A Quick Guide to DipoleCalc

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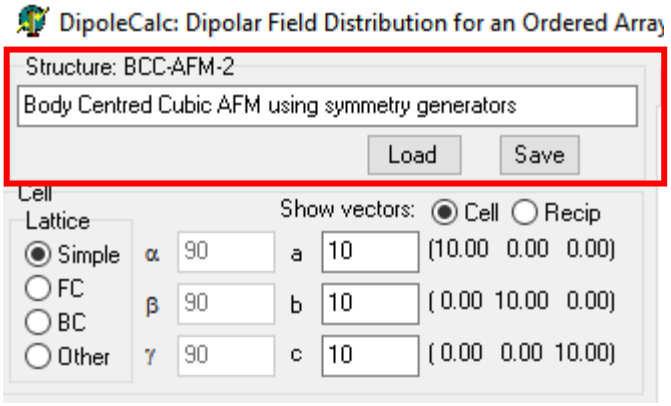
1. Introduction

   DipoleCalc is an interactive Windows program developed by Francis Pratt as a tool to enable one to explore and assess dipolar fields at potential muon sites for magnetically ordered crystalline materials.

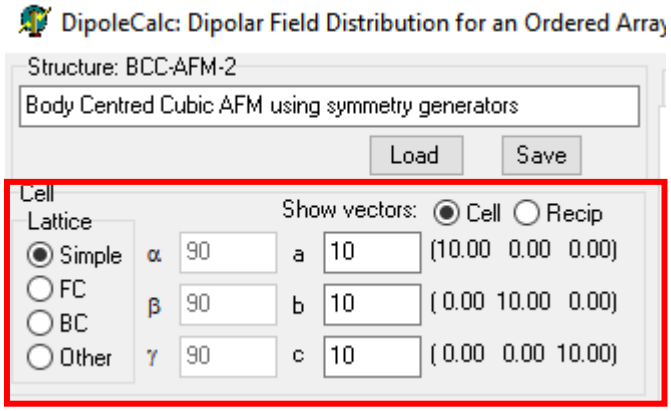
2. Saving and Loading Structures

   Structures and calculation parameters can be saved and loaded again with the save and load buttons in the 'Structure' box. The text box allows a description to included along with the structure. Structure files have the extension .str and are stored in a simple readable and editable text format.



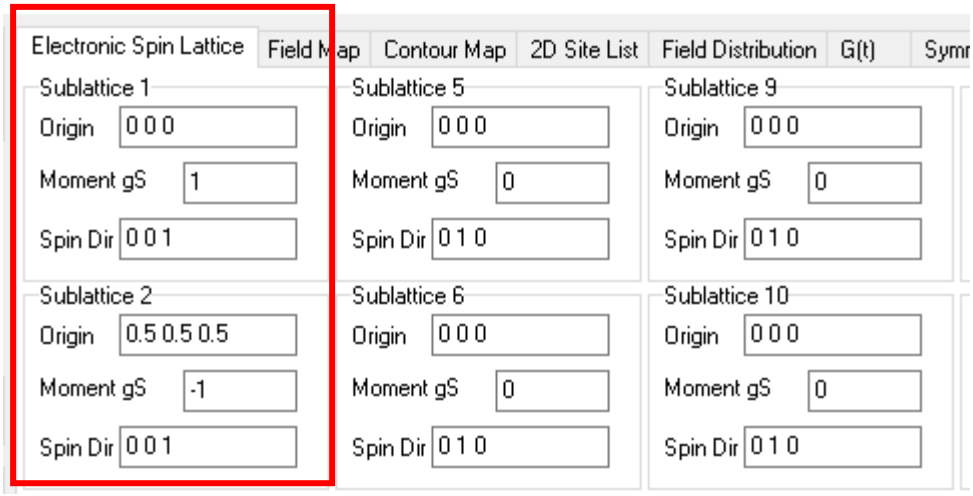
3. Defining Unit Cell Parameters

   The unit cell parameters in degrees and Ångstrom are defined in the 'Cell' box. For orthorhombic cells the 'simple' option is selected. For most other cells the 'other' option must be used. For simple FM systems the 'FC' (face-centred) or 'BC' (body-centred) options can be used. The Cartesian definition of the lattice vectors or reciprocal lattice vectors is displayed on the right.



