GSAS-II Scripting Documentation

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This is a subset of the Developer's Documentation covering the `GSASIIscriptable` package, used to create Python scripts for running GSAS-II. Note that most data structures used in GSAS-II are defined in module `GSASIIobj`, also included here.

CHAPTER

ONE

GSASIISCRIPTABLE: SCRIPTING INTERFACE

1.1 Summary/Contents

GSASIIscriptable provides routines to use an increasing amount of GSAS-II's capabilities from Python scripts, without use of the graphical user interface (GUI). GSASIIscriptable can create and access GSAS-II project (.gpx) files and can directly perform image handling, peak fits, refinements… The .gpx files are completely compatible with the GUI, so one can move back and forth between the GUI and scripting when developing scripts. This mode of code development is encouraged to get started with GSAS-II scripting.

GSASIIscriptable is normally used by writing Python commands via this module's application programming interface (API). (There is also an older mechanism where GSASIIscriptable can be accessed via shell/batch commands, see *GSASIIscriptable Command-line Interface*, called command-line mode.) Access to GSASIIscriptable via the API is used more widely than via command-line mode and offers many more features. The material below introduces and summarizes use of GSASIIscriptable via the API. Following that, detailed descriptions of all routines are provided in the *complete API documentation* section.

While the command-line mode provides access a number of features without writing Python scripts via shell/batch commands (see *GSASIIscriptable Command-line Interface*), use in practice seems somewhat clumsy. Command-line mode is no longer being developed and its use is discouraged.

GSASIIscriptable is designed around the hierarchical structure of .gpx files, that is seen in the GUI as the GSAS-II data tree. The module defines wrapper classes (inheriting from `G2ObjectWrapper`) for most GSAS-II data tree items, so most scripting is done with object-oriented code that operate on different types of data tree objects. At the top level one has a project (`G2Project`) which contains phases (`G2Phase`) powder diffraction histograms (`G2PwdrData`).

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1.2 Installation of GSASIIscriptable

GSASIIscriptable is included as part of a standard GSAS-II installation that includes the GSAS-II GUI (as described in the installation instructions). People who will will use scripting extensively will still need access to the GUI for some activities, since the scripting API does not cover all features of GSAS-II. Even if that were to be completed, there will still be some things that GSAS-II does with the GUI would be almost impossible to implement without a interactive graphical view of the project.

Nonetheless, there may be times where it does make sense to install GSAS-II without all of the Python packages needed for running the GUI, for example on a compute server or cluster. The minimal requirements for use of GSASIIscriptable are:

- python
- numpy
- scipy

GSASIIscriptable can be used without these packages, but with significantly reduced functionality, so their inclusion is highly recommended:

- PyCifRW
- requests

There are a few other packages that may be used in GSASIIscriptable, for example to import specific types of powder or image data or perform specific types of computations. They are not commonly needed, but if access is attempted, it should be obvious from error messages:

- h5py
- xmltodict
- pybaselines
- seekpath
- matplotlib
- pillow

More information on Python packages used in GSAS-II is provided in the *Scripting Requirements* section of the Requirements chapter, which also provides some installation instructions.

1.3 Accessing the GSASIIscriptable Module

When GSAS-II is installed with GSAS2MAIN or GSAS2PKG, or with the `gitstrap.py` script, or directly with git, the GSAS-II software is installed outside of Python. When the GUI is invoked, a small script or Windows batch file is used to invoke Python with a reference to a file (named `G2.py`) that starts the GSAS-II GUI. It is also possible to install GSAS-II inside Python (for example with pixi), but work on this is not yet complete or documented.

When GSASIIscriptable is used, and GSAS-II has been installed outside of Python, some mechanism is needed to provide the location of the GSAS-II files. There are two ways this can be done:

1. define the GSAS-II installation location in the Python `sys.path`, or

2. install a reference to GSAS-II inside the Python installation.

The latter method requires an extra installation step, but has the advantage that it allows writing portable GSAS-II scripts.

1.3.1 Explicit GSASIIscriptable Specification

MacOS/Linux:

The example below is for MacOS/Linux and assumes that GSAS-II has been installed in location `/Users/toby/g2main/` such that there is a directory `/Users/toby/g2main/GSAS-II/GSASII` that contains all the GSAS-II Python files such as `GSASIIscriptable.py`. Place code like this into the beginning of your script so that the location of GSAS-II files can be found:

```
import sys
sys.path.insert(0,'/Users/toby/g2main/GSAS-II') # needed to find GSASII␣
↪package
from GSASII import GSASIIscriptable as G2sc
```

Windows:

A similar example, but for Windows, assumes that GSAS-II has been installed in location `C:\Users\toby\gsas2main` such that there is a directory `C:\Users\toby\gsas2main\GSAS-II\GSASII` that contains all the GSAS-II Python files such as `GSASIIscriptable.py`. Place code like this into the beginning of your script (note that use of forward slashes is deliberate; to use back slashes, they must be doubled or placed in a raw-string, `'C:\\Users\\...'` or `r'C:\Users\...'`):

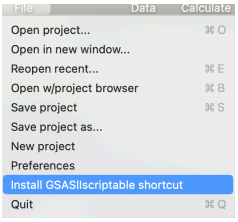
```
import sys
sys.path.insert(0,'/Users/toby/gsas2main/GSAS-II') # needed to find GSASII␣
↪package
from GSASII import GSASIIscriptable as G2sc
```

Note that the directory that is placed in the path is the one that contains the `GSASII` directory. Previously, this path contained this directory, but now is its parent.

1.3.2 Install GSASIIscriptable Location Into Python

As an alternative to defining the location of GSAS-II in every script, you can define the location of GSAS-II inside Python *once*, but note that this must be done for each version of Python, if you plan to use GSAS-II scripting with more that one. If you have more than one version of GSAS-II installed, only one can be defined for a Python installation, but the previous method, where `sys.path` is modified, can be used with all of the GSAS-II installions.

There are three different ways to use GSAS-II to define a location for GSASIIscriptable. You can choose the method that is easiest for you.



1. The most easy option is to invoke the "Install GSASIIscriptable shortcut" command in the GSAS-II GUI File menu.

   This performs the same actions as below, but since the location of both Python and the GSAS-II files are defined within the GUI, no additional input is needed.

