Scatty: Quick-start guide

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Scatty is a program that rapidly calculates magnetic diffuse-scattering patterns from atomistic models of disordered crystals. Suitable atomistic models might be generated, for example, from (reverse) Monte Carlo or molecular dynamics simulations. Scatty calculates diffuse scattering arising from three different types of disorder: compositional/occupational, displacive/positional, and magnetic. For further information on the scientific problems to which Scatty is relevant, please see the associated manuscript "Ultrafast calculation of diffuse scattering from atomistic models". For information on how to use Scatty, please read on!

Scatty makes use of the fast Fourier transform code of R. L. Singleton [1], adapted from `fftn.c` and translated from Fortran 66 to C by Mark Olesen and John Beale, and available from `https://jblevins.org/mirror/amiller/.`

1 Installation

Scatty is distributed as Fortran90 source code, so it is necessary to compile it on your computer before you can run it. If you don't have a Fortran90 compiler, you can download the free gfortran compiler from

```
http://gcc.gnu.org/wiki/GFortranBinaries
```

Once you have installed gfortran, open a Terminal window (Mac) or command prompt (Windows), navigate to the folder where `scatty.f90` is located, and type

```
make
```

to compile the program. Alternatively, you may type

```
gfortran singleton.f90 scatty.f90 -o scatty -O3
```

and replace `gfortran` with the name of your Fortran compiler, if necessary. A program called `scatty` should then appear in the folder. To run Scatty on Mac or Linux, type in a Terminal window

```
./scatty [title]
```

where *[title]* is the same title used in the file names. On Windows, type in a command prompt

```
scatty [title]
```

2 Input files

Two files are needed to run Scatty: a file containing parameters needed to calculate the scattering pattern, and the atomisitic configuration(s) that contain lists of atomic coordinates and/or magnetic-moment orientations. Both should be in ASCII plain-text format. Their formats are given below.

2.1 Atomisitic configurations

The atomisitic configuration ("supercell") should have the file name

```
[title]_atoms_01.txt
```

or

*[title]*_spins_01.txt

where *[title]* is a name of your choice. The `atoms` and `spins` names are interchangeable and will be read in the same way, regardless of whether the file actually contains atoms, magnetic moments, or both. To improve the statistical accuracy of the scattering calculation, we strongly recommend that you average the calculated scattering patterns over many (e.g., 10 to 1000) independent configurations; this can be done by providing additional configurations in the same folder, named *[title]*`_atoms_02.txt` and so on. The `atoms` file contains a list of capitalised keywords usually followed by some numbers. The keywords can occur in any order, and additional comments can be added to the input file. Some keywords are required, and a few others are optional. The keywords and their possible values are are given below:

TITLE The title of the simulation.

CELL A list of the lattice parameters a, b, c in Angstrom units, followed by a list of the cell angles α, β, γ in degrees.

BOX The number of crystallographic unit cells in the supercell, given as three integers corresponding to the number of unit cells along the crystallographic axes.

SITE The fractional coordinates of the *average* position of a site in the crystallographic unit cell. Each site is given on a new line, with the keyword `SITE` followed by the x, y, z fractional coordinates. The number of `SITE` lines should equal the number of sites in the crystallographic unit cell. (Scatty does not know symmetry, so all atoms in the unit cell must be given, not just those in the asymmetric unit.)

OCC A list of element symbols, where each element symbol is followed by a real number specifying the *average* occupancy of the site by the given element. The element symbols and occupancies should be separated by spaces (e.g., `OCC Na 0.5 Li 0.5`). Neutron-scattering lengths and atomic X-ray form factors for the various elements are stored internally in Scatty. In general, the number of `OCC` lines must equal the number of `SITE` lines, and the `OCC` lines must be given in the same order as the `SITE` lines. For convenience, however, two exceptions to this are possible. First, if only one OCC line is given, Scatty will apply the same occupancy to all sites. Second, the `OCC` lines may optionally be omitted if only magnetic scattering is calculated; Scatty will then assume that each site is fully occupied by a single type of magnetic ion with magnetic properties specified by extra lines (see below).

ATOM The position and chemical identity of an atom in the supercell. The number of `ATOM` lines is equal to the number of atoms in the supercell. The format is as follows. First, a list of four integers identifies the atom's average position by giving first the number of its site within the unit cell, which can take integer values from `1` to the number of `SITE` lines, followed by the (R_1, R_2, R_3) components of the lattice vector $\mathbf{R} = R_1\mathbf{a} + R_2\mathbf{b} + R_3\mathbf{c}$, which can take integer values from `0` to `BOX - 1`. This is followed by three real numbers giving the (u_1, u_2, u_3) components of the atom's displacement vector $\mathbf{u} = u_1\mathbf{a} + u_2\mathbf{b} + u_3\mathbf{c}$ away from its average position. Finally, the atom's chemical identify is specified by giving its element symbol, which should be one of the elements given on the `OCC` line.

