GSAS-II Help information

A compilation of HTML pages into PDF

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From https://advancedphotonsource.github.io/GSAS-II-tutorials/help/

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1. Help for GSAS-II

This and the web pages referenced below, provide documentation for use of the GSAS-II graphical user interface (GUI). The information is organized largely to follow the different sections of the GUI and is usually accessed via the "Help" features in GSAS-II: Help on specific sections of GSAS-II can be accessed from the "?" button (yellow on some computers) in the upper right corner of the data window, or from the Help command. The GSAS-II graphics window and in other locations of the program also offer access to context-specific help information.

A single file containing all GSAS-II web pages is available as a PDF document (note: ~100 pages, please don't print it.)

An index on the topics covered in these help pages is given below.

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2. GSAS-II Tutorials

The best way to learn about how different sections of GSAS-II is used is to work through some of the tutorials. The best way to access the tutorials is through the **Help/Tutorials** menu command, because once a tutorial has been selected, this will both open the tutorial instructions in a web browser and will download any input files needed to run the tutorial. It is also possible to access the tutorials via a separate web page.

Each tutorial demonstrates a different aspect of GSAS-II; when significant new capabilities are added to GSAS-II it is common to create a new tutorial. Note that it is unlikely that any one person will use all the features of GSAS-II, so it is not necessary to run through all of them. New users are suggested to look at some of the introductory tutorials and then pick more advanced topics as needs arise.

3. GSAS-II GUI Organization

The GSAS-II GUI uses three windows, which are described below. The main window has two parts. To the left is the "Data Tree" and to the right is the "Data Window". A second window, called the "Plots Window" is used for graphics such as plots of data or display of three-dimensional structures. The third window, the Console window, is used to show output from the program.

3.1 GSAS-II Data Tree

The data tree shows contents of a GSAS-II project (which can be read or saved as a .gpx file) in a hierarchical view. Clicking on any item in the tree opens that information on the right side of the window in the "Data Editing" section, where information in that item can be viewed or edited. For example, the "Sample Parameters" item under a 'PWDR' entry contains information about how data were collected, such as the sample temperature. The arrow keys (up & down) move the selection to successive entries in the data tree; both the data window and the associated plot (if any) will change.

3.1.1 What can I do here?

The leftmost entries in the GSAS-II menu provide access to many features of GSAS-II. Other menu items will change depending on what type of entry is selected in the data tree. The menu commands that do not change and are described in the main menu commands documentation.

3.2 GSAS-II Data Window

Different information is displayed in the Data Editing Window, depending on which section of the data tree is selected. For example, clicking on the "Notebook" entry of the data tree brings up the Notebook editing window, as documented elsewhere.

3.3 GSAS-II Graphics Window

This window presents all the graphical material as a multipage tabbed set of plots utilizing the matplotlib python package. Each page containing a graph or plot has a tool bar with these controls:

The first eight icons have the following functions: **Home**, **Back**, **Forward**, **Pan**, **Zoom**, **Save**, **Key Press** and **Help**, respectively and are described below. The remainder (yellow arrows) move or rescale the plot. The last "P" allows preparation of a publication quality plot. The meaning of these icons are as follows:

- **Home** - returns the plot to the initial view/scaling
- **Back** - returns the plot to the previous view/scaling
- **Forward** - reverses the action in the previous press(es) of the Back button
- **Pan** - allows you to control panning across the plot (press left mouse button & drag) and zooming (press right mouse button & drag),
- **Zoom** - allows you to select a portion of the plot (press left mouse button & drag for zoom box) for the next plot.
- **Save** - allows you to save the currently displayed plot in one of several graphical formats suitable for printing or insertion in a document.
-  - Shows a menu of key press commands that can be used to interact with the plot. These actions can be initiated from the menu.
-  - accesses GSASII help on the specific plot type.
- "<" - Shifts the plot to the left, relative to the axes
- ">" - Shifts the plot to the right, relative to the axes
- "^" - Shifts the plot up, relative to the axes
- "v" - Shifts the plot down, relative to the axes
- "<>" - Zooms in on the plot (magnifies) along the horizontal (x) direction to show more details.
- "><" - Zooms out on the plot (demagnifies) along the horizontal (x) direction.
-  - Zooms in on the plot (magnifies) along the vertical (y) direction to show more details.
-  - Zooms out on the plot (demagnifies) along the vertical (y) direction.
-  - prepare a fancy publishable version of the current plot (PWDR plots only)

For 3-dimensional structure drawings there will be below the toolbar may be a status bar that on the left may show either an instruction for a keyed input or a pull down selection of keyed input; on the right may be displayed position dependent information that is updated as the mouse is moved over the plot region.

3.4 GSAS-II Console Window

This is a "terminal" or "cmd.exe" window that shows simple text. It is used for output from the program and in some cases error messages may appear here.

3.4.1 What can I do here?

You can never type anything into this window. It is for output from GSAS-II only. If something is not working properly, you may find some useful information here. Please do include the contents of this window when reporting a bug.

4. GSAS-II Main menu commands

The menubar has two types of entries. The "Main" menu commands, described here, are present regardless of what data tree entry is selected. In addition, most data tree items have menu items specific to that entry. Those menu commands are described with the data tree entry.

4.1 **File** Menu

- **Open project...** - Open a previously saved GSAS-II project file (files are named as <project>.gpx) from a file browser. Note that a native file browser is used on all platforms except Linux unless the Configuration variable `G2FileBrowser` is set. If you currently have a project file open, you are asked if you want to "Save & Overwrite" as the contents of the current project may be lost in this operation. If you say "Yes" the current project will be saved before the next project is read; if you say "No" any changes to the current project will be discarded; "Cancel" will cancel the Open action, as if the menu command had not been entered.

> **Note**
>
> Note that as files are saved during a structure refinement, copies of the previous version are saved as backup files, named as <project>.bak<i>.gpx, where <i> starts as 0 and is increased after each save operation. NB: you may open a backup .gpx file (e.g. <project>.bak3.gpx) to return to a previous version of your project, but if you do so, it is best to immediately use the Save As... menu command (you may wish to use the same named as before to overwrite the current version or select a new name.) If you forget specify a project name, then <project>.bak3 will be considered the project name and backups will then be named <project>.bak3.bak0.gpx, etc.

- **Open in new window...** - Open a previously saved GSAS-II project file without closing the current project.
- **Reopen recent...** - Provides a list of recently used GSAS-II project file that can be opened. Otherwise behaves the same as **Open project**.
- **Open w/project browser.** - Opens a special file browser for GSAS-II .gpx files that shows some information about the status of the last refinement in that file. Useful where many different versions of a fit have been tried on the same or similar data. Otherwise behaves the same as **Open project**.
- **Save project** - Save the current project. If this is a new project that has not yet been saved, you will be prompted for a new name in a file dialog (you may optionally change the directory in that dialog). If the file exists, you will be asked if it is OK to overwrite it. Once a file name has been used to read or save a project, the name is shown after 'Loaded Data:' in the first item in the data tree.
- **Save Project as...** - Save the current project in a specified project file. You will be prompted for a new name in a file dialog (you may optionally change the directory in that dialog). If the file exists, you will be asked if it is OK to overwrite it. The current project will be now named as the saved project name.
- **New Project** - Creates a new empty project. You will be given a chance to save the current version of the open project. If not saved, any changes made to the current project since the last save will be discarded.
- **Preferences** - Provides access to GSAS-II configuration settings, as described in the Configuration variables description.
- **Install GSASIIscriptable shortcut** - Modifies the current Python installation so that GSASIIscriptable can be accessed without providing a full path, as discussed in the Scripting docs.
- **Quit** - Exit the GSAS-II program. You will be asked if the project should be saved or not (Cancel aborts the quit). You can also exit GSAS-II by pressing the red X in the upper right (Windows) or left (Mac). Pressing the red X on the console window will kill the GSAS-II run without any save.

If the Configuration variable `debug` is set to `True` these menu items will also be included in the file menu:

- **IPython console** - Opens a iPython debugging session; requires that the IPython package be installed into the current Python interpreter.
- **wx.inspection tool** - Open the wxPython window inspection debugging tool.
- **Reopen current** - Rereads the current .gpx file, discarding any changes that have been made but not saved.

4.2 **Data** Menu

- **Read Powder Pattern Peaks...** - Read in a list of powder pattern peak positions as either a d-spacing or 2θ position table; these can be used in GSAS-II powder pattern indexing. They are distinguished by their order (highest d or smallest 2θ first in table).

- **Sum or average powder data** - Forms the sum of previously read powder patterns (PWDR tree entries); you can supply a multiplier for each. Can be used to accumulate data, subtract background/sample-container patterns, etc. Patterns used to form the sum must be of identical range and step size. Result is a new PWDR entry added to the GSAS-II data tree.
- **Sum image data** - Form the sum of previously read 2-D images; you can supply a multiplier for each. Can be used to accumulate data, subtract background/sample-container patterns, etc. Images used to form the sum must be of identical size and source. Result is a new IMG entry in the GSAS-II data tree, and a GSAS-II image file is written for future use as a Python pickle file.
- **Add new phase** - This begins the creation of a new phase in the data tree (under Phases). You are first prompted in a dialog box for a name to be assigned to the new phase. Then the Phase/General tab is opened for this new phase, where you should first select the phase type, then enter the space group symbol and then the lattice parameters. Finally, move to the atoms tab where atoms can be inserted or imported. Note that inserted atoms are labeled as H atoms. You must edit the atom to set the element type and the coordinates.

> **Note**
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> Nonstandard space group symbols (such as "F 21 21 21") are permitted in GSAS-II and are sometimes to be preferred, but to be recognized correctly, space group names must have spaces between the axial fields (e.g. use 'P n a 21' not 'Pna21'). Standard space groups names will be parsed properly even when spaces are not provided, but this is not done with non-standard space group names. Also note that GSAS-II requires that space groups use the "Origin 2" setting for centrosymmetric space groups where that choice is offered. Origin 2 puts the centre of symmetry at the origin and forces structure factors to real rather than complex numbers.

- **Delete phase entries** - This will remove a phase from the data tree. A dialog box will present the list of phases; pick one (or more) to delete.
- **Rename tree entry** - Rename a histogram entry. This should only be done before the histogram is used in any phases: e.g. only rename data immediately after reading.
- **Delete data entries** - This will remove a data (e.g. PWDR) item from the data tree. A dialog box with a list of choices for histograms is presented; it has filter capability to ease this process. Be sure to remove histograms from all phases before deleting them from the tree.
- **Delete plots** - This will remove plots from the plot window. A dialog box with a list of choices for plots is presented.
- **Delete sequential result entries** - This will remove any sequential results from the tree. A dialog box with a list of choices for entries is presented.
- **Expand tree item** - This will show child entries for specified type of items (IMG, PWDR, etc.)
- **Move tree item** - Move classes of Tree items (IMG, PWDR, Phase, etc.) around in the tree. Individual top-level tree items can be moved using the right mouse button.

4.3 Calculate Menu

- **Setup PDFs** - This is the first step in computing a pair distribution function (PDF). This creates the controls for each powder pattern selected in the dialog box, but does not compute the PDF, which must be done from PDF tree entries. See PDF Controls for information on the PDF input.
- **View LS parms** - This shows a dialog box where the status and value of every parameter used in your project can be viewed. The parameter names are of the form `p:h:name:id` where 'p' is the phase index, 'h' is the histogram index and 'id' is the item index (for atoms). 'name' indicates the type of parameter, as defined in developer's docs. Indexes all begin with '0' (zero). The total number of refined parameters is shown at the top of the list. Optionally only those parameters that are refined can be viewed. The "Ref" column shows a "R" for parameters that are refined; a "C" for parameters where values are generated from a constraint. If shown as blank, the parameter value is fixed.

  Clicking on a row of the table brings up a window where **parameter limits** may be set. One may set a lower limit value, an upper limit value or both. When a parameter value refines to value outside the limit, the parameter is set to that limit value and the refinement flag for the parameter is subsequently ignored.

> **Note**
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> Note that for atom positions, the variables associated with coordinate values (named as `p::Aw:n`, where p is the phase number, n is the atom number and w is x, y or z) is not a refinable parameter, but the shift in the value is. The refined parameters are 'p::dAw:n'. The reason this is done is that by treating an atom position as (Ax+dAx,Ay+dAy,Az+dAz) where the "d" values indicate shifts from the starting position. Shifts are refined rather than the x, y, or z values as this this simplifies symmetry constraints. As an example, suppose we have an atom on a symmetry constrained site, `x,1/2-x,z`. The process needed to enforce this symmetry constraint, so that if x moves positively y has to move negatively by the same amount would be messy. With refinement of shifts, all we need to do is constrain the dAy to be equal to the negative of dAx (`0::dAy:n = -1 * 0::dAx:n`).

Also, one can set here parameters that will be logged into the Notebook, so the values can be tracked and plotted across a refinement. Right-click to toggle the log setting. Note that individual log settings will override the the `LogAllVars` preference setting (see Configuration variables).

- **Refine (Sequential refine)** - This performs the refinement (Pawley/Rietveld/LeBail or single crystal) fit according to the controls set in the Controls data tree item. This menu item name will be "Refine" unless the datasets to be used in a sequential refinement have been selected in the Controls data tree item, at which point the name will appear as "Sequential refine".

  When a PWDR histogram item is selected in the data tree, or a child tree item of a PDWR histogram is selected in the tree when Refine is used, the plot of that histogram will be updated after each cycle of refinement.

  Once the refinement is completed, you will be offered the chance to load the results of the fit or to reject them, in which case no parameters will be changed. If the fit is rejected, it is possible to change settings or refinement flags and try a different set of options and try again. The dialog asking to load or Cancel the last refinement will show a table of parameters and how they changed in the refinement. Clicking on a parameter will show a plot of how the latest value follows the previous results, if that parameter is being logged in the Notebook.

  After the refinement results are reloaded, each plot will be updated to reflect the new refinement values, if the plot has a defined update process or will be closed as the plot contents are presumed to be obsolete and need to be manually recreated to be valid.

- **Compute partials** - The term "phase partial intensities" is used to designate keeping separate track of the intensity contribution from each phase separately. When this is used, a zero-cycle refinement (meaning no parameters values are changed) where the contributions from each phase (phase partial intensities) are written for each histogram and each phase in that histogram into a single file named <project>`.partials` where <project> is the GSAS-II project (.gpx) name. This file is intended for internal use in GSAS-II and will be deleted if additional refinements are performed (as the information in them is then obsolete; use this menu command to recreate them if needed.) When the .partials file is created, the user can then choose to export the intensity information in a series of ASCII files named <project>_part_N.csv, which can be read by spreadsheets and most scientific software.

- **Parameter impact** - This shows the parameters that will have the greatest improvement to the reduced χ^2 for the fit if refined. See Toby, JAC 57, 175-180 (2024).

- **Evaluate Expression and s.u.** - This allows an expression to be entered based on multiple GSAS-II parameters that computes a value and its standard uncertainty. The uncertainty computation will use the covariance matrix and thus accounts for correlation or anti-correlation in the parameters. An example for how this might be used would be for computing the total amount along with uncertainty for an element that occurs with several refined occupancies.

- **Setup Cluster Analysis** - Uses unsupervised machine learning to group PWDR entries into groups (clusters) that share the most similarity. See the tutorial on this for more information.

- **Run Fprime** - This run the utility routine Fprime, which displays real and imaginary components of the x-ray form factors for user-selected elements, as a function of wavelength/energy. Allows for an informed choice of wavelength for resonant x-ray scattering experiments.

- **Run Absorb** - This runs the utility routine Absorb that displays the x-ray absorption for a user selected sample composition as a function of wavelength/energy. Allows determination of the maximum sample size before absorption corrections are needed or where diffraction intensities will be severely reduced by x-ray absorption.

- **Run PlotXNFF** - This runs the utility routine PlotXNFF which displays the x-ray, neutron, electron and magnetic form factors for a selected element. This imcludes resonant (if any) neutron scattering lengths for all isotopes of a selected element. It also displays the x-ray and magnetic neutron form factors for all valences (if any) for this element.

4.4 **Import** Menu

A special set of modules, known as importers, is used to read information into GSAS-II from external files. The importers that are found by GSAS-II at runtime are used to configure the import menus. Import modules are usually fairly easy to create and thus new formats are relatively easy to support. See the GSAS-II Import Modules section of the Programmers documentation for more information on this. Note that most menus include a "**guess format from file**" option. This attempts to determine the file format by matching the file extension and a cursory examination of the file contents to the importer(s) to be tried. On occasion, this command may not succeed in correctly determining a file format. If it fails, retry by selecting the correct format from the list.

While we are not able to reproduce this, with some locale settings (particularly CJK ones?), GSAS-II will not be able to read UTF-8 files that have a BOM (Byte Order Mark). If you find that you are unable to read a data file in GSAS-II, you may wish to try stripping the BOM from the file.

- **Image** - Read in one or more 2D powder diffraction images (multiple patterns can be selected). A submenu appears with choices for import of data. Each entry when selected with the mouse shows further submenus with specific imports that are available. Any of these files can be accessed from a zip file. GSAS-II can read many different image file formats including MAR345 files, Quantum ADSC files, and tiff files from Perkin-Elmer, Pilatus, and GE. See the image importers code docs for a full list of the supported formats. Although many of these formats have data fields that should contain important information for the measurement (e.g. wavelength), these are rarely filled in correctly by the data acquisition software. Thus, you should have separately noted this information as it will be needed. In some cases, this information may be in a separate "metadata" file; GSAS-II will look for this and attempt to open it as well as the image file.

> **Note**
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> gain maps can be imported but they must be integer values as 1000*the gain value (where the gain is typically ~1); if a gain map is used, GSAS-II will rescale the gain map by 1/1000 and apply it to the image.

- **Phase** - Creates a new phase by reading unit cell/symmetry/atom coordinate information. GSAS-II can read information from several different format files; see the phase importers code docs for a full list of the supported formats. In all cases, after selecting an importer, a file open dialog is opened to locate the file. If the selected file has more than one phase, a dialog is shown with the choices; only one can be chosen. To import more than one phase from a .EXP file, repeat the import command. After selecting a phase, a dialog box is shown with the proposed phase name. You can change it if desired.

  Some notes on more commonly used formats are below. Other formats currently available for import include JANA .m50, ICDD .str & RMCProfile .rmc6f files.

  - **GSAS.EXP** - This reads one phase from a GSAS/EXPGUI (old) experiment file (<name>.EXP).
  - **PDB file** - This reads macromolecular phase information from a Protein Data Base file (<name>.PDB or <name>.ENT). Be careful that the space group symbol on the 'CRYST1' record in the PDB file follows the GSAS-II conventions (e.g. with spaces between axial fields).
  - **CIF file** - This reads one phase from a Crystallographic Information File (<name>}.CIF (or <name>.cif).
  - **GSAS-II .gpx file** - This reads one phase from a GSAS-II project file (<name>.gpx).
  - **SHELX ins & res** - note that SHELX files do not contain the space group symbol; you must set it on the new phase's General tab after import.
- **Powder Data** - Reads a powder diffraction data set in a variety of formats. Results are placed in the GSAS-II data tree as 'PWDR <filename>'. After selecting an importer, a file open dialog is opened to locate the file. If the selected file has more than one histogram (dataset), a dialog is shown with the choices; multiple datasets can be selected.

  Information needed for processing a powder diffraction data set, such as data type, calibration constants (such as wavelength) and default profile parameters and after most importers are run a second file open dialog is opened to locate a separate instrument parameter file with this information. This may be a GSAS/EXPGUI (old) instrument parameter file (file extension is usually `.prm`, `.ins` or `.inst`) or a GSAS-II created file, with extension `.instparm`. If no instrument parameter file is available, press the "Cancel" button on the file open dialog and you will be offered some default options that may be a good starting point, but ideally will be used to perform a calibration and a .instparm file with appropriate instrumental terms will be created. (See the "Create Instrument Parameter File..." tutorial.)

> **Note**
>
> Note that It is possible to apply systematic changes to the 2θ, intensity or weight values. This is done by adding a Python command(s) to the instrument (.instprm) parameter file. See here for an example.

  - **CIF file** - This reads one powder pattern (histogram) from a Crystallographic Information File (<name>.CIF).
  - **GSAS-II .gpx file** - This reads powder patterns from a previously created GSAS-II gpx project file.
  - **GSAS .fxye files** - This reads powder patterns (histograms) from the powder data file formats used in the GSAS/EXPGUI (old) program. GSAS file types of STD, ESD, FXY and FXYE are recognized. Neutron TOF data with a 'TIME-MAP' are also recognized. Note that for CW data, 2θ values are in "centidegrees" (degrees*100).
  - **TOPAS .xye files** - This format is a simple 3-column (2-theta, intensity & σ) text file.
  - **other supported formats** - Bruker .brml & .RAW; FullProf .dat; Panalytical .xrdml; Comma-separated .csv; Rigaku .ras & .txt. See the powder data importers code docs for a full list of the supported formats.

Note that this menu contains three separate "special" import items:

- **Simulate a dataset** - This creates a histogram with initially all zero intensity values that will be filled with calculated intensity values later, when the Calculate/Refine menu command is used. The user will specify the range of data to be used (2θ or TOF) and the instrument parameters to be used in the computation. One or more crystalline phases must assigned to the histogram to perform a crystallographic simulation. When the "Refine" menu command is initially used, the intensities are computed from these phases and both the "observed" and "calculated" intensity values are set from these computed values, with superimposed "random" noise added to the "observed" where the variance in intensity is computed with $\sigma = \sqrt{(I)}$. (N.B. to decrease the impact of the noise, increase the histogram scale factor.) Once Refine is used, the "observed" values are not changed, but the "calculated" values will change based on the current instrument, sample and phase parameters. To reset the "observed" intensity values back to zero and recompute them, use the "Edit range" button on the "PWDR" tree item.
- **Auto Import** - This brings up a window that reads in powder diffraction files as they are added to a directory. The file extension must determine the importer that will be used and a filter pattern is specified to determine which files will be read (e.g. use "*June23*.fxye" so that only files that contain the string "June23" will be read.
- **Fit Instr. profile from fundamental parms...** - This option is used to compute instrument parameters from a set of fundamental parameters that describe a constant wavelength (most likely Bragg-Brentano) powder diffraction instrument. The user must first specify the data range to be used and then a set of FP (fundamental parameter) values. The FP values and a source spectrum can be supplied using a nomenclature similar to Topas and described separately. They will then be converted to the SI units and parameter names used in the NIST FPA code. Alternately a file can be supplied with the parameter values used directly in that program. With this input, a series of peaks are computed across the specified data range and the Instrumental Parameters that determine the instrumental profile (U, V, W, X, Y and SH/L) are determined from those peaks. These values are then saved in an instrument parameter file that can be used when reading in new datasets or for pattern simulation.

- **Structure Factor** - Creates a new single crystal data entry (histogram) from a variety of file types. Results are placed in the GSAS-II data tree as "HKLF <filename>". Note that since it cannot be determined if SHELX format `.hkl` contains F or F^2 values, do not use "guess format from file" with SHELX format files. Information on some supported formats is provided below. There are also specific importers for incommensurate or twinned single crystal data as well as data from specific neutron diffractometers. See the Single crystal importers code docs for a full list of the supported formats.
  - **HKL F file** - This reads structure factors [as F and $\sigma(F)$ values] from a SHELX format .hkl file. You must know the file contains structure factors (as F values), as the file itself has no internal indication of this.
  - **HKL F**2 file** - This reads squared structure factors [as F^2 and $\sigma(F^2)$ values]. You must know the file contains squared structure factors (F^2 values), as the file itself has no internal indication of this.
  - **CIF file** - This reads structure factors from a CIF `.CIF` / `.cif` or `.FCF` / `.fcf` format file. The CIF data names indicates which form of structure factors (F or F^2 values) are supplied.
- **Small Angle Data** - Reads small angle scattering data from files. Results are placed in the GSAS-II data tree as 'SASD <filename>'. The data are in 'QIE' form as q-stepped data of intensities in 2 columns or optionally with $\sigma(I)$ in 3 columns. Data may be preceded by comment records. Importers are for x-ray or neutron data with q in $\AA^{-1}$ or nm^{-1}; data will be stored in $\AA^{-1}$. The data type is either 'LXC' or 'LNC' (for X-ray and neutron, respectively).
- **Reflectometry Data** - Reads x-ray or neutron reflectometry data from files. Results are placed in the GSAS-II data tree as 'REFD <filename>'. The data are in 'QIE' form as q-stepped data of intensities in 2 columns or optionally with $\sigma(I)$ in 3 columns. The data are in 'QIE' form as q-stepped data of intensities and optional sig(I) as 3 (or) 2 columns. Data may be preceded by comment records. The data type is either 'RXC' or 'RNC' (for X-ray and neutron, respectively)
- **Powder Peak Position Data** - Reads ordered peak positions as 2θ or d-spacing from .txt files. Results are placed in the GSAS-II data tree as 'PKS <filename>'. The data format consists of optional comments (each line starts with '#') followed by positions in a single column. Peak positions must be sorted and their order indicates if the values are 2θ or d-spacing. If the position of the first peak is larger than the last peak, they positions are interpreted as d-spacings, otherwise as 2θ. A second column of intensities is optional.
- **PDF G(R) Data** - Reads pair distribution data for possible analysis by PDFfit from within GSAS-II.

4.5 **Export** Menu

A special set of modules, known as exporters, is used to write information from GSAS-II to external files. The exporters that are found by GSAS-II at runtime are used to configure the export menus. Export modules are usually fairly easy to create and thus new formats are relatively easy to support.

See the [GSAS-II Export Modules](https://gsas-ii.readthedocs.io/en/latest/exports section of the Programmers documentation for more information on this.

- **Entire project as** - At present there are several supported formats for all information in a GSAS-II project. One is a full CIF file, which brings up a separate window where information such as ranges for bond distances and angles can be selected. Note that when a project contains more than one histogram or phase, a multiblock CIF must be created. Two `.csv` (column-separated-value) forms suitable for cutting/pasting into manuscripts or creating spreadsheets. The "bracket notation" uses crystallographic notation [e.g. 1.234(5) indicates a value of 1.234 with a standard uncertainty of 0.005] and the other `.csv` format places standard uncertainty values in a separate column. The JSON "dump" provides a sort-of human readable (ASCII) version to the contents of a project (`.gpx`) file. GSAS-II cannot at present read anything from this file.
- **Phase as** - The contents of a phase (unit cell, space group, coordinates, etc.) can be exported in a variety of formats, including a simplified CIF file that contains only the unit cell, symmetry and coordinates.
- **Powder data as** - Powder data can be exported in number of formats. Note that this menu can also be used to export reflection lists from Rietveld and Pawley fits.
- **Small angle data** - This is exported only as a csv text file.
- **Reflectometry Data** - This is exported only as a csv text file.
- **Single crystal data as** - Single crystal reflection lists can be exported as text files or as a simplified CIF file that contains only structure factors.
- **Image data** - This exports selected images as a portable networks graphics format (PNG) file. Alternately, the image controls and masks can be written for selected images. If strain analysis has been performed on images, the results can also be exported here as a spreadsheet (.csv file).
- **Maps as** - Fourier maps can be exported here.
- **Export all Peak Lists...** - This allows peak lists from selected powder histograms to be written to a simple text file. There will be a heading for each PWDR GSAS-II tree item and columns of values for position, intensity, sigma and gamma follow.
- **Export HKLs** - This allows single crystal reflection lists from selected histograms to be written to a file.
- **Export MTZ file** - This exports macromolecular structure information in a commonly recognized format for input to other macromolecular packages.
- **Export PDF...** - This allows computed PDFs peak lists from selected histograms to be written as two simple text files, {name}.gr and {name}.sq, containing g(r) and S(Q), respectively as 2 columns of data; a header on each indicated the source file name and the column headings. The file is named based on the name of the PDF entry in the GSAS-II data tree.

4.6 **Help** Menu

The help menu offers access to this documentation, the GSAS-II tutorials, as well as options to select the version of GSAS-II that is used. Note that the update, regress and switch options will appear as inactive (greyed out) if you do not have write access to the directory where GSAS-II is installed and will not appear in the menu if the git program needed to make updates is not available to GSAS-II.

- **Check for updates** - When GSAS-II starts, if Internet access is available, a check is made to see if newer versions of GSAS-II are available. If so, it is downloaded as a background task. This menu command will check to see if a newer version has been downloaded and will offer the choice to install that. While it is not necessary to update GSAS-II every day (in fact on some days there may be multiple updates provided) it is recommended that updates be made at least monthly. Please do not report a bug in GSAS-II without first updating to the most recent version.
- **Regress to old GSAS-II version** - This allows the GSAS-II version to be set back to an older version. This might be useful to confirm that a result obtained previously is reproduced in the latest code or to avoid a bug that has inadvertently been introduced. Note that if there is some aspect of a newer version of GSAS-II that needs to be avoided, please report this, preferably by creating a new GitHub issue or at least post this on the GSAS-II mailing list. The likelihood is that the feature you like will be lost or the bug you found will not be addressed, if not reported
- **Switch to/from branch** - On occasion the GSAS-II developers will create trial versions of GSAS-II to try out new ideas or test changes before they are incorporated into the "main" release. These trial versions are called branches. Use this if working with the developers to test out a feature available in a test branch. This only appears in the menu the Configuration variable `debug` is set to `True` .

* **Add packages for more functionality** - GSAS-II runs in Python and requires several Python packages as well. Additional Python packages are optional, but sections of GSAS-II will not operate without them (as an example, to read Bruker `.brml` files, a package for interpreting XML, *xmltodict* is used. If this has not been installed, the Bruker `.brml` importer cannot be run. As GSAS-II runs, it makes note of optional Python packages that are

not present but could be useful. This menu command can be used to install those packages. If there are no uninstalled optional packages, this option will be greyed out.

- **Tutorials** - GSAS-II offers more than 50 tutorials on different aspects of the program. If this menu command is used, one see a list of tutorials, select to view a tutorial, optionally downloading the input files needed to run the tutorial.
- **Help on GSAS-II** - Opens an index file to these web pages with GSAS-II documentation.
- **Help on current data tree item** - Opens this GSAS-II documentation for the currently selected data tree item. A yellow help button on each section of the GUI will perform the same action.
- **Citation information** - If you use GSAS-II please cite Toby, B. H., & Von Dreele, R. B. (2013). “GSAS-II: the genesis of a modern open-source all purpose crystallography software package”. * Journal of Applied Crystallography, *46**(2), 544-549. doi:10.1107/S0021889813003531, but there are many specialized features of GSAS-II that utilize other's software that should also be cited. This menu item provides a list of all the works that one may want to consider citing through use of GSAS-II.

5. Data tree items

5.1 GSAS-II data tree overview

GSAS-II creates projects that are saved in `.gpx` files. The GSAS-II Data Tree, which is shown on the left side of the main GSAS-II window shows a hierarchical index to the contents of a project. This index will usually have all of the entries listed below on the Universal Data Tree Items page, which are found in all types of GSAS-II projects and will also have at least one entry representing some sort of experimental data (or simulation) -- called a histogram -- and will likely have one or more phase entries.

When you click on an entry in the data tree, the right side of the GUI, the GSAS-II Data Window will show the associated information with that section of the `.gpx` file, you may have access to additional menu commands and visualization information related to the selected data tree item may be shown in the GSAS-II Graphics Window.

Most of the subsequent sections of the GSAS-II help documentation describe: what the values shown in the GUI mean and what actions can be performed using the GUI, the menu commands and actions available for each type of data tree item, as well as any graphics that will be displayed and actions that can be performed graphically.

5.1.1 Data tree Histogram items

These constitute the data sets ("Histograms") to be used by GSAS-II for analysis. These are shown in the data tree as top-level entries where the prefix indicates the data type. The name in the data tree is usually followed by a descriptive term or file name. Most histogram types have information divided into sections, where each section is placed into a child (subdata) tree entry under the main histogram data entry. Selection of the main data tree item for a histogram may not produce much information in the data window but usually does provide visualization of the data in the graphics window. The histogram data prefixes are listed below and are described in subsequent sections of this help information.

- **PWDR**: Powder Diffraction data
- **HKLF**: Single Crystal data
- **PDF**: Pair Distribution Functions (derived from data)
- **IMG**: 2D Diffraction Images
- **SASD**: Small Angle data
- **REFD**: Reflectometry data
- **PKS** Powder Diffraction peak lists

5.1.2 Data tree Phase information

A GSAS-II phase is the description of a crystal structure, including unit cell parameters, symmetry and atom coordinates. Each phase is placed in the data tree as a child (subdata) tree entry in the phase. Note that while phases do not have any special prefix and do not have child entries in the data tree, the phase information is separated into sections through the use of tabs on the upper part of the data window. The tabs are listed here and each tab is documented separately.

5.1.3 Phase/Histogram Linking

Note that there is no limit to the number of phase and histogram entries that may be placed a project file, beyond that the computer being used must have enough memory to hold this information. Also, all the histogram and phase entries in project need not be utilized. Every phase can be linked to zero, one or more histograms. A single-crystal dataset can only be linked to one phase (or none), but a powder diffraction dataset can be linked to any number of phases, including zero. A phase that is not linked to a histogram is not used in refinements. Likewise, a histogram that is not linked to a phase is also not used. Deleting unlinked entries from a `.gpx` file is possible, but is not recommended as it may introduce problems; these are bugs that are hard to track down.

