

Magnetic Diffuse Scattering using Spinvert and Spinteract

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August 7, 2026

Installation

During this tutorial, we'll use four main programs:

- SPINVERT, which fits spin configurations to powder magnetic diffuse-scattering data;
- SPINCORREL, which calculates spin-pair correlation functions;
- SCATTY, which calculates magnetic and structural single-crystal diffuse scattering patterns;
- SPINTERACT, which fits magnetic interactions to powder or single-crystal magnetic diffuse-scattering data.

To get the most out of this tutorial, you'll need a scientific plotting program that allows you to plot graphs from text files in x, y, error format, and to plot matrices as 2D colour plots. If you don't have such a program already, I recommend installing the following program:

- VEUSZ: A simple and free program to plot data. Available from <https://veusz.github.io>

To install these programs, first unzip the archive **Summer2026_SpinHarmony_Tutorial.zip** to a convenient location on your computer (your tutorial folder).

The next steps depend on your operating system:

- On **Windows** or **Mac**, navigate to the `programs_win` or `programs_mac` subfolder in your tutorial folder. Copy all the program files to every subfolder within each exercise folder (names containing `ex1`, `ex2`, etc). This is necessary because the program files must always be in the same folder as the input data files for your refinements. That's it – you can now start the exercises below.
- On **Linux**, and on some older **Mac** machines, the procedure is slightly more complicated, as it's necessary first to compile the programs from source code on your own computer. To do this, follow these steps:
 1. If you don't already have a Fortran compiler installed, download and install the free gfortran compiler for your Mac system from <https://github.com/fxcoudert/gfortran-for-macOS/releases>
 2. Navigate (using the `cd` command) to the `programs_mac/spinvert_source` folder. Type `make` (and press enter). Five program files should appear (`spinvert`, `spincorrel`, `scatty`, `spinplot`, `ice_rules`). Copy all these program files to all the subfolders in the folders with names beginning with `Spinvert` (e.g., `spinvert_ex1_spinice/ising_spins`, `spinvert_ex2_Gd2Sn207`, `spinvert_ex3_MnO/fit_volume`).
 3. Open a Terminal window, and navigate (using the `cd` command) to the `programs_mac/minuit` subfolder in your tutorial folder. Type `make` (and press enter). A file called `lminuit.a` should appear. Copy this file to the `programs_mac/spinteract_source` folder.
 4. Navigate (using the `cd` command) to the `programs_mac/spinteract_source` folder. Type `make` (and press enter). A program file called `spinteract` should appear. Copy this program file to the `spinteract_ex4_Gd2Sn207` and `spinteract_ex5_MnO` folders.
 5. You're now ready to proceed to the exercises below. If you're more interested in `Spinvert`, start from exercise 1. If you're more interested in `Spinteract`, start from exercise 4.

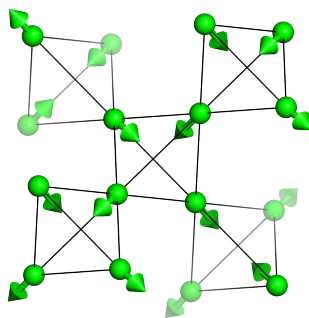


Figure 1: Pyrochlore lattice and spin-ice arrangement.

1 Spinvert: Ice rules in spin ice from powder data

Spin ices are magnetic materials with a pyrochlore structure, such as $\text{Ho}_2\text{Ti}_2\text{O}_7$. The magnetic ions – typically lanthanides, in this case Ho^{3+} – are located at the corners of a network of corner-sharing tetrahedra (Fig. 1). The space group is cubic $Fd\bar{3}m$, and the magnetic ions occupy the $16d$ Wyckoff position. Magnetically, the spins possess a strong Ising-like anisotropy, which constrains them to point either towards or away from the centres of the tetrahedra of the pyrochlore network. These directions correspond to cubic $\langle 111 \rangle$ axes (body diagonals; see Fig. 1). The magnetic interactions in spin ices are overall ferromagnetic at the nearest-neighbour distance. At low temperature (in practice, less than a few K), the interactions start to constrain the spin orientations such that each tetrahedron has two spins “in” (towards its centre) and two spins “out” (away from its centre). This is called the “ice rule”.

