H^2 q^2\right) \\
l_H &= \sqrt{\frac{2A}{\mu_0 M_0 H_i}} \\
p(q) &= \frac{M_0}{H_{eff}(q)}
\end{aligned}
$$

Perpendicular Scattering Geometry:

$$
\begin{aligned}
R_H(q) &= \frac{p^2}{4}\left(2 + \frac{1}{\sqrt{1+p}}\right) \\
R_M(q) &= \frac{\sqrt{1+p} - 1}{2}
\end{aligned}
\qquad
\begin{aligned}
S_H(q) &= \frac{8\pi b_H^2 \xi_H^3 \langle |H_p|^2 \rangle}{(1 + q^2\xi_H^2)^2} \\
S_M(q) &= \frac{8\pi b_H^2 \xi_M^3 \langle |M_z|^2 \rangle}{(1 + q^2\xi_M^2)^2} \\
\frac{d\Sigma_M}{d\Omega}(q) &= R_H S_H + R_M S_M \\
\frac{d\Sigma_{res}}{d\Omega}(q) &= 0.9\,\frac{d\Sigma_M}{d\Omega}(q, H_0^{max}) \\
\frac{d\Sigma}{d\Omega}(q) &= \frac{d\Sigma_{res}}{d\Omega} + R_H S_H + R_M S_M
\end{aligned}
$$

Parallel Scattering Geometry:

$$
\begin{aligned}
R_H(q) &= \frac{p^2}{2}
\end{aligned}
\qquad
\begin{aligned}
S_H(q) &= \frac{8\pi b_H^2 \xi_H^3 \langle |H_p|^2 \rangle}{(1+q^2\xi_H^2)^2} \\
\frac{d\Sigma_M}{d\Omega}(q) &= R_H S_H \\
\frac{d\Sigma_{res}}{d\Omega}(q) &= 0.9\,\frac{d\Sigma_M}{d\Omega}(q, H_0^{max}) \\
\frac{d\Sigma}{d\Omega}(q) &= \frac{d\Sigma_{res}}{d\Omega} + R_H S_H
\end{aligned}
$$

UNIVERSITÉ DU LUXEMBOURG