5.2 Universal Data Tree Items

The data tree items listed below will appear in every GSAS-II project once any histogram or phase has been placed in the project.

5.2.1 Notebook

This window provides a log of information on what has been done in a project. Some GSAS-II operations (*e.g.*, structure refinement, Fourier map calculation & peak fitting) will add entries to the notebook. You may also place whatever text commentary you wish into the window by clicking on the "Add comment" button. The comment will be time-stamped and placed appropriate order in the log.

- Normally entries are shown in reverse chronological order ("newest-1st"), but that button allows sorting with the oldest entries first ("oldest-1st").
- The "Set filters" button allows you to select which type of entries are shown, as are selected on a list. Note that older Notebook entries were not recorded with tags that allow filtering to work.
- The "Plot" button allows plotting the progression of the overall Rw or reduced χ^2 in the refinement, or logged variables (to log a parameter see **View LS parms** in the Calculate menu or the `LogAllVars` setting in the Configuration variables).
- The "Save" button writes the contents of the Notebook as a text file named <project>-notebook.txt.

What can I do here?

Use the notebook to keep track of information related to how you use GSAS-II, what has been done or to plot the progress of the fit. When you make different copies of a fit to try out different refinement options, it will be very helpful to put a comment here to help you remember what you did.

5.2.2 Controls

This window provides access to the controls that determine how GSAS-II performs minimizations as well as few global parameters for GSAS-II. Note that many other customization settings are set as configuration variables in the File/Preferences menu. (See the Configuration variables section of the Programmer's documentation. for listing of these options.)

1. **Refinement Controls**: These controls determine how refinements are performed. The first determines the computational engine used to minimize the structure.
    - **Refinement type** - This determines how structure refinements are performed. The choices are:
        - **analytic Hessian**: This is the default option and is usually the most useful. It uses a custom-developed least-squares minimizer that uses singular-value decomposition (SVD) to reduce the errors caused by correlated variables and the Levenberg-Marquardt algorithm to up-weight diagonal Hessian terms when a refinement step fails to lower χ2.
        - **analytic Jacobian**: This uses the numpy-provided `leastsq` minimizer, which not applicable for problem with a large number of histograms as it requires much more memory than the Hessian routines. This because it creates a Jacobian matrix (J) that is shaped N x M (N parameters x M observations) that is used to create the N x N Hessian. The Hessian method creates a Jacobian matrix only for each histogram; the N x N Hessian is the made from summing the J x J^T products across the histograms
        - **numeric**: This also uses the numpy leastsq minimizer and is also not applicable for larger problems. Unlike, the "analytic Jacobian", numerical derivatives are computed rather than use the analytical derivatives that are coded directly into GSAS-II. This will be slower than the analytical derivatives and will is often less accurate which results in slower convergence. It is typically used for code development to check the accuracy of the analytical derivative formulations.
        - **Hessian SVD**: This is very similar to analytic Hessian but does not include the Levenberg-Marquardt algorithm. It can be faster but is more prone to diverge when severe correlation is present. It is possible that it might be better for single-crystal refinements.

    Note that the Jacobian refinement tools are the Fortran MINPACK `lmdif` and `lmder` algorithms wrapped in Python, as provided in the numpy/Scipy package. The Hessian routines were developed for GSAS-II based on routines in numpy and scipy and used aw well material from *Numerical Recipes* (Press, Flannery, Teulosky & Vetterling) for the Levenberg-Marquardt algorithm. The `lmdif` and `lmder` routines were written by Burton S. Garbow, Kenneth E. Hillstrom, Jorge J. Moré (Argonne National Laboratory, 1980).
    - **Min delta-M/M** - A refinement will stop when the change in the minimization function, *M*, ($M = \sum[w(I_o - I_c)^2]$) is less than this value. The allowed range is 10^{-9} to 1.0, with a default of 0.001. A value of 1.0 stops the refinement after a single cycle. Values less than 10^{-4} cause refinements to continue even if there is no meaningful improvement.
    - **Max cycles** - This determines the maximum number of refinement cycles that will be performed. This is used only with the "analytical Hessian" and "Hessian SVD" minimizers.
    - **Initial lambda** - Note that here λ is the Marquardt coefficient, where a weight of 1+λ is applied to the diagonal elements of the Hessian. When λ is large, this down-weights the significance of the off-diagonal terms in the Hessian. Thus, when λ is large, the refinement is effectively one of steepest-descents, where correlation between variables is ignored. Note that steepest-descents minimization is typically slow and may not always find the local minimum. This is only used when with the "analytical Hessian" minimizer is selected.
    - **SVD zero tolerance** - This determines the level where SVD considers derivative values to be the same. Default is 10^{-6}. Make this larger when problems occur due to correlation. This is used only with the "analytical Hessian" and "Hessian SVD" minimizers.
    - **Initial shift factor** - This provides an initial scaling ("damping") for the first cycle of refinement. Only available for "analytic Jacobian" and "numeric" minimizers.
2. **Single Crystal Refinement Settings**: A set of controls is provided for control of single-crystal refinements. These only appear when single crystal (HKLF) histograms are present in the project.
    - **Refine HKLF as F^2?** - When checked, refinements are against F^2 rather than $|F|$.
    - **Min obs/sig** - Conventional cutoff for single crystal refinements as to what reflections should be considered observed, typical values are 2.0 (2σ) or 3.0 (3σ).
    - **Min extinct.** - Reflections with extinction corrections larger than this value are ignored.
    - **Max delt-F/sig** - Removes reflections that are very poorly fit. Should be used only with extreme care, since poorly-fit reflections could be an indication that the structure is wrong.
    - **Max d-spacing** - Reflections with d-space values larger than this value are ignored.
    - **Min d-spacing** - Reflections with d-space values smaller than this value are ignored.
3. **Sequential Settings**: A set of controls is for sequential refinement. Settings here determine if a "normal" or "sequential" refinement is performed. If no datasets are selected here, then all histograms linked to phases in the project and that are flagged as "used" are included in one potentially

large (combined) refinement. However, if any number of histograms are selected here as used in a sequential fit, then each of the selected histograms is fitted in turn, which in GSAS-II is called a sequential refinement. Only the first item below is shown in "normal" mode.

- **Select datasets/Reselect Datasets** - This brings up a menu where histograms can be selected, which potentially switches between a normal and a sequential refinement. If one or more histograms are selected, a sequential refinement is used. If none are selected, then the refinement be set as "normal". The button is labeled "Select" when in normal refinement mode and "Reselect" in sequential refinement mode.
- **Reverse order?** - Normally, in a sequential refinement histograms are fit in the order they are shown in the data tree (which can be reordered by dragging tree items), but when this option is selected, the sequential fit is performed in the opposite order, with the last tree entry first.
- **Copy results to next histogram?** - When this option is selected, the fitted parameters from each refinement are copied to the next histogram, so that the starting point for each refinement will be the results from fitting the previous. This works well for parametric experiments where parameters such as the lattice parameters change gradually over the course of successive measurements. This option is usually used only for the initial refinement after a sequential fit is started and the setting is cleared once that refinement is completed. For subsequent refinements, it is usually better to start with the results from the previous fit.
- **Clear previous seq. results** - When this button is pressed, the "Sequential Results" entry with the results from the last sequential fit is deleted from the tree.

4. **Global Settings**: This is a location for parameters that apply to an entire project. At present there is only one:
   - **CIF Author** - The value provided here is used when creating a CIF of an entire project.

What can I do here?

This offers a place to change how GSAS-II performs refinements, but has no specific menu commands or graphics.

5.2.3 Covariance

This window contains residual information after the last refinement. When this tree item is selected, the GSAS-II Plots window shows '**Covariance**', with a graphical representation of the variance-covariance matrix. The text in the data window shows statistical values related to the current fit. At the bottom of this list are buttons that display a horizontal bar chart with the shift to standard uncertainty ratio for each parameter.

- The button labeled "last refinement" shows these ratios based on the differences between each parameter value from the beginning of the refinement run and the value at the end of the refinement run.
- The button labeled "last cycle" shows these ratios based on the differences between each parameter value at the beginning of the last refinement least squares cycle and the value at the end of the cycle (and the refinement run). (These "last cycle" values are only available when the Controls are set for an "analytic Hessian" refinement.)

What is plotted here?

The variance-covariance matrix as a color-coded array is shown on this page. The color bar to the right shows the range of covariances (-1 to 1) and corresponding colors. The parameter names are to the right and the parameter numbers are below the plot.

What can I do with the plot?

- Move the mouse cursor across the plot. If on a diagonal cell, the parameter name, value and standard uncertainty (esd) is shown both as a tooltip and in the right-hand portion of the status bar. If the cursor is off the diagonal, the two parameter names and their covariance are shown in the tool tip and the status bar.
- Use the Zoom and Pan buttons to focus on some section of the variance-covariance matrix.
- Press 's' – A color scheme selection dialog is shown. Select a color scheme and press OK, the new color scheme will be plotted. The default is 'RdYlGn'.
- Press 'p' – Saves the covariance values in a text file.

5.2.4 Constraints

This window shows the constraints to be used in a refinement. Constraints are divided with a tab for each type: Phase, Histogram/Phase, Histogram, Global and Sym-Generated. Note that the standard parameters in GSAS-II are divided into three classes and appear respectively on the Phase, Histogram and Histogram/Phase tabs:

- those pertaining to quantities in each phase (naming pattern `p::name`); examples include atom coordinates, thermal motion and site fraction parameters;
- those pertaining to quantities in each histogram (naming pattern `:h:name`); such parameters are those that depend only on the data set: the scale factor and profile coefficients (e.g. U, V, W, X and Y);
- and those pertaining to quantities defined for each histogram in each phase (naming pattern `p:h:name`); these parameters are quantities that can be dependent on both the phase properties and the sample or dataset used for the measurement. Examples include phase fractions and sample-broadening coefficients such as microstrain and crystallite size; they are found in the Data tab for each phase.

The following types of constraints may be specified by users:

- **Holds** - Use this to prevent a parameter from being refined. Most valuable when refinement of a parameter is selected in a group for refinement (such as x, y & z for an atom or unit cell parameters) and one must be fixed. For example, if the space group for a phase has a polar axis (e.g., the y-axis in monoclinic space group $P\,2_1$, the origin with respect to *b* is arbitrary). With a polar axis present, if an arbitrary constant is added to all atom coordinates along that axis, a completely equivalent structure is obtained. Thus in $P\,2_1$ it is not possible to refine the y coordinates for all atoms. Place a Hold on any one atom y coordinate to keep the structure from drifting up or down the y-axis during refinement.
- **Equivalence assignments** - Determines a set of parameters that should have values with a specified ratio. Atom coordinates are handled slightly different, where the ratios are specified for the applied shifts, not the actual coordinate values. Examples for typical use are sets of atoms that should be constrained to have the same displacement parameters (aka thermal motion, Uiso, etc.) or sets of profile coefficients U, V & W across multiple data sets. Note that the first selected parameter is treated as independent, and the remainder are "slaved" to that parameter as "dependent parameters." All parameters in an equivalence must be varied. If any parameter is not varied or is given a "hold," a warning is displayed and none of the parameters in the equivalence are refined.
- **Constraint Equations** - Defines a set of parameters whose sum (with possible non-unitary multipliers) will be equal to a constant. For example, a common use for this is to specify the sum of occupancies for atoms sharing a site have a sum fixed to unity or so that the sum of occupancies for an atom type that is occurs on several sites is fixed to match a composition-determined value. Note that all parameters in the equation are considered as "dependent parameters." If a parameter in a constraint equation is held or is not varied, that parameter is removed from the equation (the sum value is modified accordingly). If no parameters remain the equation is ignored.
- **New Var assignment** - These are similar to constraint equations in that they define a set of parameters and multipliers, but rather than specifying a value for the expression, a new parameter is assigned to that sum. Thus these constraints create new variable that effectively replace the original GSAS-II parameters with ones supplied by the user. This is done by replacing a degree of freedom from the original variables with a new one that modifies the parameters, where the shift is applied according to the ratio specified in the expression. This can be used to create new parameters that redefine the relationships between items such as coordinates or magnetic moments. The new parameter may optionally be named by the user. The new var expression creates a new global parameter, where that new parameter is independent, while all the parameters in the expression are considered as dependent. The setting of the refine flags for the dependent parameters is not used. Only if the new var parameter is marked as `refine` then it will be refined. However, if any dependent variable is set as "hold," the **new var** parameter will not be refined.

  New Var constraints are generated when ISODISTORT is used to develop mode distortions from a comparison of a high symmetry parent structure (e.g. cubic perovskite) with a distorted child substructure. They are implemented for the phase when a special CIF file produced by ISODISTORT from a mode distortion analysis is imported. You can select which distortion modes to refine. Refining all modes is equivalent to refining the atoms freely and then importing the resulting structure to ISODISTORT to determine the mode amplitudes.

Note that when new var and constraint equation constraints are defined, they create new global parameters. Constraints on these will be rare, but can be managed on the Globals tab. Finally, some constraints are defined automatically based on restrictions determined by space group symmetry. These constraints can be seen, but not changed, using the Sym-Generated tab. Other constraints (holds) will be created when rigid bodies are specified.

What can I do here?

Select the tab for the parameter type(s) you wish to constrain then create new parameters using the "Edit Constr." menu commands:

- **Add Hold** - Select a parameter that you wish to remain fixed. If selected, a dialog box will appear showing the list of available parameters; select one and then OK to implement it, Cancel will cancel the operation. The held parameter will be shown in the constraint window with the keyword 'FIXED'.
- **Add equivalence** - Select the independent parameters and press OK; a second dialog box will appear with only those parameters that can be made equivalent to the first one. Choose those and press OK. Cancel in either dialog will cancel the operation. The equivalenced parameters will show as an equation of the form $M1 * P1 + M2 * P2 = 0$; usually M1=1.0 and M2=-1.0 but can be changed via the 'Edit' button. The equation(s) are shown in the window tagged by 'EQUIV' to mark it as an equivalence assignment.
- **Add constraint** - If selected, a dialog box will appear with a list of the available parameters. Select one and press OK; a second dialog box will appear with only those parameters that can be used in a constraint with the first one. Choose those and press OK. Cancel in either dialog will cancel the operation. The equivalenced parameters will show as an equation of the form $M1 * P1 + M2 * P2 + \ldots = C$; the multipliers M1, M2, … and C can be changed via the 'Edit' button. The equation is shown in the window tagged by 'CONSTR' to mark it as a constraint equation assignment.
- **Add New Var** - This behaves very much like the "Add constraint" menu command except that it defines a new parameter rather than define a value for the expression. That new var parameter can optionally have a named assigned. The expression is displayed with the keyword 'New Var' to mark its type. Note that a 'Refine?' box is included for this type of constraint.
- **Make atoms equivalent** - This provides a shortcut for establishing constraints when two share a single site. Coordinates and Uiso values are constrained to be the same and site fractions are constrained to add to 1.
- **Show ISODISTORT modes** - Used after a CIF from the ISODISTORT web site is read, which will display the values for the normal modes from representational analysis from the coordinates.

In addition to menu commands, this window also offer the following actions by pressing buttons:

- **Show Errors** - this button will be active if serious errors -- that would prevent a refinement from being performed -- are encountered processing the constraints.
- **Show Warnings** - this button will be active if correctable problems are encountered in processing the constraints, such as a constraint being rejected because a parameter is not varied. These warning may indicate that the choice of which parameters will be refined is not what was planned.
- **Show Generated Constraints** - After constraints have been processed, a series of relationships are developed to determine new variables from the current parameters and "inverse" equations that determine dependent parameters from the new variables and independent parameters. This shows the resulting relationships, as well as any "Hold" variables.
- **Delete Selected** - This button will cause all the selected constraints on the current tab to be deleted.

Sequential Refinement Constraints

While all the general information on constraints (above) applies to sequential refinements, the sequential refinement is performed by fitting each histogram individually and this affects how constraints are defined and processed for parameters keyed to a particular histogram number. When sequential refinement is selected (via the Controls tree item), it becomes possible to define constraints of form `p:*:name` and `:*:name` (where "p" is a phase number and name is a parameter name). The "*" here is called a wildcard, and in a constraint or equivalence will cause that to be used for every histogram in turn.

In sequential refinement mode, two additional controls are shown in the Constraints window. The first, which is labeled wildcard use, specifies what is done when a specific histogram is referenced by number in a constraint or equivalence by number rather than by wildcard. This offers three modes:

- **Set hist # to *** - Any constraints previously specified with a specific histogram number will be changed to apply to all histograms. This is the default for new projects.
- **Ignore unless hist=*** - Any constraints previously specified with a specific histogram number will be ignored and constraints with a "*" for a histogram number will be used. Note that constraints on phase parameters (of form 'p::name' -- without a histogram number specified) will be used normally. Note that this was the operating mode for GSAS-II in earlier versions before these buttons were introduced.
- **Use as supplied** - If different constraints are to be applied to different histograms, it becomes necessary to create constraints with specific histogram numbers. In this mode, constraints specified with a specific histogram are applied only to that histogram, while wildcarded ones are applied to all histograms. Note that one should not specify two constraints on a single parameter, one with a wildcard and one with a specific histogram number, as both will be applied to the specified histogram which results in an unsatisfiable conflict.

Also included when sequential refinement is selected is a menu button labeled "Selected histogram." With this it is possible to look at constraint problems when processing a specific histogram.

5.2.5 Restraints

This window shows the restraints to be used in a refinement for each phase (if more than one). It is organized into several tabbed pages, one page for each type of restraint. Restraints are developed for an individual phase and act as additional observations to be "fitted" during the refinement.

Note that a restraint "pushes" a refinement towards a target value, but does not require that to happen (unlike a constraint). The strength of the "push" is dependent on the weighting factor and the "esd" used on the target value. The ideal use of a restraint is for an aspect of a structure that is not well-determined by the data. In this case, when the weighting of a restraint is dropped, the value of the restrained parameter may move considerably from the target value, but the quality of the fit (noted by the Rietveld plot, R-factor, reduced χ^2, etc.) is not expected to change very much. If one places a restraint that is not consistent with the model (*e.g.* is wrong), then the fit will improve significantly as the weight is decreased. Such feedback is not possible with a constraint. See below for more discussion on restraint weighting.

What can I do here?

- Select the tab for the restraint type you wish to use. Each will have the same possibilities in the 'Edit' menu.
- You can change the Restraint weight factor – this is used to scale the weights for the entire set of restraints of this type. Default value for the weight factor is 1.0.
- You can choose to use or not use the restraints in subsequent refinements. Default is to use the restraints.
- You can change the search range used to find the bonds/angles that meet your criteria for restraint.
- You can examine the table of restraints and change individual values; grayed out regions cannot be changed. The 'calc' values are determined from the atom positions in your structure, 'obs' values are the target values for the restraint and 'esd' is the uncertainty used to weight the restraint in the refinement (multiplied by the weight factor).

- Menu **Edit** – has the menu commands listed below. Note that some entries may be grayed out, if not appropriate for your phase or for the selected restraint.
  - **Add restraints** - this takes you through a sequence of dialog boxes which ask for the identities of the atoms involved in the restraint and the value to be assigned to the restraint. The esd is given a default value which can be changed after the restraints are created.
  - **Add residue restraints** - if the phase is a 'macromolecule' then develop the restraints from a selected 'macro' file based on those used in GSAS for this purpose. A file dialog box is shown directed to /GSASIImacros; be sure to select the correct file.
  - **Add MOGUL restraints** - add restraints from a file produced by the CCDC's Mercury program (using the CSD-Core/Mogul Geometry Check) or a file prepared in that style. See below for more information on importing restraints. Note that when used from the Bond tab, only "bond" entries are read and when used from the Angle tab, only "angle" entries are read.
  - **Plot residue restraints** - if the phase is a 'macromolecule' and the restraint type is either 'Torsion restraints' or 'Ramachandran restraints', then a plot will be made of the restraint distribution; torsions as 1-D plots of angle vs. pseudopotential energy and Ramachandran ones as 2-D plot of psi vs phi. In each case a dialog box will appear asking for the residue types or specific torsion angles to plot. Each plot will show the observed distribution (blue) obtained from a wide variety of high-resolution protein structures and those found (red dots) for your structure. The restraints are based on a pseudopotential (red curve or contours – favorable values at the peaks) which has been developed from the observed distributions for each residue type.
  - **Change value** - this changes the 'obsd' value for selected restraints; a dialog box will appear asking for the new value.
  - **Change esd** - this changes the 'esd' value for selected restraints; a dialog box will appear asking for the new value.
  - **Delete restraints** - this deletes selected restraints from the list. A single click in the blank box in the upper left corner of the table will select/deselect all restraints.

Restraint types

- **Bond**: Defines restraints with a target distance between pairs of atoms (which are typically bonded, but this is not required). Atom pairs to be restrained are set by performing a search and then selecting the pairs to be used.
- **Angle**: Defines restraints with a target angle for a set of three atoms. Atoms to be used are located via a search and selection.
- **Plane**: Used to restrain selected atoms to be approximately co-planar. This is most commonly used for macromolecular crystallography.
- **Chiral**: Defines a chiral volume restraint. This is unlikely to be used other than for macromolecular crystallography.
- **Chem. Comp.**: This is of use when "Frac" parameters (atom occupancies) are refined. This option allows a variety of different types of restraints to be created. More than one chemical composition restraint can be defined for a phase. Examples of how this might be used would be to "push" refinement towards an expected composition, to encourage charge balance or to conserve valences.
- **General**: This allows a quantity to be restrained that is computed from a user-supplied equation, based on GSAS-II parameters. Thus, one can create any type of restraint that is desired. This restraint is used by supplying a Python equation and then to define which GSAS-II parameter is associated with each variable in the Python equation. One also supplies the target value for the restraint. Note that it is possible to use externally defined functions that contain "if" statements, which allows restraints that enforce minimum or maximum quantities rather than target values to be defined.

Importing Restraints

For the **Add MOGUL restraints** menu command, restraints are read from a .csv file that is usually generated in the CCDC program Mercury using the CSD-Core/Mogul Geometry Check. This file has many columns, but only the first 8 are used here and a few of those do not matter. It would also be possible to produce such a file manually or cast output from another program, but make sure the .csv file follows the following instructions:

The first line in the file must be a header, which must start with "Type" (note capitalization). The rest of that initial line is ignored, but it is convenient to follow the example below.

Subsequent lines should contain:

1. The first column (Type) should be "bond" or "angle"
2. The second column (Molecule) is ignored. It can be blank, but a comma to end the field is required
3. The third column (Fragment) specifies the atoms in the distance or angle. The atoms should be separated by at least one space. For an angle the second listed atom is the one at the apex of the angle. Capitalization of the atom name must match the name used in the atoms table.
4. The fourth column (Classification) can be anything other than "No hits"
5. The fifth column (No. of hits) is ignored. It can be blank, but a comma to end the field is required
6. The sixth column (Query value) is ignored. It can be blank, but a comma to end the field is required
7. The seventh column (Mean) is the bond distance or bond angle used in the restraint, labeled "target" in the table.
8. The eighth column (Std. dev.) is the uncertainty on the bond distance or bond angle labeled "esd" in the table. Note that quantity `"Weight factor" * (obs-calc) / esd` determines the impact of the restraint, so the esd values are on an arbitrary scale.

If the columns are reorganized and the header changed to match, the code should be able to change to match, but this has not been tested. Spacing between columns does not matter and columns do not need to be aligned. With a file such as the one below, that contains both distances and angles, the file must be read in twice, using the **Add MOGUL restraints** menu command from both the Bond tab and the Angle tab to read in both sets of restraints. Blank lines are ignored. Note that only restraints between atoms within the asymmetric unit can be generated with this type of file. If symmetry or translations are needed to generate any of the atoms in the distance or angle, the **Add restraints** menu command must be used to search.

This is an example file to be used to read in restraints:

```
Type, Molecule,    Fragment,  Classification, No. of hits, Query value,  Mean,   Std. dev.
bond,   ignore,    Co1 O16,     OK,           ignore,      ignore,      2.060,     0.001
bond,   ignore,    Co1 O20,     OK,           ignore,      ignore,      2.069,     0.001

angle,  ignore,    N15 C8 C9,   OK,           ignore,      ignore,      123.38,    0.01
angle,  ignore,    C9 C10 C11,  OK,           ignore,      ignore,      116.18,    0.01
angle,  ignore,    C11 C12 N15, OK,           ignore,      ignore,      123.91,    0.02
```

Restraint Weights

There is no simple recipe for how to weight restraints, in that it varies with the problem, but one should understand is that restraints are used computationally just like any other data point, where the refinement works towards minimizing the sum of $[w * (obs_i - calc_i)/\sigma_i]^2$ where w is usually 1 and obs_i might be a powder diffraction intensity but could also be a restraint bond distance and where σ_i is the uncertainty on obs_i, which for restraints is the "esd" value. Since there are usually 10^3 to 10^4 data points and only circa 10^1 restraints, I will usually initially weight the restraints quite highly (100-10,000) since I want to start the fit with a model that closely matches the expected distances and angles.

As the refinement progresses and I have a good fit, I will then try lowering the restraint weighting. Ideally, I can set the weight on the distances & angles to zero, in which case the restraints will show me a diagnostic of how far the as-fit distances, etc. deviate from my presupposed values, but do not actually change the fit.

A weight factor of 0 may not produce a good result with complex structures and not very complex diffraction patterns. In those cases, there just is not enough information to define all the structural degrees of freedom uniquely. In that case, lowering the weighting will increase the deviations seen in the restraints with only very trivial improvements in the fit to the powder pattern. One needs to reduce the restraint weight, but only to the point where a chemically reasonable structure is still obtained. Usually, a small value for the weight is needed (around 0.1 to 10) for the final refinements, as very little "force" is needed to keep the structure in agreement with what is expected for the class of materials.

There is one important case to be aware of, and that is where the restraints are incorrect for the material being studied. If one tries to restrain, for example, a bond to a value that is wrong for the material (for example a carbon-carbon single bond where in fact a double-bond is present) and the data have enough sensitivity to determine this, then the restraints and the data will be in conflict. Lowering the restraint weighting will produce a significant improvement in the fit to the powder data as the bond distance refines away from the target value. If this occurs the restraints need to be corrected to the valid structure. This is different from the case where there is not enough information to define all the structural degrees of freedom, where the fit to the powder data improves only slightly as the restraint is down-weighted. In that latter case, there are very many structures that produce about the same quality of fit, but restraints will prejudice the fit towards models that are more expected based on what is known on the class of materials.

5.2.6 Rigid bodies

There are three different types of rigid bodies that can be used in GSAS-II, as selected by the tabs at the top of this window.

- **vector rigid bodies**, where atoms are defined in terms of multiple displacements from an origin.
- **residue rigid bodies**, where atoms are defined according to Cartesian coordinates and torsion angles. These are much more commonly used than vector rigid bodies.
- **spinning rigid bodies**, where the dynamics or disorder causes the atoms to not have specific locations in the unit cell.

Note that there are two steps in defining a rigid body. In this data item the rigid body is defined. The rigid body is then later inserted into one or more phases using the "RB Models" tab on a Phase data item. A rigid body can be inserted into more than one phase.

What can I do here?

- Select the tab for the rigid body type you wish to use.
- Once the rigid body type has been selected, use the menu commands listed below. The menu contents will depend on which type of rigid body is selected.
- Editing of some of much of the rigid body information can be done in the data window once a body is created.
    - **Add rigid body** - (Vector & Spinning rigid bodies). For vector bodies this creates a vector description of a rigid body. A dialog box asks the number of atoms (>2) and the number of vectors required to create the rigid body. An entry will be created showing a magnitude with the vector set to be applied for each vector needed to develop the rigid body.
    - **Extract from file** - (Vector & residue rigid bodies). This prepares a rigid body by reading in coordinates (typically as fractional coordinates) and then atoms are selected from the file that is read and finally the origin and axes of the Cartesian system used by the rigid body are defined.
    - **Save rigid body** - (Vector & Spinning rigid bodies). Writes the contents of a defined rigid body into a file where it can be reused in another GSAS-II project. A different format is used for vector vs. residue bodies.
    - **Read rigid body** - (Vector & Spinning rigid bodies). Creates a rigid body from a file written perviously by a "Save rigid body" command.
    - **Add translation** - (Vector rigid bodies). The Cartesian coordinates for the body are created from the sum of coordinate matrices multiplied by a value that converts the arbitrary axis lengths to Angstroms. One can sum 9 multiplier/coordinate matrix sets. This command will add an additional "translation" consisting of a multiplier and coordinates for every atom in the rigid body.
    - **Import XYZ** - (Residue rigid bodies) this reads a text file containing a set of Cartesian coordinates describing a rigid body model. Each line has atom type (e.g. C, Na, etc.) and Cartesian X, Y and Z.
    - **Save as PDB** - (Vector rigid bodies). Writes the contents of a defined rigid body as Cartesian coordinates in a PDB file.
    - **Define Torsion** - (Residue rigid bodies) this adds a variable torsion angle in an existing rigid body via a sequence of dialog boxes. The first one asks for the origin and the second asks for the pivot atom for the torsion from the nearest neighbors to the origin atom; the atoms that ride on the selected torsion are automatically found from their bond lengths.
    - **Import residues** - (Residue rigid bodies) this reads a predetermined macro file that contains standard (Engh & Huber) coordinates for the amino acids found in natural proteins along with predetermined variable torsion angle definitions.
- Once a rigid body is defined you can plot it, change its name or manipulate any torsion angle to see the effect on the plot.
- The translation magnitudes in a vector rigid body can be refined allowing some lengths within a vector rigid body to be varied.

5.3 Sequential Results data tree entry

The Sequential Results data tree entry shows a composite result from a sequential fit. It is only present after a sequential fit has been run. Note there are the following types of sequential fits in GSAS-II:

1. Rietveld: Sequential results
2. PDF: Sequential PDFfit2 results
3. Peak fit: Sequential peak fit results
4. Small angle: Sequential SASD fit results
5. Reflectometry: Sequential REFD results
6. Image (strain): Sequential strain fit results
7. Image (calibration): Sequential image calibration results

Each sequential fitting process within GSAS-II will have its own differently named set of sequential results, as listed above. When any of these tree items is selected, the window tabulates the sequential fit results. The columns are the parameter names; the naming convention is generally 'p:h:name:n' where 'p' is the phase number,' h' is the histogram number, 'name' is the parameter name, and 'n' (if needed) is the item number (e.g. atom number). The rows are the data sets used in the sequential refinement.

For a sequential Rietveld refinement, set the PWDR histograms to be used in the sequential refinement in the Controls data tree item. Note that the Calculate/Refine menu command will be renamed as "Sequential Refine." Since not all histograms need be used in a sequential Rietveld fit, after a sequential fit, histograms that have been fit will be included in the table. Previously fit histograms will not be removed unless the table is cleared (in the Controls tree item). In this way, a large sequential fit may be worked on in sections. The first column of the table will list the histogram number and the number will be shown in red if it was not fit in the last sequential refinement.

What can I do here?

- **Select a row** - a right mouse button will display the variance-covariance matrix for the refinement with that data set; a left mouse button will display its powder data fit.
- **Select a column** - this will display a plot of that parameter across the sequence of data sets. Error bars for each value are also shown. Selecting multiple columns (hold Ctrl key down for subsequent picks) will plot all as individual curves.

Menu "Columns/Rows" contents

- **Set used** - this allows you to select in a dialog which entries to use; those not used are not plotted or used in further processing.
- **Update phase from row** - this updates the phase parameters from the entries in the selected row. Normally the phase parameters at the end of a sequential fit are those obtained from the last histogram.
- **Set phase vals** - same as previous except you can pick which parameters to update.
- **Plot selected cols** - plots the selected columns (redundant as selecting the columns automatically plots them)
- **Rename selected cols** - can change column names with this
- **Save selected as text** - gives a txt file with columns of data from those selected.
- **Save selected as CSV** - gives a comma separated values (CSV) file of selected columns.
- **Compute average** - gives average(esd) for selected column values.
- **Hide columns** - you can select/deselect columns to not show in table.
- **Save all as CSV** - gives a CSV file for all table entries.

Menu "Pseudo Vars" contents

This is used to create derived results from sequentially refined parameters; new columns are the result.

- **Add Formula** - create a formula used to make a derived result.
- **Add Distance** - adds a new column for a specific interatomic distance.
- **Add Angle** - adds a new column for a specific 3-atom angle.
- **Delete** - to remove a pseudo variable formula.
- **Edit** - to change a selected formula.

Menu "Parametric Fit" contents

This is used to create fitting models for any column of sequential results.

- **Add equation** - add a parametric fitting equation. At the end of this step, it will be used to give refined values of the coefficients with esds based of a full error propagation from the variance-covariance matrices from the individual refinements.
- **Copy equation** - make a copy of a parametric equation.
- **Delete equation** - to remove a parametric equation.
- **Edit equation** - to edit an equation.
- **Fit to equation(s)** - do the fitting of the parametric equations to the data.
- Menu '**Seq export**' –
- **Project as** - choices are
- a CIF file that contains each sequential result as a separate block (with one phase) or multiple blocks, if multi-phase.
- The output files used by the Cinema: Debye-Scherrer program from Los Alamos. This is a nice tool for visual display of parametric fits. Install it before using the export option.
- **Phase as** - either a "quick" CIF or a CSV file
- **Powder as** - either a powder pattern cif, a histogram CSV file or a reflection list CSV file.
- **Save table as CSV** - same as Save all as CSV above.