In this exercise, we’ll use SPINVERT to fit spin configurations to simulated magnetic diffuse-scattering data for spin ice, and show that we can recover the ice rule by fitting to such data, even when we do not know the underlying magnetic interactions.

1. Using a Terminal or Command Prompt, navigate to the folder `spinvert_ex1_spinice/ising_spins` on your computer. Check that SPINVERT runs by typing `./spinvert` (Mac or Linux) or `spinvert.exe` (Windows). You should get the following error message: Please start the program by writing `./spinvert [input file name stem]`
2. Open the file `spinice_data.txt` in your favourite text editor. Check that you understand the format of this data file (Q in $\text{\AA}^{-1}$, Intensity, Error). Then, plot these (simulated) data in your favourite plotting program (e.g. VEUSZ).
3. Open the file `spinice_config.txt`, which defines the crystal structure and refinement parameters. Check you understand the way we’ve defined the crystal structure using the CELL and SITE lines.
4. The `SPIN_DIMENSION 1` line tells SPINVERT to constrain the spins to point parallel or antiparallel to specified axes, defined by the ANISOTROPY lines. That is, we require the spins to be Ising variables. Why do we need to use a separate ANISOTROPY line for every magnetic atom in the unit cell?
5. The MOVES line tells SPINVERT how many spin flips (in the case of Ising spins) or spin rotations (in the case of Heisenberg spins) to attempt; the number is given per spin. Make sure this line reads `MOVES 0`, and save the file.
6. Run SPINVERT by typing `./spinvert spinice` (Mac or Linux) or `spinvert.exe spinice` (Windows). On more recent versions of Windows, you may instead need to type `./spinvert.exe spinice`. Because we have set `MOVES 0`, SPINVERT will not yet attempt to fit to the data you have provided – instead, it will just create an initial spin configuration with random Ising spin orientations. For the ANISOTROPY directions you have used, this corresponds to spins directed “in” or “out” of the tetrahedra at random. This spin configuration is written to a file called `spinice_spins_01.txt`. Open this file and check that you understand its format.
7. For a single tetrahedron, how many Ising spin arrangements are possible, if each Ising spin points either “in” or “out” of the tetrahedron? How many of these possibilities satisfy the “two in, two out” ice rule? Run the program ICE_RULES by typing `./ice_rules spinice` (Mac or Linux) or `ice_rules.exe spinice` (Windows). This program writes to screen the percentage of tetrahedra that obey the “two in, two out” ice rule. What is this number? Is it the same as the number you predicted? If not, why?
8. Open `spinice_config.txt` again and change MOVES to 100. Run SPINVERT again. After a few % of the refinement is complete, stop the program by typing `Ctrl-C` and run `ice_rules` again. How have the results changed?
9. Now restart SPINVERT and allow the program to complete the 100 proposed flips per spin. Note that SPINVERT continues the refinement from the point at which you stopped it: if you’d instead like to start a new refinement, you have to delete

the existing `spinice_spins_01.txt` file from the folder. How well did your refinement do at recovering the ice rule? Compare your results with those of your neighbour, whose refinement will have been started with different random spin orientations.

10. We're now going to calculate the radial spin-pair correlation function from your refined spin configuration. This is defined as

$$\langle \mathbf{S}(0) \cdot \mathbf{S}(r) \rangle = \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^{Z_i(r)} \frac{\mathbf{S}_i \cdot \mathbf{S}_j}{\langle Z_i(r) \rangle}, \quad (1)$$

where $\mathbf{S}_i$ is a spin vector, N is the number of spins in the configuration, and $\langle Z_i(r) \rangle$ is the average number of spins that coordinate a central spin i at distance r . If all spins in the configuration are crystallographically equivalent and there are no vacancies, $\langle Z_i(r) \rangle = Z_i(r)$ is an integer. The spin-correlation function consists of a set of peaks at interatomic distances, r . The function is normalised such that perfect parallel (ferromagnetic) alignment of all spins at an interatomic distance r would yield $\langle \mathbf{S}(0) \cdot \mathbf{S}(r) \rangle = 1$, and perfect antiparallel (antiferromagnetic) alignment would yield $\langle \mathbf{S}(0) \cdot \mathbf{S}(r) \rangle = -1$. Sketch the form of the spin-correlation function you would expect for (a) a perfect ferromagnet, and (b) a perfect paramagnet.