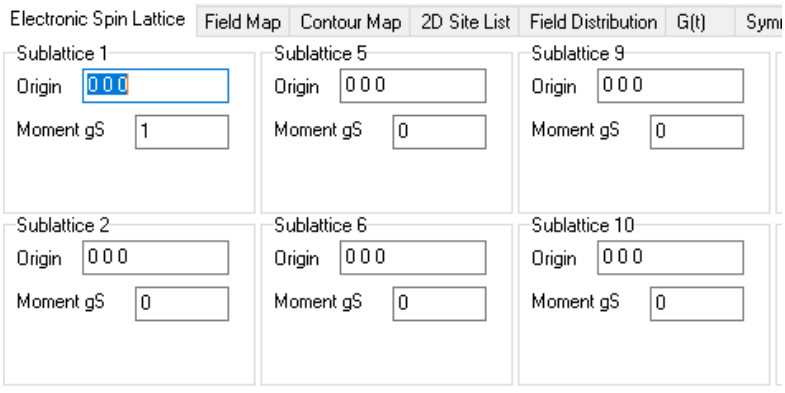
4. Spin Sublattices

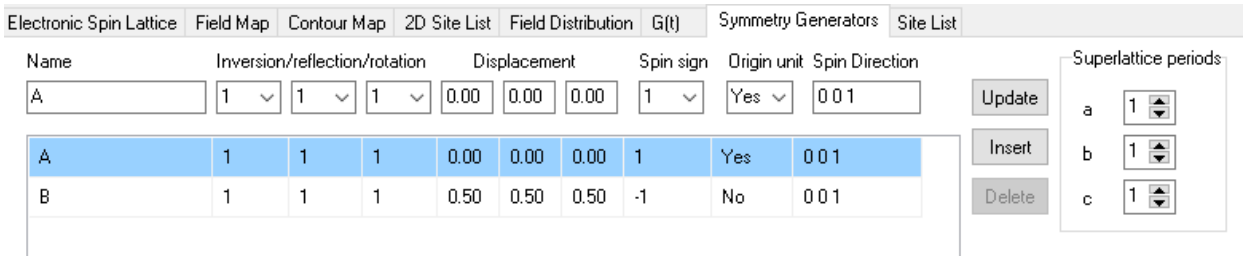
The ordered magnetic sublattices can be defined in the first tab on the top right of the window labelled 'Electronic Spin Lattice'. The position within the cell, the moment and the spin direction are defined for each sublattice. Up to 20 sublattices may be specified in this way. The example shows two sublattices defined for a simple body-centred AFM structure, with the remainder flagged as not being used by having zero moment. Sublattices can be given descriptive names by clicking the sublattice box titles.



5. Symmetry Generators

An additional way of defining magnetic sublattices is via the 'Symmetry Generators' tab page. This provides a list of symmetry operations that are to be applied to each sublattice defined in the 'Electronic Spin Lattice' page. The total number of spin elements is thus the product of the number of elements in these two pages. The examples below shows an alternative way of defining the BCC-AFM using a single sublattice and two symmetry generators. Superlattice periods can also be defined within the symmetry generators page.