What can I do with the plot?

By default, the plot shows the variation of the selected parameters across the sequence of histograms used in the sequential fit. Each point that was fitted shows as an x with a vertical bar indicating the standard error from the fit for that value. There are some key commands:

- Press "**l**" (lower case "L") – toggles display of connecting lines between the data points
- Press "**s**" – this presents a choice of parameters from the table columns to be used for the x-axis. Typically, this is used to show parameter variation with e.g. temperature.
- Press "**t**" – this provides access to all three titles of the plot.

5.4 Cluster Analysis data tree entry

The Cluster Analysis data tree entry shows parameters to perform a cluster analysis computation and results from that analysis once it has been run. This data tree entry is created in GSAS-II after the main menu command **Calculate/Setup Cluster Analysis** is used.

Cluster analysis is a suite of data survey techniques where data are grouped by some measure of their similarity. Thus, it can be used as a preliminary survey of a large number of data sets in e.g. preparation of detailed examination of representative members. In the case of powder diffraction pattern (PWDR) data or pair distribution (PDF) data, their similarity is determined by considering each pattern as a hyper-dimensional vector with one dimension for each data point and then computing some measure of how parallel pairs of these vectors are. Consequently, it can be used to survey PWDR data entries that have identical scan characteristics (e.g. instrument type, step size, radiation type, wavelength) or multiple PDF G(r) entries created with the same step sizes and using the same radiation from data collected with identical instrument configurations. The cluster analysis routines used here are from the scipy library and (if available) the scikit-learn library. If scikit-learn is absent, an attempt is automatically made to install the latter via the conda system. The scipy library provides some cluster analysis tools while the scikit-learn package provides others. If you use results from scikit-learn, please cite the following in any publication that uses it:

> "Scikit-learn: Machine Learning in Python", Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, M. and Duchesnay, E., (2011). Journal of Machine Learning Research 12, 2825-2830.

5.4.1 Cluster Analysis with scipy

Doing cluster analysis in GSAS-II requires several steps; new steps will become visible in the GUI as previous ones are completed. Redoing earlier steps may clear subsequent ones. For an example, see the tutorial, Cluster and Outlier Analysis.

In order of their appearance, the GUI commands are:

- **Select datasets** - this brings up a selection tool for PWDR (& PDF, if present) entries in the GSAS-II data tree. Your selection must be either PWDR or PDF data; otherwise, there is no check on data similarity so be careful with your selections. Multi-bank TOF data should not be mixed for cluster analysis nor should laboratory and synchrotron data. Cluster analysis on fewer than 5-10 data sets is probably not useful, but can be applied on dozens or even hundreds of data sets.
- **Data limits** - selection of data is followed by entries for the minimum and maximum data limits; the defaults are taken from the data Limits imposed on the original PWDR data or the r-range for the PDF G(r) data. The units are degrees 2θ, TOF in μs, or Å, as appropriate. Refer to any PWDR (or PDF) plot to select these values; leading background should be skipped, and the upper limit chosen from a relatively clear point where there are still significant peaks. Values will be used to give the cluster analysis input data matrix size.
- **Make Cluster Analysis data array** - this button forms the data matrix for cluster analysis; it is number of data sets times number of data points between the limits in size. the next item will appear in the GUI.
- **Select cluster analysis distance method** - there are several choices as what is meant by "distance" between all pairwise selection of data vectors (u & v). They are (as taken from scipy):
    - **braycurtis** – Computes the Bray-Curtis distance between the data vectors as

$$d(u,v) = \frac{\sum_i |u_i - v_i|}{\sum_i |u_i + v_i|}$$

    - **canberra** – Computes the Canberra distance between data vectors as:

$$d(u,v) = \sum \frac{|u_i - v_i|}{|u_i| + |v_i|}$$

    - **chebyschev** – Computes the Chebyschev distance between data vectors as:

$$d(u,v) = \max |u_i - v_i|$$

    - **cityblock** (sometimes called "Manhattan") – Computes the city block distance between data vectors as:

$$d(u,v) = \sum |u_i - v_i|$$

    - **correlation** – Computes the correlation distance between data vectors as:

$$d(u,v) = 1 - \frac{(u - \bar{u}) \cdot (v - \bar{v})}{\sqrt{(u - \bar{u})^2 (v - \bar{v})^2}}$$

    - **cosine** – Computes the cosine squared between the data vectors as:

$$d(u,v) = 1 - \frac{u \cdot v}{\sqrt{u^2 v^2}}$$

    - **euclidian** (default) – Computes the Euclidian distance between the data vectors as:

$$d(u,v) = \sqrt{\sum_i (u_i - v_i)^2}$$

    - **jensenshannon** – Computes the Jensen-Shannon distance between the data vectors
    - **minkowski** – Computes the Minkowski distance between the data vectors as:

$$d(u,v) = \sqrt[p]{\sum_i |u_i - v_i|^p}$$

where the exponent, p, = 2 by default; this is identical to the Euclidian formula. Some choices for p: 1 is the same as city block, and 10 (~ ∞) is essentially the same as Chebyschev. The others (3 & 4) give distance results that are between Euclidian (p=2) and Chebyschev (p=10 ~ ∞).

    - **seculidian** – Computes the standardized Euclidian distance between the data vectors as:

$$d(u,v) = \sqrt{\sum_i (u_i - v_i)^2 / V[x_i]}$$

where the variance, $V[x_i]$, is computed automatically as the variance in the data point values for each data position (i.e. 2θ) across the entire data array.

- **sqeuclidian** – Computes the squared Euclidian distance between the data vectors as:

$$d(u,v) = \sum_i (u_i - v_i)^2$$

Changing the method results in an automatic calculation of the distances; the Compute button is provided for convenience. The result of this calculation is displayed as the 1st plot in a plot tab named for the selected distance method; this facilitates comparison between methods for your data. Also shown in this plot tab is a 3D plot of the result of a Principal Component Analysis (PCA) of the distance data; it shows the location of each data set in this space. Clusters may be evident from this plot; variable temperature scans tend to show a complex path of distance points with cluster

grouping corresponding to phases. Since data sets may be in a series, a plot of the serial distances across the suite of data is shown; spikes in a temperature series may indicate phase changes. The GUI will be extended to show more steps in cluster analysis.

- **linkage method for hierarchical clustering** - there are several choices for linkage in determining the hierarchical relationship (if any) between the data sets and the algorithm will use the distance matrix determined above to determine the data hierarchy. The distances are used by the linkage method to group similar data into clusters; these are successively combined until just a single cluster is obtained. A dendrogram is displayed showing the progression of this clustering. Each cluster is given a mean position, s or t, to compare to the others. The linkage methods for calculating the distance (using the distance method, dist, as selected above) between each pair of clusters are:
  - **single** – computes the linkage as:

$$d(s,t) = \min(dist(u(s)_i, v(t)_j))$$

  - **complete** – computes the linkage as:

$$d(s,t) = \max(dist(u(s)_i, v(t)_j)$$

  - **average** (default) – computes the linkage as (Ns, Nt are numbers of members in cluster s & t, respectively):

$$d(s,t) = \sum_{ij} \frac{dist(u(s)_i, v(t)_j)}{N_s N_t}$$

  - **weighted** – computes the linkage when s is formed with clusters u & v and t is another cluster as:

$$d(s,t) = (dist(u,t) + dist(v,t))/2$$

  - **centroid** ("UPGMC") – computes the linkage when cs & ct are the centroids of clusters s & t, respectively as:

$$d(s,t) = (dist(c_s, c_t)$$

  - **median** ("WPGMC") – computes the linkage when ms & mt are the medians for all member pairs in clusters s & t as:

$$d(s,t) = (dist(m_s, m_t)$$

  - **ward** – computes the linkage when s is formed with clusters u & v and t is another cluster as (Nu, Ns, Nt are numbers of members in cluster u, s & t, respectively, & T=Nu+Nv+Nt):

$$d(s,t) = \sqrt{\frac{N_t + N_u}{T} dist^2(t,u) + \frac{N_t + N_v}{T} dist^2(t,v) - \frac{N_t}{T} dist^2(u,v)}$$

  Changing the linkage method results in an automatic recalculation of the hierarchical clustering; a Compute button is provided for convenience. The result of this calculation is shown as a dendrogram in the same plot tab; the 4th plot shows the percentage contribution of the leading terms in the PCA to the distance data. Usually, 2-3 terms are sufficient to describe the distribution.
- **Select number of clusters** for K-means clustering (scipy algorithm). The algorithm attempts to group the data points (e. g. as in the PCA plot) into the requested number of clusters based on Euclidian distances on a "whitened" data array (i. e. not the distance matrix). To whiten the data matrix the suite of values at each position (e. g. at each 2θ) are divided by its standard deviation; this reduces the scale of the PWDR & PDF observations to just numbers of standard deviations from zero. Use the Compute to repeat the K-means clustering; the start points are randomly selected and will sometimes yield different results. Cluster populations are shown in the GUI, clusters are colored to match the data point colors in the PCA plot.
  - **Select cluster to list members** – Shows a colored list of the data items that belong to the selected cluster.
  - **Select cluster member** (use mouse RB on item in displayed list) – Displays the PWDR (or PDF) data on the Powder Pattern plot tab for the selected item.

* **Plot selection** – changes the displayed plots: * **All** – All four plots are shown * **Distances** – Only the distance matrix is shown * **Dendogram** – Only the hierarchical dendrogram is shown. * **3D-PCA** – Only the 3D representation of the Principal Component Analysis is shown. * **Diffs** – Only the serial differences are shown.

5.4.2 Cluster Analysis with scikit-learn

The next section of the GUI only appears if the scikit-learn package is installed. It has multiple algorithms for doing clustering and detecting outliers (i. e. bad data) in the suite of PWDR or PDF patterns. Changing the method or number of clusters results in an automatic calculation; the **Compute** button is provided for convenience. There is a reminder to properly cite Scikit-learn if you use it.

- **Select clustering method** – some may also require selecting number of clusters
  - **K-Means** (requires number of clusters) – Uses the scikit-learn "K-means++" algorithm for clustering; this gives a better starting position and usually succeeds on the 1st try. It uses the "whitened" data matrix.
  - **Affinity propagation** – It uses the distance matrix computed above.
  - **Mean-shift** – It uses the "whitened" data matrix.
  - **Spectral clustering** (requires number of clusters) – It uses the "whitened" data matrix.
  - **Agglomerative clustering** (requires number of clusters) – It uses the distance matrix computed above.

For details of these methods, please see 2.3. Clustering — scikit-learn 1.1.2 documentation. After completion, Cluster populations are shown in the GUI and clusters are colored to match the data point colors in the PCA plot.

5.4.3 Outlier Analysis with scikit-learn

After selection of the PWDR or PDF data and doing the distance calculation, one can examine the distance data for possible "bad" data items. These outliers can be detected by a choice of methods that make different assumptions how the data "should" be clustered; any data that do not fall within them are flagged as outliers and are colored different in the resulting 3D PCA plot from all others that would be in clusters. Although the chosen distance method affects the appearance of the 3D PCA plot, the three outlier methods all use the original data, thus are independent of any selected distance method. The GUI is refreshed showing a listing of the outlier data; selection of any, displays that data item in the powder pattern plot tab. Any previous cluster identification, e. g. by K-means, is erased. The outlier detection methods are:

- **One-Class SVM** - Attempts to form boundaries around the clusters; outliers are items that fall outside the boundaries.
- **Isolation Forest** - Similar to the above but uses a different algorithm.
- **Local Outlier Factor** - Uses the local density of other points about each point to determine if it is within a high-density area, i. e. in a cluster, or not.

Further details of these methods can be found at 2.7. Novelty and Outlier Detection — scikit-learn 1.1.2 documentation. The current GSAS-II implementation of these methods all use the default settings for any of their respective parameters.

What can I do with the plots?

For each selection of distance method, i.e. "Euclidian", a plot tab is created with 2 or 4 plots. They are:

1. the distance matrix displayed in the same way the refinement covariance matrix is displayed (default coloring is "paired" – same parameter as the powder pattern contour plot);
2. the 3D PCA analysis plot;
3. the hierarchical dendrogram plot and
4. the PCA percent contribution plot.

Each can be zoomed independent of the others and the 1st three can be selected to show as a single plot in the tab (see **Plot selection**, above). A LB mouse selection (& hold button down) of a 3D PCA point will show the data set name in the plot status line. If clusters are determined by e. g. K-means, the 3D PCA points will be colored by cluster membership.

5.5 Phases

5.5.1 Overview on **Phase** data tree entries

Phases are placed in their own section of the GSAS-II data tree as subentries under the "Phases" entry. Note that there are no limits to how many phases may be placed in a GSAS-II project (`.gpx` file), other than as limited by available computer memory. Also, phases are only used in refinements when they are linked to histograms (datasets) so there is very little "cost" connected to including a phase that is not in use.

Phases are either created with the Data/"Add new phase" menu item (manual input) or are read in using the Import/Phase menu items. After a phase is imported, if there are histograms (datasets) present in the project, you will be offered a chance to link the imported phase to the previously imported histogram(s). Likewise, if histograms(s) are imported when phase(s) are already present, you will also be asked to link the new data to existing phases. It is also possible to link histograms to a phase later by selecting that phase in the data tree and then selecting the "Data" tab and finally using the "Edit Phase"/"Add powder histograms" menu command.

When a phase is selected from the data tree, parameters are shown for that selected phase in a tabbed window. Clicking on each tab raises the windows as documented in subsequent sections of the help documentation.

The tabs are:

- General
- Data
- Atoms
- Draw Options
- Draw Atoms
- RB Models
- Texture
- Map Peaks
- Pawley
- Layers
- Wave Data
- MC/SA
- RMC
- ISODISTORT
- Dysnomia

5.5.2 **General** phase tab

This section of the phase information provides overall parameters describing the phase such as: the phase's name, space group, the unit cell parameters and overall parameters for the atom types present in the phase. It also has the controls for Pawley intensity extraction and for computing Fourier maps for this phase. It can also has the controls for Monte Carlo/Simulated Annealing for solving structures with flexible rigid molecular bodies.

WHAT CAN I DO HERE?

1. Menu '**Compute**' – The compute menu shows computations that are possible for this phase.

Fourier map

Compute Fourier maps according to the controls set at bottom of General page.

Search map

Search the computed Fourier map. Peaks that are above 'Peak cutoff' % of the maximum will be found in this procedure; they will be printed on the console and will be shown in the "Map peaks' tab. This page will immediately be shown, and the peaks will be shown on the structure drawing for this phase as white 3-D crosses.

Charge flipping

Performs a charge flipping *ab initio* structure solution using the method of Oszlanyi & Suto (Acta Cryst. **A60**, 134-141, 2004). You will need to select a source for the reflection set and perhaps select an element for normalization by its form factor, a resolution limit (usually 0.5Å) and a charge flip threshold (usually 0.1); these are found near the bottom of the General window. There are also Test HKLs to show the progress in phasing with charge flipping cycles. They show the generally chaotic phase behavior before a solution is found; after that the phases are essentially fixed. No use is made of this information; it is just for your edification. A progress bar showing the charge flip residual is shown while the charge flip is in operation. When the residual is no longer decreasing (be patient – it doesn't necessarily fall continuously), press the Cancel button to stop the charge flipping, otherwise it will stop at 10,000 cycles. The resulting map will be positioned to properly place symmetry operators (N.B.: depends on the quality of the resulting phases; the map could be still offset by a few steps), searched for peaks and the display shifts to Map peaks to show them.

4D Charge flipping

4-Dimensional charge flipping is done for a modulated structure. Only available for phases with a 3+1 superspace group.

Clear map

This clears any Fourier/charge flip map from the project; the Fourier map controls are also cleared.

MC/SA

Perform Monte Carlo/Simulated Annealing structure solution using the model as set up in the MC/SA tab and the controls at the bottom of this tab.

Multi MC/SA

Perform multiple Monte Carlo/Simulated Annealing structure solutions, accumulating the best ones as set up in the MC/SA tab.

Transform

This allows for a change in axes, symmetry or unit cell. It is also used to create a magnetic phase from a chemical (nuclear) phase. One important transformation that can be done here is for Origin 1 settings to Origin 2 (see more extensive elsewhere).

Compare Cells

Compares two supplied unit cells for a transformation matrix that converts one to the other within supplied search tolerances using the NIST*LATTICE program. If this is used, please cite:

- V. L. Karen and A. D. Mighell, NIST Technical Note 1290 (1991). (link)
- V. L. Karen & A. D. Mighell, U.S. Patent 5,235,523. (link)

Compare polyhedra

Compares idealized polyhedra (tetrahedron & octahedron) to those obtained from a Reverse Monte Carlo run in RMCProfile.

Select magnetic/subgroup phase

Selection of the results from a magnetic subgroup analysis done in the PWDR/Unit cells list data tree item. This will generate a new magnetic phase. Can also be used to select from possible subgroups of a nonmagnetic super group for possible symmetry reduction. See the PWDR/Unit cells list description for further information.

Protein quality

Evaluate protein quality by Python versions of `errat` & `errat2` codes by Colovos, C. & Yeates, T.O. Protein Science **2**, 1511-1519 (1991).

The items in the upper part of the General page that can be changed are Phase name, Phase type, Space group, unit cell parameters & refine flag. These are described in turn:

- **Phase name** – this is the name assigned to this phase. It can be changed at any time.
- **Phase type** – this can only be set when there are no atoms in the Atoms page for this phase. Select it when the phase is initialized.
- **Space group** – this is usually set when the phase is initialized, but it can be changed later. Be careful about the impact on Atom site symmetry and multiplicity if you do. The choice of space group will set which unit cell parameters are displayed in this window.

  GSAS-II will recognize any legal space group symbol using the short Hermann-Mauguin forms, provided whitespace is placed between the axial fields (e.g. "F d 3 m" not "Fd3m", but note that "F d -3 m" is interpreted the same as "F d 3 m". Standard Space groups will also be recognized without spaces, but non-standard ones will not.

  For space groups where there is a choice of origin (e.g. F d 3 m), GSAS-II always uses the 2nd setting, the one where the center of inversion is located at the origin (see more extensive elsewhere).
- **Refine unit cell** – set this flag to refine the unit cell parameters in a Rietveld or Pawley refinement. The actual parameters refined are the symmetry allowed terms (A0-A5) in the expression

$$d^{*2} = A_0 h^2 + A_1 k^2 + A_2 l^2 + A_3 hk + A_4 hl + A_5 kl$$

where $A_0 - A_5$ correspond to elements in the reciprocal metric tensor element (**G**) where off-diagonal contributions are doubled, A0-A5 = G_{11}, G_{22}, G_{33}, $2 * G_{12}$, $2 * G_{13}$, $2 * G_{23}$

- **a, b, c, alpha, beta, gamma** – lattice parameters; only those permitted by the space group are shown. The volume is computed from the values entered.

If there are entries in the Atoms tab, then the Elements table is shown below on the General tab; you may select the isotope (only relevant for neutron diffraction experiments). The density (just above the Elements) is computed depending on this choice, the unit cell volume and the atom fractions/ site multiplicities in the entries on the Atoms page.

Next are the Pawley controls.

- **Do Pawley refinement?** – This must be chosen to perform a Pawley refinement as opposed to a Rietveld refinement for this phase. NB: you should clear the Histogram scale factor refinement flag (found in Sample parameters) for the powder data -- PWDR histogram) as it cannot be refined simultaneously with the Pawley reflection intensities.
- **Pawley dmin** – This is the minimum d-spacing to be used in a Pawley refinement. NB: be sure to set this to match the minimum d-spacing indicated by the powder pattern limits (see Limits for the powder data set).
- **Pawley dmax** – This is the maximum d-spacing for reflections in a Pawley refinement. It is usually defined by the beginning of the data collection scan and will thus remove reflections that have too large d-spacing to be seen in the scan.
- **Pawley neg. wt.** – This is the weight for a penalty function applied during a Pawley refinement on resulting negative intensities. Use with caution; initially try very small values (e.g. .01). A value of zero means no penalty is applied.

Fourier map controls are shown next on the General page. Single crystal data or a completed Rietveld or Pawley refinement is required before a Fourier map can be computed. Select the desired type of map, the source of the reflection set and the map resolution desired. The peak cutoff is defined as a percentage of the maximum and defines the lowest level considered in the peak search.

Charge flip controls are below the Fourier map controls.

- **Reflection sets** – This is the source of structure factors to be used in a charge flip calculation. These may be either a single crystal data set, or structure factors extracted from a powder pattern via a Pawley or LeBail refinement or a Rietveld refinement.
- **Normalizing element** – This is an element form factor chosen to normalize the structure factors before charge flipping. None (the default) can be selected from the lower right of the Periodic Table display shown when this is selected.
- **Map grid step** – This is the step size of the charge flip map; default is 0.25Å. The set of reflections is expanded to a full sphere and zero filled to 2X this value; this suite of reflections is then used for charge flipping.
- **k-Factor** – This is the threshold on the density map, all densities below this are charge flipped.
- **k-Max** – This is an upper threshold on the density map; all densities above this are charge flipped. In this way the "uranium solution" problem is avoided. Use k-Max = 10-12 for equal atom problems and larger for heavy atom ones (typically 2X largest atom number).
- **Test HKLs** – plot of phases for selected hkls are shown at end of charge flipping run. Just for you to look at.

Monte Carlo/Simulated Annealing controls are at the bottom of the window.

- **Reflection set from** – This is the source of structure factors to be used in a charge flip calculation. These may be either a single crystal data set, or structure factors extracted from a powder pattern via a Pawley or Lebail refinement or a Rietveld refinement.
- **d-min** - This restricts the set of reflections to be used in the MC/SA run. Suggest using no lower than 2.0.
- **MC/SA runs** – pulldown with selection of number of trials to be done.
- **MC/SA Refine** – requires a refinement of parameters over range about each test position.
- **MC/SA schedule** – This selects the schedule for the "temperature" to be used during MC/SA run. For 'fast' and 'log', coefficients control details of schedule; a plot shows the scheduled temperatures for the set of steps.
- **Annealing schedule** – This selects the beginning MC/SA "temperature", final "temperature", and number of trials at each step.

5.5.3 **Data** phase tab

This data tab serves several purposes. It is used to link histograms to the selected phase, and it allows the values and refinement flags to be set for the parameters that are defined for each histogram-phase pair, labeled as HAP parameters. [Note that some GSAS-II parameters are defined for each phase (atomic positions, for example), other parameters are defined for each histogram (scale factors and instrumental constants, for example) but the HAP parameters have values for each histogram in each phase.]

The HAP parameters include:

- the phase fraction;
- the sample contributions to peak broadening: microstrain and crystallite size;
- a LeBail intensity extraction flag;
- hydrostatic/elastic strain shifts to lattice parameters;
- corrections to peak intensities due to experimental effects (preferred orientation, extinction and disordered solvents). The data tab also implements graphical representation for some of these HAP parameter sets.

For single crystal data, the only parameters are scale, extinction and disordered solvent. There is no scale factor directly associated with the histogram.

- **Use flag** - When the Use flag is selected, the currently selected phase is included in the computation of intensities as a contribution to the selected histogram (single-crystal histograms can have only one phase; powder histograms can have any number of associated phases). When not set, the phase is not included in the selected histogram, as if it the phase and histogram had not been linked. Changing the use flag is much easier that linking and unlinking phases and histograms.
- **Start LeBail extraction** - When this is selected, intensities are set to values that are best fit using the LeBail intensity determination method rather than are computed from the atomic information for the phase. Cycling this setting will reset LeBail extracted intensities to their default (F^2 = 100).
- **Phase fraction** - Used in powder histograms: a multiplier that determines the relative amount of the selected phase to a histogram. It is proportional the number of unit cells of the phase in the sample. The number is assumed to be on an arbitrary scale; the values are mass normalized to compute phase mass (weight) fractions.

  Note that when the histogram scale factor is varied, these values are on a relative scale. Conventional practice is to vary the scale factor and to not vary the phase fraction for one phase in a histogram, but also common is to fix the histogram scale factor and refine all phase fractions. Do not refine the scale factor and all phase fractions unless a constraint is defined so the phase fractions add to 1.
- **Scale factor** - Used for single crystal data: relates F^2_{obs} to F^2_{calc}.
- **Crystallite size peak broadening** – Peaks can be broadened due to the finite size of crystallites or due to microstrain (see below). Microstrain is more common other than in nanoparticles. The broadening is computed from size factor(s) in microns (1 μm = 10^{-6} m), with the Scherrer constant assumed as unity. Sizes can be computed with a choice of three models: isotropic, uniaxial and ellipsoidal. Typical sensitivity for crystallite size is to no more than 4 μm (less for lower resolution instruments); beyond that the particles are effectively infinite for a diffraction experiment.
  - In **isotropic** broadening, crystallites are assumed to average as uniform in all directions and a single size value is supplied;
  - with **uniaxial** broadening, a preferred direction (as a crystallographic axis, such as (001) is supplied) -- note that for most crystal systems only one axis makes sense -- and two size parameters are defined, one for along the axis and one for in the perpendicular plane;
  - with **ellipsoidal**, six terms are used to define a broadening tensor that has arbitrary orientation -- this model may require constraints and is seldom needed.

  Note that size broadening is usually Lorentzian, which corresponds to a LGmix value of 1.0; if this value is between 0 and 1, both Gaussian and Lorentz size broadening is modeled and a value of 0.0 is pure Gaussian. Values less than 0 or greater than 1 make no physical sense. LGmix is not commonly refined.
- **Microstrain peak broadening** - This is computed as unitless fraction of Δd/d (or equivalently ΔQ/Q) times 10^6. Typical microstrain is ~1000, but may be significantly higher in physically processed materials. Note that the term residual stress is sometimes used for microstrain, but residual stress can be computed from microstrain when the elastic strain constants are known. Microstrain was can be computed in GSAS-II via a choice of three models: isotropic, uniaxial and generalized:
  - In **isotropic** broadening, microstrain broadening assumed to be the same in all crystallographic directions and a single value is supplied;
  - with **uniaxial** broadening, a preferred direction (as a crystallographic axis, such as 0,0,1) is supplied -- note that for most crystal systems only one axis makes sense -- and two microstrain parameters are defined, one for along the axis and one for in the perpendicular plane;
  - with **generalized**, the Nicolae Popa/Peter Stephens second-order expansion model is used and the number of terms will depend on the crystal system. It is typically possible to refine all terms when significant anisotropic strain broadening is present.

  Note that microstrain broadening is usually Lorentzian, which corresponds to a LGmix value of 1.0; if this value is between 0 and 1, both Gaussian and Lorentz size broadening is modeled and a value of 0.0 is pure Gaussian. Values less than 0 or greater than 1 make no physical sense. LGmix is not commonly refined.
- **Hydrostatic/elastic strain** – This shifts the lattice constants for the contribution of a phase into a histogram. These D_{ij} values are added to the reciprocal lattice parameter tensor terms. They must be refined in sequential refinements or where the lattice constants are slightly different in different histograms (as an example, see the Combined X-ray/CW-neutron refinement of $PbSO_4$ tutorial) or may account for changes to the lattice constants due to external stress (as occurs in a high-pressure measurement.) Note that *these values and the phase's lattice parameters (on the General tab) should not be refined at the same time*. When the values are non-zero, the lattice constants after application of these strain tensor terms is shown with these D_{ij} values.

  For cubic material, an extra term, eA (ϵ_A) with units of Å^{-2}, is included that is particularly useful in high pressure work. This accounts for the shift of peaks due to macroscopic stress along the (111) directions:

$$\Delta 2\theta = -180. * d^2 * \Delta D_{hkl,\epsilon_A} * \tan(\theta)/\pi$$

$$\Delta T = -\mathrm{difC} * d^2 * \Delta D_{hkl,\epsilon_A}/2.$$

where $\Delta 2\theta$ is in degrees and ΔT is TOF in μsec; d is d-space (Å) and

$$\Delta D_{hkl,\epsilon_A} = \epsilon_A \frac{(hk)^2 + (hl)^2 + (kl)^2}{(h^2 + k^2 + l^2)^2}$$

- **Preferred Orientation** – Preferred orientation (texture) can be treated in one of two different sections of GSAS-II, either the Preferred Orientation correction here in the Data tab, or the "Texture" tab, depending on what is desired. The Preferred Orientation correction here is typically used for crystallographic studies, where intensity corrections are desired to repair for undesired texture in the sample, while the Texture tab is used for studies where the goal is to characterize preferred orientation in a sample.

  The preferred orientation correction, here in the Phase/Data tab, can apply one of two different types of intensity corrections. One is to apply a cylindrical (wire symmetry) spherical harmonics orientational distribution function and the other is a simpler, single-parameter model, known as **March-Dollase**. Note either of these is applied to only a single histogram. This is in contrast to the model applied in the Texture tab, where the corrections from a set of spherical harmonics terms will be applied to all histograms associated with the current phase appears. Note that multiple sample orientations or detector settings are usually needed to determine texture with symmetry lower than cylindrical. Typically, the Preferred Orientation correction here is used for crystallographic studies, where intensity corrections are desired to repair for undesired texture in the sample, while the Texture tab is used for studies where the goal is to characterize preferred orientation in a sample. Note that both the Preferred Orientation and Texture corrections should not be used at the same time.

  Use of the **March-Dollase** model requires a definition of a unique axis (as a reciprocal space vector) and then a single ratio can be refined, which specifies the relative amount of excess (value >1) or depleted (value <1) crystallites in that direction. Note that there is only one choice for the unique axis for many crystal systems, such as 001 for hexagonal and tetragonal.

  The **Spherical Harmonics model** allows for a more complex probability surface (which is always constrained to match the symmetry of the crystal system and assumes a cylindrical symmetry sample.) An order parameter term is available which dictates how many terms are introduced into the model and thus the complexity of the probability surface. Note that use of this model requires that the correct value is used for Sample parameters. For the goniometer χ (chi) setting be sure to use:

  - χ = 90.0 for Debye-Scherrer or
  - χ = 0.0 for Bragg-Brentano.

  A measure of fit quality can be made by plotting the Preferred Orientation for different reflections. (Use the selection box at the at the top right to cause this to be displayed.) The MRD (multiples of random distribution) term will be 1 everywhere for a random (texture-free) sample. A value that is significantly below zero is not physically possible and indicates overfitting. The amount of the correction that has been applied to each reflection for a phase in a histogram is shown in the `Prfo` column of the "Reflection Lists" table. This should also be positive for every reflection.
- **Extinction** – This can occur when crystals/crystallites have minimal mosaic character, which results in lowering of diffraction intensities for the most intense reflections. This is not commonly seen in CW powder diffraction, but can be more apparent in neutron TOF data. For single crystal data the extinction model is more complex allowing for primary and two types of secondary extinction.
- **Disordered solvent**; Babinet A & B - This correction, using the Babinet model, is typically used to treat scattering from solvent that is not well-ordered in protein structures. It probably makes no sense in most any other application.
- **Merohedral twins** - Used for single crystal data; gives twin law transformation matrix and fraction for each twin member. These are for merohedral twins where the observed structure factors are a composite of contributions from each twin. Twin fractions are automatically constrained to sum to unity.

WHAT CAN I DO HERE?

- In this tab, menu items allow copying values or refinement flags to histograms/phases and selection of which histograms are used in the current phase.
- The plot selection items allow for three dimensional representations of the microstrain or crystallite size distributions (which are spheres for isotropic treatments); preferred orientation can be plotted as a Psi scan (a plot of relative crystallite abundance for a particular reflection as a function of azimuthal angle) or as an inverse pole figure (which shows a stereographic projection of the probability distribution for different reciprocal lattice directions as viewed down the sample cylinder axis). For no texture/preferred orientation this figure would be flat = 1.0.

5.5.4 **Atoms** phase tab

This data tab holds the table of parameters for the atoms in this crystal structure model. The menu controls allow manipulation of the values, refinement flags as well as initiation calculations of geometrical values (distances & angles) among the atoms.

Some atom operations utilize or set the "viewpoint." This is the location in the graphics window's structure drawing that is marked by crossing , red, green and blue lines.

WHAT CAN I DO HERE?

1. **Atom selection from table** - These are controlled by the mouse and the Shift/Ctrl/Alt keys. Note that for most purposes (one exception is atom reordering which requires an Alt-Left-click on the rows), selection of any cell for an atom will work equivalently with selection of the entire row. Upon selection, the atoms will turn green in the structure drawing:
    - **Left Mouse Button (LMB)** – on a row number selects the atom.
    - **Shift+LMB** – on a row number selects all atoms from last selection to the selected row (or top is none previously selected).
    - **Ctrl+LMB** – on a row number selects/deselects the atom.
    - **Alt+LMB** – on a row number selects that atom for moving; the status line at bottom of window will show name of atom selected. Use Alt+LMB again to select a target row for this atom; insertion will be before this row and the table will be updated to show the change. NB: the Draw Atoms list is not updated by this change.
2. **Double-left click a Type column heading**: a dialog box is shown that allows you to select all atoms with that type.
3. **Double-left click a refine or I/A column heading**: a dialog box will be shown with choices to be applied to every atom in the list.
4. **Editing tools** – These are controlled by the mouse (Alt ignored, Shift & Ctrl allow selection of multiple cells but no use is made of them). An individual data item can be cut/pasted anywhere including from/to another document. Bad entries are rejected (yellow background). If any entry is changed, press Enter key or select another atom entry to apply the change.
    - **Name** – can change to any text string.
    - **Type** – causes a popup display of the Periodic Table of the elements; select the element/valence desired; the atom will be renamed as well.
    - **refine** – shows a pulldown of allowed refinement flag choices to be shown; select one (top entry is blank for no refinement).
    - **x,y,z** – change atom coordinate. Fractions (e.g. 1/3, 1/4) are allowed.
    - **frac,Uiso,Uij** – change these values; fractions (e.g. 1/3, 1/4) are allowed.
    - **I/A** – select one of I(sotropic) or A(nisotropic); the Uiso/Uij entries will change appropriately.