11. Run the program `SPINCORREL` by typing `./spincorrel spinice` (Mac or Linux) or `spincorrel.exe spinice` (Windows), and plot the results. What is the sign of $\langle \mathbf{S}(0) \cdot \mathbf{S}(r) \rangle$ at the nearest-neighbour distance? Why do you think this is?
12. Now, we're going to calculate the single-crystal diffuse scattering pattern using the program `SCATTY`. Open the file `scatty_config.txt`, and check you understand the format. Which reciprocal-space plane are we calculating?
13. Run `SCATTY` by typing `./scatty spinice` (Mac/Linux) or `scatty.exe spinice` (Windows).
14. `SCATTY` writes the single-crystal scattering in several formats, depending on the software you prefer to view the results. `SCATTY` can output a text file you can open in (e.g.) `Veusz`, a `.ppm` image you can convert and view using image-editing software such as `ImageMagick`, and a Visualization Toolkit (`.vtk`) file you can view in `ParaView`. Use your preferred software to view the diffuse scattering. (In `VEUSZ`, click Data menu – Import data – 2D data, select the file using “Browse”, import the data by pressing “Import”, and finally plot it using the “Plot 2D dataset as an image” widget.)
15. You may notice that the scattering pattern looks rather noisy. This is because we've calculated the scattering from only one spin configuration. If you have time, run multiple `SPINVERT` refinements by changing the line `RUNS 1` in `spinice_config.txt` to `RUNS 20` (or however many independent refinements you'd like to perform). Then, run `SCATTY` again. It will average the calculated diffuse scattering over all the spin configurations, and you should notice an improvement in statistics.
16. (optional) So far, we've assumed that the spins are perfectly Ising. Now, we are going to check whether this information on the single-ion anisotropy is actually present in the experimental data. To do this, we'll repeat the refinement without constraining the Ising anisotropy, and then examine whether we can recover this anisotropy by fitting to the data. To do this, navigate to the folder `ex1_spinice/heisenberg_spins`. Open the file `spinice_config.txt`. How is it different to the previous example, and why?
17. (optional) Run the refinement in the folder `ex1_spinice/heisenberg_spins`.
18. (optional) Run `SPINPLOT` by typing `./spinplot spinice`. This will produce a text file called `spinice_log_spinplot.txt` that contains a stereographic projection of the distribution of spin orientations. The coordinate system in which this distribution is calculated is determined by the local axes given in the file `spinplot_config.txt`. Open this file and check you understand its format – note that the local z -axis is always a $\langle 111 \rangle$ direction, respecting the $\bar{3}m$ point symmetry of the $16d$ site in $Fd\bar{3}m$.
19. (optional) Visualise the distribution of spin orientations by plotting the file `spinice_log_spinplot.txt`. Do you observe a preference for spins to align along the local z -axis?
20. (optional) In the folder `ex1_spinice/ho2ti2o7_data`, you can find experimental data for a real spin-ice material, $\text{Ho}_2\text{Ti}_2\text{O}_7$. These data were measured at a temperature of 0.28 K using the HB-2A diffractometer at ORNL, and are discussed in this preprint: <https://arxiv.org/pdf/2601.02555>. To achieve better agreement with the experimental data, a few changes were made to the config file. A background term was fitted (`FLAT_BACKGROUND refine`); a more accurate form for the magnetic form factor was used; and the value of `WEIGHT` was increased. If you have time, run a refinement for these real data and compare the results with the simulated data we've fitted so far.

2 (Optional) Spinvert: Spin correlations of Gd₂Sn₂O₇ from powder data

In this second exercise, we'll use SPINVERT to fit spin configurations to experimental powder magnetic diffuse-scattering data for Gd₂Sn₂O₇. These data were collected using neutron polarisation analysis on the D7 instrument at the ILL at 1.1 K, just above the magnetic ordering temperature $T_N = 1.0$ K, and have been normalised in absolute intensity units of barnsr⁻¹ spin⁻¹ using measurements of a vanadium standard. Just like the spin ice example above, the magnetic Gd³⁺ ions in Gd₂Sn₂O₇ occupy a pyrochlore network of corner-sharing tetrahedra. Unlike the spin-ice case, however, we can't assume that the Gd³⁺ ions have an Ising anisotropy—instead, we expect a more isotropic spin distribution, because Gd³⁺ ions have no orbital angular momentum ($L = 0, S = 7/2$).