The following lines are only necessary if there are magnetic atoms in the simulation, and you want to calculate a magnetic neutron-scattering pattern. Please note that the current version of Scatty does not consider coupling between magnetic and displacive variables, and no Debye-Waller factor is applied to the magnetic scattering.

SPIN The position and chemical identity of a magnetic moment (spin) in the supercell. The number of `SPIN` lines is equal to the number of magnetic moments in the supercell. The format is as follows. First, a list of four integers identifies the spin's average position by giving first the number of its site within the unit cell, which can take integer values from `1` to the number of `SITE` lines, followed by the (R_1, R_2, R_3) components of the lattice vector $\mathbf{R} = R_1\mathbf{a} + R_2\mathbf{b} + R_3\mathbf{c}$, which can take integer values from `0` to `BOX - 1`. This is followed by three real numbers giving the (M_1, M_2, M_3) components of the magnetic-moment vector $\mathbf{M} = M_1\hat{\mathbf{a}} + M_2\hat{\mathbf{b}} + M_3\hat{\mathbf{c}}$. Note that magnetic-moment vectors are referred to *unit* vectors parallel to the crystallographic axes. Finally, the type of magnetic ion is specified by giving its element symbol, which should be one of the elements given on the `OCC` line. This last entry may be omitted if each site is fully occupied by a single type of magnetic ion.

FORM_FACTOR_J0 The magnetic form factor, $f_{\mathrm{mag}}(|\mathbf{Q}|)$. This is given as a list of coefficients A, a, B, b, C, c, D for the analytical approximation to the $j_0(|\mathbf{Q}|)$ integrals, which can be found in [**?**], or online at `www.ill.eu/sites/ccsl/ffacts/ffachtml.html`. If more than one type of magnetic ion can occupy the same site, the form-factor coefficients should be listed sequentially on this line, in the same order as for the `OCC` line.

C2 (optional) A value should be given for this keyword if there is a non-zero orbital contribution to the magnetic moment; otherwise `C2` may be omitted. The magnetic form factor is then given by $f_{\mathrm{mag}}(|\mathbf{Q}|) = j_0(|\mathbf{Q}|) + C_2 j_2(|\mathbf{Q}|)$, where

$C_2 = L_z/(2S_z + L_z)$ (i.e., C_2 is the ratio of the orbital moment to the total moment). Note that, for the lanthanide series, $C_2 = (2 - g_J)/g_J$, where g_J is the Landé g-factor. For transition metals with unquenched orbital momentum, an effective g-factor g_{eff} may be defined by $g_{\text{eff}} S_z = 2S_z + L_z$, from which $C_2 = (g_{\text{eff}} - 2)/g_{\text{eff}}$ (note the difference in sign compared to the lanthanide case). The default value of `C2` is 0.

FORM_FACTOR_J2 (optional) If $C_2 \neq 0$, it is necessary to specify the list of coefficients A, a, B, b, C, c, D for the analytical approximation to the $\langle j_2 \rangle$ integrals, which are given in [**?**].

In general, the number of `FORM_FACTOR_J0` lines (as well as `C2` and `FORM_FACTOR_J2` lines, if relevant) should equal the number of `SITE` lines, and be given in the same order as the `SITE` lines. However, if only one `FORM_FACTOR_J0` line is given, SCATTY will assume the same magnetic form factor for all sites.

2.2 Scattering parameters

The second file contains the parameters needed for the scattering calculation, and should have the filename

```
scatty_config.txt
```

This file contains a list of capitalised keywords (the parameters), usually followed by some numbers or a character string (the values of these parameters). The keywords can occur in any order, and additional comments can be added to the input file. The keywords and their possible values are are given below:

NAME A name for the calculation (e.g., the scattering plane to be calculated). This will be included in the filename of the output files.

CENTRE (optional) The centre of the calculated scattering pattern in reciprocal space, in reciprocal-lattice (hkl) units. The format is three real numbers, giving the components of the origin shift from $\mathbf{Q} = \mathbf{0}$. The default value is `0 0 0`.

X_AXIS The reciprocal-space vector used as the x-axis of the calculated scattering pattern. The format is 3 real numbers followed by 1 integer. The three real numbers give the components of the reciprocal-space vector relative to the origin, in reciprocal-lattice (hkl) units. The integer p specifies the number of points along the x direction. SCATTY will calculate $2p + 1$ points along this direction, extending from `ORIGIN - X_AXIS` to `ORIGIN + X_AXIS`.