2. Alternatively, using the commands modeled after the ones above, add the Python command `G2sc.installScriptingShortcut()` into your script as:

```
import sys
sys.path.insert(0,'/Users/toby/gsas2main/GSAS-II') # needed to find␣
↪GSASII package
from GSASII import GSASIIscriptable as G2sc
G2sc.installScriptingShortcut()
```

   This only needs to be done once. After the script has been run, remove the command or comment it out.

3. The third choice is to run two command-line (bash/zsh/DOS,…) commands. This assumes that the intended Python interpreter is already in the path. (If not use a conda activate command.) Note that the directory that is used is the parent of the `GSASII` directory (the directory that contains `GSASII`.)

   Here are the commands on **MacOS/Linux**:

```
% cd /Users/toby/gsas2main/GSAS-II
% python -c "import GSASII.GSASIIscriptable as G2sc; G2sc.
↪installScriptingShortcut()"
```

   On **Windows** the commands in a cmd.exe window will be similar:

```
>cd \Users\toby\gsas2main\GSAS-II
>python -c "import GSASII.GSASIIscriptable as G2sc; G2sc.
↪installScriptingShortcut()"
```

   The output from this process on Windows is shown below.

```
C:\Users\toby>gsas2main\Scripts\activate

(base) C:\Users\toby>cd gsas2main\GSAS-II

(base) C:\Users\toby\gsas2main\GSAS-II>python -c "import GSASII.GSASIIscriptable as G2sc; G2sc.installScriptingShortcut()"
3 values read from C:\Users\toby\.GSASII\config.ini
GSAS-II binary directory: C:\Users\toby\gsas2main\GSAS-II\GSASII-bin\win_64_p3.13_n2.2
Created file C:\Users\toby\gsas2main\Lib\site-packages\G2script.py
setting up GSASIIscriptable from C:\Users\toby\gsas2main\GSAS-II\GSASII
success creating C:\Users\toby\gsas2main\Lib\site-packages\G2script.py
```

Once any of the above three choices has been completed, a good test to see if GSASIIscriptable is working will be commands:

```
import G2script as G2sc
print(G2sc.ShowVersions())
```

as is shown in the image below.

```
(base) C:\Users\toby\gsas2main\GSAS-II>python
Python 3.13.3 | packaged by conda-forge | (main, Apr 14 2025, 20:31:24) [MSC v.1943 64 bit (AMD64)] on win32
Type "help", "copyright", "credits" or "license" for more information.
>>> import G2script as G2sc
setting up GSASIIscriptable from C:\Users\toby\gsas2main\GSAS-II\GSASII
3 values read from C:\Users\toby\.GSASII\config.ini
GSAS-II binary directory: C:\Users\toby\gsas2main\GSAS-II\GSASII-bin\win_64_p3.13_n2.2
>>> print(G2sc.ShowVersions())
  Python      3.13.3:  from C:\Users\toby\gsas2main\python.exe
  numpy       2.2.5:
  scipy       1.15.2:
  GSAS-II:    6c26ef37, 25-Apr-2025 15:26 (0.0 days old). Tag: #5806, v5.3.3

GSAS-II location: C:\Users\toby\gsas2main\GSAS-II\GSASII
Binary location:  C:\Users\toby\gsas2main\GSAS-II\GSASII-bin\win_64_p3.13_n2.2 (5805, v5.2.0)

>>>
```

1.3.3 When GSAS-II is Installed Inside Python

If GSAS-II is installed inside of Python, the location of the GSAS-II software is established without any changes to the path so this command should work without using any of the above:

```
from GSASII import GSASIIscriptable as G2sc
```

1.4 Application Interface (API) Summary

This section of the documentation provides an overview to API, with full documentation in the *API: Complete Documentation* section. The typical API use will be with a Python script, such as what is found in *Code Examples*. Most functionality is provided via the objects and methods summarized below.

1.4.1 Overview of Classes

Scripting class name	Description
G2Project	`G2Project`: A GSAS-II project file; provides references to objects below, each corresponding to a tree item (exception is `G2AtomRecord`)
G2Phase	`G2Phase`: Provides phase information access (also provides access to atom info via `G2AtomRecord`)
G2AtomRecord	`G2AtomRecord`: Access to an atom within a phase
G2PwdrData	`G2PwdrData`: Access to powder histogram info
G2Single	`G2Single`: Access to single crystal histogram info
G2Image	`G2Image`: Access to image info
G2PDF	`G2PDF`: PDF histogram info
G2SmallAngle	`G2SmallAngle`: Small Angle scattering histogram info
G2SeqRefRes	`G2SeqRefRes`: The sequential results table

1.4.2 Independent Functions

A small number of Scriptable routines do not require existence of a G2Project object.

method	Use
`ShowVersions()`	Shows Python and GSAS-II version information
`GenerateReflections()`	Generates a list of unique powder reflections
`SetPrintLevel()`	Sets the amount of output generated when running a script
`installScriptingShortcut()`	Installs GSASIIscriptable within Python as G2script

1.4.3 Class `G2Project`

All GSASIIscriptable scripts will need to create a `G2Project` object either for a new GSAS-II project or to read in an existing project (.gpx) file. The table below is not complete but does contain the most commonly used methods in this object:

method	Use
`save()`	Writes the current project to disk.
`add_powder_histogram()`	Used to read in powder diffraction data into a project file.

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method	Use
add_simulated_powder_histogram()	Defines a "dummy" powder diffraction data that will be simulated after a refinement step.
add_image()	Reads in an image into a project.
add_phase()	Adds a phase to a project
add_PDF()	Adds a PDF entry to a project (does not compute it)
add_single_histogram()	Used to read in a single crystal diffraction dataset into a project file.
add_SmallAngle()	Adds a small-angle scattering histogram to a project
histograms()	Provides a list of histograms in the current project, as *G2PwdrData* or as *G2Single* objects.
histogram()	Finds a histogram from an object, name or random id reference, returning a a *G2PwdrData* or *G2Single* object.
histType()	Determines the histogram type from an object, name or random id reference.
phases()	Provides a list of phases defined in the current project, as *G2Phase* objects
phase()	Finds a phase from an object, name or random id reference, returning a a *G2Phase* object.
images()	Provides a list of images in the current project, as *G2Image* objects
image()	Finds an image from an object, name or random id reference, returning a a *G2Image* object.
pdfs()	Provides a list of PDFs in the current project, as *G2PDF* objects
seqref()	Returns a *G2SeqRefRes* object if there are Sequential Refinement results
do_refinements()	This is passed a list of dictionaries, where each dict defines a refinement step. Passing a list with a single empty dict initiates a refinement with the current parameters and flags. A refinement dict sets up a single refinement step (as described in *Project-level Parameter Dict*). Also see *Refinement recipe*.
set_refinement()	This is passed a single dict which is used to set parameters and flags. These actions can be performed also in *do_refinements()*.
get_Variable()	Retrieves the value and esd for a parameter
get_Covariance()	Retrieves values and covariance for a set of refined parameters
set_Controls()	Set overall GSAS-II control settings such as number of cycles and to set parameter limits. This is also used to set up a sequential fit. (Also see *get_Controls()* to read values.)
get_LastFitResults()	Retrieves the shifts and sigma values from the last least-squares cycle
imageMultiDistCalib()	Performs a global calibration fit with images at multiple distance settings.
get_Constraints()	Retrieves *constraint definition* entries.
add_HoldConstr()	Adds a hold constraint on one or more variables
add_EquivConstr()	Adds an equivalence constraint on two or more variables