1. Navigate to the folder `spinvert_ex2_gd2sn2o7`.
2. Open the file `gd2sn2o7_config.txt`. Why have we used `SPIN_DIMENSION 3`? Note that we've also changed the $\langle j_0 \rangle$ magnetic form factor coefficients to the values for Gd³⁺ – you can find this information for most magnetic ions at www.ill.eu/sites/ccsl/ffacts/.
3. Run SPINVERT.
4. Look at the fit to data. Do you think it is good enough? If not, increasing the value of `WEIGHT` in `gd2sn2o7_config.txt` and repeating the refinement—note that you'll first need to delete your existing `gd2sn2o7_spins_xx.txt` files, or start again in a new folder. The value of `WEIGHT` corresponds to W in the function

$$\chi^2 = W \sum_Q \left[\frac{I_{\text{calc}}(Q) - I_{\text{expt}}(Q)}{\sigma(Q)} \right]^2$$

that is minimised during the refinement, so a larger value of W corresponds to a reduction in the uncertainty assigned to each data point.

5. Once you have refined several spin configurations, repeat the analysis you did above for spin ice: calculate the spin-correlation function using `SPINCORREL`, the single-crystal diffuse scattering using `SCATTY`, and the spin-orientation distribution function using `SPINPLOT`.
6. Compare and contrast the results for Gd₂Sn₂O₇ with those for spin ice. Is the spin anisotropy Ising-like (easy axis) or XY-like (easy plane)? Based on your analysis, do you think the magnetic interactions are likely to be ferromagnetic or antiferromagnetic?
7. Open one of the `gd2sn2o7_spins_xx.txt` files, and find the value of `SCALE` – this is the refined value of the overall intensity scale factor. If your experimental data are correctly normalised in absolute units of barnsr⁻¹ spin⁻¹, this value should refine to the squared magnitude of the effective magnetic moment. For a spin-only magnetic moment such as Gd³⁺, this is given by

$$\mu^2 = g^2 S(S+1). \quad (2)$$

Compare the refined value of `SCALE` with the expected value of μ^2 for Gd³⁺. Do you think the agreement is reasonable? Discuss possible reasons for any discrepancies.

8. (optional) This paper <https://doi.org/10.1107/S1600576725003632> explains how the magnetic diffuse-scattering intensities can be placed in absolute intensity units using Rietveld refinement to the nuclear Bragg profile, using the nuclear Bragg peaks as an internal intensity standard. I recommend this approach to data normalisation, especially if you use a temperature subtraction (low – high temperature) to isolate the magnetic diffuse scattering. Accurate intensity normalisation is essential if temperature-subtracted data are used in Spinvert.

3 Spinvert: Spin correlations of MnO from single-crystal data

We'll now study the frustrated antiferromagnet, MnO. In this material, magnetic Mn^{2+} ions occupy a face-centred cubic lattice. Above its long-range magnetic ordering temperature of 118 K, MnO is cubic and paramagnetic. The single-crystal diffuse scattering data we'll be using were collected at 160 K using the SXD diffractometer at ISIS (data are from Paddison et al., *Phys. Rev. B* **97**, 014429 (2018)).