Y_AXIS The reciprocal-space vector used as the y-axis of the calculated scattering pattern (format as above), and the corresponding number of points.

Z_AXIS The reciprocal-space vector used as the z-axis of the calculated scattering pattern (format as above), and the corresponding number of points.

If `X_AXIS`, `Y_AXIS`, and `Z_AXIS` are all of non-zero length, SCATTY will calculate a scattering volume (this may take several minutes, depending on how many points are to be calculated). If any one of `X_AXIS`, `Y_AXIS`, or `Z_AXIS` is given as `0 0 0`, the scattering plane defined by the two non-zero vectors is calculated. In the same way, giving only one non-zero vector will calculate the scattering along the specified line. Please note that all the non-zero axes specified here should be mutually orthogonal; SCATTY will give a warning message if this does not seem to be the case.

RADIATION The type of incident radiation for the scattering simulation, indicated by a single character: either `X` for X-ray scattering, `N` for neutron scattering, or `E` for electron scattering.

EXPANSION_MAX_ERROR (optional) One real number x, giving the maximum acceptable error in the Taylor expansion of $\exp(\mathrm{i}\mathbf{G} \cdot \mathbf{u})$, where $\mathbf{G}$ is a wavevector and $\mathbf{u}$ is an atomic displacement (see "Ultrafast calculation of diffuse scattering from atomistic models"). This should be a number much smaller than unity. If the `atoms` files include displacive disorder, `EXPANSION_MAX_ERROR` and/or `EXPANSION_ORDER` must be given. The way in which the maximum-error constraint $|\epsilon| \leq x$ is implemented depends on whether `EXPANSION_ORDER n` is also given:

- If `EXPANSION_ORDER n` is **not** given, then the order n of the Taylor expansion is determined at each $|\mathbf{G}|$ by the requirement that $|\epsilon| \leq x$;
- If `EXPANSION_ORDER n` is given, then where the n-th order Taylor expansion of $\exp(\mathrm{i}\mathbf{G} \cdot \mathbf{u})$ could yield an error $|\epsilon| > x$, SCATTY will replace the Taylor expansion with direct calculation of $\exp(\mathrm{i}\mathbf{G} \cdot \mathbf{u})$, to ensure that $|\epsilon| \leq x$.

In most cases, the calculation will run fastest if you specify `EXPANSION_MAX_ERROR` **and do not specify** `EXPANSION_ORDER`**.** The possible exception is for supercells that contain large displacements, because a very large number of terms in the Taylor expansion can then be required to obtain reasonable accuracy (e.g., for displacements of $\sim$0.5 Å and typical $|\mathbf{G}_{\max}| \sim 15\,\text{Å}^{-1}$, a maximum error $|\epsilon| < 0.05$ would require an expansion to order 20). In such cases, it may be preferable to specify `EXPANSION_ORDER` as well as `EXPANSION_MAX_ERROR`.

EXPANSION_ORDER (optional) One integer n, specifying the number of terms included in the Taylor expansion of $\exp(\mathrm{i}\mathbf{G}\cdot\mathbf{u})$, where $\mathbf{G}$ is a wavevector and $\mathbf{u}$ is an atomic displacement (see "Ultrafast calculation of diffuse scattering from atomistic models"). If the `atoms` files include displacive disorder, `EXPANSION_ORDER` and/or `EXPANSION_MAX_ERROR` must be given. If `EXPANSION_MAX_ERROR` is given, n is the *maximum* number of terms included in the Taylor expansion (see `EXPANSION_MAX_ERROR` above).

REMOVE_BRAGG (optional) If this keyword is given, Scatty will remove nuclear Bragg peaks from the scattering calculation. If given, it should be followed by one of the letters `P`, `I`, `F`, `R`, `A`, `B`, `C`, or `H` to specify the centring of the crystallographic unit cell. This keyword has no effect for magnetic scattering.

WINDOW (optional) The value of m in the Lanczos interpolation formula, which is an integer ≥ 2 (see "Ultrafast calculation of diffuse scattering from atomistic models"). The default value is 3. If `WINDOW 0` is given, nearest-neighbour interpolation is used instead of Lanczos resampling.

CUTOFF (optional) The value of m' in the Lanczos interpolation formula (see "Ultrafast calculation of diffuse scattering from atomistic models"). The default value is 2.

SUM (optional) A character string giving the summation type in real space. The options are `PARALLEL` (sum over atom pairs within a parallelepiped) or `SPHERE` (sum over atom pairs within a sphere). The default value is `PARALLEL`.

MAG_ONLY (optional) If this keyword is given, nuclear scattering will be excluded from the calculation, and only magnetic scattering will be calculated. This is useful to compare calculations with data measured using xyz neutron polarisation analysis, which can allow magnetic and nuclear diffuse scattering to be separated.