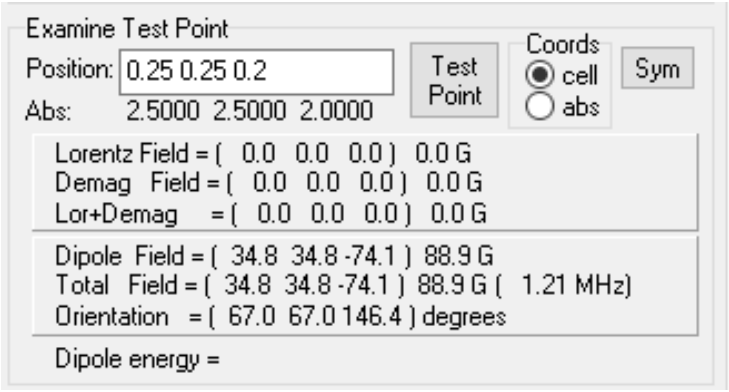


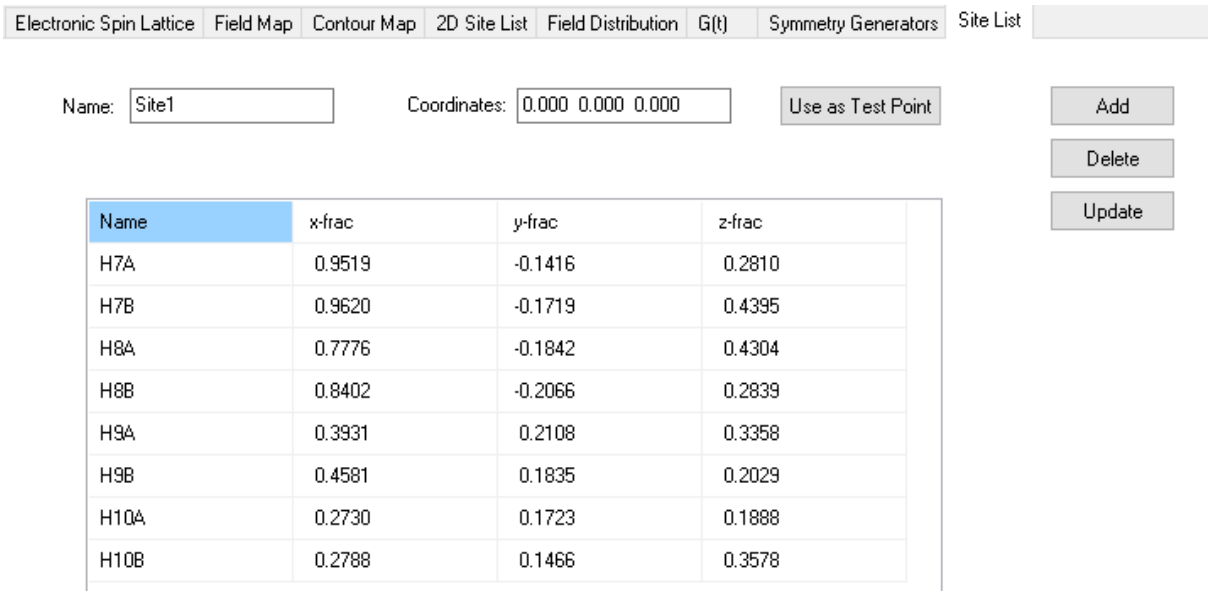
6. Cut-off, sampling and demagnetization

   The 'Sampling and Demagnetization' box defines the cutoff radius for the dipolar sum, the grid resolution used for 2D and 3D scans and the demagnetization factor that applies in the case of a ferromagnet.

7. Test Points and the Site List

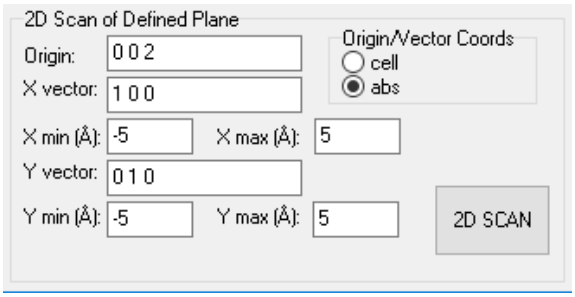
   The 'Examine Test Point' box is used to test the dipolar field vector and precession frequency at individual sites within the magnetic structure. A set of site positions can be maintained via the 'Site List' tab and used as test points.