continues on next page

Table 1 – continued from previous page

method	Use
add_EqnConstr()	Adds an equation-type constraint on two or more variables
add_NewVarConstr()	Adds an new variable as a constraint on two or more variables
ComputeWorstFit()	Determines the parameters that will have the greatest impact on the fit if refined
get_Frozen()	Find variables where parameters have refined out of the parameter limit ranges. Note that parameter limits are set using *set_Controls()*.
set_Frozen()	Adds or removes variables from the list where parameters have refined outside of their limits. Note that parameter limits are set using *set_Controls()*.

1.4.4 Class `G2Phase`

Another common object in GSASIIscriptable scripts is *G2Phase*, used to encapsulate each phase in a project, with commonly used methods:

method	Use
set_refinements()	Provides a mechanism to set values and refinement flags for the phase. See *Phase parameters* for more details. This information also can be supplied within a call to *do_refinements()* or *set_refinement()*.
clear_refinements()	Unsets refinement flags for the phase.
set_HAP_refinements()	Provides a mechanism to set values and refinement flags for parameters specific to both this phase and one of its histograms. See *Histogram-and-phase parameters*. This information also can be supplied within a call to *do_refinements()* or *set_refinement()*.
clear_HAP_refinements()	Clears refinement flags specific to both this phase and one of its histograms.
getHAPvalues()	Returns values of parameters specific to both this phase and one of its histograms.
copyHAPvalues()	Copies HAP settings between from one phase/histogram and to other histograms in same phase.
HAPvalue()	Sets or retrieves values for some of the parameters specific to both this phase and one or more of its histograms.
atoms()	Returns a list of atoms in the phase
atom()	Returns an atom from its label
add_atom()	Adds an atom to a phase
histograms()	Returns a list of histograms linked to the phase
get_cell()	Returns unit cell parameters (also see *get_cell_and_esd()*)
export_CIF()	Writes a CIF for the phase
setSampleProfile()	Sets sample broadening parameters
clearDistRestraint()	Clears any previously defined bond distance restraint(s) for the selected phase
addDistRestraint()	Finds and defines new bond distance restraint(s) for the selected phase
setDistRestraintWeight()	Sets the weighting factor for the bond distance restraints
Origin1to2Shift()	Shifts the atom coordinates from an Origin 1 setting to the Origin 2 setting

1.4.5 Class `G2PwdrData`

Another common object in GSASIIscriptable scripts is *G2PwdrData*, which encapsulate each powder diffraction histogram in a project, with commonly used methods:

method	Use
set_refinements()	Provides a mechanism to set values and refinement flags for the powder histogram. See *Histogram parameters* for details.
clear_refinements()	Unsets refinement flags for the powder histogram.
residuals()	Reports R-factors etc. for the powder histogram (also see *get_wR()*)
add_back_peak()	Adds a background peak to the histogram. Also see *del_back_peak()* and *ref_back_peak()*.
fit_fixed_points()	Fits background to the specified fixed points.
set_background()	Sets a background histogram that will be subtracted (point by point) from the current histogram.
calc_autobkg()	Estimates the background and sets the fixed background points from that.
getdata()	Provides access to the diffraction data associated with the histogram.
reflections()	Provides access to the reflection lists for the histogram.
Export()	Writes the diffraction data or reflection list into a file
add_peak()	Adds a peak to the peak list. Also see *Peak Fitting*.
set_peakFlags()	Sets refinement flags for peaks
refine_peaks()	Starts a peak/background fitting cycle, returns refinement results
Peaks	Provides access to the peak list data structure
PeakList	Provides the peak list parameter values
Export_peaks()	Writes the peak parameters to a text file
Limits()	Reads or sets the region of data used in fitting (histogram limits)
Excluded()	Reads or sets regions of powder data that will be ignored
ComputeMassFracs()	Reports mass (weight) fractions and their uncertainties

1.4.6 Class `G2Single`

A less commonly-used object in GSASIIscriptable scripts is *G2Single*, which will encapsulate each single crystal diffraction histogram in a project. At present, very few methods are provided:

method	Use
set_refinements()	Provides a mechanism to set refinement flags for the single crystal histogram. See *Histogram parameters* for details.
clear_refinements()	Unsets refinement flags for the single crystal powder histogram.
Export()	Writes the reflection list into a file

1.4.7 Class `G2Image`

When working with images, there will be a *G2Image* object for each image (also see *add_image()* and *images()*).

method	Use
Recalibrate()	Invokes a recalibration fit starting from the current Image Controls calibration coefficients.
Integrate()	Invokes an image integration All parameters Image Controls will have previously been set.
GeneratePixelMask()	Searches for "bad" pixels creating a pixel mask.
setControl()	Set an Image Controls parameter in the current image.
getControl()	Return an Image Controls parameter in the current image.
findControl()	Get the names of Image Controls parameters.
loadControls()	Load controls from a .imctrl file (also see *saveControls()*).
loadMasks()	Load masks from a .immask file.
setVary()	Set a refinement flag for Image Controls parameter in the current image. (Also see *getVary()*)
setCalibrant()	Set a calibrant type (or show choices) for the current image.
setControlFile()	Set a image to be used as a background/dark/gain map image.
getControls()	Returns the Image Controls dict for the current image.
setControls()	Updates the Image Controls dict for the current image with specified key/value pairs.
getMasks()	Returns the Masks dict for the current image.
setMasks()	Updates the Masks dict for the current image with specified key/value pairs.
getImage()	Returns the image array for the current image.
IntThetaAzMap()	Computes the set of 2theta-azimuth mapping matrices to integrate the current image.
IntMaskMap()	Computes the masking map for the current image for integration.
MaskThetaMap()	Computes the 2theta mapping matrix to determine a pixel mask.
MaskFrameMask()	Computes the Frame mask needed to determine a pixel mask.
TestFastPixelMask()	Returns True if fast pixel masking is available.
clearImageCache()	Clears a saved image from memory, if one is present.
clearPixelMask()	Clears a saved Pixel map from the project, if one is present.
loadPixelMask()	Loads a Pixel map from an array