5. Menu '**Edit Atoms**' - The edit menu shows operations that can be performed on your selected atoms. The command will operated on the atoms selected prior with the left mouse button. If no atoms have been selected, a window will open to allow atoms to be selected.

    - **On selected atoms...** -

        a. **Refine selected** – A popup dialog box appears; select refinement flags to apply to all selected atoms.

        b. **Modify parameters** – A popup dialog box appears with a list of atom parameter names; select one to apply to all selected atoms. Name will rename selected atoms according to position in table [e.g. Na(1) for Na atom as 1st atom in list in row '0']. Type will give periodic table popup; selected element valence will be used for all selected atoms and atoms names will be changed. I/A will give popup with choices to be used for all selected atoms. x,y,z will give popup for shift to be applied to the parameter for all selected atoms. Uiso and frac will give popup for new value to be used for all selected atoms.

        c. **Set viewpoint** – Set the viewpoint to be position of 1st selected atom

        d. **Move atom to viewpoint** – Move a single atom to the viewpoint location.

        e. **Insert atom** – insert an H atom (name= Unk) at 0,0,0 before the selected atom, it is also drawn as an H atom in the structure plot (small white ball). The atom can then be edited to change the type, coordinates, etc.

        f. **Insert viewpoint** – insert an H atom (name= Unk) before the selected atom with coordinates matching the location of the viewpoint, it is also drawn as an H atom in the structure plot.

        g. **Calc H atoms** – insert H-atoms in standard positions bonded to the selected atoms. The positions used will be computed based on bonding patterns for the selected atoms.

        h. **Delete atom** – selected atoms will be deleted from the atom list; they should also vanish from the structure drawing.

        i. **Transform atoms** – A popup dialog box appears; select space group operator/unit cell translation to apply to the selected atoms. You can optionally force the result to be within the unit cell and optionally generate a new set of atom positions. You may also invert a noncentrosymmetric structure. NB: many of these operations only make sense if all atoms are selected, but this is not enforced.

        j. **Select all** – Selects all atoms for further changes. Atoms in drawing will turn green.

        k. **Select from list** – A popup appears allowing selection of atoms for further changes. Selected atoms will turn green.

        l. **Append atom** – add an H atom (name= Unk) at 0,0,0 to the end of the atom table, it is also drawn as an H atom in the structure plot.

        m. **Append viewpoint** – add an H atom (name= Unk) to the end of the atom table with coordinates matching the location of the viewpoint; it is drawn as an H atom in the structure plot.

        n. **Update H atoms** – Reset H-atoms according to bonding geometry; only applies to H-atoms initially placed via Calc H-atoms. Usually used after running a structure refinement.

        o. **Assemble molecule** – move atoms to create single molecule, not appropriate for extended structures.

        p. **Collect atoms** – move atoms to be closest to selected position

        q. **Reload draw atoms** – reload drawing atoms from current atom list. Generally needed after a refinement.

        r. **Reimport atoms** – resets the coordinates to values from any importable phase file (e.g. CIF, `.gpx`,...)

6. Menu '**Compute**' –

    - **Show Distances & Angles** – compute distances and angles with esds (if possible) for selected atoms. A popup dialog box will appear with distance angle controls. NB: if atoms have been added or their type changed, you may need to do a Reset of this dialog box before proceeding.
    - **Save Distances & Angles** – same as the prior menu command, but writes the distance & angle result to a file with extension `.disagl`.
    - **Histogram bonds and angles** – plots histograms of bond lengths & angles about selected atoms.
    - **Apportion atom frac** – after selection of a 2nd element; this determines from atomic number and neutron scattering length the atom fractions of each type for selected atoms and presents results on the console.
    - **Density** – calculate density
    - **ISODISTORT mode values** – when a structure has been imported from ISODISTORT, this will compute the mode displacements for the current atom positions and display them in a popup window.

WHAT CAN I DO WITH THE PLOT?

A drawing of the crystal structure will be displayed in the Graphics Window only if the Draw Options or Draw Atoms tab has been visited first prior to selecting the Atoms tab. When back at the Atoms tab, the following actions and keypress commands are available, when use of the mouse buttons changes the view of the structure and can be used to select atoms. On a Mac with a one-button mouse, some alternate actions must be used

- **Left drag**: Holding down left button rotates axes around screen x & y
- **Right drag**: Holding down right button translates the fractional coordinates assigned to the viewpoint (which is kept at the center of the drawing). The structure will appear to translate. The viewpoint can also be entered directly in the Draw Options..
- **Middle drag**: Holding down center button rotates axes around screen z (direction perpendicular to screen).
- **Mouse Wheel**: Rotating the scroll wheel changes "camera distance" (zoom in/out)
- **Shift+Left Click**: Holding down the shift key while clicking on an atom with the left mouse button causes that atom to be selected (Shift + a Right click does the same). Any previously selected atoms will be reset. If two atoms are overlapped in the current view, then the top-most atom will usually be selected. Only atoms in the asymmetric unit can be selected from the plot in this way.
- **Shift+Right click**: Holding down the shift key while clicking on an atom with the right mouse button causes the atom to be selected if previously unselected and unselected if previously selected. Any previously selected atoms will be continue to be selected so shift-right click can be used to add atoms to the selection list. If two atoms are overlapped in the current view, then the top-most atom will usually be selected. Only atoms in the asymmetric unit can be selected from the plot in this way. (On a Mac, control+mouse click is an alternate way to do this.)
- **Key n**: Pressing the "n" key selects the next atom in the displayed atom list.
- **Key p**: Pressing the "p" key selects the previous atom in the displayed atom list.
- **Key c**: Pressing the "c" key sets the plot viewpoint at unit cell center. Also resets n/p selection item to the 1st atom.
- **Key s**: Pressing the "s" key brings up a (large) selection of color schemes for the slice contours. Default – "RdYlGn" (Green – positive, red – negative & yellow – zero).
- **Key k**: Pressing the "k" key cycles through the possible slice contouring options (none, lines, colors, lines+colors)
- **Key m**: Pressing the "m" key for an incommensurate structure creates a movie file of the change in the structure along the 4th dimension (tau). Movie controls are found in the GSAS-II Configuration Variables. Requires the imageio python package be available for import – it is not normally available in the GSAS-II version of python.
- **Key +**: Pressing the "+" (or "=") key steps the viewpoint in positive drawing z-direction (toward viewer). If structure is incommensurate, "+" steps the structure and map through the 4th dimension (+tau).
- **Key -**: Pressing the "-" key steps the viewpoint in negative drawing z-direction (away from viewer). If structure is incommensurate, "-" steps the structure and map through the 4th dimension (-tau).

5.5.5 *Draw Options*

WHAT CAN I DO HERE?

The Draw Options window provides access to a number of items that control how the structure is displayed. If a map is available (Fourier/charge flipping), one can display a 10Åx10Å contoured slice centered at the viewpoint. Contouring done as lines, colors or lines & colors combined. 3-D contouring is also available as green (red for negative density) map grid points. One can also draw individual or stack of hkl planes across unit cell.

WHAT IS PLOTTED HERE?

A drawing that shows the atoms of the crystal structure is generated. The way that the structure is displayed is determined according to the controls in this page as well as the atoms selected and their settings on the Draw Atoms page.

WHAT CAN I DO WITH THE PLOT?

Use of the mouse buttons and key presses when viewing a crystal structure changes the view of the structure; this is described on the Atoms tab.

5.5.6 *Draw Atoms* phase tab

Visiting this tab causes a drawing of the crystal structure to be displayed in the Graphics Window

The contents of this tab is a list of the atoms that are displayed. These may be rendered as lines, van der Waals radii balls, sticks, balls & sticks, ellipsoids & sticks or polyhedra. Bonds, as shown in the structure drawing, are determined by the atomic radii settings. There are four menus for this tab:

- **Edit** allows modification of the list of atoms to be rendered,
- **Compute** gives some options for geometric characterization of selected atoms,
- **Restraints** allows definition of 4 different types of restraints on the structure and
- **Rigid body** allows selection of atoms that form a previously defined rigid body.

WHAT CAN I DO HERE?

The commands and operations here determine what atoms are included in the structure drawing and how those atoms are displayed. Note that options for display type are by atom, so van der Waals, ball & stick and polyhedral display, for example, can all be mixed in a single display. Note that when atoms are added to the list, the anisotropic thermal displacement parameters (Uij) for atoms created by symmetry operations will be transformed as appropriate. Note that any atom positions that duplicate atoms already in the list are not retained.

There are two convenient ways to use the capabilities here. Select atoms and then select a menu item, typically from the **Edit Figure** menu. Alternately, right-click on the table and you will be offered a list of commands that can be performed on the selected atoms.

ATOM SELECTION

Atoms may be selected by a number of methods:

1. **Atom Selection from table**: select individual atoms by a left click of the mouse when pointed at the left most column (atom numbers) of the atom display; hold down the Ctrl key to add to your selection; a previously selected atom will be deselected; hold down Shift key to select from last in list selected to current selection. A selected atom will be highlighted (in grey) and the atoms will be shown in green on the plot. Selection without the Ctrl key will clear previous selections. A double left click in the (empty) upper left box will select or deselect all atoms.
2. **Atom Selection from drawing**: select an atom by a left click of the mouse while holding down the Shift key and pointed at the center of the displayed atom, it will turn green if successful and the corresponding entry in the table will be highlighted (in grey); any previous selections will be cleared. To add to your selection, use the right mouse button (Shift down); if a previously selection is reselected it is removed from the selection list. NB: beware of atoms that are hiding behind the one you are trying to select they may be selected inadvertently. You can rotate the structure anytime during the selection process.
3. **Double left click a Name, Type and Sym Op column heading**: a dialog box is shown that allows you to select all atoms with that characteristic. For example, selecting the Type column will show all the atom types; your choice will then cause all those atoms to be selected.
4. **Double left click a Style, Label or Color column**: a dialog box is shown that allows you to select a rendering option for all the atoms. For Color a color choice dialog is displayed that covers the entire color spectrum. Choose a color by any of the means available, press the "Add to Custom Colors", select that color in the Custom colors display and then press OK. NB: selecting Color will make all atoms have the same color and for Style "blank" means the atoms aren't rendered and thus the drawing will not show any atoms or bonds!
5. **Select from list** menu command (see below). A list of atoms is displayed and one can select using checkmark buttons. This will be offered automatically when a menu command requires selected atoms and none have been selected.

Note that on a Mac with a one-button mouse, some alternate actions must be used for selection.

MENU 'EDIT FIGURE' CONTENTS

The edit menu shows operations that can be performed on your selected atoms. If you have not selected any atoms using any of the menu items, you will be presented with a window where you can select atoms.

Many of the options below can also be accessed after selecting one or more atoms by right-clicking the mouse on the table.

- **Atom style** – select the rendering style for the selected atoms
- **Atom label** – select the item to be shown as a label for each atom in selection. The choices are: none, type, name or number. (NB: atom labelling slows drawing response time).
- **Atom color** – select the color for the atom; a color choice dialog is displayed that covers the entire color spectrum. Choose a color by any of the means available, press the "Add to Custom Colors", select that color in the Custom colors display and then press OK.
- **Reset atom colors** – return the atom color back to their defaults for the selected atoms.
- **Edit atom radii** – modify atom radii used in the bond assignment algorithm.
- **View point** – position the plot view point to the first atom in the selection. The view point is shown as crossing red, blue and green lines and this is placed at the center of the plot diagram in all three dimensions.
- **Select from list** – select atoms from a popup list of names.
- **Add atoms** – using the selected atoms, additional atoms are added to the bottom of the list after applying your choice of symmetry operator and unit cell translation to the *selected atom* coordinates. Through use of this command, usually after the **Fill unit cell** and/or **Complete molecule** commands, makes it possible to display multiple unit cells.
- **Add sphere of atoms** – fill in all atoms that fall within a sphere of selected radius about selected atom(s).
- **Add box of atoms** – Not yet implemented
- **Transform draw atoms** – apply a symmetry operator and unit cell translation to the set of selected atoms; they transformed atoms will replace the original atoms in the draw atoms list.
- **Fill CN-sphere** – using the atoms currently in the draw atom table, find all atoms that belong in the coordination sphere around the selected atoms via unit cell translations. NB: symmetry operations are not used in this search; do **Fill unit cell** first.
- **Fill unit cell** - using the atoms currently selected from the draw atom table, find all atoms that fall inside or on the edge/surface/corners of the unit cell. This operation is frequently performed before Fill CN-sphere.
- **Complete molecule** – beginning with a selected atom, transform other atoms to equivalent positions that form a contiguous molecule. Not appropriate for continuous structures (a warning will appear if the command is not completing)
- **Create void map** – by using a grid of probe positions, locate points outside of normal contact distances within a structure. Result is a mesh of small blue points in structural voids. These could indicate possible locations of missing solvent molecules or voids in porous materials.
- **Delete atoms** – Remove selected atoms from the draw atom table. If you remove all atoms, the table is then refilled from the Atoms table. You should do this operation after any changes to the contents of the Atoms table, e.g. if atoms are added or deleted.
- **Update draw atoms** – refresh the drawn atom positions from the Atoms list, You should do this operation after any changes to the contents of the Atoms table, e.g. by a structure refinement. This operates on all atoms and ignores any previous atom selection.
- **Load selected atoms** - refresh the selected atom positions in the draw atoms list from the Atoms list.

MENU 'COMPUTE' CONTENTS

The compute menu gives a choice of geometric calculations to be performed with the selected atoms. You must select the appropriate number of atoms for these to work and the computation is done for the atoms in selection order.

- **View pt. dist.** - this calculates distance from view-point to all selected draw atoms; result is given on the console window.
- **Dist. Ang. Tors.** – when 2-4 atoms are selected, a distance, angle or torsion angle will be found for them. The angles are computed for the atoms in their selection order. The torsion angle is a right-hand angle about the A2-A3 vector for the sequence of atoms A1-A2-A3-A4. An estimated standard deviation is given for the calculated value if a current variance-covariance matrix is available. The result is shown on the console window; it may be cut & pasted to another application (e.g. Microsoft Word).
- **Best plane** – when 4 or more atoms are selected, a best plane is determined for them. The result is shown on the console window; it may be cut & pasted to another application (e.g. Microsoft Word). Shown are the atom coordinates transformed to Cartesian best plane coordinates where the largest range is over the X-axis and the smallest is over the Z-axis with the origin at the unweighted center of the selection. Root mean square displacements along each axis for the best plane are also listed. The Z-axis RMS value indicates the flatness of the proposed plane. NB: if you select (e.g. all) atoms then Best plane will give Cartesian coordinates for these atoms with respect to a coordinate system where the X-axis is along the longest axis of the atom grouping and the Z-axis is along the shortest distance. The origin is at the unweighted center of the selected atoms.

MENU 'RESTRAINTS' CONTENTS

Individual restraints may be generated by selecting atoms and the corresponding restraint type from the menu.

- **Add bond restraint** – for selected atom pair (A-B).
- **Add angle restraint** – for selected atom triple (A-B-C)
- **Add plane restraint** – for selected 4 or more atoms
- **Add chiral restraint** – for selected 4 atoms; chiral atom first followed by 3 other atoms; if selected in righthand sequence, chiral volume will be > 0.

MENU 'RIGID BODY' CONTENTS

- **Define rigid body**' - Assign a previously defined rigid body to selected atoms.

WHAT IS PLOTTED HERE?

A drawing that shows the atoms of the crystal structure is generated. The atoms are displayed according to the controls in the in this page as well as options on the Draw Options page.

WHAT CAN I DO WITH THE PLOT?

Use of the mouse buttons and key presses when viewing a crystal structure changes the view of the structure; this is described on the Atoms tab.

5.5.7 **RB Models** phase tab

A rigid body is a collection of atoms that is treated as a group in GSAS-II. The position and orientation of the group can be refined and some other simplified parameters can also be varied, such as dihedral angles. Use of a rigid body requires two actions. First the rigid body must be defined for the project, see the Rigid bodies tree item for details on that. Then the rigid body must be inserted into a phase, which is done here, from the phases's RB Models tab. In this process, a number of parameters are defined for each body that determine how the rigid body is placed in the cell: the location in the cell for the rigid body origin, a rotation angle and orientation vector. These can be modified while being visualized, using the mouse by holding down the Alt key.

WHAT CAN I DO HERE?

A rigid body can be inserted into a phase using the "Locate & Insert Rigid Body" command in the "Edit Body" menu.

Once a body has been inserted into a structure, this tab provides access to the rigid body placement parameters, as well controls that determine how the rigid body is refined. Note that the selected rigid body can be positioned and oriented in the unit cell by holding down the Alt key (option on Mac) while "dragging" the mouse (moving the mouse while holding a mouse button down.) Dragging the mouse without the Alt key repositions the view of the cell.

WHAT CAN I DO WITH THE PLOT?

Use of the mouse buttons when viewing a crystal structure changes the view of the structure. On a Mac with a one-button mouse, some alternate actions must be used.

- **Left drag**: Holding down left button rotates axes around screen x & y
- **Right drag**: Holding down right button translates the fractional coordinates assigned to the viewpoint (which is kept at the center of the plot). The structure will appear to translate. The viewpoint can also be entered directly in the Draw Options.
- **Middle drag**: Holding down center button rotates axes around screen z (direction perpendicular to screen).
- **Mouse Wheel**: Rotating the scroll wheel changes "camera distance" (zoom in/out).

Use of the Alt key causes the above mouse movements to reposition the rigid body rather than change the view of the crystal structure. This can be done when the rigid body is being added to a model or later by selecting the body.

When the rigid body is being initially inserted into a structure, both the rigid body and the crystal structure are displayed. The rigid body will be displayed with a "Balls-and-Sticks" model but bonds will be drawn in green. It is useful to plan for this by preselecting the atoms in the Draw Atoms list and to have atoms displayed as "Sticks" or "Balls-and-Sticks" etc. so that it is easy to differentiate positions of atoms already in the model from the new rigid body location.

When the rigid body has already been placed in the model, the rendering of the structure works a bit differently. As the rigid body is repositioned via Alt+mouse drag, all atoms in the Draw Atoms array are deleted and only the atoms in the asymmetric unit are displayed. The mode used to draw them will depend on the selection made on this window; (the default selection is "Balls-and-Sticks".) When the mouse button is released, if the "Fill cell" option is selected, the symmetry replicants of the atoms in the asymmetric falling inside the unit cell are placed into the Draw Atoms array.

Actions to reposition the rigid body in either mode are:

- **Alt+Left drag**: Holding Alt (Opt on Mac) while dragging the mouse with the left button down rotates the rigid body around screen x & y axes
- **Alt+Middle drag**: Holding Alt while dragging the mouse with the middle button down rotates the rigid body around screen z (out of screen) axis. On the Mac hold down the Alt and Command buttons together.
- **Alt+Right drag**: Holding Alt while dragging the mouse with the right button down (use Control+Opt on Mac with a single-button mouse) translates the rigid body in the screen x & y directions (rotate the plot to see and move in the rigid body in the third direction.) Selecting the "Lock" checkbox next to the origin location, or unselecting the "Refine?" button locks the origin from being changed via mouse dragging when the location should be fixed by symmetry.

5.5.8 **Texture** phase tab

This tab is used to control settings used for a texture study of a material. This type of characterization usually requires diffraction data recorded with multiple detector orientations (the number of orientations will depend on sample and material symmetry). Do not confuse this with applying a preferred orientation correction (found in the "Data" tab) in a structural study. The sample orientation relative to the detector axes is specified here and the detector orientation is specified for each histogram as goniometer omega, chi, phi and azimuth values (details below). These values must be specified.

Texture analysis using GSAS-II employs spherical harmonics modeling, as described by Bunge, "Texture Analysis in Materials Science" (1982), and implemented by Von Dreele, J. Appl. Cryst., **30**, 517-525 (1997) in the original GSAS program. The even part of the orientation distribution function (ODF) via the general axis equation

$$A(x,y) = 1 + \sum_{L=2}^{N_L} \frac{4\pi}{2L+1} \sum_{m=-L}^{L} \sum_{n=-L}^{L} C_L^{mn} k_L^m(y) k_L^n(h)$$

is used to give the intensity corrections due to texture. The two harmonic terms, $k_L^m(y)$ and $k_L^n(h)$, take on values according to the sample and crystal symmetries, respectively, and thus the two inner summations are over only the resulting unique, nonzero harmonic terms. These unique terms are automatically selected by GSAS-II according to the space group symmetry and the user chosen sample symmetry. The available sample symmetries are cylindrical, 2/m, mmm and no symmetry. The choice of sample symmetry profoundly affects the selection of harmonic coefficients. For example, in the case of cylindrical sample symmetry (fiber texture) only $k_L^0(y)$ terms are nonzero so the rest are excluded from the summations and the set of C_L^{0n} coefficients is sufficient to describe the effect on the diffraction pattern due to texture. The crystal harmonic factor, $k_L^n(h)$, is defined for each reflection, h, *via* polar and azimuthal coordinates (ϕ, β) of a unit vector coincident with h relative to the reciprocal lattice. For most crystal symmetries, ϕ is the angle between h and the n-th order major rotation axis of the space group (usually the c-axis) and β is the angle between the projections of h and any secondary axis (usually the a-axis) onto the normal plane. In a similar way the sample harmonic factor, $k_L^m(y)$, is defined according to polar and azimuthal coordinates (ψ, γ) of a unit vector coincident with the diffraction vector relative to a coordinate system attached to the external form of the sample. For example, in the case of a rolled steel plate having mmm symmetry, the polar angle, Ψ, is frequently measured from the normal direction (ND, parallel to K_s) and g is then measured from the rolling direction (RD, parallel to I_s) in the TD (transverse direction, parallel to J_s) - RD plane. Thus, the general axis equation becomes

$$A(\phi,\beta,\psi,\gamma) = 1 + \sum_{L=2}^{N_L} \frac{4\pi}{2L+1} \sum_{m=-L}^{L} \sum_{n=-L}^{L} C_L^{mn} k_L^m(\psi,\gamma) k_L^n(\phi,\beta)$$

Note that this version of the general axis equation differs from that shown in Von Dreele (1997) in that the assignment of m and n are reversed.

In a diffraction experiment the crystal reflection coordinates (ϕ, β) are determined by the choice of reflection index (hkl) while the sample coordinates (Ψ, γ) are determined by the sample orientation on the diffractometer. To define the sample coordinates (ψ, γ), we have defined an instrument coordinate system (I, J, K) such that K is normal to the diffraction plane and J is coincident with the direction of the incident radiation beam toward the source. We further define a standard set of right-handed eulerian goniometer angles (ω, χ, ϕ) so that ω and ϕ are rotations about K and χ is a rotation about J when $\omega = 0$. Finally, as the sample may be mounted so that the sample coordinate system (I_s, J_s, K_s) does not coincide with the instrument coordinate system (I, J, K), we define three eulerian sample rotation offset angles $(\omega_s, \chi_s, \phi_s)$ that describe the rotation from (I_s, J_s, K_s) to (I, J, K). The sample rotation angles are defined so that with the goniometer angles at zero ω_s and ϕ_s are rotations about K and χ_s is a rotation about J. The zeros of these three sample rotation angles can be refined as part of the Rietveld analysis to accommodate any angular offset in sample mounting. For the specific case of cylindrical sample symmetry, the cylinder axis is coincident with Ks as is the 2-fold in 2/m sample symmetry. After including the diffraction angle, 2θ, and a detector azimuthal angle, A, the full rotation matrix, M, is

$$M = -\theta A \omega \chi (\phi + \phi_s) \chi_s \omega_s$$

By transformation of unit Cartesian vectors (100, 010 and 001) with this rotation matrix, the sample orientation coordinates (ψ, γ) are given by

$$cos(y) = M \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

and

$$tan(\gamma) = M \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} / M \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

The harmonic terms, $k_L^m(\psi,\gamma)$ and $k_L^n(\phi,\beta)$, are developed from (those for $k_L^m(\psi,\gamma)$ are similar)

$$k_L^n(\phi,\beta) = \frac{1}{\sqrt{2\pi}} e^{in\beta} \bar{P}_L^n(cos\phi)$$

where the normalized associated Legendre functions, $\bar{P}_L^n(x)$, are defined via a Fourier expansion as

$$\bar{P}_L^n(cos\phi) = \sum_{s=0}^{L} a'^{ns}_L sin(s\phi)$$

for n even and

$$\bar{P}_L^{ns}(cos\phi) = \sum_{s=0}^{L} a'^{ns}_L sin(s\phi)$$

for n odd. Each sum is only over either the even or odd values of s, respectively, because of the properties of the Fourier coefficients, a'^{ns}_L. These Fourier coefficients are determined so that the definition

$$\bar{P}_L^n(cos\phi) = \bar{P}_L^n(x) = \sqrt{\frac{(L+n)!}{(L-n)!}} \sqrt{\frac{2L+1}{2}} \frac{(-1)^{L-n}}{2^L L!} (1-x^2)^{-n/2} \frac{d^{L-n}}{dx^{L-n}} (1-x^2)^L$$

is satisfied. Terms of the form $cos(n\beta)\bar{P}_L^n(cosn\beta)$ and $sin(n\beta)\bar{P}_L^n(cos\phi)$ are combined depending on the symmetry and the value of n (or m) along with appropriate normalization coefficients to give the harmonic terms $k_L^n(\phi,\beta)$ and $k_L^m(\psi,\gamma)$. For cubic crystal symmetry, the term $k_L^n(\phi,\beta)$ is obtained directly from the Fourier expansion

$$k_L^n(\phi,\beta) = \sum_{j=0}^{L} B_L^{nj} \bar{P}_L^n(cos\phi) cosn\beta$$

using the coefficients, B_L^{nj} , as tabulated by Bunge (1982).

The Rietveld refinement of texture then proceeds by constructing derivatives of the profile intensities with respect to the allowed harmonic coefficients, C_L^{mn}, and the three sample orientation angles, ω_s, χ_s, ϕ_s Ws, Cs, Fs, all of which can be adjustable parameters of the refinement. Once the refinement is complete, pole figures for any reflection may be constructed by use of the general axis equation, the refined values for C_L^{mn} and the sample orientation angles ω_s, χ_s, ϕ_s.

$$J = 1 + \sum_{L=2}^{N_L} \frac{1}{2L+1} \sum_{m=-L}^{L} \sum_{n=-L}^{L} |C_L^{mn}|^2$$

The magnitude of the texture is evaluated from the texture index by

If the texture is random then J = 1, otherwise J > 1; for a single crystal J = ∞.

In GSAS-II the texture is defined in two ways to accommodate the two possible uses of this correction. In one, a suite of spherical harmonics coefficients is defined for the texture of a phase in the sample; this can have any of the possible sample symmetries and is the usual result desired for texture analysis. The other is the suite of spherical harmonics terms for cylindrical sample symmetry for each phase in each powder pattern

("histogram") and is usually used to accommodate preferred orientation effects in a Rietveld refinement. The former description allows refinement of the sample orientation zeros, ω_s, χ_s, ϕ_s, but the latter description does not (they are assumed to be zero and not refinable). The sample orientation angles, ω, χ, ϕ are specified in the Sample Parameters table in the GSAS-II data tree structure and are applied for either description.

Some useful examples:

1. Bragg-Brentano laboratory powder diffractometer

The conventional arrangement of this experiment is to have a flat sample with incident and diffracted beams at equal angles (theta) on opposite sides of the sample. The sample is frequently spun about its normal to improve powder statistics and impose cylindrical symmetry on any preferred orientation (texture). Thus, the diffraction plane (source, diffraction vector & detector) contains the K-vector which is parallel to the diffraction vector and $\omega, \chi, \phi = 0$.

2. Debye-Scherrer diffractometer with point detector(s)

The usual arrangement here is to have a capillary sample perpendicular to the diffraction plane. The capillary may be spun about its cylinder axis for powder averaging and to impose cylindrical symmetry on the texture which is perpendicular to the diffraction plane. Thus, $\omega, \phi = 0$ and $\chi = 90$.

3. Debye-Scherrer diffractometer with 2D area detector

The area detector is presumed to be directly behind the sample with the incident beam somewhere near the center of the detector. The detector axes are defined (for a synchrotron) with the X-axis toward the synchrotron ring and the Y-axis vertical "up"; one views the detector image as if looking from the x-ray source. The sample is assumed to be a capillary (which may be spun to impose cylindrical symmetry), although other sample shapes may be used, and is aligned with the cylinder axis horizontal. Integration of the image from a series of "caked" slices gives a set of powder patterns, each assigned an azimuthal angle where zero is along the X-axis. Thus, at azimuth=0 the diffraction plane is horizontal and contains the cylinder axis so ω, \chi, ϕ = 0.

WHAT CAN I DO HERE?

1. Menu '**Texture/Refine** texture' – refines the spherical harmonics texture model using the previously determined values of Prfo for all histogram reflection sets as demonstrated in 2DTexture tutorial.
2. **Texture settings** - The texture index, J is shown on the 1st line.
    - The Texture model can be chosen from ['cylindrical', 'none', 'shear - 2/m', or 'rolling – mmm'].
    - The Harmonic order (even integer 0-34), refine flag & show coefficients flag are next.
    - The Texture plot type is one of:
        - **Axial pole distribution** which simulates the intensity of a reflection during a phi scan.
        - **pole figure** where a projection of the probability of finding a pole (hkl) is plotted as a function of sample orientation.
        - **inverse pole figure** where a projection of the probability of finding all poles (hkls) is plotted for a selected sample orientation.
        - **3D pole distribution** that shows the probability of finding a pole (hkl) is plotted as a function of sample orientation.

    For Axial distribution, pole figure and 3D pole distribution one must next select the hkl of the desired pole, for Inverse pole figure one must select a sample direction (typically 0 0 1).

    One can choose the contour (pole & inverse pole figures) color scheme (default "Paired") and make a CSV file of the image for import into other software.

    - The spherical harmonics coefficients are shown next; they may be edited. They may be cleared by setting harmonic order to zero and then back to desired value.
    - The sample orientation angle zeros $(\omega_s, \chi_s, \phi_s)$ are shown with their individual refinement flags.

5.5.9 **Map peaks** phase tab

This gives the list (magnitude, x y & z) of all peaks found within the unit cell from the last Fourier/charge flip map search, sorted in order of decreasing peak magnitude. In the crystal structure plot, each peak position,shown as a white to dark gray cross; the shade is determined from the magnitude for the peak relative to the maximum peak magnitude; some are connected by white sticks as possible bonds. Negative peaks are shown in orange.

WHAT CAN I DO HERE?

- **Peak Selection from table**: select individual atoms by a left click of the mouse when pointed at the left most column (atom numbers) of the atom display; hold down the Ctrl key to add to your selection; a previously selected atom will be deselected; hold down Shift key to select from last in list selected to current selection. A selected atom will be highlighted (in grey) and the atoms will be shown in green on the plot. Selection without the Ctrl key will clear previous selections. A left click in the (empty) upper left box will select or deselect all atoms.
- **Select the mag column** – the entries will be sorted with the largest at the top.
- **Select the dzero column** – the entries will be sorted with the smallest (distance from origin) at the top.
- **Select the dcent column** – the entries will be sorted with the smallest distance from the unit cell center at the top.
- Menu '**Map peaks**' –
  - **Move peaks** – this copies selected peaks to the Atoms tab and the Draw Atoms tab. They will be appended as new atoms to the end of each list each with the name 'UNK' and the atom type as 'H'. They will also be drawn as small white spheres at their respective positions in the structure drawing. If inclusion of an atom into the model is appropriate, you should next go to the Atoms tab and change the atom type to whatever element you desire; it will be renamed automatically.
  - **View point** – this positions the viewpoint (large 3D RGB cross) at the 1st selected peak.
  - **View pt. dist.** – this calculates distance from viewpoint to all selected map peaks.
  - **Hide/Show bonds** – toggle display of lines (bonds) between peaks
  - **Calc dist/ang** – if 2 peaks are selected, this calculates the distance between them. If 3 peaks are selected this calculates the angle between them; NB: selection order matters. If selection is not 2 or 3 peaks this is ignored. Output is on the console window.
  - **Equivalent peaks** – this selects all peaks related to selection by space group symmetry.
  - **Invert peak positions** – inversion through cell center of map and all positions.
  - **Roll charge flip map** – popup allows shifting of the map & all peak positions by unit cell fractions; can be along combinations of axes.
  - **Unique peaks** – this selects only the unique peak positions amongst those selected; a popup allows selection of atom subset closest to x=0, y=0, z=0 origin or center.
  - **Save peaks** – saves the peak list as a csv file.
  - **Delete peaks** – this deletes selected peaks. The shading on the remaining peaks is changed to reflect any change in the maximum after deletion.
  - **Clear peaks** – this deletes all the peaks in the map peak list; they are also removed from the crystal structure drawing plot.