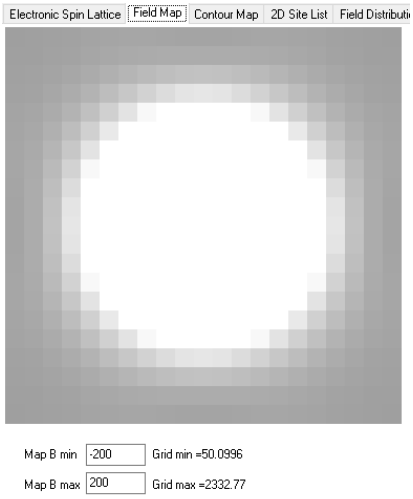


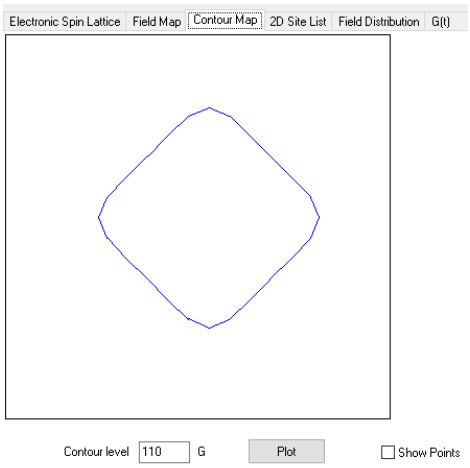


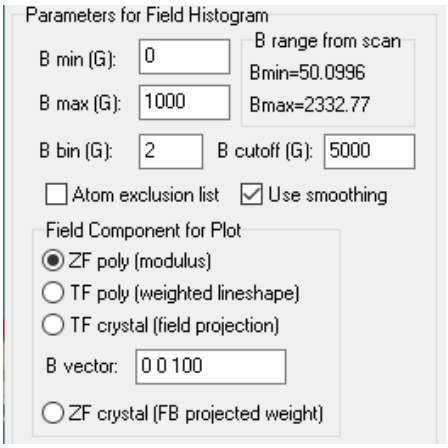
8. 2D Scan of a Defined Plane

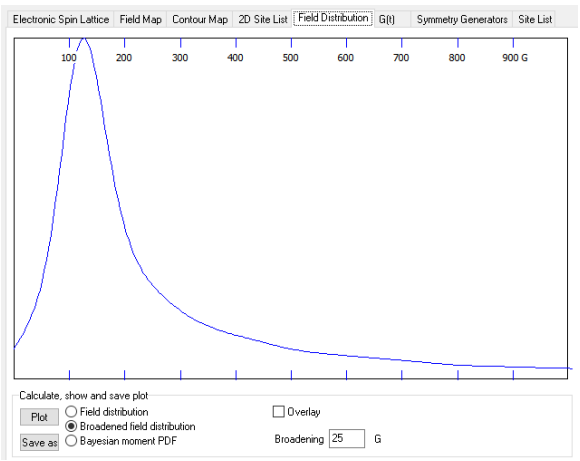
If it is desired to map the dipolar field within the lattice then options to scan over a 2D plane and over the full 3D lattice are offered. The '2D Scan of Defined Plane' box is used to make a 2D scan. An origin and scan vectors must be defined before making the scan. After the scan is complete the data may be viewed via three alternative tab pages 'Field Map' , 'Contour Plot' and 'Field Distribution'. The range and binning for the field distribution plot are specified in the 'Parameters for Field Histogram' box. Broadening can be applied to the field distribution to smooth out the sampling noise.