TEMP_SUBTRACT (optional) If this keyword is given, a ideal paramagnetic background is subtracted from the calculated magnetic scattering intensity. This keyword should be given if the calculated magnetic scattering pattern is being compared to experimental magnetic diffuse-scattering data obtained by low–high temperature subtraction. Please note that the magnetic scattering pattern will contain both negative and positive intensities in this case.

SYMMETRY (optional) If this keyword is given, Scatty will symmetrise the calculated scattering patterns. For systems showing only short-range correlations, the symmetry of the scattering pattern should be the same as the Laue symmetry of the crystal. Hence, the options that can follow the `SYMMETRY` keyword are the 11 Laue classes:

- `m-3m`
- `m-3`
- `6|mmm`
- `6|m`
- `-3m` (hexagonal axes are assumed)
- `-3` (hexagonal axes are assumed)
- `4|mmm`
- `4|m`
- `mmm`
- `2|m`
- `-1`

Due to the finite size of the spin configurations, atomistic simulations do not reproduce the Laue symmetry exactly, so it is often possible to obtain a large improvement in apparent statistics by symmetrising. Of course, one should check before using this option that the scattering pattern actually possesses the expected symmetry!

SUPERCELL_BRAGG_OUTPUT (optional) Writes a legacy Visualisation Toolkit file containing the intensities of the supercell Bragg peaks, which can be read in free software for three-dimensional data visualisation, such as ParaView (*www.paraview.org*) and MayaVi (*http://mayavi.sourceforge.net*). Axes are labelled in reciprocal-lattice units.

PPM_OUTPUT (optional) Writes an image file in .ppm format, a simple image format that stores pixel information in plain text. It is possible to convert .ppm images into standard formats (e.g., .gif or .png) using an image-editing program such as ImageMagick (*www.imagemagick.org*). This option is only available for two-dimensional plots.

PPM_RANGE (optional) If the option to write a .ppm image is selected, this keyword may be given to specify the minimum and maximum intensity values shown on the image (two real numbers, minimum followed by maximum). By default, the minimum and maximum intensities in the calculated plane are used.

PPM_COLOURMAP (optional) If the option to write a .ppm image is selected, this keyword may be given to specify the colourmap. The options are:

- `default`: By default, Scatty uses the "cool-to-warm" colourmap used in the ParaView program. This map has been designed for scientific visualisation in order to be easily interpreted and aesthetically pleasing [**?**].
- `heat`: Black-red-yellow-white colourmap.
- `jet`: The "rainbow" colourmap used in Matlab.
- `grey1`: Greyscale with a black background.
- `grey2`: Greyscale with a white background.

3 Output files

The default output files written by Scatty are

- *[title]*`_`*[name]*`_scatty_info.txt`, which contains the parameters used for the calculation;
- *[title]*`_`*[name]*`_sc_list.txt`, which gives a list of scattering intensities in the format h, k, l, intensity;
- *[title]*`_`*[name]*`_sc.txt`, which gives a grid of scattering intensities that can be read by image-plotting software (this file is only written if a scattering plane is calculated);
- *[title]*`_`*[name]*`_sc.vtk`, which is a legacy Visualisation Toolkit file that can be read in popular free software for three-dimensional data visualisation, such as ParaView (*www.paraview.org*) and MayaVi (*http://mayavi.sourceforge.net*). Axes are labelled by their wave-vector components (in Å^{-1} units) along the mutually-orthogonal directions;

If the `PPM_OUTPUT` keyword is given in `scatty_config.txt`, Scatty also outputs

- *[title]*`_`*[name]*`_sc.ppm`, which is a .ppm image file.

If the `SUPERCELL_BRAGG_OUTPUT` keyword is given in `scatty_config.txt`, Scatty also outputs

- *[title]*`_`*[name]*`_sc_supercell.vtk`, which contains the intensities of the supercell Bragg peaks.

4 Update history

- 14 October 2022: Current version. Introduced option for calculation of electron scattering. Fixed bug when EXPANSION_MAX_ERROR and EXPANSION_ORDER keywords are both given. Changed code to double precision.
- 9 July 2019: Fixed bug reading input files containing a single OCC line but multiple sites.
- 21 November 2018: Publication version. Included error checking of input files. Introduced EXPANSION_MAX_ERROR keyword.
- 31 October 2018: Pre-publication. Changed normalisation from barn per unit cell to barn per atom.
- 12 September 2018: Pre-publication. Original version.

References

[1] R. Singleton, *IEEE Trans. Audio and Electroacoustics* **17**, 93 (1969).