1.4.8 Class G2PDF

To work with PDF entries, object *G2PDF*, encapsulates a PDF entry with methods:

method	Use
export()	Used to write G(r), etc. as a file
calculate()	Computes the PDF using parameters in the object
optimize()	Optimizes selected PDF parameters
set_background()	Sets the histograms used for sample background, container, etc.
set_formula()	Sets the chemical formula for the sample

1.4.9 Class G2SmallAngle

To work with Small Angle (currently only SASD entries), object *G2SmallAngle*, encapsulates a SASD entry. At present no methods are provided.

1.4.10 Class G2SeqRefRes

To work with Sequential Refinement results, object *G2SeqRefRes*, encapsulates the sequential refinement table with methods:

method	Use
histograms()	Provides a list of histograms used in the Sequential Refinement
get_cell_and_esd()	Returns cell dimensions and standard uncertainties for a phase and histogram from the Sequential Refinement
get_Variable()	Retrieves the value and esd for a parameter from a particular histogram in the Sequential Refinement
get_Covariance()	Retrieves values and covariance for a set of refined parameters for a particular histogram

1.4.11 Class G2AtomRecord

When working with phases, *G2AtomRecord* methods provide access to the contents of each atom in a phase. This provides access to atom values via class "properties" that can be used to get values of much of the atoms associated settings, as below. Most can also be used to set values via "setter" methods. See the *G2AtomRecord* docs and source code.

method/prope	Use
label	Reference as `<atom>.label` to get or set label value for atom
type	Reference as `<atom>.G2AtomRecord.type` to get or set the atom type
element	Reference as `<atom>.G2AtomRecord.element` to get the element symbol associated with an atom (change with `<atom>.G2AtomRecord.type`, see *type*)
refinement_flags	Reference class property `<atom>.G2AtomRecord.refinement_flags` to get or set the refinement flags associated with an atom
coordinates	Reference as `<atom>.G2AtomRecord.coordinates` to get or set the three coordinates associated with an atom
occupancy	Reference class property `<atom>.G2AtomRecord.occupancy` to get or set the site occupancy associated with an atom
mult	Reference as `<atom>.G2AtomRecord.mult` to get an atom site multiplicity (value cannot be changed in script)
ranId	Reference as `<atom>.G2AtomRecord.ranId` to get an atom random Id number (value cannot be changed in script)
adp_flag	Reference as `<atom>.G2AtomRecord.adp_flag` to get either 'U' or 'I' specifying that an atom is set as anisotropic or isotropic (value cannot be changed in script)
uiso	Reference pseudo class variable `<atom>.G2AtomRecord.uiso` to get or set the Uiso value associated with an atom

1.5 Refinement parameters

While scripts can be written that setup refinements by changing individual parameters through calls to the methods associated with objects that wrap each data tree item, many of these actions can be combined into fairly complex dict structures to conduct refinement steps. Use of these dicts is required with the *GSASIIscriptable Command-line Interface*. This section of the documentation describes these dicts.

1.5.1 Project-level Parameter Dict

As noted below (*Refinement parameter types*), there are three types of refinement parameters, which can be accessed individually by the objects that encapsulate individual phases and histograms but it will often be simplest to create a composite dictionary that is used at the project-level. A dict is created with keys "set" and "clear" that can be supplied to `set_refinement()` (or `do_refinements()`, see *Refinement recipe* below) that will determine parameter values and will determine which parameters will be refined.

The specific keys and subkeys that can be used are defined in tables *Histogram parameters*, *Phase parameters* and *Histogram-and-phase parameters*.

Note that optionally a list of histograms and/or phases can be supplied in the call to `set_refinement()`, but if not specified, the default is to use all defined phases and histograms.

As an example:

```
pardict = {'set': { 'Limits': [0.8, 12.0],
                    'Sample Parameters': ['Absorption', 'Contrast', 'DisplaceX'],
                    'Background': {'type': 'chebyschev-1', 'refine': True,
                                   'peaks':[[0,True],[1,1,1]] }},
          'clear': {'Instrument Parameters': ['U', 'V', 'W']}}
my_project.set_refinement(pardict)
```

1.5.2 Refinement recipe

Building on the *Project-level Parameter Dict*, it is possible to specify a sequence of refinement actions as a list of these dicts and supplying this list as an argument to `do_refinements()`.

As an example, this code performs the same actions as in the example in the section above:

```
pardict = {'set': { 'Limits': [0.8, 12.0],
                    'Sample Parameters': ['Absorption', 'Contrast', 'DisplaceX'],
                    'Background': {'type': 'chebyschev-1', 'refine': True}},
          'clear': {'Instrument Parameters': ['U', 'V', 'W']}}
my_project.do_refinements([pardict])
```

However, in addition to setting a number of parameters, this example will perform a refinement as well, after setting the parameters. More than one refinement can be performed by including more than one dict in the list.

In this example, two refinement steps will be performed:

```
my_project.do_refinements([pardict,pardict1])
```

The keys defined in the following table may be used in a dict supplied to `do_refinements()`. Note that keys `histograms` and `phases` are used to limit actions to specific sets of parameters within the project.

key	explanation
set	Specifies a dict with keys and subkeys as described in the *Specifying Refinement Parameters* section. Items listed here will be set to be refined.
clear	Specifies a dict, as above for set, except that parameters are cleared and thus will not be refined.
once	Specifies a dict as above for set, except that parameters are set for the next cycle of refinement and are cleared once the refinement step is completed.
skip	Normally, once parameters are processed with a set/clear/once action(s), a refinement is started. If skip is defined as True (or any other value) the refinement step is not performed.
output	If a file name is specified for output is will be used to save the current refinement.
histograms	Should contain a list of histogram(s) to be used for the set/clear/once action(s) on *Histogram parameters* or *Histogram-and-phase parameters*. Note that this will be ignored for *Phase parameters*. Histograms may be specified as a list of strings [('PWDR …'),…], indices [0,1,2] or as list of objects [hist1, hist2].
phases	Should contain a list of phase(s) to be used for the set/clear/once action(s) on *Phase parameters* or *Histogram-and-phase parameters*. Note that this will be ignored for *Histogram parameters*. Phases may be specified as a list of strings [('Phase name'),…], indices [0,1,2] or as list of objects [phase0, phase2].
call	Specifies a function to call after a refinement is completed. The value supplied can be the object (typically a function) that will be called or a string that will evaluate (in the namespace inside `iter_refinements()` where `self` references the project.) Nothing is called if this is not specified.
callargs	Provides a list of arguments that will be passed to the function in call (if any). If call is defined and callargs is not, the current <tt>G2Project</tt> is passed as a single argument.