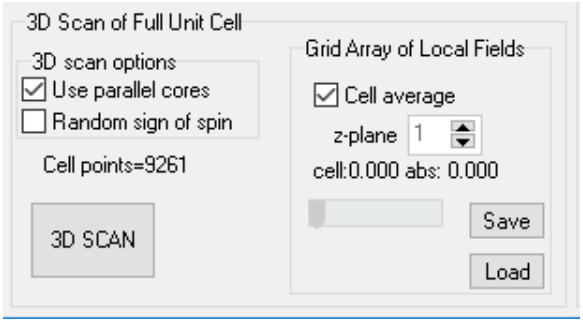


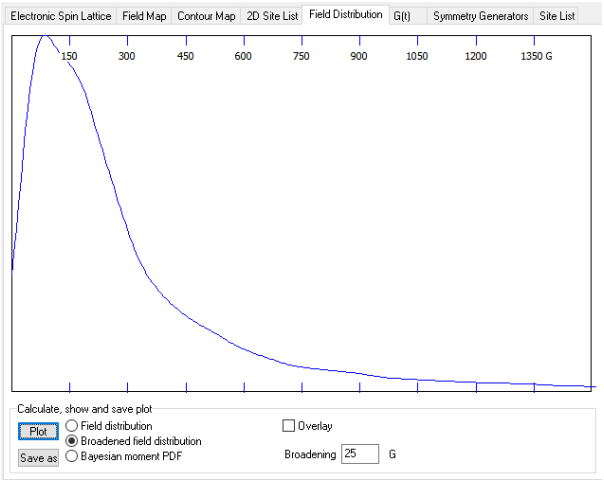


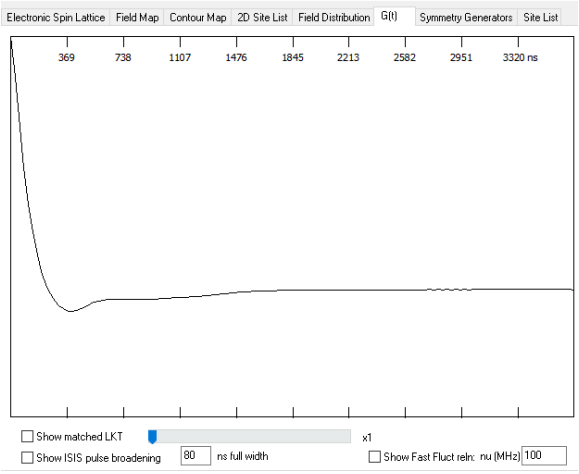


9. 3D Scan of the Full Cell

To map the dipolar field within the entire magnetic cell the '3D Scan of Full Unit Cell' box is used. If a multicore processor is available then there is an option to speed up the calculation with parallel processing. After the calculation is complete, there is an option to view the cell averaged field distribution or alternatively view the results as a series of planes with different z-values. The grid array of local field vectors can be saved and reloaded later.