5.5.10 **Pawley reflections** phase tab

This gives the list of reflections used in a Pawley refinement; for them to be used the 'Do Pawley refinement' flag must be set (see the General tab), otherwise they are ignored.

WHAT CAN I DO HERE?

- Menu '**Operations**' –
  - **Pawley settings** – allows setting of Pawley parameters as shown on the General tab.
  - **Pawley create** – this creates a new set of Pawley reflections, over writing any preexisting Pawley set. They are generated with d-spacings larger than the limit set as 'Pawley dmin' in the General tab for this phase. By default, the refine flags are not set and the Fsq(hkl) = 100.0.
  - **Pawley estimate** – this attempts an estimate of Fsq(hkl) from the peak heights of the reflection as seen in the 1st powder pattern of those shown as 'Use' in the Data tab for this phase.
  - **Pawley update** – process Pawley reflection set for negative intensities. These are set to ½ its absolute value for noncentrosymmetric space groups (0.3 otherwise); the refine flag is turned off. One should repeat Pawley refinement and then do Refine all and an additional refinement. Repeat as needed to remove negative intensities. Set Pawley neg. wt. (see Pawley settings) to further suppress negatives.
  - **Refine all** – sets all refine flags
  - **Refine none** – clears all refine flags
  - **Toggle selection** – toggles all refine flags
- You can change the refine flags either by clicking on the box or by selecting one and then selecting the column (a single click on the column heading). Then type 'y' to set the refine flags or 'n' to clear the flags. You should not refine those reflections that are below the lower limit or above the upper limit of the powder pattern otherwise you will have singular matrix errors in your Pawley refinement (adds to the refinement time as bad parameters are removed). Reflections that fall inside excluded regions may also result in refinement singularities.
- You can delete an individual reflection from the Pawley set by selecting its row (will be highlighted) and then pressing the Delete key (this is not reversable & only deletes the 1st one selected).
- You can change the individual Fsq(hkl) values by selecting it, typing in the new value and then pressing enter or selecting somewhere else in the table.

5.5.11 **Layers** phase tab

This is used to set up stacking fault models for simulations of x-ray diffraction patterns. See for example the Diamond stacking faults tutorial. The computations are done by a modified version of DIFFaX. See M.M.J. Treacy, J.M. Newsam and M.W. Deem, Proc. Roy. Soc. Lond. **433A**, 499-520 (1991) for more information on DIFFaX and please cite this if you use this section of GSAS-II.

WHAT CAN I DO HERE?

1. Menu '**Operations**' –
    - **Load from DIFFaX file** – load parameters from a DIFFaX input file
    - **Copy phase cell** – copy the lattice parameters from a selected phase (usually transformed from average unit cell)
    - **Simulate pattern** – run DIFFaX to simulate selected pattern
    - **Fit pattern** – refine stacking fault parameters to fit observed pattern (not available yet)
    - **Sequence simulations** – do a sequence of simulations incrementing a selected stacking fault parameter
2. Show a plot of the 2D diffraction pattern for the stacking model – look for streaks.
3. Select Laue symmetry
4. Reference unit cell – filled by Copy phase cell and is the stacking fault block dimensions (NB: refine inactive)
5. Layer width (a & b) – outer dimensions of crystallite; used for broadening calculations (NB: refine inactive)
6. Next are descriptions of the layers to be used in the calculations. They can be created atom-by-atom or imported from another GSAS-II gpx file. If a layer is already present, then the new layer can be the same; give it a different name.
7. The layers stack according to probability rules – these are presented in tables in the next section
8. You can specify specific layering sequences as a sequence of layer numbers (begins with 1).
9. Finally, you can set the type of sequence and the number of layers to use in the simulation

You can draw the layer structures as well as sequences of layers to check on how they fit together; see the Plot boxes for this.

5.5.12 **Wave Data** phase tab

This tab displays the modulation functions used for incommensurate structures; it will not appear if the structure is commensurate (i.e. 3D). They include modulations on atom site fractions, positions and thermal motion parameters. If the structure is magnetic, atom moment modulation parameters are also shown.

WHAT CAN I DO HERE?

1. Select an atom from the Atoms list; the pulldown shows them by name. The display will show the assigned modulations, if any.
2. Add a modulation wave and define its type; window will be redrawn showing allowed coefficients (white background) and symmetry fixed or dependent coefficients (gray background).
3. Select a modulation wave to refine. Holds can be used to fix individual coefficients (see Constraints).
4. Delete a modulation wave.
5. If a 4D map is available (Fourier or charge flip), a contour plot showing density modulation along tau for a selected 3D axis of the selected atom. The +/- keys can be used to adjust the phase offset of the map so it matches the calculated modulation curve.

5.5.13 **MC/SA** phase tab

This tab displays Monte Carlo/Simulated Annealing model parameters and results. Each rigid body is described by a location (fractional x,y,z) and a quaternion description for the orientation (rotation angle & 3D vector) along with possible bond torsion angles on side chains. Each parameter has a defined range. The MC/SA controls on the General tab further limit the MC/SA run. Selection of a result shows a drawing of the structure with unit cell contents for visualization.

WHAT CAN I DO HERE?

1. Modify the preferred orientation model (currently not operational)
2. **MC/SA** Menu –
    - **Add atom** – add an isolated atom to the MC/SA model
    - **Add rigid body** – add a previously defined rigid body, which may have adjustable internal torsion angles.
    - **Clear rigid bodies** – removes rigid bodies from the MC/SA model
    - **Clear results** – clears table of MC/SA results from a previous set of MC/SA trials.

5.5.14 **RMC** phase tab

This tab is used for access to three different programs, RMCProfile, fullrmc and PDFfit, that are used for fitting structural models to pair distribution functions (PDF). RMCProfile and fullrmc are "big box" modelling routines and PDFfit is a "small box" modelling routine. Select the program you wish to use from radio button at the top of the window. Three different windows are displayed depending on that selection.

Tutorials for using RMCProfile and PDFfit can be accessed from the Tutorials menu item in the GSAS-II Help menu. These routines all run as stand-alone applications which are initiated by GSAS-II. When finished, GSAS-II processes their output files to update parameters that are within the GSAS-II project. The two big box routines can have very long running times; they run as separate console programs. GSAS-II is active while they are running and can "interrogate" them for intermediate results. PDFfit has a short running time and GSAS-II is "locked out" until it finishes; its result can be examined after.

WHAT CAN I DO HERE?

Operations Menu –

- **Setup RMC** – this builds the input files and python script (if needed) for running the selected PDF modeling program.
- **Execute** – this executes the chosen program in a new console which will vanish when finishes (after a "press any key" command). When finished, GSAS-II will extract results and place them in appropriate places in the project.
- **Stop run** – only valid for fullrmc; stops the RMC run & saves progress so it can be continued later.
- **Plot** – this displays the resulting graphical output from the PDF modeling run. For RMCProfile and fullrmc this can be 5 or more plots, for PDFfit it is only the observed and calculated G(r) plot with a difference curve.

For each program, the setup page is similar. There is a block for "metadata" items for your convenience; they have no impact on the calculations. Next is timing controls for the big box programs (PDFfit has none). Then is structural information and finally the data section for the patterns to be fitted. The big box programs are for only single runs while PDFfit can be used to process a sequence of G(r) data collected as a function of, e.g., temperature (giving Sequential PDFfit2 results).

FULLRMC

The fullrmc program is a large-box pair distribution function modeling library developed by Bachir Aoun [Fullrmc, a Rigid Body Reverse Monte Carlo Modeling Package Enabled with Machine Learning and Artificial Intelligence", B. Aoun, Jour. Comp. Chem. (2016), 37, 1102-1111. DOI: 10.1002/jcc.24304]. Extensive information about fullrmc is found, including a number of explanatory videos, along with older source code on GitHub: https://bachiraoun.github.io/fullrmc/. Note that the GSAS-II implementation is not compatible with the open-source version of fullrmc, but rather the new version 5.0 must be used, which is distributed as a compiled versions for 64-bit Intel-compatible processors running Windows, Linux and MacOS from website https://github.com/bachiraoun/fullrmc/tree/master/standalones. Note that an even newer and more powerful version of fullrmc is available for cloud computing by subscription at https://fullrmc.com.

When fullrmc is selected in this tab, GSAS-II will locate an executable for fullrmc using the GSAS-II configuration variable `fullrmc_exec`, which if defined points to a Python image with fullrmc. Otherwise GSAS-II will look in the following places, in the order specified, for a Python image for a file named `fullrmc5*64bit` (MacOS or Linux) or `fullrmc5*.exe` (Windows):

1. The location where GSAS-II is installed,
2. The location where Python is installed,
3. The location where the GSAS-II binaries are found,
4. the current default location
5. and all directories in the system path.

RMCPROFILE

The RMCProfile program fits large-box atomic models to x-ray & neutron PDF and S(Q) "data" as well as other types of observations. When RMCProfile is selected in this tab, GSAS-II will see if an RMCProfile executable can located using the GSAS-II configuration variable `rmcprofile_exec`, which if defined should have the name of the RMCProfile program. If that is not defined, the following locations are searched:

1. The location where GSAS-II is installed,
2. The location where Python is installed,
3. The location where the GSAS-II binaries are found,
4. the current default location
5. and all directories in the system path.

PDFFIT2

The PDFfit2 program fits small-box atomic models to x-ray & neutron PDFs. When PDFfitis selected in this tab, GSAS-II will see if PDFfit2 can be loaded as a package in the current Python installation (use of PDFfit2 in this manner is not recommended as this invites conflicts in the packages used by GSAS-II and PDFfit2) if that fails, GSAS-II will attempt to use a Python executable for PDFfit2 using the GSAS-II configuration variable `pdffit_exec`, which if defined points to a Python image with PDFfit2fullrmc. Optionally, if the Python installation used with GSAS-II uses conda (which is the case for the gsas2main installer), GSAS-II can download and install a separate conda environment with PDFfit2 installed.

5.5.15 **ISODISTORT** phase tab

This displays the setup for using the web-based application, ISODISTORT, to identify the possible mode distortions of a parent structure. To use it you must be connected to the internet. Two ISODISTORT Methods are supported in GSAS-II:

- Method 1: identifies all possible subgroups that result from simple mode distortions that are associated with a single irreducible representation.
- Method 4: is more useful in that it finds the mode decomposition of a parent structure to give a specified distorted structure and is set up to find only atom displacement modes.

See help pages for ISODISTORT for more information. The ultimate product of using ISODISTORT is a special CIF file with constraints describing the mode distortions; this is imported into GSAS-II to form a new phase with these constraints.

WHAT CAN I DO HERE?

If this is a freshly created phase (not an imported ISODISTORT CIF) then you can choose the Method (4 is default) and select parent structure and distorted child structure (for Method 4).

If you chose Method 1 & run ISODISTORT, a table of possible substructures is displayed; a CIF file with mode distortion constraints can be produced from your selection. The table can be filtered by crystal class.

If this is a phase imported from an ISODISTORT CIF file, the mode displacements are shown with sliders to allow visualization of the displacements in a drawing of the crystal structure (prepare this first before trying a slider). A structure refinement using this phase will employ the mode distortions as constraints on the atom coordinates; there should be as many as there are free variable coordinates in the structure. The values (in Å) represent the largest atom shift associated with the mode; shown is a list of atom coordinates affected by each mode.

- **Operations** menu –
  - **Run ISODISTORT** – run this from the web site with the controls as shown.
  - **Make cif file** – active after table from Method 1 is displayed; generate CIF file by ISODISTORT web site with mode distortion constraints.
  - **Make PDFfit phase** – active when mode distortions are shown. Makes new phase specific for fitting PDF data via PDFfit2.
  - **Show modes** – active when mode distortions are shown. Displays mode names & values.
  - **Show relationships** - active when mode distortions are shown. Displays constraint equations associated with mode distortions.

5.5.16 **Dysnomia** phase tab

This is displayed if the **Use Dysnomia** box in the General tab is checked. Dysnomia is a maximum entropy method for improving Fourier density maps. The Dysnomia tab provides access to controls used in its operation.

WHAT CAN I DO HERE?

- **Operations** menu –
  - **Load from Dysnomia file** – as previously saved set of controls.
  - **Save Dysnomia file** – saves data needed to run Dysnomia
  - **Run Dysnomia** – execute the routine from GSAS-II (not a separate console). Replaces existing map with one improved by maximum entropy.

5.6 Type **IMG** data tree entries: 2-D Images

An `IMG` data tree entry is created whan a 2D diffraction image is imported into a GSAS-II project. Note that unlike every other type of entry in the GSAS-II data tree, images are not self-contained. The actual contents of the image is read from the original file whenever the image is needed, but all other settings utilized in image processing other than the image itself are stored inside the project. If the `.gpx` file is moved to another computer, if it contains images, the image files must also be moved.

A `IMG` data tree entry is always accompanied by four child tree entries, labeled **Comments**, **Image Controls**, **Masks** and **Stress/Strain**. There is also some information in the parent `IMG` entry.

When a 2D diffraction image (prefix `IMG`) or one of its children is selected from the data tree, the image is displayed as a color contoured picture. At a minimum, a small 'X' shows the currently defined location of the incident beam on the image plane (NB: it could be off to one side or the other depending on detector location, or even outside of the image). Optionally, the integration limits are shown as an interior arc, an outer arc and green (beginning 2θ limit) and red (ending 2θ limit) as well as “cake” section limits (dashed lines) connecting the two. These are set in Image Controls. There may be a frame mask (green) that encloses the area used for subsequent integration or other analysis. Red outlines and pixels indicated selected areas/pixels that are excluded (masked) from further use; the settings for these are found in Masks.

5.6.1 Parent IMG data tree entry

The data window for the main `IMG` data tree entry shows some controls, most of which are rarely modified (e.g., pixel dimensions) and are usually obtained via the image importer from either the image header or a metadata file associated with the image. It is the user's/instrument scientist's responsibility to ensure the accuracy of these values. When they are wrong, the image cannot be used.

What can I do here?

- A number of calibration values are shown for the placement and dimensions of the detector. They can be changed here. (*Caution:* you do need to know what their true value is; you do not want to invalidate data by incorrectly changing these values.)
- **Polarization:** you can determine the x-ray beam polarization for your detector. This requires an image with scattering from a purely isotropic amorphous sample (a glass slide mounted perpendicular to the incident beam is recommended) with the detector close to the sample so that the scattering angle at the edge of the detector is at least 35° 2θ; better is > 40° 2θ. A frame mask is recommended to remove detector edge effects. The image should be as free as possible (except for beam stop) from shadows and obstructions and normal to the incident beam. The detector orientation should have been previously calibrated with a known reference material (e.g., LaB_6 or Si). Use the **Calibrate?** button to start the Polarization process, as below.
  - **Calibrate?** (Polarization) - This begins the calibration procedure (Von Dreele & Xi, 2021) for the x-ray beam polarization, which integrates a 4° 2θ wide ring sampling area with and without an arc mask positioned about 90° azimuth (top of image) with selected polarization values. The integrations match with the correct polarization value. You will be asked for a 2θ position for the sampling mask; choose a value at least 2° 2θ less than the maximum 2θ seen for all edges inside the frame mask. The process takes about 5 min to complete, so be patient.

5.6.2 Comments

This window shows whatever comment lines found in a “metadata” file when the image data file was read by GSAS-II. If you are lucky, there will be useful information here (e.g., sample name, date collected, wavelength used, etc.). With some types of files, this window will be blank. The text is read-only. It will be transferred over to diffraction patterns when the image is integrated and can be used to set parametric values (in Sample Parameters) associated with the diffraction pattern.

What can I do here?

Nothing.

5.6.3 Image Controls

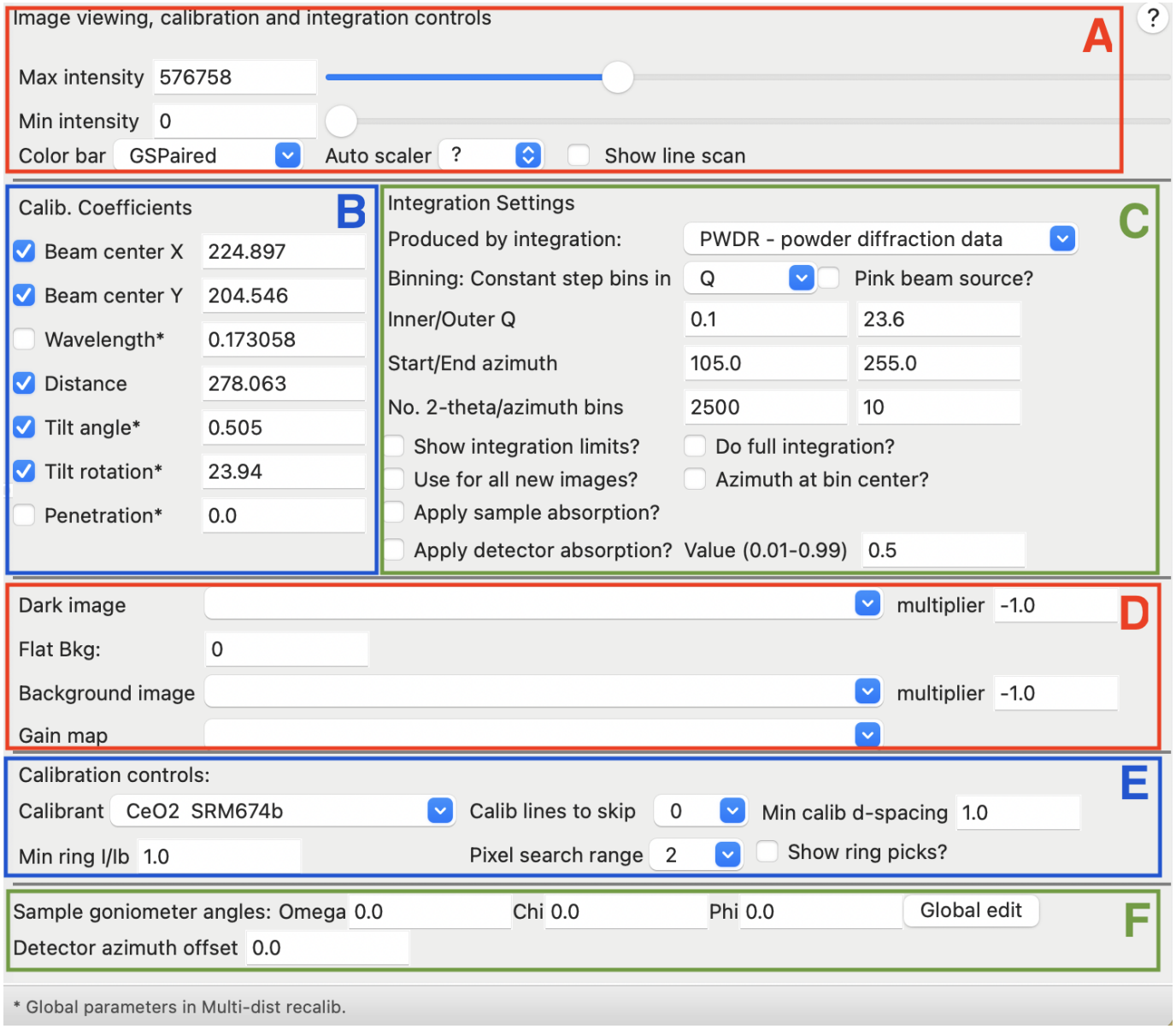
The image controls data window displays a number of settings and options that include calibration values needed to convert pixel locations to two-theta and azimuth, values used to integrate the image, settings that adjustment the image, settings used when performing image calibration and sample setting angles.

What can I do here?

- Perform image calibration with data from a standard
- Create a gain map (requires multiple images)
- Integrate images

Window organization

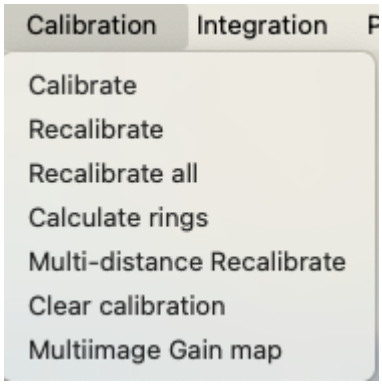
The window used for Image Controls contains a large number of settings and controls, as shown below. The sections of the window are outlined below with colored boxes and labeled that are described further, also below.



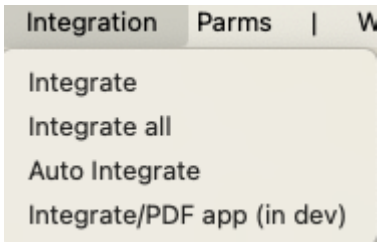
- A. The **Image controls** section at the top has controls that determine how the image is displayed. These settings do not affect computations from the image.
- B. The **Calibration coefficients** have the results from an image calibration and are used to determine the 2θ value for each pixel in the image.
- C. The **Integration coefficients** determine how image integration is performed. Show integration limits will show lines on the image, but does not change the integration results.
- D. Image corrections: It is possible to subtract images from the current image to account for pixels that provide non-zero results even when not illuminated (Dark image); or a constant value that is subtracted from all pixels (Flat Bkg), as well as subtract an image with scattering from the instrument or sample container (Background image). It is also possible to adjust for pixel-by-pixel detector response with a gain map.
- E. The **Calibration controls** determine the process used to search for diffraction rings when the detector calibration is used. The "Show ring picks" check button determines if the located ring positions are displayed, but does not affect the computation.
- F. The **Sample goniometer angles** reflect positioning of a sample. They are not used for calibration, but will be transferred to powder patterns generated from the image during image integration. The Global edit button provides a single window where setting angles for all images can be changed.

Menu commands

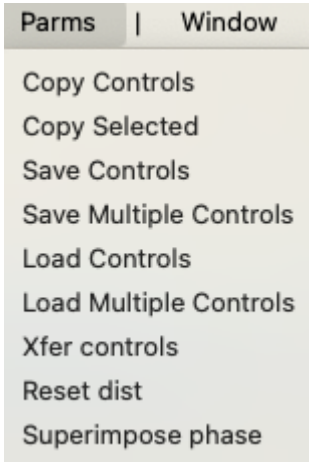
Three sets of menu commands are associated with the Image Controls tree item. The first, **Calibration**, provides commands to perform calibration from an image (where the calibration values are fitted from a diffraction pattern image taken with a calibrant).



The Integration menu provides the ability to radially integrate an image to provide one or more powder diffraction patterns (requires that calibration parameters must be set first.)



Finally, the Parms menu has commands allow the values on the window to be saved to a file, read from a file or copied to other images. The "Xfer controls" menu command differs from the "Copy Controls" command in that integration range for the current image is scaled when applied for other images based on the detector distances.



Calibration parameters definitions

The detector coordinate system has **x** horizontal and **y** vertical with (0,0) located at the lower left, looking from the sample position. The **z** axis is defined as **z** = **x** × **y**, which points from the detector towards the sample. When a detector is rotated from this position, the detector azimuthal offset describes the angle applied to rotate the detector clockwise (as viewed from the sample position) from the orientation with **x** horizontal and **y** vertical. The beam center position in GSAS-II is in mm, measured from the bottom left corner of the detector.

COMPARISON TO OTHER SOFTWARE

Note that calibration parameters used in GSAS-II are closely related to those used by the pyFAI and Fit2D programs, but add 90 to the GSAS-II tilt plane rotation (labeled as "Rotation" in GSAS-II) to obtain the pyFAI value. The beam center location in pyFAI is defined the the same way as in GSAS-II, except that in pyFAI the units are pixels rather than in mm.

$$X_{GSAS-II}/size_X = X_{pyFAI}$$

and

$$Y_{GSAS-II}/size_Y = Y_{pyFAI}$$

For Fit2D, the center is also in mm, but measured from the bottom left, so

$$X_{GSAS-II}/size_X = X_{Fit2D}$$

and

$$Y_{max} - Y_{GSAS-II}/size_Y = Y_{Fit2D}$$

where Y_{max} is the detector size in pixels and $size_X$ and $size_Y$ are the pixel size in mm along the appropriate direction.

5.6.4 Masks

The information on the **Masks** window are used to determine what parts of an image will not be included in the integration, typically used due to detector irregularities, shadows of the beam stop, single-crystal peaks from a mounting, cosmic rays, etc.

Note that the top section of the window repeats some of the display controls from the **Image Controls** window. These are duplicated so that the image can be viewed under different conditions without needing to switch between the different data items.

Sections of the image may removed from integration by one or all of the following options.

- The **Upper/Lower Thresholds** designate the allowed values for pixels to be considered valid. Typically detectors will set pixels that are in margins between segments etc. and are not in use to have negative intensity values, so a threshold of 0 causes these pixels to be ignored. Likewise, malfunctioning pixels or those picking up anomalous signals, such as cosmic rays, may have exceptionally high intensity values that should also be ignored.
- **Pixel masking** excludes individual pixels that have intensities that are significantly higher or lower than the median intensity across single 2θ value. The controls for the pixel mask search determine the threshold for exclusion, which is expressed as a multiple of the median-based standard deviation for the 2θ ring; the minimum and maximum 2θ value to be used in the search; and if the search should replace any previous pixel map search(es) or should be added to the previous pixel mask search. This latter control, when "Clear..." is turned off, allows the sensitivity for exclusion to be varied for different 2θ ranges. Finally, a button allows a previous pixel mask to be cleared.
- Specific geometrical regions of the detector can be designated to be ignored using menu commands or with keyboard/mouse shortcuts.

There are five types of geometrical masks:

- **Spot masks**: exclude a circle with a selected center and diameter in image coordinates (mm).
- **Ring masks**: excludes a specific Bragg reflection (a ring placed relative to the image center). The location and thickness of the ring are specified in degrees 2-theta.
- **Arc masks**: exclude a section of a Bragg reflection, similar to a ring mask, except that in addition to the location and thickness of the ring, the mask has a starting and ending azimuthal angle.
- **Polygon masks**: exclude an arbitrary region created by line segments joining a series of points specified in image coordinates (mm). Pixels inside the polygon mask are not used for integration.
- **Frame mask**: excludes an arbitrary region created by line segments joining a series of points specified in image coordinates (mm). Typically, a point is placed near each corner of the image. Only pixels inside the frame mask are used for integration. Only one frame mask can be defined.

What can I do here?

Masks of each type are created using the appropriate menu commands and then clicking as described in the section on "What can I do with the plot?" below, or by using keyboard shortcuts, also described in that section.

What is plotted here?

The image is shown, as described above. Note that the frame mask, if defined, is displayed in green, while the other types of masks are shown in red.

What can I do with the plot?

There are menu commands to create masks as well as keyboard shortcuts. If a menu command is used, then use left and right mouse clicks as described below. Note that on a Mac with a one-button mouse, some alternate actions must be used.

1. **Spot masks**: excludes inside a circular region of the image.

   - **Create Spot masks** after a menu command by clicking on the location on the image that should be masked. There are also two ways to create spot masks with the keyboard:
     - Press the 's' key and then left-click successively on multiple locations for spot masks. Press the 's' key again or right-click to stop adding spot masks.
     - Alternately, move the mouse to the position for a new spot mask and press the 't' key. (Note that this can be used while the plot is in Zoom or Pan mode.)

     The default size for newly-created spot masks is determined by the `Spot_mask_diameter` configuration variable or 1.0 mm, if not specified.
   - **Edit Spot mask location** by left-clicking inside or on the edge the of the mask and then drag the spot mask to a new location.
   - **Edit Spot mask radius** by right-clicking inside the mask and then dragging to change the mask size.

2. **Ring masks**: excludes inside a ring of selected width that follows constant 2θ as determined by the calibration (e.g. a Bragg diffraction ring).

   - **Create Ring masks** with a menu command and then by left-clicking on the mask center; Or, by pressing the 'r' key and then left-clicking. (Right-click to cancel.)

     The default thickness for newly-created ring masks is determined by the `Ring_mask_thickness` configuration variable or 0.1 degrees (2θ) if not specified.
   - **Edit Ring mask location** by left-clicking on either the inner or outer circle and drag the circle to the new radius.
   - **Edit Ring mask thickness** by right-clicking either on the inner or outer circle and drag the the circle change spacing between the inner and outer circle.

3. **Arc masks**: excludes inside an arc of constant 2θ, similar to a ring mask, except that in addition to the location and thickness of the ring, the mask has a starting and ending azimuthal angle.

   - **Create Arc masks** with a menu command and then by left-clicking on at the mask center; Or, by pressing the 'a' key and then left-clicking. (Right-click to cancel.)

     The default size for newly-created ring masks is determined by configuration variables:
     - thickness: `Ring_mask_thickness` (0.1 degrees 2θ if not specified) and
     - azimuthal range: `Arc_mask_azimuth` (10.0 degrees if not specified.)
   - **Edit Arc mask location** by left-clicking on either the inner or outer circle and drag the circle to the new radius. Alternately, left-click on the upper or lower arc limit (the straight lines) and drag them to rotate the center of the arc azimuthal range to a new position.
   - **Edit Arc mask thickness** or range by right-clicking either on the inner or outer circle and drag the the circle change spacing between the inner and outer circle. Alternately, right-click on the upper or lower arc limit (the straight lines) and drag them to change the arc azimuthal range.

4. **Polygon masks**: excludes inside an arbitrary region created by line segments joining a series of points specified in image coordinates (mm). Pixels inside the polygon mask are not used for integration.

   - **Create Polygon masks** with a menu command and then by left-clicking successively on the vertices of the polygon shape surrounding pixels to be excluded. After the last point is defined, right-click anywhere to close the mask. Alternately, press the 'p' key and then left-click, as before, to define the mask and right-click anywhere to close the mask.
   - **Edit Polygon mask** by left-clicking on any point at a vertex in the polygon mask and drag that point to a new position. If the vertex is dragged to the same position as any other vertex in the mask the dragged point is deleted.
   - **Add a point to Polygon mask** by right-clicking on any vertex and dragging. A new point is added to the mask immediately after the selected point at the position where the mouse is released.

5. **Frame mask**: excludes outside an arbitrary region created by line segments joining a series of points specified in image coordinates (mm). Typically, a point is placed near each corner of the image. Only pixels inside the frame mask are used for integration. Only one frame mask can be defined.
    - **Create a Frame mask** with a menu command and then by left-clicking successively on the vertices of a polygon. After the last point is defined, right-click anywhere to close the frame mask. Alternately, press the 'f' key and then left-click, as before, to define the mask and right-click anywhere to close the mask. Note that if a Frame mask already exists, using the 'f' key or the "Create Frame" menu item causes the existing frame mask to be deleted.
    - **Edit the Frame mask** by left-clicking on any point at a vertex in the frame mask and drag that point to a new position. If the vertex is dragged to the same position as any other vertex in the mask the dragged point is deleted.
    - **Add a point to the Frame mask** by right-clicking on any vertex and dragging. A new point is added to the mask immediately after the selected point at the position where the mouse is released.
6. **Pixel mask**: excludes individual pixels that are found in a pixel mask search, which looks for pixels that have intensities that are higher or lower by a threshhold than the median intensity for all pixels in a ring with the same two-theta value. By default this mask contains no pixels, but pixels are added using a search.
    - **Search to add to the pixel mask** using either the Operations->"Pixel mask search" or the Operations->"Multi-IMG pixel mask search" menu commands. This searches for pixels that have intensities that are significantly higher or lower than the median intensity for all pixels in a ring having the same two-theta value. The threshold for exclusion is determined by the standard deviation for the pixels in the ring multiplied by a user-supplied value.

5.6.5 Stress/Strain

This allows one to evaluate strain typically induced by a pure axial load (e.g. no shear) on a polycrystalline sample (e.g. a steel bar). This strain will distort the Bragg diffraction rings seen by the 2D detector. This follows the method of He & Smith (Baoping Bob He & Kingsley Smith, (1997). Adv. in X-Ray Anal. **41**, 501.) to determine the 3 unique terms of the axial strain tensor. One can examine the results as a series of diffraction line d-spacings vs azimuth angle; if no strain, these are straight, otherwise they will show a single sinusoidal variation with maxima at the maximum strain direction (90° & 270°) for a tension load. The signs are reversed for a compression load. One can also examine the local intensity variation as multiples of a random distribution (**MRD**) due to texture. Before embarking on this analysis be sure that your detector is *carefully calibrated* for orientation and position; you are looking for very slight variations in ring shape which may be biased by inadequate detector calibration. Commonly, the calibrant (typically CeO_2) is painted on one sample surface (be sure to note if in front or back of sample!) and the sample ½ thickness is used in the Sample delta-z box (significant only for residual stress analysis).

What can I do here?