An example that performs a series of refinement steps follows:

```
reflist = [
        {"set": { "Limits": { "low": 0.7 },
                  "Background": { "no. coeffs": 3,
                                  "refine": True }}},
        {"set": { "LeBail": True,
                  "Cell": True }},
        {"set": { "Sample Parameters": ["DisplaceX"]}},
        {"set": { "Instrument Parameters": ["U", "V", "W", "X", "Y"]}},
        {"set": { "Mustrain": { "type": "uniaxial",
                                "refine": "equatorial",
                                "direction": [0, 0, 1]}}},
        {"set": { "Mustrain": { "type": "uniaxial",
                                "refine": "axial"}}},
        {"clear": { "LeBail": True},
         "set": { "Atoms": { "Mn": "X" }}},
        {"set": { "Atoms": { "O1": "X", "O2": "X" }}},]
my_project.do_refinements(reflist)
```

In this example, a separate refinement step will be performed for each dict in the list. The keyword "skip" can be used to specify a dict that should not include a refinement. Note that in the second from last refinement step, parameters are

both set and cleared.

1.5.3 Refinement parameter types

Note that parameters and refinement flags used in GSAS-II fall into three classes:

- **Histogram**: There will be a set of these for each dataset loaded into a project file. The parameters available depend on the type of histogram (Bragg-Brentano, Single-Crystal, TOF,…). Typical Histogram parameters include the overall scale factor, background, instrument and sample parameters; see the *Histogram parameters* table for a list of the histogram parameters where access has been provided.
- **Phase**: There will be a set of these for each phase loaded into a project file. While some parameters are found in all types of phases, others are only found in certain types (modulated, magnetic, protein…). Typical phase parameters include unit cell lengths and atomic positions; see the *Phase parameters* table for a list of the phase parameters where access has been provided.
- **Histogram-and-phase** (HAP): There is a set of these for every histogram that is associated with each phase, so that if there are `N` phases and `M` histograms, there can be `N*M` total sets of "HAP" parameters sets (fewer if all histograms are not linked to all phases.) Typical HAP parameters include the phase fractions, sample microstrain and crystallite size broadening terms, hydrostatic strain perturbations of the unit cell and preferred orientation values. See the *Histogram-and-phase parameters* table for the HAP parameters where access has been provided.

1.6 Specifying Refinement Parameters

Refinement parameter values and flags to turn refinement on and off are specified within dictionaries, where the details of these dicts are organized depends on the type of parameter (see *Refinement parameter types*), with a different set of keys (as described below) for each of the three types of parameters.

1.6.1 Histogram parameters

This table describes the dictionaries supplied to *`set_refinements()`* and *`clear_refinements()`*. As an example,

```
hist.set_refinements({"Background": {"no. coeffs": 3, "refine": True},
                      "Sample Parameters": ["Scale"],
                      "Limits": [10000, 40000]})
```

With *`do_refinements()`*, these parameters should be placed inside a dict with a key `set`, `clear`, or `once`. Values will be set for all histograms, unless the `histograms` key is used to define specific histograms. As an example:

```
gsas_proj.do_refinements([
    {'set': {
        'Background': {'no. coeffs': 3, 'refine': True},
        'Sample Parameters': ['Scale'],
        'Limits': [10000, 40000]},
    'histograms': [1,2]}
                          ])
```

Note that below in the Instrument Parameters section, related profile parameters (such as U and V) are grouped together but separated by commas to save space in the table.

key	subkey	explanation
Limits		The range of 2-theta (degrees) or TOF (in microsec) range of values to use. Can be either a dictionary of 'low' and/or 'high', or a list of 2 items [low, high] Available for powder histograms only.
	low	Sets the low limit
	high	Sets the high limit
Sample Parameters		Should be provided as a **list** of subkeys to set or clear refinement flags for, e.g. ['DisplaceX', 'Scale'] Available for powder histograms only.
	Absorption	
	Contrast	
	DisplaceX	Sample displacement along the X direction (Debye-Scherrer)
	DisplaceY	Sample displacement along the Y direction (Debye-Scherrer)
	Shift	Bragg-Brentano sample displacement
	Scale	Histogram Scale factor
Background		Sample background. Value will be a dict or a boolean. If True or False, the refine parameter for background is set to that. Available for powder histograms only. Note that background peaks are not handled via this; see *ref_back_peak()* instead. When value is a dict, supply any of the following keys:
	type	The background model, e.g. 'chebyschev-1'
	refine	The value of the refine flag, boolean
	'no. coeffs'	Number of coefficients to use, integer
	coeffs	List of floats, literal values for background
	FixedPoints	List of (2-theta, intensity) values for fixed points
	'fit fixed points'	If True, triggers a fit to the fixed points to be calculated. It is calculated when this key is detected, regardless of calls to refine.
	peaks	Specifies a set of flags for refining background peaks as a nested list. There may be an item for each defined background peak (or fewer) and each item is a list with the flag values for pos,int,sig & gam (fewer than 4 values are allowed).
Instrument Parameters		As in Sample Parameters, provide as a **list** of subkeys to set or clear refinement flags, e.g. ['X', 'Y', 'Zero', 'SH/L'] Available for powder histograms only.
	U, V, W	Gaussian peak profile terms
	X, Y, Z	Lorentzian peak profile terms
	alpha, beta-0, beta-1, beta-q,	TOF profile terms
	sig-0, sig-1, sig-2, sig-q	TOF profile terms
	difA, difB, difC	TOF Calibration constants
	Zero	Zero shift
	SH/L	Finger-Cox-Jephcoat low-angle peak asymmetry
	Polariz.	Polarization parameter
	Lam	Lambda, the incident wavelength
Single xtal		As in Sample Parameters, provide as a **list** of subkeys to set or clear refinement flags, e.g. […]. Available for single crystal histograms only.
	Scale	Single crystal scale factor
	BabA, BabU	Babinet A & U parameters
	Eg, Es, Ep	Extinction parameters
	Flack	Flack absolute configuration parameter

1.6.2 Phase parameters

This table describes the dictionaries supplied to *set_refinements()* and *clear_refinements()*. With *do_refinements()*, these parameters should be placed inside a dict with a key `set`, `clear`, or `once`. Values will be set for all phases, unless the `phases` key is used to define specific phase(s).

key	explanation
Cell	Whether or not to refine the unit cell.
Atoms	Dictionary of atoms and refinement flags. Each key should be an atom label, e.g. 'O3', 'Mn5', and each value should be a string defining what values to refine. Values can be any combination of 'F' for site fraction, 'X' for position, and 'U' for Debye-Waller factor
LeBail	Enables LeBail intensity extraction.