1. Navigate to the folder `spinvert_ex3_MnO/fit_hk0_plane`.
2. To start with, we'll try fitting experimental single-crystal data measured in a single scattering plane, $(hk0)$. These data are provided in the file `MnO_hk0_xtal_data_01.vtk`. When used with Spinvert, this file format requires that the data are binned in a parallelepiped with axes parallel to $[100]^*$, $[010]^*$, and $[001]^*$. The file contains a header giving the ORIGIN in (hkl) space and the spacing along each of the axes (both in reciprocal-lattice units), followed by a list of intensity values (with the $[100]^*$ index varying fastest). This is the recommended file format because it contains sufficient meta-data and enables faster calculation. However, it's also possible to provide data in a plain-text format containing a list of `h,k,l,intensity,uncertainty` values.
3. Open the file `MnO_hk0_config.txt`. The information in this file is very similar to the previous examples, except we've changed the SITE lines to reflect the face-centred cubic lattice occupied by the Mn^{2+} ions and some keywords are now prefaced by XTAL_.
4. Run SPINVERT. Once the program has read the single-crystal data, it writes a file called `MnO_hk0_xtal_data_img_01.txt` which contains the input data as a matrix. Plot this matrix as a colour plot (heat map) in your preferred plotting program. (In VEUSZ, click Data menu – Import data – 2D data, select the file using “Browse”, import the data by pressing “Import”, and finally plot it using the “Plot 2D dataset as an image” widget.) Note that it's necessary to remove (“punch”) nuclear Bragg peaks from the data before attempting to fit to them using Spinteract. This has already been done for the data sets we're using here.
5. Once the program has finished, plot the file called it writes a file called `MnO_hk0_xtal_fit_img_01.txt` in the same way. You should find that the fit agrees very well with the data.
6. If a model is physically reasonable, it should be able to make predictions. So, as a sanity check on the results, it's a good idea to try to calculate some quantity that was not included in the fit. To do this, use Scatty to calculate the $(hk0.48)$ scattering plane (a suitable `scatty_config.txt` file is included in the folder). Experimental data in the $(hk0.48)$ scattering plane are shown in Fig. 2:

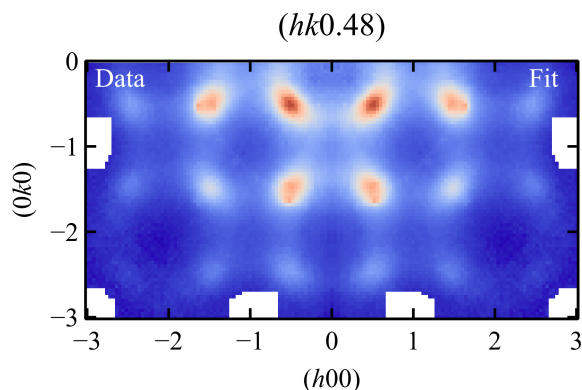


Figure 2: Experimental data for MnO in the $(hk0.48)$ scattering plane.

You'll notice that the calculated $(hk0.48)$ from the Spinvert model fails to predict many of the features of the data shown in Fig. 2. This is because the experimental data we provided was not sufficient to constrain the model effectively, since it contained no information about the scattering outside of the $(hk0)$ plane. For this reason, it's strongly recommended to fit to a volume of diffuse scattering data when performed single-crystal refinements in Spinvert, or alternatively, to fit powder data together with a single-crystal plane. Otherwise, the model may not be sufficiently well constrained.

7. Navigate to the folder `spinvert_ex3_MnO/fit_volume`. This folder contains a large volume of single-crystal data measured on MnO. Repeat the Spinvert refinement and Scatty calculation and check that the results look better.

4 Spinteract: Spin Hamiltonian of $\text{Gd}_2\text{Sn}_2\text{O}_7$ from powder data

We'll use the program SPINTERACT [*J. Phys.: Condens. Matter* **35**, 495802 (2023)] to refine magnetic interaction parameters to powder magnetic diffuse-scattering data for the frustrated antiferromagnet $\text{Gd}_2\text{Sn}_2\text{O}_7$. These data were collected using neutron polarisation analysis on the D7 instrument at the ILL at 1.1 K, just above the magnetic ordering temperature $T_N = 1.0$ K, and have been normalised in absolute intensity units of $\text{barn sr}^{-1} \text{spin}^{-1}$ using measurements of a vanadium standard. The magnetic Gd^{3+} ions in $\text{Gd}_2\text{Sn}_2\text{O}_7$ occupy a pyrochlore network of corner-sharing tetrahedra. The Spinteract program provides direct information about the magnetic *interactions* of the material. As such, it is different to magnetic reverse Monte Carlo programs (such as Spinvert), which provide information only about the magnetic *correlations*. Also, unlike Spinvert, Spinteract does not use a “box” of spins in real space – instead it uses a field-theory approximation to calculate the magnetic diffuse scattering pattern directly from the magnetic interaction parameters.