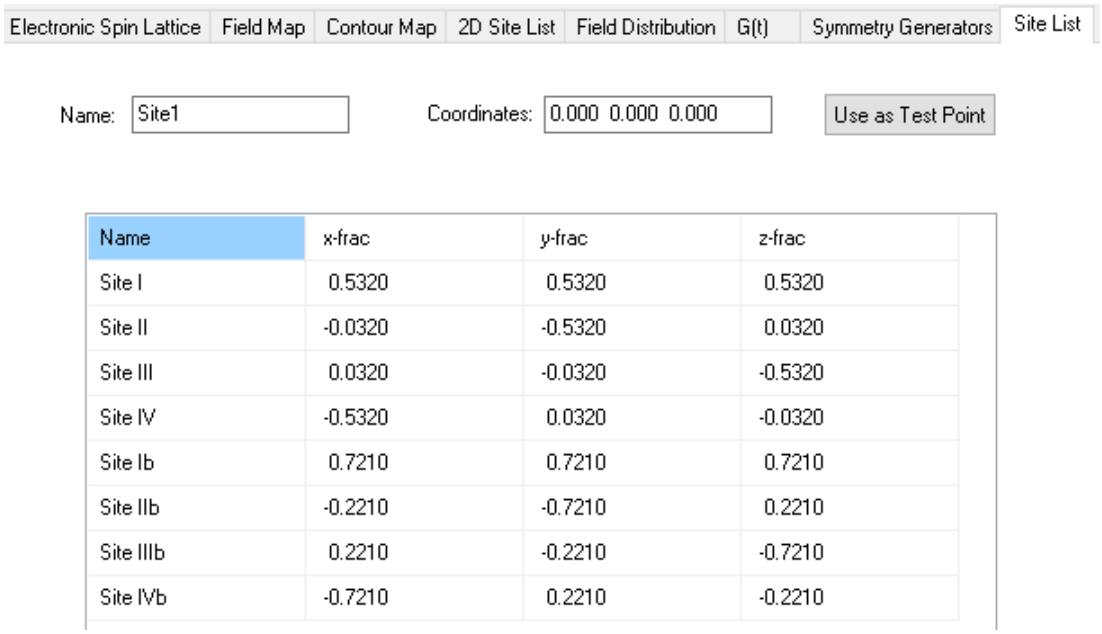




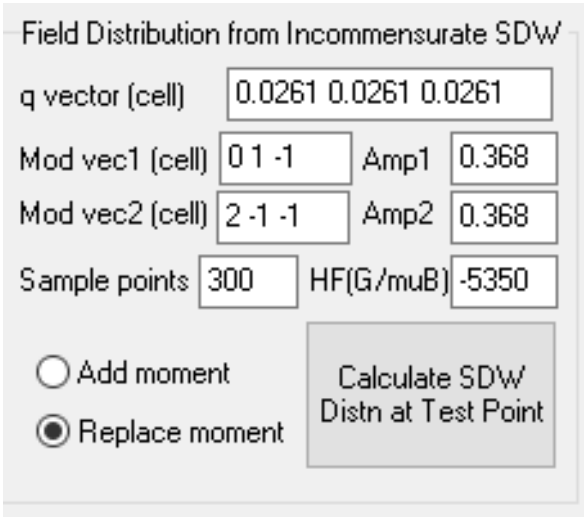


10. SDW Modulated Spin Systems

The field distribution at the test point from an incommensurate periodic modulation of the moments by a spin density wave can be simulated using the 'Field Distribution from Incommensurate SDW' box. The q vector of the modulation is defined and the direction and amplitude of modulation is defined either by a single modulation vector for the case of a linear SDW or by a pair of modulation vectors acting in quadrature for the case of a helical SDW. The modulation can be chosen to either add to the existing moments or replace them. A modulated contact hyperfine term acting in addition to the dipolar fields can also be specified in units of Gauss per Bohr magneton.

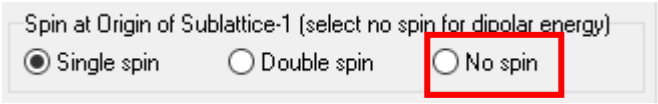


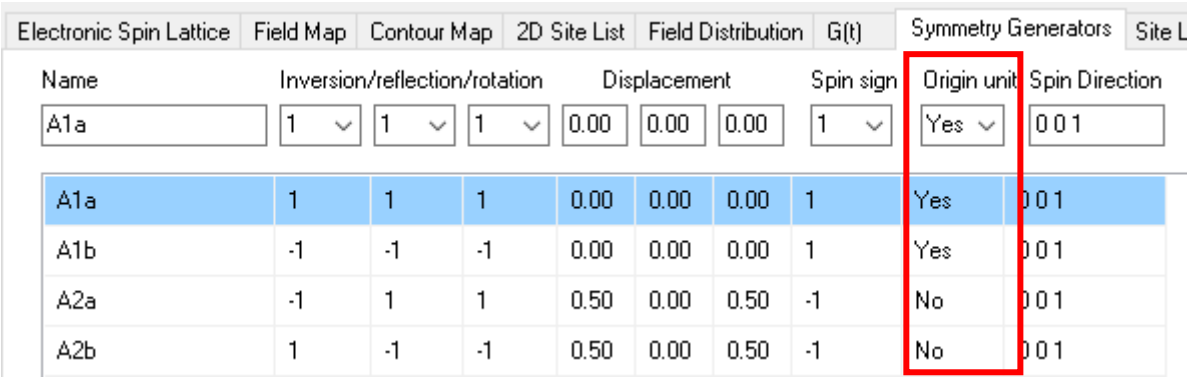
Name	x-frac	y-frac	z-frac
Site I	0.5320	0.5320	0.5320
Site II	-0.0320	-0.5320	0.0320
Site III	0.0320	-0.0320	-0.5320
Site IV	-0.5320	0.0320	-0.0320
Site Ib	0.7210	0.7210	0.7210
Site IIb	-0.2210	-0.7210	0.2210
Site IIIb	0.2210	-0.2210	-0.7210
Site IVb	-0.7210	0.2210	-0.2210