1.6.3 Histogram-and-phase parameters

This table describes the dictionaries supplied to *set_HAP_refinements()* and *clear_HAP_refinements()*. When supplied to *do_refinements()*, these parameters should be placed inside a dict with a key `set`, `clear`, or `once`. Values will be set for all histograms used in each phase, unless the `histograms` and `phases` keys are used to define specific phases and histograms.

key	subkey	explanation
Babinet		Should be a **list** of the following subkeys. If not, assumes both BabA and BabU
	BabA	
	BabU	
Extinction		Boolean, True to refine.
HStrain		Boolean or list/tuple, True to refine all appropriate D_{ij} terms or False to not refine any. If a list/tuple, will be a set of True & False values for each D_{ij} term; number of items must match number of terms.
Mustrain		
	type	Mustrain model. One of 'isotropic', 'uniaxial', or 'generalized'. This should be specified to change the model.
	direction	For uniaxial only. A list of three integers, the [hkl] direction of the axis.
	refine	Usually boolean, set to True to refine. or False to clear. For uniaxial model, can specify a value of 'axial' or 'equatorial' to set that flag to True or a single boolean sets both axial and equatorial.
Size		
	type	Size broadening model. One of 'isotropic', 'uniaxial', or 'ellipsoid'. This should be specified to change from the current.
	direction	For uniaxial only. A list of three integers, the [hkl] direction of the axis.
	refine	Boolean, True to refine.
	value	float, size value in microns
Pref.Ori.		Boolean, True to refine
Show		Boolean, True to refine
Use		Boolean, True to refine
Scale		Phase fraction; Boolean, True to refine
PhaseFraction		PhaseFraction can also be used in place of Scale for the routines that access HAP parameters: *HAPvalue()*, *setHAPvalues()*, *copyHAPvalues()*, *set_refinement()*, *do_refinements()*, *clear_HAP_refinements()* and *set_HAP_refinements()*.

1.6.4 Histogram/Phase objects

Each phase and powder histogram in a *G2Project* object has an associated object. Parameters within each individual object can be turned on and off by calling *set_refinements()* or *clear_refinements()* for histogram parameters; *set_refinements()* or *clear_refinements()* for phase parameters; and *set_HAP_refinements()* or *clear_HAP_refinements()*. As an example, if some_histogram is a histogram object (of type *G2PwdrData*), use this to set parameters in that histogram:

```
params = { 'Limits': [0.8, 12.0],
           'Sample Parameters': ['Absorption', 'Contrast', 'DisplaceX'],
           'Background': {'type': 'chebyschev-1', 'refine': True}}
some_histogram.set_refinements(params)
```

Likewise to turn refinement flags on, use code such as this:

```
params = { 'Instrument Parameters': ['U', 'V', 'W']}
some_histogram.set_refinements(params)
```

and to turn these refinement flags, off use this (Note that the `.clear_refinements()` methods will usually will turn off refinement even if a refinement parameter is set in the dict to True.):

```
params = { 'Instrument Parameters': ['U', 'V', 'W']}
some_histogram.clear_refinements(params)
```

For phase parameters, use code such as this:

```
params = { 'LeBail': True, 'Cell': True,
           'Atoms': { 'Mn1': 'X',
                      'O3': 'XU',
                      'V4': 'FXU'}}
some_histogram.set_refinements(params)
```

and here is an example for HAP parameters:

```
params = { 'Babinet': 'BabA',
           'Extinction': True,
           'Mustrain': { 'type': 'uniaxial',
                         'direction': [0, 0, 1],
                         'refine': True}}
some_phase.set_HAP_refinements(params)
```

Note that the parameters must match the object type and method (phase vs. histogram vs. HAP).

1.7 Access to other parameter settings

There are several hundred different types of values that can be stored in a GSAS-II project (.gpx) file. All can be changed from the GUI but only a subset have direct mechanism implemented for change from the GSASIIscriptable API. In practice all parameters in a .gpx file can be edited via scripting, but sometimes determining what should be set to implement a parameter change can be complex. Several routines, *getHAPentryList()*, *getPhaseEntryList()* and *getHistEntryList()* (and their related get…Value and set.Value entries), provide a mechanism to discover what the GUI is changing inside a .gpx file.

As an example, a user in changing the data type for a histogram from Debye-Scherrer mode to Bragg-Brentano. This capability is not directly exposed in the API. To find out what changes when the histogram type is changed we can create a short script that displays the contents of all the histogram settings:

```
gpx = G2sc.G2Project('/tmp/test.gpx')
h = gpx.histograms()[0]
for h in h.getHistEntryList():
    print(h)
```

This can be run with a command like this:

```
python test.py > before.txt
```

(This will create file `before.txt`, which will contain hundreds of lines.)

At this point open the project file, `test.gpx` in the GSAS-II GUI and change in Histogram/Sample Parameters the diffractometer type from Debye-Scherrer mode to Bragg-Brentano and then save the file.