1. Navigate to the folder `spinteract_ex4_gd2sn2o7` on your computer.
2. The experimental powder data is contained in the text file `Gd2Sn207_powder_data_01.txt`. Spinteract is able to fit to multiple data sets (powder and single-crystal) simultaneously, though we won't use this capability here.
3. Look at the text file `Gd2Sn207_config.txt`. This file defines the crystal structure and refinement parameters using keywords (which can be in any order). The essential keywords are:

TITLE The title of the refinement (text string).

CELL A list of the lattice parameters a, b, c in Angstrom units, followed by a list of the cell angles α, β, γ (six real numbers).

CENTRING The centring of the unit cell (one character). Options are P (primitive), I (body-centred), F (face-centred), R (rhombohedral), A-centred, or C-centred.

SITE The fractional coordinates of a magnetic atom in the unit cell. Each magnetic atom is given on a new line, with the keyword SITE followed by the x, y, z fractional coordinates (three real numbers). **Note:** Fractional coordinates related by centring operations [that is, $(x, y, z) + (0, \frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}, 0)$, or $(\frac{1}{2}, 0, \frac{1}{2})$] are generated internally by the program, and should not be given. Taking the example of the pyrochlore lattice, only the following four coordinates should be given when using Spinteract: $(0, 0, \frac{1}{2})$, $(0, \frac{1}{4}, \frac{3}{4})$, $(\frac{1}{4}, 0, \frac{3}{4})$, and $(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$.

SPIN_DIMENSION The dimensionality of the spins (one integer):

- | | |
|---|--|
| 1 | Ising spins |
| 2 | XY spins |
| 3 | Heisenberg (isotropic) spins. This is the option we'll use for $\text{Gd}_2\text{Sn}_2\text{O}_7$, because Gd^{3+} is a spin-only ion with only small single-ion anisotropy. |

LOCAL_AXES These lines define an orthogonal local axis system $\mathbf{x}, \mathbf{y}, \mathbf{z}$ for every site in the unit cell. They are only needed if the system is magnetically anisotropic.

FORM_FACTOR_J0 The magnetic form factor, $f(Q)$, for the magnetic ion—we've already used values appropriate for Mn^{2+} here. This is given as a list of seven real numbers A, a, B, b, C, c, D for the analytical approximation to the $j_0(Q)$ integrals, which can be found online at www.ill.eu/sites/ccsl/ffacts/ffachtml.html.

BZ_POINTS Three integers, specifying the number of samples in the first Brillouin zone. Larger numbers yield more accurate results in a longer time. Values between 20 20 20 and 50 50 50 usually work well.

POWDER_TEMPERATURE The measurement temperature in Kelvin. Here, it is 1.1 K. **Note:** Interactions will also be reported in Kelvin units.

POWDER_TEMP_SUBTRACT If a high temperature data set has been subtracted to remove nonmagnetic scattering, this line must be included and the high temperature given. This is not the case for the data we're using, however.

POWDER_SCALE refine This tells the program to refine an overall intensity scale factor. This is almost always necessary, since data are not typically reported in absolute intensity units. There are options to refine a flat or linear-in- Q background, too, but we won't use them here.

4. When $\text{Gd}_2\text{Sn}_2\text{O}_7$ was first studied, it was suggested it might realise a simple model of nearest-neighbour Heisenberg interactions on the pyrochlore lattice,

$$H_{\text{trial}} = -\frac{1}{2} \sum_{i,j \in \text{n.n.}} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (3)$$

where the sum is taken over nearest neighbour spin pairs. Note the conventions that Spinteract uses. The inclusion of a factor 1/2 means that interactions between pairs of spins are counted only once. The spins $\mathbf{S}_i$ are treated as classical vectors

with unit magnitude. The unit of the interactions is Kelvin. If $J_1 > 0$, the energy is minimised when neighbouring spins are parallel; thus, positive values of J_1 indicate ferromagnetic interactions. There is no consensus in the literature about any of these conventions (e.g., some authors double-count pairwise interactions, report energies in meV, take spins as having a length of S , and define $J < 0$ as ferromagnetic). For this reason, it's a good idea to check the conventions carefully when comparing values from different sources.