11. Spin at the origin

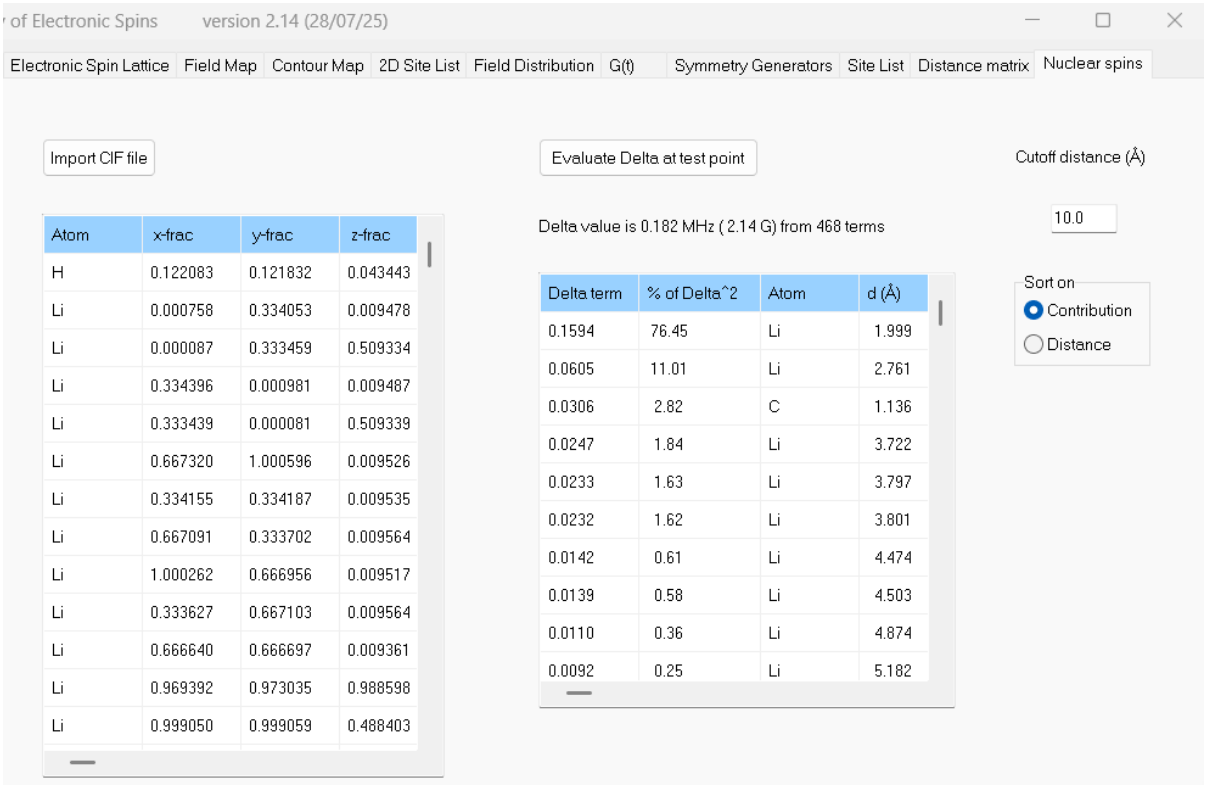
It is sometimes useful to be able to switch off the spin at the origin of Sublattice-1. One reason is to calculate the dipolar stabilisation energy of a spin structure. After turning off the spin, taking a test point at the origin will calculate the dipolar field seen at the origin and the corresponding dipolar stabilisation energy. Another reason for switching off the spin is to account for molecular singlet formation when a muonium spin pairs up with a molecular radical spin. To allow for the spin being delocalised over one or more molecules, the Symmetry Generators page enables the assignment of whole sublattice groups (e.g. molecules) to the 'Origin unit'. These groups of sites then all switch off together when 'No spin' is selected.





12. Nuclear Spins

The final tab allows an analysis to be made of the dipolar contributions from nuclear spins to a muon site. The structure file is imported from a CIF file via the 'Import CIF File' button and the Delta value at the test point representing the muon is evaluated via the 'Evaluate Delta at test point' button. The site is typically estimated by an external calculation using Density Functional Theory (DFT). The terms contributing to Delta can be sorted either on their size or on the distance of the nucleus from the test site. The nuclear contribution terms automatically take into account the natural abundance of different isotopes.



13. Output Files

A number of files are automatically saved in the working directory. Bdist.dat is the unbroadened field distribution, Bdistb.dat is the broadened field distribution and timedomain.dat is the relaxation function for the case of stopping at all points in the distribution. The field distribution may also be saved as a named file using the 'Save as' button.

14. Examples

A few example structures are included, starting with a simple cubic ferromagnetic structure stored in folder 'cubic FM'.

A second example is a body-centred-cubic antiferromagnetic structure in folder 'BCC-AFM'. Two ways of defining the same structure are illustrated: 'BCC-AFM-sublattice.str' uses two sublattices and 'BCC-AFM-symmetry.str' uses one sublattice and two symmetry generators.

A more complicated example is given in folder 'Molecular AFM' where the sublattice page is used to define a spin density that is delocalised across a molecule and the symmetry generators page is used to define the eight molecules in the magnetic cell. The site list page is used to define proton sites for estimating the proton NMR spectrum.

The final example is MnSi which is an incommensurate SDW system with a helical spin modulation. Both left-handed and right-handed structures are included, only one helicity is found to be consistent with muon experiments.