Rerun the previous script creating a new file:

```
python test.py > after.txt
```

Finally look for the differences between files `before.txt` and `after.txt` using a tool such as diff (on Linux/OS X) or fc (in Windows).

in Windows:

```
Z:\>fc before.txt after.txt
Comparing files before.txt and after.txt
***** before.txt
       fill_value = 1e+20)
, 'PWDR Co_PCP_Act_d900-00030.fxye Bank 1', 'PWDR Co_PCP_Act_d900-00030.fxye Ban
k 1'])
(['Comments'], <class 'list'>, ['Co_PCP_Act_d900-00030.tif #0001 Azm= 180.00'])
***** AFTER.TXT
       fill_value = 1e+20)
, 'PWDR Co_PCP_Act_d900-00030.fxye Bank 1', 'PWDR Co_PCP_Act_d900-00030.fxye Ban
k 1', 'PWDR Co_PCP_Act_d900-00030.fxye Bank 1']

(['Comments'], <class 'list'>, ['Co_PCP_Act_d900-00030.tif #0001 Azm= 180.00'])
*****

***** before.txt
(['Sample Parameters', 'Scale'], <class 'list'>, [1.276313196832068, True])
(['Sample Parameters', 'Type'], <class 'str'>, 'Debye-Scherrer')
(['Sample Parameters', 'Absorption'], <class 'list'>, [0.0, False])
***** AFTER.TXT
(['Sample Parameters', 'Scale'], <class 'list'>, [1.276313196832068, True])
(['Sample Parameters', 'Type'], <class 'str'>, 'Bragg-Brentano')
(['Sample Parameters', 'Absorption'], <class 'list'>, [0.0, False])
*****
```

in Linux/Mac:

```
bht14: toby$ diff before.txt after.txt
103c103
< , 'PWDR Co_PCP_Act_d900-00030.fxye Bank 1', 'PWDR Co_PCP_Act_d900-00030.fxye Bank 1
↪'])
---
> , 'PWDR Co_PCP_Act_d900-00030.fxye Bank 1', 'PWDR Co_PCP_Act_d900-00030.fxye Bank 1
↪', 'PWDR Co_PCP_Act_d900-00030.fxye Bank 1'])
111c111
< (['Sample Parameters', 'Type'], <class 'str'>, 'Debye-Scherrer')
---
> (['Sample Parameters', 'Type'], <class 'str'>, 'Bragg-Brentano')
```

From this we can see there are two changes that took place. One is fairly obscure, where the histogram name is added to a list, which can be ignored, but the second change occurs in a straight-forward way and we discover that a simple call:

```
h.setHistEntryValue(['Sample Parameters', 'Type'], 'Bragg-Brentano')
```

can be used to change the histogram type.

1.8 Code Examples

Contents for Scripting Examples

1.8.1 Accessing GSASIIscriptable

As discussed in the *Accessing the GSASIIscriptable Module* section of this chapter, GSAS-II is commonly installed outside of a Python installation, which means that Python must be instructed on how to access the GSASII package. In *that section* three methods are provided for defining G2sc as the location of the GSASIIscriptable module. The scripting examples below all assume that one of choices for import statements has been executed to provide access to GSASIIscriptable.

1.8.2 Status Information

To find information on Python, Python packages and the GSAS-II version, one can call the `ShowVersions()` function. This will show versions and install locations.

```
print(f'Version information:\n{G2sc.ShowVersions()}')
```

which produces output like this:

```
setting up GSASIIscriptable from /Users/toby/G2/git/g2full/GSAS-II/GSASII
Version information:
  Python      3.11.9:  from /Users/toby/py/mf3/envs/py311/bin/python
  numpy       1.26.4:
  scipy       1.13.0:
  IPython     8.22.2:
  GSAS-II:    641a65, 24-May-2024 10:16 (0.5 days old). Last tag: #5789
```

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```
GSAS-II location: /Users/toby/G2/git/g2full/GSAS-II/GSASII
Binary location:  /Users/toby/G2/git/g2full/GSAS-II/GSASII-bin/mac_arm_p3.11_n1.26
```

1.8.3 Peak Fitting

Peak refinement is performed with routines *add_peak()*, *set_peakFlags()* and *refine_peaks()*. Method *Export_peaks()* and properties *Peaks* and *PeakList* provide ways to access the results. Note that when peak parameters are refined with `refine_peaks()`, the background may also be refined. Use *set_refinements()* to change background settings and the range of data used in the fit. See below for an example peak refinement script, where the data files are taken from the "Rietveld refinement with CuKa lab Bragg-Brentano powder data" tutorial (in https://advancedphotonsource.github.io/GSAS-II-tutorials/LabData/data/).

```
import os
datadir = os.path.expanduser("~/Scratch/peakfit")
PathWrap = lambda fil: os.path.join(datadir,fil)
gpx = G2sc.G2Project(newgpx=PathWrap('pkfit.gpx'))
hist = gpx.add_powder_histogram(PathWrap('FAP.XRA'), PathWrap('INST_XRY.PRM'),
                                fmthint='GSAS powder')
hist.set_refinements({'Limits': [16.,24.],
      'Background': {"no. coeffs": 2,'type': 'chebyschev-1', 'refine': True}
                     })
peak1 = hist.add_peak(1, ttheta=16.8)
peak2 = hist.add_peak(1, ttheta=18.9)
peak3 = hist.add_peak(1, ttheta=21.8)
peak4 = hist.add_peak(1, ttheta=22.9)
hist.set_peakFlags(area=True)
hist.refine_peaks()
hist.set_peakFlags(area=True,pos=True)
hist.refine_peaks()
hist.set_peakFlags(area=True, pos=True, sig=True, gam=True)
res = hist.refine_peaks()
print('peak positions: ',[i[0] for i in hist.PeakList])
for i in range(len(hist.Peaks['peaks'])):
    print('peak',i,'pos=',hist.Peaks['peaks'][i][0],'sig=',hist.Peaks['sigDict']['pos
↪'+str(i)])
hist.Export_peaks('pkfit.txt')
#gpx.save()  # gpx file is not written without this
```

1.8.4 Pattern Simulation

This shows two examples where a structure is read from a CIF, a pattern is computed using a instrument parameter file to specify the probe type (neutrons here) and wavelength.

The first example uses a CW neutron instrument parameter file. The pattern is computed over a 2θ range of 5 to 120 degrees with 1000 points. The pattern and reflection list are written into files. Data files are found in the Scripting Tutorial.