Menu Operations -

- **Append d-zero** – this adds a d-spacing value to the stress strain ring list; this also can be done by picking a ring from the plot.
- **Fit stress/strain** – this fits the three unique axial strain tensor elements (ε11, ε22 & ε12) for each ring to the local ring maxima at 1 mm intervals about each ring. Results display on console and table. The fitted d-zero is calculated from the mean d-spacings found for the ring & given as d-zero ave and can be compared to the d-zero value for any residual stress/strain.
- **Plot intensity distribution** – this makes an MRD plot with azimuth for each ring.
- **Save intensity distribution** – this saves the intensity distribution curves as a simple text file
- **Update d-zero** – this updates the d-zero values with the d-zero ave ones thus removing any effect of residual stress/strain.
- **All image fit** – this performs the Fit stress/strain operation for a selected sequence of images. NB: the stress/strain data should be copied to all other images before doing this. Results are reported in Sequential strain fit results.
- **Copy stress/strain** – this copies the stress/strain data from the current image to other selected images in preparation for doing an All image fit.
- **Save stress/strain** – this saves the current stress/strain data to a file with .strsta extension.
- **Load stress/strain** – this loads previously saved stress/strain data from a file with .strsta extension.
- **Load sample data** – this opens a metadata file containing sample load data.

What is plotted here?

The Strain plot shows the variation of d-spacing for each selected ring with azimuth angle. If there is no strain the points will scatter about a straight line. If there is strain, the points will describe a negative “cosine” curve if the sample is under tension or a positive “cosine” curve if the sample is under compression. If the fit has been done, a calculated curve will be shown along with a dashed black line for the fitted average d-spacing of the calculated curve. This average is either the mean (“Poisson mean” = False) or the Poisson mean which is ¼ or ¾ of the interval from d-min to d-max depending on the comparison between ε11 & ε22. Detector calibration errors will distort these curves.

The Ring intensities plot shows the local intensities as MRD taken at 1mm intervals about the circumference of each ring.

What can I do with the plot?

The Strain plot is best examined line by line by zooming in on each. The deviations are quite small and can not be discerned over the full d-spacing range. You should examine the calibration lines to ensure they are straight.

The Ring intensities plot will respond to the following key strokes:

- Key '**l**' – this progressively shifts the RMD lines to the left
- Key '**r**' – this progressively shifts the RMD lines to the right
- Key '**u**' – this progressively shifts the RMD lines up
- Key '**d**' – this progressively shifts the RMD lines down
- Key '**o**' – this resets the shifts to zero
- Key '**g**' – this toggles display of a grid on the plot
- Key '**s**' – this saves all the plot data as a CSV file.

5.7 Powder (PWDR)

5.7.1 Overview on **PWDR** (Powder Diffraction) data tree entries

This is where to find information on the Tree item in GSAS-II associated with powder diffraction (labeled PWDR) and its associated subitems. Note that GSAS-II uses the label of "histogram" for datasets of any type (single-crystal, powder,...) Powder diffraction histograms are added to a project using the Import/"Powder Data" menu items. After data are read, if there are phases present, you will be offered a chance to link the imported histograms to the previously imported phase(s). Likewise, if phase(s) are imported after histograms you will also be asked to link the new phase(s) to existing histograms. It is also possible to add histograms to a phase later by selecting that phase in the data tree and then selecting the "Data" tab and finally using the "Edit Phase"/"Add powder histograms" menu command. Note that there is no limit to the number of histograms that can be included in a GSAS-II project (other than as limited by available computer memory) and histograms that are not linked to at least one phase are ignored in refinements.

Each powder diffraction dataset has a main (parent) entry and a number of children (subdata tree items) in the tree:

- Comments
- Limits
- Background
- Instrument Parameters
- Sample Parameters
- Peak List
- Index Peak List
- Unit Cells List
- Reflection Lists

Clicking on the parent or on the subdata tree items, as well as main (parent) entry for the histogram allows access to different parameters associated with the dataset and offers different menu commands. With the exception of the Instrument Parameters subdata tree item, which produces a different type of plot, showing peak widths, each PWDR subdata tree item produces similar plots of the powder diffraction histogram, with different variations:

- By selecting the Limits entry, range of data used, as well as possible excluded regions, can be set.
- Selecting Reflection Lists allows display of reflection indices (hkl values) for a selected phase. Letting the mouse rest unmoved at the position of a reflection in 2θ, TOF, Q, etc. (the vertical position does not matter) will cause these to be displayed. After a short delay a "tool tip" will appear with indices for any reflections close to the lateral mouse position.
- Selecting Background allows a mouse to be used to define fixed points, where a background curve can be fitted to those points.
- Selecting Peak List allows positions of peaks to be defined for use in direct peak fitting.
- Selecting Unit Cells List can show the positions of reflections for an arbitrary set of unit cell parameters, optionally with space group extinctions applied.
- Selecting Instrument Parameters produces a different type of plot, which shows peak widths as a function of Q rather than the powder diffraction histogram.

WHAT ARE THE GENERAL OPTIONS FOR THE PLOT?

PLOT SCALING

When the histogram is displayed by clicking on a data tree entry, the axes are initially scaled to fit the selected histogram. The plot can be rescaled a number of ways:

-  Clicking on the "Zoom" button allows you to trace out a box to use as new limits for the plot. Use a left-mouse drag to draw a box to enclose the region to be displayed. Note that when this mode is selected, other actions with the mouse (such as dragging plot elements, peak picking, etc.) cannot be performed.
-  Clicking on "Pan" button allows the limits to be repositioned: by dragging with the left mouse button, or increase or decrease the scaling: by dragging with the right button either vertically or horizontally (control+left also works on Macs). Note that when this mode is selected, other actions with the mouse cannot be performed.
-  The "Home" button resets the scale to allow the data to fit into the plot. Note that a stack of scaling values are stored. Clicking left arrow provides access to a previous scaling values and then the right button returns to later values.
- Pressing the "s" key with the graphics window active causes the plot to enter "sqrt" plotting mode, where intensity values are shown as $\sqrt{I}$. This also causes the tickmarks and difference plot positions to be repositioned to their initial locations. Pressing the key again exits "sqrt" plotting mode. Pressing this key twice is a convenient way to reset the plotting scaling and tickmark positioning.
-  An alternative to remembering what key to press is to use the "K" button which provides a menu of all defined key strokes and allows the action to be selected from that menu, so "sqrt" plotting mode can also be selected using this button.
- When the main data tree item is selected, tickmarks and the difference plot location can be selected by dragging the plot item (using the left mouse button) to the desired location.
- To specify exact values for plot limits, one can use the Commands/"Set plot limits..." menu command (with the main PWDR data tree item only.) One can select which limits are to b specified in the window that is opened, so it is possible to scale only the "x" axis.
-  The eight yellow "V" buttons can be used to reposition or rescale the plot axes. The four to the left reposition the plot limits but do not change the range. The "V" points in the direction the data move relative to the axes. The next two change the x-axis scaling and the final two change the y-axis scaling. The first of each pair zooms in (decreasing the plot range). The advantage of using these buttons over the "Zoom" and "Pan" buttons is that these controls will not interfere with other mouse actions, while "Zoom" and "Pan" mode need to be toggled off before other mouse actions are possible.

Histogram selection

Once a first histogram has been selected, the plot scaling and difference/tickmark positioning is usually retained unchanged when selecting other histograms from the data tree, but only when the histogram type is the same. This allows one to zoom in on a region of a pattern and then look at that region in a series of histograms. If this is not the desired behavior, use the "!" key command to set default settings for histograms. When moving from x-ray to neutron data, for example, the scaling etc. is reset.

Histogram defaults

It is also possible to define default scaling/appearance settings for a histogram. Use the commands above to define the scaling, as well as position difference & tickmark items (and then press the "!" key (or access from the "K" button). The current display settings for the histogram are saved and these settings will be used when the histogram is redisplayed by clicking on a data tree entry. This is of particular value when working with several histograms having different Q and/or intensity ranges. Note that the default settings for a histogram are saved in the project (.gpx) file.

PLOT ACTIONS

Here is a list of things that one can do with the plot of diffraction patterns from the PWDR entry and some of its subdata tree entries.

For all plots

- **Move mouse**: As the mouse cursor is moved across the plot, the plot status line will show the cursor position as 2θ (or TOF), d-spacing, Q and the intensity.
- **Press keyboard keys** - See below. The "s" and "w" modes are commonly used.
- **Create a Publication-ready plot** - Press the green "P" button to generate a customizable version of the displayed plot that can be exported at high resolution, as discussed below.

For specific datatree items

Display/edit histogram information: Each PWDR subdata tree entry offers access to different sections of the histogram data and settings. In the Data Window one can see this information, plot it and in many cases, edit information associated with the histogram.

- **Drag tickmarks** - Select any tickmark and while holding the left mouse button down, move them to where you want them to be displayed (press the s key for Sqrt(I) mode to reset to the defaults). With multiple phases, selecting the 2nd phase, etc. changes the vertical spacing between phases. tickmarks can be dragged only when the main PWDR or Reflection Lists tree items are selected.
- **Drag the difference curve** - When the "normal" obs-calc plot is shown (as opposed to the "w" mode plot where (obs-calc)/sigma is displayed, select any point in the difference curve and while holding the left mouse button down move the curve to where you want it to be displayed (press the s key for Sqrt(I) mode to reset it to the default). The difference curve can be dragged only when the main PWDR or Reflection Lists tree items are selected.
- **Highlight reflection positions** - By selecting the "Reflection Lists" tree item and a phase, if the mouse is moved to the region of a reflection in that phase, a "tool tip" (temporarily displayed text) with the indices for nearby reflections is displayed.
- **Label reflection positions** - Right-clicking on a reflection tickmark (in the PWDR and "Reflection Lists" plots) will cause an hkl label with the indices for nearby reflection(s) to be displayed. Once a reflection label is shown, it can be dragged to a new position vertically with the left mouse button. Right-clicking on the label will delete it. All hkl labels can be deleted with a menu command. The hkl labels, including their positions, are saved in the GSAS-II project (.gpx) file.

PLOT KEY COMMANDS

The following key press characters have defined actions. These actions can also be initiated from the Key Press button on the plot toolbar. Not all actions are available for all PWDR subdata tree items.

For Single-Histogram line plots

- **a: add magnification region** - Adds a magnification region to the plot and sets the magnification amount to x2. This can be edited (or deleted) in the table that is shown when the main PWDR tree entry is selected.
- **b: subtract background** - Subtracts the fitted background from the powder pattern. Pressing this again turns the mode off.
- **c: contour on/off** - with multiple powder profiles, a contour plot is shown of the observed intensities (see below)
- **f: toggle reflection tickmarks** - Reflection positions can be indicated when the main PDWR tree entry is selected, or when the "Reflection Lists" entry is selected by display of vertical lines. These lines can be shown as tickmarks: short lines or a thin vertical line the full length of the plot. The 'f' key toggles between three modes: short lines, thin lines or no lines.
- **g: grid lines** - Toggle drawing vertical and horizontal grid lines at all axis label positions. Applies to all plot modes.
- **m: toggle single/multiple plot** - In single mode, this will show only the one selected from the data tree. In multiple “waterfall” mode, all selected data are shown (see below).
- **n: log(I) on/off** - changes the y-axis to be the log10 of the intensity; difference curve is not shown for log(I) on.
- **L: legend contents** - toggle removal of the labels for obs, calc, etc (only phase names for tickmarks may remain, as determined by the **f** key).
- **p: plot partials** - plots the partial contributions from each phase, if they have been computed (using Calculate/Compute partials) in addition to the
- **q: toggle Q plot** - changes the x-axis to Q (in $Å^{-1}$). This will put multiple powder patterns taken at different wavelengths/types on the same x-axis scale.
- **s: Sqrt(I) on/off** - changes the y-axis to be the square-root of the intensity. The tickmark and the difference curve location is reset.
- **t: toggle d-space plot** - changes the x-axis to d-space (in Å). This will put multiple powder patterns taken at different wavelengths/types on the same x-axis scale.
- **T: toggle plot title** - Removes or returns the plot title
- **v: Save CSV output** - exports the contents of the plot as a .csv file for use in plotting and spreadsheet programs.

- **w: toggle diff plot mode** - for the pattern selected from the data tree, this will replace the difference (obs-calc) curve with the differences divided by their standard uncertainty (esd) values [(obs-calc)/sigma], which shows the significance of the deviations in the fit of the pattern. (Recommended for proper evaluation of the differences). In this mode both plots have separate zoom control.
- **x: show excluded region** - Normally all observed data is plotted. When the "x" key is pressed, data inside excluded regions are not shown.
- **X: cumulative** χ^2 - Superimposes a cumulative** χ^2 plot that shows the data regions most contributing to the disparities in the fit.
- **+,=: no selection** - This is a three-way toggle. In the default mode, observed points are shown as blue "+" signs (the color can be changed in preferences) and the fitted pattern as a green line. Pressing this once adds a line for the observed points and pressing it again removes the "+" signs and for single histogram plots removes the difference curve.
- **.: scaling diagnostic** - When the '.' key is pressed, data are plotted as intensity*weight. Normally this = 1.0 for CW data and proportional to incident spectrum for normalized neutron TOF data. Does not include effect of selected weight factor but is equal to number of detectors in multidetector data. (not in menu)
- **!: save plot parameters as default** - When the "!" key is pressed, the current display settings for the histogram are saved and these settings will be used when the histogram is displayed by clicking on a data tree entry. To reset the scaling, use either the "s" key (sqrt plotting mode) twice or press the "Home" button to the left on the Matplotlib toolbar.

For specific data tree items

- **e: set excluded region** - Defines a new excluded region: press the "e" key with the mouse on one side of the region. Move the mouse to the other side and press "e" again. The region markers (magenta dashed lines) can be dragged to new positions. Available only when the Limits tree entry is selected.
- **d: highlight next peak** - Selects a peak in the table, or the next peak. Available only when the Peak List or Index Peak List tree entries are selected.
- **u: highlight previous peak** - Selects a peak in the table, or the previous peak. Available only when the Peak List or Index Peak List tree entries are selected.

For Waterfall Plots (with more than one powder pattern)

- **m: toggle single/multiple plot** - In single mode, this will show only the one histogram selected from the data tree. In multiple “waterfall” mode, all selected histograms are superimposed (see **F** for selection); offset options (below) can be used to shift them. The mode for display of the selected dataset is determined by the **+** (or **=**) key (see below).
- **F: select data** - Allows a subset of the powder patterns to be plotted, rather than all.
- **n: log(I) on/off** - changes the y-axis to be the log10 of the intensity; difference curve is not shown for log(I) on.
- **L: legend contents** - toggles addition of histogram names in the plot legend for waterfall plots. Names are the histogram label or the data tree name, if the former is not set. See **f** for inclusion of phase names via tickmarks in the legend.
- **s: Sqrt(I) on/off** - changes the y-axis to be the square-root of the intensity. The tickmark location is reset.
- **+,=: no selection** - With waterfall plots, this is a four-way toggle. As before, in the default mode, observed points are shown as blue "+" signs (the color can be changed in preferences) and the fitted pattern as a green line. Pressing this once adds a line for the observed points, pressing it again removes the "+" signs. The additional mode for waterfall plots removes the calculated plot from the display and shows the histogram name as the histogram label or the data tree name, if the former is not set. ('+' and '=' do exactly the same thing).
- **/: normalize** - For multiple powder profiles, all diffraction datasets are normalized so that the maximum intensity is 1 (only as displayed, the stored values are not changed).

Waterfall Plot Offsets

- **l: offset left** - For a waterfall plot of multiple powder profiles, increase the offset so that later plots are shifted more to the left relative to previous plots.
- **r: offset right** - For a waterfall plot of multiple powder profiles, increase the offset to the right (or decrease the left offset.)
- **d,D: offset down** - For a waterfall plot of multiple powder profiles, increase the offset down. (D does the same as d but to a much larger amount)
- **u,U: offset up** - For a waterfall plot of multiple powder profiles, increase the offset up. (U does the same as u but to a much larger amount)
- **o: reset offset** - For a waterfall plot of multiple powder profiles, reset to initial state (no offsets.)

For Contour Plots

- **c: contour on/off** - if multiple powder profiles, then a contour plot is shown of the observed intensities. Data sets of differing length are padded/trimmed to match the 1st pattern.

- **F: select data** - Allows a subset of the powder patterns to be plotted, rather than all.

Contour Plots Display Options

- **S: set color Scheme** - Select the color map used for contour plots. Default is 'Paired', black/ white options are 'Greys' and 'binary' (for black on white) or 'gray' (for white on black). Some others can be very colorful (but not all are useful!).
- **d: lower contour max** - This lowers the level chosen for the highest contour color.
- **D: lower contour min** - This lowers the level chosen for the lowest contour color; can be negative.
- **u: raise contour max** - This raises the level chosen for the highest contour color
- **U: lower contour min** - This lowers the level chosen for the highest contour color
- **i: interpolation method** - This changes the method used to represent the contours. If selected a dialog box appears with all the possible choices. Default is 'nearest'; the other useful choice is 'bilinear', this will smooth out the contours.
- **t: temperature on/off** - Show “temperature” for y-axis; valid only if temperature is varied across data sequence and evenly spaced.
- **s: toggle sqrt(I) plot** - Show sqrt(intensity) in contour plot

For display of reflections from magnetic unit space groups

These two key commands allow one to step through the output from k-SUBGROUPSMAG in Unit Cells List that are marked “Keep”.

- **j: show next; clear Keep flag** - Show the next magnetic space group in the list, clearing the "Keep" flag for the currently displayed space group. Use this to remove magnetic substructures from consideration that don't satisfy the reflection extinction conditions.
- **k: show next** - Show the next magnetic space group in the list. The "Keep" flag for the currently displayed space group is unchanged.

PUBLICATION PLOTS

When the green "P" button is pressed, a copy of the current powder diffraction plot is presented in a separate window. This can only be done with plots of a single histogram, not for waterfall or contour plots. The separate plot offers GUI controls to modify aspects of the plot, for example by changing colors, line widths, plot limits the contents or size of displayed text. The displayed plot, including any changes made, can be exported in a number of formats. These include a number of bitmap formats (JPEG, PNG, TIFF,...) that can then be imported into other programs; several formats offer vector graphics (Postscript, PDF, SVG), that will render at whatever resolution is desired, which can be of great value for posters or other applications where pixilation would be problematic; other formats are intended to be read into other software: Input for the Grace, Igor Pro and Origin programs is offered, as well as a generic .csv file that can be used with custom software. Note that Igor Pro and Origin are commercial products. (Origin export is only available on Windows and requires that Origin 2021 or later be installed on the computer where GSAS-II is installed.) The Grace program is open-source, runs on all major computing platforms, and is available in several versions.

Publication .csv contents

The `.csv` file consists of 10 or more columns (depending on the number of phases included in the histogram). The columns are described below, noting that N is the total number of phases and if there are M data points in the histogram, will be M datapoints in each column except in the Phase, tick-pos, and Axis-limits columns.

1) Used: Indicates if the data point is inside the plot limits or is excluded from the fit. A value of 1 means the values are used and 0 means the data point is not used.

2) X: The x-values from the plot in the units used in the plot (2theta, Q,...). The units are noted in the header.

3) Obs: The observed diffraction intensity. This may be modified by scaling options or background subtraction, if that has been selected for the plot.

4) Calc: The computed diffraction intensity. This will usually be zero if "Used" is 0.

5) Bkg: The computed background value at the current "X" location, This will usually be zero if "Used" is 0.

6) Diff: The plotted difference curve. This will have the offset used in the plot.

6+i) Phase i: This has the reflection positions (tickmarks) in the same units as used for "X". There will be far fewer values for this than for the previous columns.

7+N) tick-pos: The name of each phase followed by the vertical position used to display the tickmarks for each phase. There will be 2N of these values.

8+N) diff/sigma: The uncertainty-weighted difference plot [(Obs-Calc)/sigma where sigma is the statistically expected uncertainty in the obs values, i.e. the standard uncertainty values]. Note that values where "Used" is 0 are meaningless, as the Calc value is 0, but the Obs and sigma values are from the data.

9+N) Axis-limits: Has four values, x-min, x-max, y-min and y-max as used as the limits for the plot.

5.7.2 **PWDR** parent data tree (Powder Diffraction)

When a powder diffraction dataset (prefix 'PWDR') is selected from the data tree or for most of the subdata tree items, the dataset is plotted. The observed data points are shown as blue crosses and where fit, the calculated pattern is shown as a green line; the background is shown as red line. The difference curve is shown as a cyan line. These colors can be changed through configuration variables `Obs_color`, `Calc_color`, `Diff_color`, and `Bkg_color`.

Reflection positions are shown with small vertical lines. The data window shows statistical fit information if the pattern has been used in any fitting (peak fits, Rietveld, LeBail or Pawley fitting). The “Weight factor” is a multiplier on the data point weights; normally 1.0 but could be adjusted, e.g., to provide better balance in a combined data refinement. A data “Surprise” (S) factor is also shown. It is defined here as:

$$S = \frac{1}{N}\left[\sum \ln\left(\frac{\hat{I}^2}{(I-\hat{I})^2}\right)\right] - 1$$

where the sum is over the points (N) in the profile delimited by the Limits (see below). The surprise factors thus give an indication of the excursions of the data points from their mean ($\hat{I}$) and is best viewed for a sequence of data and not between instruments or of different materials. Data with few sharp peaks will have small surprise factors while patterns with many peaks may have larger surprise factors. An increasing timed sequence of data collections will show an initial rise & then level surprise factor perhaps indicating when sufficient data has been collected. Phase changes in a temperature sequence may show as abrupt shifts in the surprise factor.

WHAT CAN I DO HERE?

"Commands" Menu Commands

- **Error Analysis** – this produces a 'normal probability' plot for the refinement result as bounded by the limits. The slope and intercept of the curve in the central region (-1 < / < 1) are shown on the plot status line. The slope is the GOF for the best fit set of data points (~68% of the data).

WHAT IS PLOTTED HERE?

The powder patterns that are part of your project are shown in the graphics window. They can be displayed as a stack of powder patterns, just a single pattern, or as a contour image of the peak intensities, or be plotted individually. What can be done here will depend on how many patterns are shown as well as what mode is selected. Note that the tickmarks and difference curve positions can be customized, as discussed below.

WHAT CAN I DO WITH THE PLOT?

There are a huge number of options that can be used with the plot to change different aspects of how pattern(s) are plotted. The controls are largely the same for graphics associated with the main PWDR Powder Histograms tree entry and most subdata tree entries. See the overview section for the plot actions and key press commands.

5.7.3 PWDR **Comments** subdata tree item (Powder Diffraction)

This window shows whatever comment lines (usually preceded by "#", but this depends on the data format) found when the powder data file was read by GSAS-II. If you are lucky, there will be useful information here (e.g. sample name, date collected, wavelength used, etc.). If not, this window will be blank. The text is read-only. Nothing is plotted and there are no menu commands for this tree item.

5.7.4 PWDR **Limits** subdata tree item (Powder Diffraction)

This subdata tree entry window controls the limits in position to be used in any fitting for this powder pattern. The "original" values are obtained from the minimum & maximum values in the powder pattern. The "new" values determine the range of data that will be used in fitting, Tmax and Tmin. Tmin and Tmax will be either 2θ (deg.) for CW data or time (μsec) for TOF data.

You can also designate areas of the pattern that should be "excluded", meaning that they will not be included in the refinement. This should be be done when there is a well-understood reason why that region is expected to have spurious intensities (such as scattering from a furnace). For the computed pattern (shown as a green line from a fit, no computed pattern is shown for data in an excluded region.

WHAT CAN I DO HERE?

You can change the 'new' values for Tmin and Tmax as needed. Change the upper (Tmax) and lower (Tmin) values by clicking on the appropriate vertical line and dragging it to the right or left, or by typing values into the data window, or using the "Set lower limit" or "Set upper limit" commands in the "Edit Limits" menu and then click on a point in the pattern.

You can add an excluded region using the "Add excluded region" command in the "Edit Limits" menu and then click on a point in the pattern. This creates region at that point. Edit the region by dragging the magenta lines or by editing the values in the data window.

"EDIT LIMITS" MENU COMMANDS

Copy: This copies the limits shown for the selected pattern to other powder patterns. After using this menu command, a dialog box (Copy Parameters) will appear showing the list of available powder patterns, you can copy the limits parameters to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.

Add excluded region: Select this menu item and click on a data point. A pair of magenta lines is drawn to indicate a range that should be excluded. The magenta lines can be dragged, as described below.

Set lower limit/**Set upper limit**: These menu items are used to select a location in the pattern to set as Tmin or Tmax. After using the menu command, click on a point in the pattern at the appropriate location.

Cancel Set: Resets the "Add excluded region", "Set lower limit" or "Set upper limit" command so that no change is made.

WHAT IS PLOTTED HERE?

The plot is the largely the same as for the parent PWDR Powder Histograms tree entry with the same plot actions and same key press commands, except that tickmarks and the obs-calc position cannot be dragged. What is unique to the plot associated with the Limits subdata tree entry is that the entire pattern is shown, including data outside the limits and regions that are ignored. Also, vertical lines are displayed for the fitting limits: green for the lower Tmin value and red for the upper Tmin value. Excluded regions are displayed with pairs of magenta vertical lines. All these vertical lines can be dragged to set limits or change excluded regions.

WHAT CAN I DO WITH THE PLOT?

- The upper and lower Tmin values can be changed by clicking on the appropriate vertical line and dragging it to the right or left.
- A of a limit drag beyond the end of the pattern will reset that limit to the original value.
- Excluded regions can be created here from the menu or with a "e" keypress and modified by dragging the lines, as needed.

5.7.5 PWDR **Background** subdata tree item (Powder Diffraction)

This window shows the choice of background functions and coefficients to be used in fitting this powder pattern. There are four types of background contributions available here that are summed, so they can be used together, but use care when introducing too many degrees of freedom into background fitting. Note that as numbers are changed in this window, the background is recomputed, so it is possible to visualize the effect of different values and options.

1. The most commonly used option is a continuous empirical function, with function choices:

    - "chebyschev",
    - "chebyschev-1",
    - "cosine",
    - "lin interpolate",
    - "inv interpolate" &
    - "log interpolate".

    The latter three "interpolate" functions select fixed points with spacing that is equal, inversely equal or equal on a log scale of the x-coordinate. The set of magnitudes at each point then comprise the background variables. All terms are refined when the refine is selected. Note that 'chebyschev-1' is a better choice than 'chebyschev'.

- A set of Debye diffuse scattering equation terms of the form:

$$Background = \sum_i A_i \frac{\sin QR_i}{QR_i} e^{-U_i Q^2}$$

  where Q = 2π/d and A_i, R_i & U_i can be individually selected for refinement as desired and the range for i is determined by the selected number of terms.
- A set of individual background peaks can be added, These use the pseudo-Voigt profile function as their shapes. Their parameters are "pos" (peak position), "int" (integrated intensity), "sig" (Gaussian width) & "gam" (Lorentzian width); each can be selected for refinement, but it is uncommon to fit both both sig and gam. The default values for sig & gam (=0.10) are for very sharp peaks. For typical background use, values of 100 to 10,000 for sig are more common. You may adjust them accordingly to the kind of peak you are trying to fit before trying to refine them. It is common to use these with the 'chebyschev-1' function, where a small number of terms allows the chebyschev-1 to fit a smooth, slowly-varying, function and the background peaks account for broad "lumps" in the pattern, such as what arises from Kapton.
- Subtract an experimentally measured background. The experimentally measured background points are scaled by a multiplier that can be refined to account for sample absorption effects.

WHAT CAN I DO HERE?

"BACKGROUND" MENU COMMANDS

- **Copy** – this copies the background parameters shown to other selected powder histograms. If used, a dialog box (Copy Parameters) will appear showing the list of available powder patterns, you can copy the background parameters to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.
- **Copy flags** – this copies only the refinement flags shown to other selected powder patterns. If used, a dialog box (Copy Refinement Flags) will appear showing the list of available powder patterns, you can copy the refinement flags to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.
- **Save** – saves the background values to a file so the can be used in a different GSAS-II project (`.gpx` file).
- **Load** – Reads in background values from a file created with the Save command.

"FIXED POINTS" MENU COMMANDS

- **Add** – When this is selected, it is marked as checked. In this mode clicking on the pattern will add a background point (marked as a large red diamond) to the pattern. This will be used with the "Fit Background" menu command or button.
- **Move** – When this is selected, it is marked as checked. In this mode background points can be dragged to new positions.

- **Delete** – When this is selected, it is marked as checked. In this mode clicking on a background point will delete it
- **Clear** – Deletes all fix background points
- **Fit Background** – When this is used, the refined terms in the background functions are refined to best fit the fixed background points. Note that the "Fit to fixed bkg" button does the same thing as this menu command, but is more convenient.

Things you can do here:

1. You can select a different Background function from the pulldown tab.
2. You can choose to refine/not refine the background coefficients.
3. You can select the number of background coefficients to be used (1-36). You should use the minimum required.
4. You can change individual background coefficient values. Enter the value then press Enter or click the mouse elsewhere in the Background window. This will set the new value.
5. You can introduce one or more Debye scattering terms into the background. For each one you should enter a sensible value for 'R' – an expected interatomic distance in an amorphous phase is appropriate. Select parameters to refine; usually start with the 'A' coefficients.
6. You can introduce single Bragg peaks into the background. For each you should specify at least the starting position. Select parameters to refine; usually start with the 'int' coefficients. Set the "sig" value manually to give a breadth that visually seems to match the pattern. You may need to increase "int" significantly to see the effect of changing "sig" in the plot.
7. You can select an experimentally measured background pattern from those in the GSAS-II data tree and scale it with a multiplier.
8. You can place fixed background points on the pattern and then fit background coefficients to fit them. If this is done, it is possible to postpone the Rietveld fitting of the background until the late stages of the fit. This can greatly simply fitting of patterns with messy background intensities and that have poorly fit models, by allowing you to concentrate on improving the model. Note that the tutorial Fitting the Starting Background using Fixed Points shows how this is done.
9. You can automatically generate fixed background points across the pattern using the "Compute auto background" button. This creates a smooth function that will tend to ignore sharp peaks.

    - There are two functions available, "arpls" and "iarpls"; you can choose the one that works best for you.
    - The "log(Lambda)" term is a spline coefficient that determines how much the background can "wiggle" (have sharper variations). As this is moved, the resulting background function is shown.

    To complete the operation, one can either use

    - "Set Fixed Points & Fit", which creates fixed background points across the entire pattern and then fits the refined background terms.
    - "Define Fixed Bkg histogram" creates a histogram of fixed background points and sets this to be subtracted from the current pattern.

    Note that this computation is done with the `pybaselines` package, which must be installed into Python to use this feature.

Any modification of the background representation will be immediately applied to the calculated pattern so you can see its effect.

WHAT IS PLOTTED HERE?

The plot is the largely the same as for the parent PWDR Powder Histograms tree entry with the same plot actions and same key press commands, except that tickmarks are not shown and the obs-calc position cannot be dragged. Specific to this plot are fixed background points. These can be added, deleted and moved. Once that is done the background parameters for the selected function can be fitted to the fixed points. NB: the number of fixed points must exceed the number of background parameters to be fitted. Not recommended for fitting sharp Bragg peak backgrounds unless sufficient fixed points are selected across each Bragg peak.

5.7.6 PWDR **Instrument Parameters** subdata tree item (Powder Diffraction)

This window shows the instrument parameters for the selected powder data set. Note that the preferred method for use of GSAS-II is that these parameters are fitted only to calibration materials. The parameters fit from the calibrant then defines a set of values unique to that instrumental configuration; these values are not refined when fitting samples. The plot window shows the corresponding resolution curves.

- Solid lines are for the default values (in parentheses),
- dashed lines from the refined values and
- '+' fitted widths for individual entries in the Peak List.

Curves that fall below zero will generate a warning in the plot title, coefficients should be adjusted to ensure every dashed line curve is zero or above.

WHAT CAN I DO HERE?

"OPERATIONS" MENU COMMANDS

A single menu is provided with the selection of instrument parameters.

- **Calibrate**: performs calibration of position dependent instrument coefficients from indexed peak positions.
- **Reset profile**: resets the values for the instrument parameters to the default values shown in parentheses for each entry.
- **Load profile...**: loads a GSAS-II instrument parameter file (name.instprm), replacing the existing instrument parameter values. All refinement flags are unset.
- **Save profile...**: saves the current instrument parameter values in a simple text file (name.instprm); you will be prompted for the file name – do not change the extension. This file may be edited but heed the warning to not change the parameter names, the order of the parameter records or add new parameter records as this will invalidate the file. You may only change the numeric values if necessary. You can change or add comment records (begin with '#').
- **Save all profile...**: saves multibank histogram instrument parameters into a single instprm file. Suitable for neutron TOF instruments.
- **Copy**: this copies the instrument parameters shown to other selected powder patterns. If used, a dialog box (Copy parameters) will appear showing the list of available powder patterns, you can copy the instrument parameters to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation. The copy will only work for instrument parameters that are commensurate with the one that is shown, e.g. single radiation patterns will not be updated from Kα1α2 ones.
- **Copy flags**: this copies the instrument parameter refinement flags shown to other selected powder patterns. If used, a dialog box (Copy refinement flags) will appear showing the list of available powder patterns, you can copy the instrument parameter refinement flags to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation. The copy will only work for instrument parameters that are commensurate with the one that is shown, e.g. single radiation patterns will not be updated from Kα1α2 ones.
- **Set one value**: this is used to set a single selected instrument parameter for the current selected PWDR histogram. Once changed, the new value can be copied to selected other histograms. There is also an "Edit in table" option. When that is used, the value can be set individually (likewise for the refine flag) for every selected histogram. Note that the "down arrow" button in the table is used to copy the selected value to all histograms below.
- **Show multiple**: Displays instrument parameters for all histograms similar to the current selected histogram in a single table.