5. We're now going to set up a refinement of the value of J_1 against our powder data. To do this, open the file `gd2sn2o7_params.txt`. This "parameters file" is where we define the parameters to be refined, and their initial values. An example is shown below. The file contains a title line, followed by a line for each parameter that is to be refined. Each parameter line contains four columns, each of which must have a width 10 characters (I apologise for this pernickety aspect of the program). The first column gives the **number** of the parameter. The second column gives the **name** of the parameter. The third column gives the **initial (guess) value** of the parameter. The fourth column gives the **initial (guess) uncertainty** of the parameter value. The parameter name `J_ISO 1` tells the program that we want to include isotropic interactions `J_ISO` between spins that are nearest neighbours (the first shell of neighbours). Similarly, `J_ISO 2` correspond to next-nearest neighbour interactions (the second shell of neighbours), and so on. Finally, the file ends with a blank line followed by the lines `MIGRAD` and `RETURN` or `END` (see below).

```

Test
1      J_ISO 1  450.00  50.0
2      J_ISO 2  250.00  50.0
3      J_ISO 3  250.00  50.0
MIGRAD
RETURN

```

Figure 3: Example parameters file for Spinteract showing format requirements. This example includes Heisenberg (isotropic) interactions up to third-nearest neighbours.

In our case, the file `gd2sn2o7_params.txt` specifies a single parameter, called `J_ISO 1`. This defines an isotropic (Heisenberg) interaction between nearest-neighbour spins.

6. Run the refinement by typing `./spinteract Gd2Sn2O7` (Mac) or `spinteract.exe Gd2Sn2O7` (Windows). When the refinement is complete, plot the fit (text file ending `_fit_01.txt`). Do you think the fit is good enough?
7. If the fit does not agree well with the data, it is possible to refine additional parameters, to try and improve it. Modify the parameters file to refine also a next-nearest-neighbour interaction, and re-run the program (you may want to copy the files to a new folder so you don't overwrite your previous work). Does the fit look acceptable?
8. So far, we've considered only Heisenberg exchange interactions. However, if exchange interactions are small and magnetic moments are large, the long-ranged magnetic dipolar interaction may also be significant. The magnitude of this interaction at the nearest-neighbour distance is given (in Kelvin units) by $D_{\text{dip}} = \mu_0 \mu_B^2 \mu^2 / 4\pi k_B |\mathbf{r}_{\text{nn}}|^3$, where the nearest-neighbour distance $|\mathbf{r}_{\text{nn}}| = 3.691 \text{ \AA}$ in $\text{Gd}_2\text{Sn}_2\text{O}_7$, and the magnetic moment length $\mu = g\sqrt{S(S+1)}$ with spin $S = 7/2$. Calculate the value of D_{dip} in $\text{Gd}_2\text{Sn}_2\text{O}_7$. Is it comparable to the exchange interactions you refined?
9. Perform a refinement including D_{dip} , by using the parameter name `DIPOLAR` in the parameters file. Since the value of D_{dip} is fixed by the magnetic moment length and the crystal structure, it should not be refined. To hold its value fixed, add the line `FIX n` above the line `MIGRAD`, where n is the parameter number of the dipolar interaction.
10. Look at the fit you get. Is the dipolar interaction important here?
11. Spinteract writes a file called `gd2sn2o7_results.tex` containing the refined values of the interaction parameters, and other useful information about the refinement. This file is in LaTeX format for easy integration into publications. If you have LaTeX editor, have a look at the refined interaction values on the last page of this file. If you don't have a LaTeX editor, you can find the same values at the end of the plain-text file `gd2sn2o7_minuit_output.txt`.

5 Spinteract: Spin Hamiltonian of MnO from single-crystal data

We'll now study the frustrated antiferromagnet, MnO. In this material, magnetic Mn^{2+} ions occupy a face-centred cubic lattice. Above its long-range magnetic ordering temperature of 118 K, MnO is cubic and paramagnetic. The single-crystal diffuse scattering data we'll be using were collected at 160 K using the SXD diffractometer at ISIS (data are from Paddison et al., *Phys. Rev. B* **97**, 014429 (2018)).