Note that you can change any of the instrument coefficients and the instrument peak widths plot will be updated to show the effect of the change on overall peak widths. Note that while the software does allow you to refine any of the instrument coefficients, refinement of these terms is discouraged, except for generating instrumental profiles for calibration. NB: In certain circumstances some refinement choices are ignored: e.g. Zero is not refined (or used) during peak fitting. Also, some parameter choices may lead to unstable refinement, e.g. combining refinement of Lam (wavelength) and lattice parameter. In Rietveld fitting, examine the 'Covariance' display for highly correlated parameters.

WHAT IS PLOTTED HERE?

This plot shows the contributions to the powder pattern peak widths as ΔQ/Q (=Δd/d) vs. Q for the Gaussian and Lorentzian parts of the profile function, in addition to the overall widths. The solid curves are based on the default values of U, V, W, X and Y shown in the Instrument Parameters window (shown in parentheses; these are the values for the instrument contribution that were set when the powder pattern was first read in to GSAS-II.) The dashed values are based on the refined values, if different. If individual peak fitting has been performed, the values of 'sig' & 'gam' for those

individually-fit peaks are plotted as '+'; these are computed from the fitted values of U, V, W, X and Y as well as any sig or gam values that are individually refined. For neutron TOF, the curves include those for the α and β coefficients.

Care should be taken that coefficients do not generate negative peak widths at any point in the pattern where peaks are present. Negative values are not mathematically or physically possible; if encountered in fitting, the corresponding peaks may be ignored.

5.7.7 PWDR **Sample Parameters** subdata tree item (Powder Diffraction)

This window shows the various sample-dependent parameters for the selected powder pattern. Some are related to the measurement conditions, such as diffractometer setting angles, or the data collection temperature. Others, such as the histogram scale factor, adjust the fit to match the collected data. The presence of a refine button indicates that a parameter can be refined (all others are fixed.) All values shown in this window can be edited.

Note that the last three parameters (named internally as `FreePrm` *X*, *X*=1,2,3), which are labeled by default as "Sample humidity", "Sample Voltage" and "Applied Load" are fields where the labels that can be changed. If changed in one histogram, the same label is used for all histograms. Thus, a total of six parametric variables are available, including the more common variable of temperature, pressure and time. Also, note when a label `FreePrm` is changed to "ParmName", the Comments tree item for each PWDR histogram is searched for a matching "*ParmName*=value" or "*ParmName*:value" pair (i.e. the string "ParmName" will be looked for within the label+value pairs in the comments, ignoring differences in letter case between the two label strings). Thus if the Sample Parameters label is specified as "focus", then a Comments string of "/Instrument/BeamFocus_at_sample=10" will be matched. When found, the value is converted to a float and saved as the value for the newly-labeled Sample Parameter. Also, note the similar action in the "Set from comments" command, below.

Be sure the correct instrument type is selected (Debye-Scherrer or Bragg-Brentano). Also, ensure the goniometer radius is correct (in mm) so that sample displacements are properly scaled (in μm).

WHAT CAN I DO HERE?

In this window you can change parameters associated with a histogram or set them to be refined.

- The histogram scale factor is usually refined.
- For **Debye-Scherrer** mode the "**Sample X displacement**" is also usually refined but the "**Sample Y displacement**" *can only be refined when data are collected over a two-theta range that extends to much greater than 90 degrees* (typically for CW Neutron). Note that while in the past it was common to vary the $2\theta_0$ (**Zero**) Instrument Parameter, the "Sample X displacement" is almost always a much better parameter to fit. "Sample X displacement" should never be refined with Zero, with the possible exception of a calibrant where the lattice parameters are fixed.
- For **Bragg-Brentano** mode the "**Sample displacement**" is the displacement of the sample from the diffractometer circle in μm. This almost always refined. The $2\theta_0$ (**Zero**) Instrument Parameter is almost never refined with Bragg-Brentano data. For low-Z samples "**Sample transparency**" is usually refined instead of "**Sample displacement**". Only if data are collected over a very wide 2θ range should both be refined together.
- Sample absorption should not be refined when all atomic displacement parameters (Uiso or Uij values) are varied, as the correlation is very high.
- "Surface roughness" parameters are not usually refined, unless the sample has high absorption and negative Uiso values are obtained for heavy atoms.

The remaining parameters are non-refinable and may be needed for texture or parametric studies. They may be edited in the window or may be changed for all histograms with the menu commands described below.

"COMMAND" MENU COMMANDS

- **Set scale** - Rescales a pattern by multiplying by the current scale factor. Scale factor is then set = 1.0.
- **Load** - This loads sample parameters from a previously saved `.samprm` file.
- **Save** - This saves the sample parameters to a file with the extension `.samprm`. A file dialog box will appear to ask for the name of the file to be written.
- **Copy** - This copies the sample parameters shown to other selected powder patterns. If used, a dialog box (Copy parameters) will appear showing the list of available powder patterns, you can copy the sample parameters to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.
- **Copy selected...** - This copies only the sample parameter that are selected to other selected powder patterns but is otherwise similar to "Copy".
- **Copy flags** - This copies the sample parameter refinement flags shown to other selected powder patterns. If used, a dialog box (Copy refinement flags) will appear showing the list of available powder patterns, you can copy the sample parameter refinement flags to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.
- **Set one value** - This is used to set a single selected sample parameter for a selected set of PWDR histograms. The same value can be used for all histograms or a dialog can be used to provide a table where you can set the values differently for each of selected histograms.

- **Load all** - Reads a file containing a table of sample parameters and copies them to matching PWDR entries. The file will look something like the example below.

  Note that the first line(s) in the file can be a header, but each header line must start marked with a hash (#). A header is not required. "Columns" in the table are separated by one or more delimiters (which may be a comma, tab or space). Note that columns do not need to be aligned, as long as each entry is spaced by at least one delimiter. The first column in the table is used to look up PWDR entries where the initial space-delimited string after the PWDR tag ("myfile" in "PWRD myfile AZM=180...") must match the table. Subsequent columns can then be mapped to sample parameters or can be ignored, using a dialog window.

```
#filename       temperature pressure ignore-me  humidity
LaB6_dc250.tif      100          1      test       .2
LaB6_dc300.tif      150          1      test       .25
```

- **Rescale all** - Allows a series of selected PWDR histograms to be put on a common scale by integrating them over a specific two-theta region and then scaling them so that the integration range will match the first pattern.
- **Set from comments** - The histogram comments section, depending on the importer used to read in the powder data (or image that data is derived from) often contains values that are recorded by the diffraction instrument. These are recorded in the comments as "Label=value" or "Label:value". This command can be used to scan the comments and transfer them to the sample parameters. This is done by selecting a sample parameter, as well as a "Label" found in the comments. One then specifies the histograms where the value will be located and the parameter will be set. Alternately, one can specify an equation to be used to set the chosen sample parameter as a function of one or more "Label" values. This command can be used to set any of the Sample Parameter values, but this is particularly useful for parametric variables and for sample setting angles. Note that a similar action is possible by changing the name of one of the "free parameters," as described above.

5.7.8 PWDR **Peak List** subdata tree item (Powder Diffraction)

The Peak List data tree entry is used to fit diffraction peaks at refined or user-supplied positions (not generated from a unit cell). Peak positions and intensities may be selected for individual refinement. There are four modes available here for treatment of peak widths:

1. Gaussian (σ^2) and Lorentzian (Γ) peak widths may be varied individually.
2. The width values may be generated from the the appropriate profile terms in the Instrument Parameters tree item (U, V & W for σ^2; X & Y for Γ), where those terms may optionally be refined.
3. It is possible to mix refinement of XY terms and fit a few individual (Γ) peak widths, but this is not possible with the UVW terms. When any individual (σ^2) peak widths are fit, it is not possible to refine the U, V or W terms. Note that when individual widths are refined, the fitted values override the values that would be generated from the UVW/XY terms, except as noted in the next mode.
4. It is possible to turn off the setting of individual (σ^2 or Γ peak width values) peak width If are refined, then those value(s) in the table are used as the refinement starting point. If values are not refined, then normally the unvaried widths are determined from the appropriate Instrument Parameters profile terms and are placed in the table prior to fitting. When the "Gen unvaried widths" menu item is turned off, the unvaried peak with values are not computed from the Instrument Parameters; this must be turned on (the default mode) to vary Instrument Parameters.

Note that the Gaussian full-width at half-maximum is given by:

$$FWHM_G = \sqrt{8 * \ln 2 * \sigma^2}$$

while the Lorentzian full-width at half-maximum is just Γ:

$$FWHM_L = \Gamma$$

The σ^2 values (peak variances) are in units of centidegrees^2 (centidegrees are degrees*100) for CW data or microseconds^2 for TOF data; Γ has units of centidegrees or microseconds. Except in very unusual circumstances, instrumental broadening is Gaussian and will be a slowly-changing function of Q. However, sample broadening is strictly Lorentzian and while sample broadening may only vary with Q, it can also vary from peak to peak if the sample is a mixture of phases, or anisotropic peak broadening is present. Thus, it makes sense to fit Gaussian widths only using the U, V & W terms and indeed the software will not allow those terms to be varied if *any* individual peak σ^2 terms are varied, as this usage would not make sense physically. This is different for X & Y and individual peak Γ values. The refinement of X & Y, while fitting of *some* individual peak Γ values is allowed and this can make sense physically, but note that one should have a sufficient number of peaks that are not being fit individually and these peaks should be distributed over a wide range in Q when X & Y are fit simultaneously.

For peak fitting, the background is generated using the parameters in the Background data tree entry. Also, the range of data used in the fit is set from the Limits tree item. In both cases these are the same values that are used in Rietveld fits. Note that optionally the parameters on the Background and in the Instrument Parameters tree items may be refined during peak fitting, but in the case of U, V & W, these values cannot be refined if any individual σ^2 values are fit.

WHAT CAN I DO HERE?

There are three ways to interact with Peak List data tree item: through its menu, labeled Peak Fitting, through interaction with the peak list table, and through interactions with the plot.

The following interactions are available with the peak table:

- You can change individual peak coefficient values. Enter the value then press Enter or Tab or click the mouse elsewhere in the Peak List window. This will set the new value.
- You can change the individual refine flags by clicking on the individual check boxes.
- You can change all refine flags in a column by clicking on a single flag and then click on the column label above. (The entire column should then be highlighted in blue.) Type 'y' to set the refine flags or 'n' to clear the flags. You can also change flags for an entire column by double-clicking on the column label, which brings up a menu where "Y" or "N" can be selected.
- You can delete peaks in the Peak List by selecting a row by clicking on the row label to the left (multiple selection of rows is allowed). Selected rows will be highlighted in the plot (see below). Then press the Delete or backspace key. (Note that peaks can also be deleted from the plot, see below.)
- You can highlight a peak in the plot by double-clicking on the row label (to the left) for a peak.
- Pressing "d" in the plot window causes the next peak in the table (or the first if none are selected) to be selected and causes that peak to be highlighted in the plot; pressing "u" causes the previous peak in the list to be highlighted.

MENU COMMANDS: "COMMAND" MENU

The menu for Peak Fitting contains the following commands:

- **Set sel. ref flags** - If one or more rows of peaks are selected by clicking on the peak label to the left, this menu item can be used to set the refinement flags for the selected reflections.
- **Set all ref flags** - This sets refinement flags for all peaks in the table.
- **Auto search** - This fills the table with peak positions. These are selected based on peak tops that are substantially above background. Noisy data will give spurious peaks, and small peaks or shoulders will necessarily not be found. Examine results & modify as needed.
- **UnDo** - Resets peak parameters, background and instrument parameter values varied in the last peak fitting refinement back to their original values. Use this to recover from a failed refinement. Note: only one previous refinement is saved, so this cannot be pressed twice to return to the refinement before the previous.
- **PeakFit** - Performs a least squares fit of the peaks in Peak List to the data. Any peak parameters, background parameters and instrument parameters with refine checked will be varied in this refinement. The refinement will proceed until convergence. We suggest you vary the peak intensities along with the background first (the default), then vary the position and instrument parameters after. The order will depend on how poor is the initial estimate of the instrument parameters (U, V, W, X, Y & SH/L). To determine how to proceed, examine in detail the powder pattern difference curve displayed in the GSASII Plots window. If individual peaks show peak widths that are widely different, their individual σ^2 and Γ parameters may be refined. If the refinement results in negative peak coefficients, these will be highlighted in red. If this happens, you should use the UnDo menu item (above) to return to the refinement and reconsider your choice of parameters to be varied.
- **Peakfit one cycle** - Perform a single cycle of least squares refinement. This can be used in difficult cases to get a refinement started toward convergence.
- **Reset sig and gam** - This resets the values of σ^2 and Γ in the table to those computed from the instrument parameters U, V, W, X & Y.
- **Peak copy** - Copy the current set of peaks to other histogram(s).
- **Seq PeakFit** - Fit peaks for multiple histograms; results will be in Sequential peak fit results.
- **Clear peaks** - This removes all the peaks from the Peak List.
- **Move selected peak** - A peak may be moved using the following process: select it in the table by clicking on its label (to left), use this menu item. The peak line will then follow movement of the mouse in the plot window. Click with the left mouse button to set a new position. Click with the right mouse button to delete that peak. Click outside the axes to abort the move and return to the previous position. (Note that peak movement is also possible with the plot window, see below.)
- **Gen unvaried widths** - This determines how σ^2 and Γ values are treated when unvaried. When this item is checked (the default mode), unvaried Gaussian (σ^2) and Lorentzian (Γ) peak widths will be generated from the the appropriate profile terms in the Instrument Parameters tree item (U, V & W for σ^2 X & Y for Γ). This allows those Instrument Parameters to be refined. If this mode is changed and the "Gen unvaried widths" mode is unchecked the the σ^2 and Γ peak widths are used as supplied, but then it is not possible to refine Instrument Parameters. This mode will not affect σ^2 and Γ values that have their refine flag checked.

WHAT IS PLOTTED HERE?

The plot is the largely the same as for the parent PWDR Powder Histograms tree entry with the same plot actions and same key press commands. Specific to this plot are the peak positions that are shown as vertical dashed blue lines. To show that a peak is selected, it is highlighted in yellow and the blue line is made wider. The upper and lower data limits are shown as red and green dashed vertical lines, respectively, and can be dragged to change the fitting range.

WHAT CAN I DO WITH THE PLOT?

For all actions involving mouse clicks such as those below, be sure that the Zoom/Pan buttons are not selected on the Plot window, as the mouse will be used for zooming or panning, not the desired action.

- You can add peaks to the Peak list using the mouse on the plot by: position the cursor pointer onto a cross for an observed point and pressing the left mouse button. The selected peak will be added to the Peak List in the appropriate position to keep peaks sorted and a blue vertical line will be plotted on that position. We recommend that you begin picking peaks from the right side of the pattern; that way the tool tip won't be in your way as you select peaks.
- You can delete peaks using the mouse on the plot by positioning the pointer on the blue line for the peak to be deleted and then pressing the right mouse button. The blue line should vanish, and the corresponding peak will be removed from the Peak List.
- You can move a Peak List item using the mouse on the plot: position the pointer on the blue line for the peak you wish to move and then hold the left mouse button down, dragging the line to the desired position. When the mouse button is released, the peak line will be drawn in the new position.
- The fit limits can be changed from the plot either here or in the Limits data tree. Change the upper and lower Tmin/Tmax values by clicking on the appropriate vertical line and dragging it to the right or left.
- Highlight each peak in the list successively using the "d" keyboard key to move down the list or "u" to move up the list.

"EXTRA PEAK" MODE

When working with full-pattern fits, it is sometimes useful to pay attention only to the peaks that are not being indexed and fit by the full pattern fit. One reason for this may be to learn more about a phase that is not currently being fit or with magnetic scattering, one may have fit the chemical ("nuclear") structure and one needs to identify the additional peaks that are seen at a temperature below a magnetic phase transition in order to understand the lowered symmetry of the magnetic lattice. Similarly one may wish to explore a phase transition lowering of symmetry. In "Extra Peak mode", individual peak fitting is performed not on the diffraction data, but rather on the "difference curve," the observed pattern with the computed pattern subtracted. A separate peak list is kept for these "extra peaks". This "Extra Peak Mode" can be entered either from pressing the button labeled "Switch to In "Extra Peak mode", or by using the checkmark menu button in the "Peak Fitting" menu labeled "Add impurity/subgrp/magnetic peaks."

5.7.9 PWDR **Index Peak List** subdata tree item (Powder Diffraction)

This window shows the list of peaks that will be used for indexing (see Unit Cells List). It must be filled with peaks from the Peak List (using the Operations->Load/Reload menu command) before indexing can proceed. When indexing is completed, this display will show the resulting hkl values for every indexed reflection along with the calculated d-spacing ('d-calc') for the selected unit cell in Unit Cells List. .

WHAT CAN I DO HERE?

- Double-clicking on a row of the table causes that row to be selected and causes that peak to be highlighted in the plot.
- Pressing "d" in the plot window causes the next peak in the table (or the first if none are selected) to be selected and causes that peak to be highlighted in the plot; pressing "u" causes the previous peak in the list to be highlighted.
- You may designate that individual peaks not be used in the indexing by process by unchecking the corresponding "use" box.

"OPERATIONS" MENU COMMANDS

- **Load/Reload** – loads the peak positions & intensities from the Peak List to make them available for the indexing routine. The d-obs value is obtained from Bragg's Law after applying the Zero correction shown on the Instrument Parameters table to the position shown here.
- **Save** – saves a csv version of this table.
- **Export to PreDict** – saves the table in a format that can be used by PreDict, an updated version of the DICVOL program.
- **Refine Cell** – optimizes the unit cell parameters shown at the bottom of the window to best-fit the peak list.

WHAT IS PLOTTED HERE?

The plot is the largely the same as for the parent PWDR Powder Histograms tree entry with the same plot actions and same key press commands. Specific to this plot are the peak positions that are shown as vertical solid blue lines. To show that a peak is selected, it is highlighted in yellow and, if "use" is selected, the blue line is made wider. The upper and lower data limits are shown as red and green dashed vertical lines, respectively. Tickmarks are not shown. Limits cannot be dragged from this data tree item.

WHAT CAN I DO WITH THE PLOT?

- Highlight each peak in the list successively using the "d" or "u" keyboard keys.

5.7.10 PWDR **Unit Cells List** subdata tree item (Powder Diffraction)

This tree item has several purposes, it can be used to perform autoindexing and it can be used to show the positions of peaks from unit cells which may be results from autoindexing or may be entered from a phase or manually. It can be used to refine unit cell parameters. It can also be used to search for cells/symmetry settings related to a specified unit cell & space group.

WHAT CAN I DO HERE?

The actions that can be performed with this tree item are:

1. Autoindexing
2. Visualizing reflection positions
3. Symmetry exploration
4. Cell fitting

AUTOINDEXING

For autoindexing, the peaks in the Index Peak List are used. Select one or more Bravais lattice types to use and use the "Cell Index/Refine"/"Index Cell" menu command to start indexing. Output will appear on the console and a progress bar dialog will appear which tracks trial volume. A **Cancel** button will terminate indexing for the Bravais lattice being searched; one may need to press it more than once to fully terminate the indexing process. Console output shows possible solutions with a computed **M20** for each; good solutions are indicated by high **M20** values. **X20** gives number of unindexed lines out of the 1st 20 lines and **Nc** gives total number of reflections generated for each solution.

- **Max Nc/Nobs**: – this controls the extent of the search for the correct indexing. This may need to be increased if an indexing trial terminates too quickly. It rarely needs to be changed.
- **Start Volume**: – this sets an initial unit cell volume for the indexing. It rarely needs to be changed.
- Select "**try**" in the table to display the reflection positions the selected unit cell/space group (as described below).
- Select "**keep**" in the table for a cell that should be preserved when an additional indexing run is tried; all without that are erased before the indexing trial begins.

Use the "**Index Cell**" menu command to search for a unit cell that matches the peaks in the Index Peak List

UNIT CELL DISPLAY

To display a unit cell, possibly with space group extinctions, enter the unit cell here. Optionally enter space group information here as well. The values can be typed into the appropriate boxes (note that the Bravais class determines which cell parameters are available) or use the "Cell Index/Refine"/"Load Phase" menu command to read this information from a phase that has been read into a project or from a file (such as a CIF) using the "Cell Index/Refine"/"Import Cell" menu command. Note that the values in the unit cell parameter boxes can be specified as Python equations, thus entering "*2" after a value will double it and "/2" will divide it by two.

To change the displayed extinctions, first set a Bravais class, which determines the unit cell type (see list below), and then optionally select a space group (by default the highest symmetry space group for the class is selected). As any change is made to the unit cell values or the symmetry, the display of reflection positions shown in the plot window is immediately updated. The "Show hkl positions" button also forces an update of the plot, but this is normally not needed.

Reflection positions are displayed as dashed vertical lines. Reflections will normally be shown as orange, but green lines are used instead in 3+1 superspace groups for reflections with non-zero components in the fourth dimension ("superlattice lines"). If the "Show extinct" option is selected, then reflections that are generated by the unit cell, but must be zero in intensity due to the selected space group are shown with blue dashed lines. This slows computations somewhat. Note that the speed of reflection display is determined by the number of reflections that are computed, so reducing the range of data used by changing the diffraction Limits will speed the refresh of the display when values/symmetry is changed.

The reflection indices (hkl values) can be displayed by moving the mouse cursor over a reflection line and waiting ("hovering"). After a short delay, the indices for all nearby reflections are shown temporarily as a "tool tip". If multiple reflections are closely spaced, the reflection indices will be listed in the order that reflections occur, but extinct reflections are shown after non-extinct. Also, if multiple extinct reflections occur at the same location, only the first of them is used.

SYMMETRY EXPLORATION

For symmetry exploration, once a phase/cell has been loaded, the following commands in available in the "Cell Index/Refine" menu to explore related unit cells and space groups. Use the:

- The "**Load Phase**" menu command copies a selected solution to the Unit cell values;
- The "**Copy Cell**" menu command copies a selected solution to the Unit cell values; the Bravais lattice shown for the choice is copied. Press **Show hkl positions** to generate the allowed reflection positions, which are visually superimposed on the displayed powder pattern to visually confirm the indexing. Pay particular attention to any unmatched peaks in the pattern. A **Space group** can be selected from the pulldown box to remove reflections based on space group extinctions and visually eliminate possibilities. The **Try All?** button tests all compatible space groups from the pull down against the peak set. The results are displayed and one can select the “best” one based on the listed criterion.
- "Run SUBGROUPS" menu item to generate lower symmetry space groups for the loaded phase;
- "Cell Symmetry Search" menu item to find higher symmetry unit cells equivalent to the current cell.
- "Run k-SUBGROUPSMAG" menu item to find magnetic subgroups (with neutron data) commands from the
- "Transform Cell" command in that menu can perform many common lattice transformations, apply a user-supplied cell transformation or create a magnetic phase.

Note that "Run SUBGROUPS", "Cell Symmetry Search" and "Run k-SUBGROUPSMAG" access the Bilbao Crystallographic Server. If you use them please cite: Bilbao Crystallographic Server I: Databases and crystallographic computing programs, M. I. Aroyo, J. M. Perez-Mato, C. Capillas, E. Kroumova, S. Ivantchev, G. Madariaga, A. Kirov & H. Wondratschek Z. Krist. 221, 1, 15-27 (2006) (DOI and Determining magnetic structures in GSAS-II using the Bilbao Crystallographic Server tool k-SUBGROUPSMAG, R.B. Von Dreele & L. Elcoro, Acta Cryst. B80, x-x (2024) (DOI.

OPTIMIZE A CELL

To optimize a cell to fit the indexed peaks in the Index Peak List, use the "Cell Index/Refine"/"Refine Cell" menu command. The results will be placed in the Indexing Result table with 'use' selected.

CREATE PHASE

The "Make new phase" command creates a new phase from the selected unit cell and chosen space group. A dialog box will appear asking for a name for this phase. See the new entry under Phases and the new lattice parameters will be in the General window for that phase.

WHAT CAN I DO WITH THE PLOT?

The plot is the largely the same as for the parent PWDR Powder Histograms tree entry with the same plot actions and same key press commands, except that tickmarks are not shown and the obs-calc position cannot be dragged. The fit limits can be changed from the plot either here or in the Limits data tree. Change the upper and lower Tmin values by clicking on the appropriate vertical line and dragging it to the right or left. Reducing the maximum Q value (TOF min or 2θ max) can greatly speed the time needed to compute reflections from a unit cell.

VISUALIZATION LAUE CLASSES

GSAS-II offers space groups in the following Laue classes when visualizing reflection positions from a unit cell. Note that symmetry classes in italics are redundant, but are included as choices for convenience:

- Cubic: Fm3m, Im3m & Pm3m
- Rhombohedral: R3-H (hexagonal axes)
- Hexagonal: P6/mmm
- Tetragonal: I4/mmm, P4/mmm
- Orthorhombic: Fmmm, Immm, Ammm, *Bmmm*, *Cmmm*, Pmmm
- Monoclinic: *I2/m*, *A2/m*, C2/m, P2/m (b-unique)
- Triclinic: P1, *C1*

5.7.11 PWDR **Reflection Lists** subdata tree item (Powder Diffraction)

This window shows the reflections for the chosen phase (selected by the tab at top) found in this powder data set. It is generated by a Rietveld (including Pawley and LeBail) refinement. Reflection d-spaces are generated directly from lattice parameters but 2θ (or TOF) values will incorporate corrections, such as for sample displacement, zero, etc. The values of various correction factors, I100, size and mustrain terms for each are also shown.

The powder diffraction reflection list shows the reflection widths, accounting for instrumental as well as sample effects (the latter can be anisotropic), where the columns labeled as "sig2" and "gam" show the Gaussian and Lorentzian components for the width. The "sig2" value is the variance of the Gaussian contribution to the peak (σ^2), while "gam" is the full-width at half maximum (FWHM) for the Lorentzian component, Γ. Note that the Gaussian full-width at half-maximum is given by $$FWHM = \sqrt{8\sigma^2 \ln 2}$$ while Γ is the Lorentzian FWHM. The σ^2 values (peak variances) are in units of centidegrees^2 (centidegrees are degrees*100) for CW data or microseconds^2 for TOF data; Γ has units of centidegrees or microseconds.

5.7.12

WHAT CAN I DO HERE?

- The indices (hkl values) for reflections can be displayed by letting the mouse rest at the position of a reflection in 2θ, Q, etc. in the PWDR plot (the vertical position does not matter) for reflections in the phase selected as a tab in the data window. A "tool tip" with the reflection indices will be displayed for any reflections close to the lateral mouse position.
- Right-clicking on a reflection tickmark will cause an hkl label with the indices for nearby reflection(s) to be displayed. Once a reflection label is shown, it can be dragged to a new position vertically with the left mouse button. Right-clicking on the label will delete it. All hkl labels can be deleted with a menu command. The hkl labels, including their positions, are saved in the GSAS-II project (.gpx) file.

"REFLECTION LIST" MENU COMMANDS

Note that some of these commands are more useful for `HKLF` (single crystal) histograms.

- **Select phase** – if there is more than one phase; you can select another phase; the window title will show which phase is shown. You can also simply select the tab for the desired phase.
- **Plot 1D HKLs** – shows a stick diagram scaled to Fc2 for the reflection for the selected phase
- **Plot HKLs** – shows a HKL layer with rings scaled to F or F2 for Fo and Fc. +/- steps through the layers and h,k or l selects the orientation – see K box for all the possible commands.
- **Plot 3D HKLs** – shows a 3D representation of the unique part reciprocal space points for this phase. The save as/key item in the plot status bar shows the various commands for modifying this plot.
- **Wilson statistics** – displays a Wilson plot for the intensities.
- **Show/hide extinct reflections** – can exclude space group extinctions from the list (not valid for PWDR data).

5.8 Type HKLF data tree entries: Single Crystal

Single-crystal datasets are read into GSAS-II using the Import/Structure Factor menu command, since the histogram is a table of structure factors. Note that GSAS-II can fit a structure (phase entry) to a one single crystal histogram, but it is also possible to fit a phase to multiple single-crystal histograms (which might be collected at different wavelengths) or even a combination of single-crystal and powder datasets (as might be the case with a laboratory single-crystal measurement combined with a neutron powder diffraction histogram.)

What can I do here?

You can change the weight factor. This is a multiplier on all of the reflection weights in this histogram. Rarely needs to be changed. Use of 1 for all datasets provides optimal statistical weighting, unless there is systematic error present.

Menu Commands

- **Error Analysis** - this produces a 'normal probability' plot for the refinement result as bounded by the limits. The slope and intercept of the curve in the central region (-1 < / < 1) are shown on the plot status line. The slope is the GOF for the best fit set of data points (~68% of the data).
- **Merge HKLs** - this combines equivalent/duplicate reflections according to space group and some options to make a unique and averaged set of structure factors.
- **Plot 1D HKLs** - shows a stick diagram scaled to F_c^2 for the reflection for the selected phase
- **Plot HKLs** (the default plot) - shows a HKL layer with rings scaled to F or F^2 for F_o and F_c.
    - +/- steps through the layers
    - h,k or l selects the orientation
    - see K box for all the possible commands.
- **Plot 3D HKLs** - shows a 3D representation of the unique part reciprocal space points for this phase. The save as/key item in the plot status bar shows the various commands for modifying this plot.

5.8.1 Instrument Parameters

This window shows the histogram type (SXC or SNC, for x-ray and neutron, respectively) and the wavelength. You may change the wavelength or radiation type but rarely will need to do so.

5.8.2 Reflection List

This window shows the reflections for this single crystal data set.

What can I do here?

- Menu '**Reflection List**' – some items are useful for SHKL (single crystal) histograms.
  - **Select phase** – if there is more than one phase; you can select another phase; the window title will show which phase is shown. You can also simply select the tab for the desired phase.
  - **Plot 1D HKLs** – shows a stick diagram scaled to F_c^2 for the reflection for the selected phase
  - **Plot HKLs** (the default plot)– shows a HKL layer with rings scaled to F or F^2 for F_o and F_c.
    - +/- steps through the layers
    - h,k or l selects the orientation
    - see K box for all the possible commands.
  - **Plot 3D HKLs** – shows a 3D representation of the unique part reciprocal space points for this phase. The save as/key item in the plot status bar shows the various commands for modifying this plot.
  - **Wilson statistics** – displays a Wilson plot for the intensities.
  - **Show/hide extinct reflections** – can exclude space group extinctions from the list

What is plotted here?

By default, the plot will show a l=0 layer of reflections on a square grid as rings proportional to F_o (blue), F_c (green) and a central dot (green or red) proportional to $(\mathrm{F}_\mathrm{o} - \mathrm{F}_\mathrm{c})$.

What can I do with the plot?

The "K" box in the plot controls shows the 14 keystroke controls for the plot – they are generally self-explanatory.

5.9 Type PDF data tree entries: Pair Distribution Functions

A PDF entry is created from a powder histogram (PWDR entry) using the Setup PDFs entry in the Calculate menu. Alternately, a PDF entry can also be imported as G(r) from a file. When this item is selected, the S(Q) function or G(r) function (if imported) is plotted, see below. The main PDF data tree item displays the same window as the PDF Controls, below.

5.9.1 PDF Controls

This window provides parameters for computing the pair distribution function [PDF, G(r)] from the I(Q) function. This can only be done when a chemical formula and appropriate control values are provided. If so, clicking on this menu item causes the I(Q), S(Q), F(Q) and G(r) functions to be plotted, as described below.

The **Optimize PDF** button can be used to refine the values of the "Flat Bkg", "Background ratio" and "Ruland width" parameters to best agree with the $-4 * \pi * r$ line that is plotted for r < Rmin. Rmin should be set to a distance below the shortest expected interatomic distance for the material.

What can I do here?

The PDF parameters can be changed, triggering recomputation of the I(Q), S(Q), F(Q) and G(r) functions.

Available menu commands are:

- **Add element** - Adds a new element to the chemical formula by clicking on a periodic table. Note that the number of atoms of this type in the empirical formula must still be entered.
- **Delete element** - Removes a previously-entered element from the chemical formula.
- **Copy Controls** - Copies the current PDF control values to other PDF data entries
- **Load Controls** - Replaces the current PDF control values with values read from a file (see Save controls).
- **Save Controls** - Saves the current PDF control values into a file.
- **Compute PDF** - Recomputes the PDF for the current entry. This is usually done automatically when values are changed, but if not, this can be forced with this menu item.
- **Compute all PDFs** - Recomputes the PDFs for all selected PDF entries. This is usually done after Copy Controls is used. By default, PDFs are optimized to reduce the low G(r) region, but this can be turned off.

What is plotted here?

When a chemical formula and appropriate control values are provided, clicking on this menu item causes the I(Q), S(Q), F(Q) and G(r) functions to be plotted, as described separately, below.

What can I do with the plot?