1. Navigate to the folder `spinteract_ex5_MnO` in your user area.
2. Open the files `MnO_config.txt` and `MnO_params.txt`, and check that you understand their format. Here, we're fitting to two scattering planes, $(hk0)$ and the $(hk0.48)$, and constraining the profile parameters (scale and background) to be the same for both using the keyword `XTAL_COMMON_PROFILE`.
3. For single-crystal data, the data files are called `MnO_xtal_data_01.txt`, `MnO_xtal_data_02.txt`, and so on. These files simply contain a list of h, k, l , intensity, uncertainty values (with every data point on a new line). Since we're considering diffuse scattering, h, k , and l , will generally have non-integer values.
4. Edit the file `MnO_params.txt` so that it contains a single, isotropic exchange parameter corresponding to antiferromagnetic interactions between nearest neighbours, and save the file.
5. Run SPINTERACT by typing `./spinteract MnO` (Mac or Linux) or `spinvert.exe MnO` (Windows).
6. Spinteract should have written two files called `MnO_xtal_data_img_01.txt` and `MnO_xtal_data_img_02.txt`. These contain the experimental data, now written as grids suitable for plotting. Plot these matrices as colour plots (heat maps) in your preferred plotting program. (In VEUSZ, click Data menu – Import data – 2D data, select the file using “Browse”, import the data by pressing “Import”, and finally plot it using the “Plot 2D dataset as an image” widget.) Note that it's necessary to remove (“punch”) nuclear Bragg peaks from the data before attempting to fit to them using Spinteract. This has already been done for the data sets we're using here.
7. After a little while, Spinteract will report that the fit is done, and write files called `MnO_xtal_fit_img_01.txt` and `MnO_xtal_fit_img_02.txt`. These are the fits to experimental data, for the optimized value of J_1 . Plot these files and decide whether the fit is good enough. If you think the fit isn't yet good enough, also refine a next-nearest neighbour interaction by adding an appropriate line to the file `MnO_params.txt`, and run Spinteract again. You should then obtain a fit similar to the one shown in Fig. 4 below.

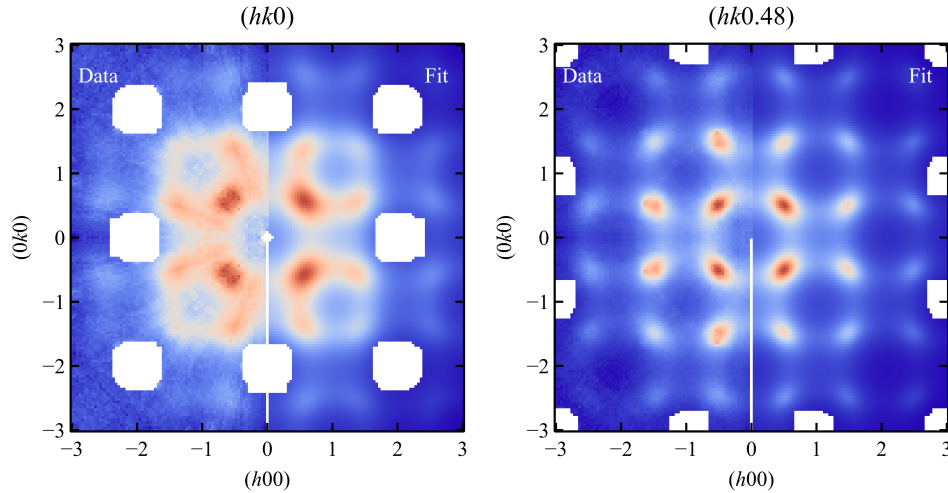


Figure 4: Plot of MnO data and fit using Veusz.

8. (optional) It's a good idea to try several refinements with different initial parameter values, in case your initial choice of starting values led the refinement into a false minimum. If you have time, try doing so, and see if you find any false minima.
9. The values of the magnetic interactions can be used to calculate the Curie-Weiss temperature, which for the conventions of Eq. 3 can be expressed as

$$\theta_W = \frac{1}{3} \sum_n J_n Z_n, \quad (4)$$

where the coordination number $Z_1 = 12$ and $Z_2 = 6$ for the FCC lattice. This is a useful sanity check, since an independent experimental estimate of the Curie-Weiss temperature is often available from laboratory magnetic characterization data (e.g., bulk susceptibility). Calculate θ_W for your fitted values of J_1 and J_2 , and compare it with the experimental value of approximately -500 K.

10. Is J_1 or J_2 of larger magnitude in MnO?