For each of the plots, the following keyboard shortcuts are available:

- **c: contour on/off** - if multiple PDFs are available, then a contour plot is shown for the displayed function. All data sets must be the same length as the first one to be included in the contour plot.
- **m: toggle multiple plot** - for multiple PDFs, this will show only the one selected from the data tree. The offset options are not active. Or all selected items will be plotted on a single axis.
- **s: toggle single plot** - for multiple PDFs, this will show only the one selected from the data tree. The offset options are not active. Or all selected items will be plotted on a single axis.
- **f: select data** - Allows only some PDFs to be plotted, rather than all.
- **t: toggle legend** - provides a legend with the line type and name for each PDF.
- **l: offset left** - for a waterfall plot of multiple powder profiles, increase the offset so that later plots are shifted more to the left relative to previous plots.
- **r: offset right** - for a waterfall plot of multiple powder profiles, increase the offset to the right (or decrease the left offset.)
- **d: offset down** - for a waterfall plot of multiple powder profiles, increase the offset down.
- **u: offset up** - for a waterfall plot of multiple powder profiles, increase the offset up.
- **o: reset offset** - for a waterfall plot of multiple powder profiles, reset to no offset.

5.9.2 I(Q) Function

This shows the I(Q) function. See the PDF Controls for information on menu commands and plot options.

5.9.3 S(Q) Function

This shows the S(Q) function. See the PDF Controls for information on menu commands and plot options.

5.9.4 F(Q) Function

This shows the F(Q) function. See the PDF Controls for information on menu commands and plot options.

5.9.5 G(r) Function

This shows the PDF, G(r) function. See the PDF Controls for information on menu commands and plot options.

5.10 Type SASD data tree entries: Small Angle Scattering

5.10.1 Comments

This window shows whatever comment lines found above the QIE table when the small angle data file was read by GSAS-II. If you are lucky, there will be useful information here (e.g. sample name, date collected, wavelength used, etc.). If not, this window will be blank. The text is read-only.

5.10.2 Limits

This window shows the limits in position to be used in any fitting for this small angle scattering data. The 'original' values are obtained from the minimum & maximum values in the data. The 'new' values determine the range of data that will be used in fitting. Units are in Q (Å $^{-1}$).

What can I do here?

You can change the "new" values for Tmin and Tmax as needed. Change the upper and lower Tmin values by clicking on the appropriate vertical line and dragging it to the right or left or by typing values into the data window.

Menu '**Edit Limits**'

- **Copy** - this copies the limits shown to other selected small angle patterns. If used, a dialog box (Copy Parameters) will appear showing the list of available small angle patterns, you can copy the limits parameters to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.

5.10.3 Instrument Parameters

This window shows the relevant instrument parameter for small angle data; namely a wavelength to relate Q to scattering angle (2θ). It is not refinable.

What can I do here?

1. Menu '**Operations**' –
    - **Copy** – this copies the instrument parameter shown to other selected small angle data. If used, a dialog box (Copy parameters) will appear showing the list of available small angle data, you can copy the wavelength to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.
2. You can change the wavelength.

5.10.4 Substances

This window shows the substances that make up the small angle scattering sample. By default, “vacuum” and “unit scatterer” are included; others can be added as needed. The desired substances must be added to Sample Parameters (below) before their use in constructing scattering models for small angle data analysis.

What can I do here?

1. Menu '**Edit substance**' –
    - **Load substance** – select from a suite of various substance predefined by GSAS-II as defined in GSASII/Substances.py. You may add to this list by adding a file, UserSubstances.py, by following the substance format as described in Substances.py. Place your UserSubstances.py in the GSAS-II directory.
    - **Reload substances** – this recomputes the scattering contrast data for the substances.
    - **Add substance** – this allows one to enter a new substance that is not among the previously defined ones. Give it a name, element composition and volume/density; GSAS-II will compute the scattering contrast data for it.
    - **Copy substances** – this allows one to copy these defined substances to other small angle data histograms.
    - **Delete substance** – this allows one to remove any substance but not vacuum or unit scatterer.
    - **Add elements** – this allows one to add new element types to a selected substance.
    - **Delete elements** – this allows one to remove elements from a substance.
2. You can edit the composition by changing the number of each kind of element and change the sum of atomic volumes or the material density.

5.10.5 Sample Parameters

This window shows the various sample-dependent parameters for the selected small angle pattern. All values shown in this window can be edited. Note that the last three parameters (named `FreePrm`X, X=1,2,3) have labels that can be changed. If changed in one histogram, the same label is used for all histograms. When a label is changed, the Comments tree item for each SASD histogram is searched for a matching "Label=value" pair (differences in letter case between the two label strings is ignored). When found, the value is converted to a float and saved as the appropriate Sample Parameter. The last two items define the two components of a small angle scattering sample. One comprises the objects of interest while the other is the marix they are embedded in. The small angle pattern then results from the shape and scattering contrast between the two materials.

What can I do here?

Command Menu - In this window you can change parameters associated with a histogram. This histogram scale factor is ignored for SASD. Remaining parameters are of use for parametric studies and may be changed with the menu commands described here.

- **Set scale** - Rescales a pattern by multiplying by the current scale factor. Scale factor is then set = 1.0. Useful for stitching together partial SASD scans
- **Load** - This loads sample parameters from a previously saved .samprm file.
- **Save** - This saves the sample parameters to a file with the extension '.samprm'. A file dialog box will appear to ask for the name of the file to be written.
- **Copy** - This copies the sample parameters shown to other selected SASD patterns. If used, a dialog box (Copy parameters) will appear showing the list of available SASD patterns, you can copy the sample parameters to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.
- **Copy selected...** - This copies only the sample parameter that are selected to other selected SASD patterns but is otherwise similar to "Copy".
- **Copy flags** - (Not valid for SASD).
- **Set one value** - This is used to set a single selected sample parameter for a selected set of SASD histograms. The same value can be used for all histograms or a dialog can be used to provide a table where you can set the values differently for each of selected histograms.
- **Load all** - Reads a file containing a table of sample parameters and copies them to matching SASD entries. The file will look something like the example here:

```
#filename       temperature pressure ignore-me  humidity
LaB6_dc250.tif      100          1      test       .2
LaB6_dc300.tif      150          1      test       .25
```

Note that the first line(s) in the file can be a header, but each header line must start marked with a hash (#). A header is not required. "Columns" in the table are separated by one or more delimiters (which may be a comma, tab or space). Note that columns do not need to be aligned, as long as each entry is spaced by at least one delimiter. The first column in the table is used to look up SASD entries where the initial space-

delimited string after the SASD tag ("myfile" in "SASD myfile AZM=180...") must match the table. Subsequent columns can then be mapped to sample parameters or can be ignored, using a dialog window.

- **Rescale all** - Allows a series of selected SASD histograms to be put on a common scale by integrating them over a specific Q region and then scaling them so that the integration range will match the first pattern. (May not be valid for SASD)

5.10.6 Models

Small angle scattering models in GSAS-II have four different forms:

- **Size Dist.** – this represents the size distribution for particles of a selected shape (usually “spheroid”, but others possible) via maximum entropy or the Interior-Point Gradient (IPG) method. The result is a volume distribution of particle diameters in Å.
- **Particle Fit** – this gives the best fit of a suite of models for each component of the sample. Each model is chosen from a suite of possible descriptions, each with parameters that describe the shape, size (as a radius, Å) and magnitude.
- **Pair Distance** – this is used as the preliminary step in creating a “beads” model for the shape of a protein and gives the distribution of all interatomic vectors within the protein.
- **Shapes** – after a Pairs Distance distribution has been obtained, this develops a bead model for the protein shape that best satisfies the pair distance distribution using the SHAPES python algorithm developed by J. Badger.

What can I do here?

Menu **Models** –

- **Add** – this adds a distribution to a Particle Fit model
- **Fit** – this does the fitting of the model to the small angle data or bead model to the Pair Distance distribution (Shapes only).
- **Undo** – reverses the last fit operation. Can only be done once for a given fit result.
- **Sequential Fit** – does the fit to a sequence of SAD data. All must have the same model description.
- **Copy** – this copies the current model description to other SASD histograms
- **Copy flags** – this copies refinement flags from the current model to other SASD histograms with the same model.

5.11 Type **REFD** data tree entries: Reflectometry Data

5.11.1 Comments

This window shows whatever comment lines found above the QIE table when the reflectometry data file was read by GSAS-II. If you are lucky, there will be useful information here (e.g. sample name, date collected, wavelength used, etc.). If not, this window will be blank. The text is read-only.

5.11.2 Limits

This window shows the limits in position to be used in any fitting for this reflectivity pattern. The 'original' values are obtained from the minimum & maximum values in the reflectivity pattern. The 'new' values determine the range of data that will be used in fitting. Units are Q(Å-1) for CW data.

What can I do here?

You can change the "new" values for Tmin and Tmax as needed. Change the upper and lower Tmin values by clicking on the appropriate vertical line and dragging it to the right or left or by typing values into the data window.

Menu '**Edit Limits**'

- **Copy** - this copies the limits shown to other selected powder patterns. If used, a dialog box (Copy Parameters) will appear showing the list of available powder patterns, you can copy the limits parameters to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.

5.11.3 Instrument Parameters

This window shows the relevant instrument parameter for reflectivity data; namely a wavelength needed to properly calculate resonant scattering factors for x-rays or neutrons for the substances used in the reflectometry sample. It is not refinable.

What can I do here?

1. Menu '**Operations**' –
2. **Copy** – this copies the wavelength shown to other selected reflectivity data. If used, a dialog box (Copy parameters) will appear showing the list of available reflectivity data, you can copy the wavelength to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.
3. You can change the wavelength.

5.11.4 Substances

This window shows the substances that make up the reflectometry sample. By default, "vacuum" and "unit scatterer" are included; others can be added as needed. The reflectometry model is then constructed from layers of these substances.

What can I do here?

1. Menu '**Edit substance**' –
2. **Load substance** – select from a suite of various substance predefined by GSAS-II as defined in GSASII/Substances.py. You may add to this list by adding a file, UserSubstances.py, by following the substance format as described in Substances.py. Place your UserSubstances.py in the GSAS-II directory.
3. **Reload substances** – this recomputes the scattering contrast data for the substances.
4. **Add substance** – this allows one to enter a new substance that is not among the previously defined ones. Give it a name, element composition and volume/density; GSAS-II will compute the scattering contrast data for it.
5. **Copy substances** – this allows one to copy these defined substances to other small angle data histograms.

6. **Delete substance** – this allows one to remove any substance but not vacuum or unit scatterer.
7. **Add elements** – this allows one to add new element types to a selected substance.
8. **Delete elements** – this allows one to remove elements from a substance.
9. You can edit the composition by changing the number of each kind of element and change the sum of atomic volumes or the material density.

5.11.5 Sample Parameters

This window shows the various sample-dependent parameters for the selected reflectometry pattern. All values shown in this window can be edited. Note that the last three parameters (named `FreePrm` X, X=1,2,3) have labels that can be changed. If changed in one histogram, the same label is used for all histograms. When a label is changed, the Comments tree item for each REFD histogram is searched for a matching "Label=value" pair (differences in letter case between the two label strings is ignored). When found, the value is converted to a float and saved as the appropriate Sample Parameter.

What can I do here?

Command Menu - In this window you can change parameters associated with a histogram. This histogram scale factor is ignored for REFD. Remaining parameters are of use for parametric studies and may be changed with the menu commands described here.

- **Set scale** - Rescales a pattern by multiplying by the current scale factor. Scale factor is then set = 1.0. Useful for stitching together partial REFD scans
- **Load** - This loads sample parameters from a previously saved .samprm file.
- **Save** - This saves the sample parameters to a file with the extension '.samprm'. A file dialog box will appear to ask for the name of the file to be written.
- **Copy** - This copies the sample parameters shown to other selected REFD patterns. If used, a dialog box (Copy parameters) will appear showing the list of available powder patterns, you can copy the sample parameters to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.
- **Copy selected...** - This copies only the sample parameter that are selected to other selected REFD patterns but is otherwise similar to "Copy".
- **Copy flags** - (Not valid for REFD).
- **Set one value** - This is used to set a single selected sample parameter for a selected set of REFD histograms. The same value can be used for all histograms or a dialog can be used to provide a table where you can set the values differently for each of selected histograms.
- **Load all** - Reads a file containing a table of sample parameters and copies them to matching REFD entries. The file will look something like the example here:

```
#filename       temperature pressure ignore-me  humidity
LaB6_dc250.tif      100          1      test       .2
LaB6_dc300.tif      150          1      test       .25
```

  Note that the first line(s) in the file can be a header, but each header line must start marked with a hash (#). A header is not required. "Columns" in the table are separated by one or more delimiters (which may be a comma, tab or space). Note that columns do not need to be aligned, as long as each entry is spaced by at least one delimiter. The first column in the table is used to look up REFD entries where the initial space-delimited string after the REFD tag ("myfile" in " REFD myfile AZM=180...") must match the table. Subsequent columns can then be mapped to sample parameters or can be ignored, using a dialog window.

- **Rescale all** - Allows a series of selected REFD histograms to be put on a common scale by integrating them over a specific Q region and then scaling them so that the integration range will match the first pattern. (May not be valid for REFD)

5.11.6 Models

A reflectometry model is composed of a sequence of layers beginning with the medium ("superphase") as the top layer in which the incident and scattered radiation paths are located (usually "vacuum" = air or other gasses) and ending with the bottom layer ("substrate") upon which the sample layers have been deposited. The substrate is considered to be "infinite" in thickness. The sample layers in between are each defined as a particular substance with a thickness and upper surface "roughness". The surface roughness describes the possibility of an interlayer mixing with the previous layer. Their scattering density can also be scaled and could include polarized magnetic neutron scatterers. The layer sequence is defined so that complex or multiple layers can be defined.

What can I do here?

Command Menu –

- **Fit** – This attempts a refinement by one of 4 different methods of the reflectometry model to the data.
- **Undo** – This reverses the result of a bad refinement; can only be done once.
- **Sequential fit** – This attempts a fit for a sequence of REFD patterns; each has their own model description so one should ensure they are all similar.
- **Copy** – Copy the present model to other REFD patterns.
- **Plot** – Plot the scattering length density (SLD) with respect to the distance from the top surface in Å. Results from multiple REFD fits can be superimposed

5.12 Type PKS data tree entries: Powder Diffraction Peaks

Powder diffraction peaks are read with the Data/"Read Powder Pttern Peaks" menu command. Powder peaks can only be used for indexing of the peak positions for possible unit cells.

5.12.1 Comments

This window shows whatever comment lines (preceded by "#") found when the peaks data file was read by GSAS-II. If you are lucky, there will be useful information here (e.g. sample name, date collected, wavelength used, etc.). If not, this window will be blank. The text here is read-only.

5.12.2 Limits

This window shows the limits in position to be used in indexing from these peak positions. The 'original' values are obtained from the minimum & maximum 1st & last position. The 'new' values determine the range of data that will be used in fitting. Units are 2θ.

What can I do here?

You can change the "new" values for Tmin and Tmax as needed. Change the upper and lower Tmin values by clicking on the appropriate vertical line and dragging it to the right or left or by typing values into the data window.

Menu "Edit Limits" contents

- **Copy** - this copies the limits shown to other selected powder patterns. If used, a dialog box (Copy Parameters) will appear showing the list of available peaks list patterns, you can copy the limits parameters to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.

5.12.3 Instrument Parameters

This window shows the relevant instrument parameters for a peaks list; namely a wavelength and zero needed to relate d-spacing to 2θ. Neither are refinable.

What can I do here?

1. Menu '**Operations**' – (many are irrelevant & will probably be removed at some point; only useful ones will be mentioned below).
    - **Reset profile** – resets the values for the instrument parameters to the default values shown in parentheses for each entry.
    - **Load profile...** - loads a GSAS-II instrument parameter file (name.instprm), replacing the existing instrument parameter values. All refinement flags are unset.
    - **Save profile...** - saves the current instrument parameter values in a simple text file (name.instprm); you will be prompted for the file name – do not change the extension. This file may be edited but heed the warning to not change the parameter names, the order of the parameter records or add new parameter records as this will invalidate the file. You may only change the numeric values if necessary. You can change or add comment records (begin with '#').
    - **Copy** – this copies the instrument parameters shown to other selected powder patterns. If used, a dialog box (Copy parameters) will appear showing the list of available powder patterns, you can copy the instrument parameters to any or all of them; select 'All' to copy them to all patterns. Then select 'OK' to do the copy; 'Cancel' to cancel the operation.
2. You can change any of the instrument coefficients

5.12.4 Index Peak List

This window shows the list of peaks that will be used for indexing (see Unit Cells List). It was filled when the import of the peaks list was done. It shows 2θ position as input or calculated from provided d-spacing and wavelength given in Instrument Parameters. Note that peaks from a neutron TOF pattern could be entered here as d-spacings in descending order and a suitable wavelength used in the Instrument Parameters. When indexing is

completed, this display will show the resulting hkl values for every indexed reflection along with the calculated d-spacing ('d-calc') for the selected unit cell in Unit Cells List.

What can I do here?

1. You may deselect individual peaks from indexing by unchecking the corresponding 'use' box.

5.12.5 Unit Cells List

This tree item has several purposes, it can be used to perform autoindexing and it can be used to show the positions of peaks from unit cells which may be results from autoindexing or may be entered from a phase or manually. It can be used to refine unit cell parameters. It can also be used to search for cells/symmetry settings related to a specified unit cell & space group.

What can I do here?

For autoindexing, the peaks in the Index Peak List are used. Select one or more Bravais lattice types to use and use the "Cell Index/Refine"/"Index Cell" menu command to start indexing. Output will appear on the console and a progress bar dialog will appear which tracks trial volume. A Cancel button will terminate indexing; it may need to be pressed more than once to fully terminate the indexing process. Console output shows possible solutions with a computed M20 for each; good solutions are indicated by high M20 values. X20 gives number of unindexed lines out of the 1st 20 lines and Nc gives total number of reflections generated for each solution.

The "Copy Cell" menu command copies a selected solution to the Unit cell values; the Bravais lattice shown for the choice is copied. Press **Show hkl positions** to generate the allowed reflection positions, which are visually superimposed on the displayed powder pattern to visually confirm the indexing. Pay particular attention to any unmatched peaks in the pattern. A Space group can be selected from the pulldown box to remove reflections based on space group extinctions and visually eliminate possibilities.

- Max Nc/Nobs: – this controls the extent of the search for the correct indexing. This may need to be increased if an indexing trial terminates too quickly. It rarely needs to be changed.
- Start Volume: – this sets an initial unit cell volume for the indexing. It rarely needs to be changed.
- Select "keep" in the table for a cell that should be preserved when an additional indexing run is tried; all without that are erased before the indexing trial begins.

To display a unit cell, optionally with space group extinctions, set a Bravais class (see list) to determine a unit cell type, optionally select a space group (by default the highest symmetry space group for the class is selected) and enter the unit cell parameters. Or use the "Cell Index/Refine"/"Load Phase" menu command to read this information from a phase that has been read into a project or from a file (such as a CIF) using the "Cell Index/Refine"/"Import Cell" menu command.

For symmetry exploration, once a phase/cell has been loaded, use the "Run SUBGROUPS", "Cell Symmetry Search" or "Run k-SUBGROUPSMAG" commands from the "Cell Index/Refine" menu. These commands look for: subgroups, lower symmetry cells or magnetic subgroups, respectively. Also note the "Transform Cell" command in that menu that can perform many common lattice transformations, apply a user-supplied cell transformation or create a magnetic phase.

To optimize a cell, to fit the peaks in the Index Peak List, use the "Cell Index/Refine"/"Refine Cell" menu command. The results will be placed in the Indexing Result table with 'use' selected.

Other: The "Make new phase" command creates a new phase from the selected unit cell and chosen space group. A dialog box will appear asking for a name for this phase. See the new entry under Phases and the new lattice parameters will be in the General window for that phase.

6. Miscellaneous information

6.1 Macintosh notes:

GSAS-II can be run on Windows, Linux and Macintosh/OS X computers, but the GUI follows the native style of the window manager where it is run, so GSAS-II will look more like a Mac application on that platform and more like a Windows application there. On Windows and some versions of Linux, the menu bars appears on top of the main window. On the Mac, the menu appears at the location that has been configured for menus (usually at the top of the screen). At present, two versions of GSAS-II are provided. One is for older, Intel CPUs and the other for "Apple Silicon" (ARM or M1, M2,...) CPUs. Eventually only ARM CPUs will be supported. At present, the Intel version will run on ARM machines under Rosetta, but eventually Rosetta will also go away.

GSAS-II defines actions for both the left and right and middle buttons assuming that a three-button mouse is available. If a two or three-button mouse is used with a Mac, the "extra" mouse buttons will work as intended. If using a Mac touchpad or single-button mouse, clicking the touchpad or pressing the mouse button will generate a "left button" click. Hold down the control-key to generate a "right button" click or for a right-button drag, hold down control while pressing on the mouse button or touchpad. I do not know how to generate a middle-button click or drag with a single-button mouse, but with a MacBook touchpad, pressing with two fingers generates the equivalent of a right-mouse drag and moving two fingers without pressure is the equivalent of a middle-button drag action.

6.2 Windows notes:

When GSAS-II is installed through most of the conventional installation methods, the `GSASII\install\MakeBat.py` file is run and this creates two "Windows .bat" files that can be used to make running GSAS-II easier as well as making some minor Windows registry changes. This script can be run manually by people who are installing GSAS-II directly from GitHub.

The `MakeBat.py` script creates a file named `RunGSASII.bat` file, which is placed in the directory where GSAS-II is installed and a shortcut to this file is placed on the Windows desktop. The shortcut can be moved, renamed etc. Clicking on this file or shortcut will start GSAS-II.

Another file, `2Reset2FreshGSASII.bat` is created in the same directory. Ideally, this will not be needed, but might be of use if GSAS-II cannot be started due to changes made in the files locally or because we have put out a bad version. By double-clicking on the `2Reset2FreshGSASII.bat` file, the `gitstrap.py` script that is used to install GSAS-II will be updated to the latest version and then run that in a mode that will reset any changes that have been made to the GSAS-II files on your computer. It will also rerun the `MakeBat.py` script.

6.3 Configuration Variables:

GSAS-II provides a number of configuration settings that can be changed via variables that can be set and saved. These are controlled in the File/ Preferences menu item (on Mac the Preferences menu is found in the usual place on Macs, in the main application menu as well as in the File menu). These settings are saved for subsequent runs in a file named `config.ini` in the user's `.GSASII` directory. More information, including a list of the available configuration variables and their use can be found in the `config_example.py` file or the Configuration variables section of the Programmer's documentation.

6.4 Programmers' documentation

The routines and classes used within GSAS-II are documented in a set of [web pages]((https://gsas-ii.readthedocs.io/en/latest) and in a PDF document with >400 pages. This documentation is created from the Python source code files using Sphinx. There is also an abbreviated form of the documentation intended for people developing scripting applications only, or as a PDF.

6.5 Origin 1 -> Origin 2 Transformations

An important transformation may be needed in certain cases for space groups that have two alternate origin settings listed here. These are centrosymmetric space groups where the highest symmetry point in the structure does not contain a center of symmetry. Origin 1 places the origin at the highest symmetry setting while Origin 2 places the origin at a center of symmetry (creating a -x,-y,-z symmetry operator, which means that reflection phases can only be 0 or π.) GSAS-II requires use of the Origin 2 settings because computations are much faster and simpler without

complex structure factors. Alas, the literature contains a number of structures reported in Origin 1, where the origin choice may not be clearly communicated. (The CIF standard does not require that origin choice be indicated.) When a structure is imported that uses any of the space groups where an origin choice is possible, a message is shown in GSAS-II notifying the user that they must confirm that the origin choice is correct and then provides the opportunity to change origins.

Example: An example of what can go wrong is illustrated with the structure of anatase. The space group is $I\ 4_1/a\ m\ d$. The coordinates for the two origin choices are:

6.5.1 Origin 1

Atom	X	Y	Z
Ti	0	0	0
O	0	0	0.208

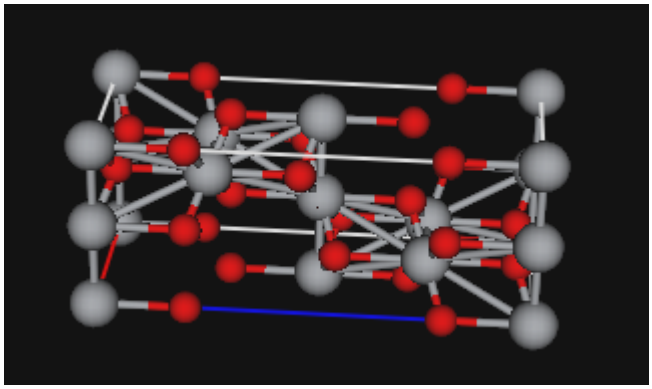
6.5.2 Origin 2

Atom	X	Y	Z
Ti	0	1/4	-1/8
O	0	1/4	0.083

Note that the Origin 2 coordinates are shifted by by addition of (0,1/4,-1/8) relative to those in Origin 1 (the values in the GSASIIspc.spg2origins array).

GSAS-II always uses the symmetry operators for Origin 2; if the structure is input incorrectly with the coordinates set for Origin 1, there are several obvious signs of problems:

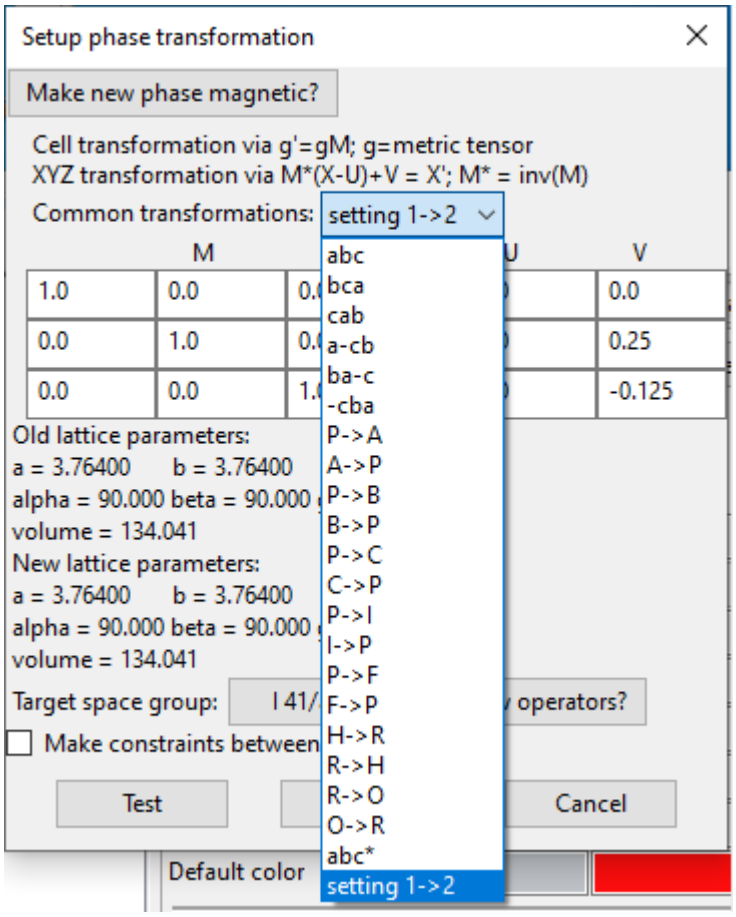
- the site symmetries and multiplicities are wrong, often giving an incorrect chemical formula,
- the interatomic distances are incorrect
- a plot of the structure is improbable, as below:



In this case incorrect multiplicities gives rise to a density of 7.9 g/cc, double the correct value. Impossible interatomic distances of 1.88Å for Ti-Ti, and 1.39Å for Ti-O are seen. The unit cell contents with the wrong space group operators is shown above.

With coordinates that match the space group operations, the correct Ti-O distances are 1.92Å and 1.97Å and the shortest Ti-Ti distance is 3.0Å. (Note that interatomic distances can be computed in GSAS-II using the Phase's Atoms tab and the Compute/"Show Distances & Angles" menu item.)

Transform Origin: To transform a space group setting from Origin setting 1 to 2, use the Transform option in the Compute menu of a Phase's General tab and then select the last option in the "Common transformations" pulldown menu, which will be setting 1->2 for space groups where both origins are available, as shown to the right. The transformation matrix will be set to the identity and the "V" vector will have the required origin shift loaded. Press OK. The changes can be seen by selecting the Atoms tab.



6.6 Fundamental Parameters as used to derive instrumental parameters

This describes the FPA terms used to determine instrumental parameters in the "Fit Instr. profile from fundamental parms...". These follow the general usage in the Topas program. They are converted to the values needed by the NIST code. Parameters names are listed in bold, followed by units in parentheses and are then described.

6.6.1 Basic Bragg-Brentano parameters

- **divergence (degrees)** - Angle in equatorial plane describing the sample illumination for a Bragg-Brentano instrument
- **soller_angle (degrees)** - Angular limit for divergence in equatorial plane as limited by Soller collimator(s)
- **Rs (mm)** - Diffractometer radius: source to sample and sample to detector distance
- **filament_length (mm)** - Length of x-ray filament when used in “line-focus” (filament oriented along the axial direction)
- **sample_length (mm)** - Illuminated sample length in axial direction. Typically the same as filament_length.
- **receiving_slit_length (mm)** - Length of the receiving slit in axial direction. Typically the same as filament_length.
- **LAC_cm (cm^{-1})** - : The linear absorption coefficient adjusted for the sample packing density.
- **sample_thickness (mm)** - Thickness of sample measured along the radial direction in the equatorial plane
- **convolution_steps (none)** - The number of steps used for convolution for each step in the diffraction pattern. This results in more smooth convolutions.
- **source_width (mm)** - Width of x-ray filament in projection in the equatorial plane.
- **tube-tails_L-tail (mm)** - Width for x-ray intensity occurring beyond the Wehnelt shadow as a projection in the axial direction and measured in the positive two-theta direction.
- **tube-tails_R-tail (mm)** - Width for x-ray intensity occurring beyond the Wehnelt shadow as a projection in the axial direction and measured in the negative two-theta direction.

- **tube-tails_rel-I (none)** - Fractional of x-ray intensity found in the tube tails vs. the main peak. Note that tube tails are modeled as a step function.

6.6.2 Point detector parameter

- **receiving_slit_width (mm)** - Width of receiving slit placed in front of detector or possibly the diffracted beam monochromator (analyzer) measured in the equatorial plane

6.6.3 Linear position-sensitive detector parameter

- **SiPSD_th2_angular_range (degrees)** - Angular (two-theta) range in equatorial plane that the entire Si PSD subtends (not implemented in Topas)

6.6.4 Incident-beam monochromator (IBM) parameters

- **src_mono_mm (mm)** - Distance between the x-ray source (filament) and the monochromator, measured in the equatorial plane
- **focus_mono_mm (mm)** - Distance from monochromator crystal to focus slit, measured in the equatorial plane
- **passband_mistune (none)** - Offset for the tuning of the IBM to the center of the reference line of the spectrum, as a fraction of the IBM bandwidth
- **mono_src_proj_mn (micron)** - Bandwidth setting for the monochromator as set by the projection width of the xray source on the monochromator along beam direction and in the equatorial plane
- **passband_shoulder (none)** - Width of transition region from high-intensity, roughly flat region of the x-ray tube output to the to the tube tails region as a fraction of the IBM bandwidth
- **two_theta_mono (degrees)** - The full diffraction angle of the IBM crystal. This will be double the Bragg two-theta angle for the monochromator
- **mono_slit_attenuation (none)** - The attenuation of the Cu K alpha 2 source lines relative to the K alpha 1 lines as determined by the focal slit

If you use this, please cite M.H. Mendenhall, K. Mullen & J.P. Cline (2015), J. Res. of NIST, 120, p223. DOI: 10.6028/jres.120.014. If the incident beam monochromator model is used, please also cite: M.H. Mendenhall, D. Black & J.P. Cline (2019), J. Appl. Cryst., 52, p1087. DOI: 10.1107/S1600576719010951.

6.7 Applying corrections when reading powder data:

A special parameter can be added manually to a `.instparm` instrument parameter that will apply systematic changes to the position (usually 2θ), intensity or weight values. An example showing how this is done follows:

```
#GSAS-II instrument parameter file; manually edited by B.H.Toby to show how to use CorrectionCode
Lam:0.72768
SH/L:0.002
...
Polariz.:0.99
Type:PXC
Bank:1

CorrectionCode:'''# Example 2theta correction (applied via numpy array correction; fast!)
print('2theta before', rd.powderdata[0][:3],'...',rd.powderdata[0][-2:])
TT = rd.powderdata[0]
rd.powderdata[0] += 0.06038972 - 0.001500277 * TT + 7.389e-06 * TT**2
print('2theta after', rd.powderdata[0][:3],'...',rd.powderdata[0][-2:])
'''
#
# alternate example. This applies a correction point-by-point in a loop
#
#CorrectionCode:'''#apply 2theta correction in a loop
#print '2T before', rd.powderdata[0][:3],'...',rd.powderdata[0][-3:]
#for i,TT in enumerate(rd.powderdata[0]):
#    rd.powderdata[0][i] += 0.06038972 - 0.001500277 * TT + 7.389e-06 * TT**2
#print('2T after', rd.powderdata[0][:3],'...',rd.powderdata[0][-3:])
#'''
```