```
import os
datadir = "/Users/toby/software/G2/Tutorials/PythonScript/data"
PathWrap = lambda fil: os.path.join(datadir,fil)
gpx = G2sc.G2Project(newgpx='PbSO4sim.gpx') # create a project
phase0 = gpx.add_phase(PathWrap("PbSO4-Wyckoff.cif"),
```

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```
        phasename="PbSO4",fmthint='CIF') # add a phase to the project
# add a simulated histogram and link it to the previous phase(s)
hist1 = gpx.add_simulated_powder_histogram("PbSO4 simulation",
            PathWrap("inst_d1a.prm"),5.,120.,Npoints=1000,
            phases=gpx.phases(),scale=500000.)
gpx.do_refinements()   # calculate pattern
gpx.save()
# save results
gpx.histogram(0).Export('PbSO4data','.csv','hist') # data
gpx.histogram(0).Export('PbSO4refl','.csv','refl') # reflections
```

This example uses bank#2 from a TOF neutron instrument parameter file. The pattern is computed over a TOF range of 14 to 35 milliseconds with the default of 2500 points. This uses the same CIF as in the example before, but the instrument is found in the TOF-CW Joint Refinement Tutorial tutorial.

```
import os
cifdir = "/Users/toby/software/G2/Tutorials/PythonScript/data"
datadir = "/Users/toby/software/G2/Tutorials/TOF-CW Joint Refinement/data"
gpx = G2sc.G2Project(newgpx='/tmp/PbSO4simT.gpx') # create a project
phase0 = gpx.add_phase(os.path.join(cifdir,"PbSO4-Wyckoff.cif"),
        phasename="PbSO4",fmthint='CIF') # add a phase to the project
hist1 = gpx.add_simulated_powder_histogram("PbSO4 simulation",
            os.path.join(datadir,"POWGEN_1066.instprm"),14.,35.,
            phases=gpx.phases(),ibank=2)
gpx.do_refinements([{}])
gpx.save()
```

1.8.5 Simple Refinement

GSASIIscriptable can be used to setup and perform simple refinements. This example reads in an existing project (.gpx) file, adds a background peak, changes some refinement flags and performs a refinement.

```
datadir = "/Users/Scratch/"
gpx = G2sc.G2Project(os.path.join(datadir,'test2.gpx'))
gpx.histogram(0).add_back_peak(4.5,30000,5000,0)
pardict = {'set': {'Sample Parameters': ['Absorption', 'Contrast', 'DisplaceX'],
                   'Background': {'type': 'chebyschev-1', 'refine': True,
                                  'peaks':[[0,True]]}}}
gpx.set_refinement(pardict)
```

1.8.6 Sequential Refinement

GSASIIscriptable can be used to setup and perform sequential refinements. This example script is used to take the single-dataset fit at the end of Step 1 of the Sequential Refinement tutorial and turn on and off refinement flags, add histograms and setup the sequential fit, which is then run:

```
import os,glob
datadir = os.path.expanduser("~/Scratch/SeqTut2019Mar")
PathWrap = lambda fil: os.path.join(datadir,fil)
# load and rename project
gpx = G2sc.G2Project(PathWrap('7Konly.gpx'))
gpx.save(PathWrap('SeqRef.gpx'))
```

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```
# turn off some variables; turn on Dijs
for p in gpx.phases():
    p.set_refinements({"Cell": False})
gpx.phase(0).set_HAP_refinements(
    {'Scale': False,
     "Size": {'type':'isotropic', 'refine': False},
     "Mustrain": {'type':'uniaxial', 'refine': False},
     "HStrain":True,})
gpx.phase(1).set_HAP_refinements({'Scale': False})
gpx.histogram(0).clear_refinements({'Background':False,
                'Sample Parameters':['DisplaceX'],})
gpx.histogram(0).ref_back_peak(0,[])
gpx.phase(1).set_HAP_refinements({"HStrain":(1,1,1,0)})
for fil in sorted(glob.glob(PathWrap('*.fxye'))): # load in remaining fxye files
    if '00' in fil: continue
    gpx.add_powder_histogram(fil, PathWrap('OH_00.prm'), fmthint="GSAS powder",phases=
↪'all')
# copy HAP values, background, instrument params. & limits, not sample params.
gpx.copyHistParms(0,'all',['b','i','l'])
for p in gpx.phases(): p.copyHAPvalues(0,'all')
# setup and launch sequential fit
gpx.set_Controls('sequential',gpx.histograms())
gpx.set_Controls('cycles',10)
gpx.set_Controls('seqCopy',True)
gpx.refine()
```

1.8.7 Image Processing

A sample script where an image is read, assigned calibration values from a file and then integrated follows. The data files are found in the Scripting Tutorial.

```
import os
datadir = "/tmp"
PathWrap = lambda fil: os.path.join(datadir,fil)

gpx = G2sc.G2Project(newgpx=PathWrap('inttest.gpx'))
imlst = gpx.add_image(PathWrap('Si_free_dc800_1-00000.tif'),fmthint="TIF")
imlst[0].loadControls(PathWrap('Si_free_dc800_1-00000.imctrl'))
pwdrList = imlst[0].Integrate()
gpx.save()
```

This example shows a computation similar to what is done in tutorial Area Detector Calibration with Multiple Distances

```
import os,glob
PathWrap = lambda fil: os.path.join(
    "/Users/toby/wp/Active/MultidistanceCalibration/multimg",
    fil)

gpx = G2sc.G2Project(newgpx='/tmp/img.gpx')
for f in glob.glob(PathWrap('*.tif')):
    im = gpx.add_image(f,fmthint="TIF")
# image parameter settings
```

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```
defImgVals = {'wavelength': 0.24152, 'center': [206., 205.],
  'pixLimit': 2,  'cutoff': 5.0, 'DetDepth': 0.055,'calibdmin': 1.,}
# set controls and vary options, then fit
for img in gpx.images():
    img.setCalibrant('Si    SRM640c')
    img.setVary('*',False)
    img.setVary(['det-X', 'det-Y', 'phi', 'tilt', 'wave'], True)
    img.setControls(defImgVals)
    img.Recalibrate()
    img.Recalibrate() # 2nd run better insures convergence
gpx.save()
# make dict of images for sorting
images = {img.getControl('setdist'):img for img in gpx.images()}
# show values
for key in sorted(images.keys()):
    img = images[key]
    c = img.getControls()
    print(c['distance'],c['wavelength'])
```

1.8.8 Image Calibration

This example performs a number of cycles of constrained fitting. A project is created with the images found in a directory, setting initial parameters as the images are read. The initial values for the calibration are not very good, so a *Recalibrate()* is done to quickly improve the fit. Once that is done, a fit of all images is performed where the wavelength, an offset and detector orientation are constrained to be the same for all images. The detector penetration correction is then added. Note that as the calibration values improve, the algorithm is able to find more points on diffraction rings to use for calibration and the number of "ring picks" increase. The calibration is repeated until that stops increasing significantly (<10%). Detector control files are then created. The files used for this exercise are found in the Area Detector Calibration Tutorial (see Area Detector Calibration with Multiple Distances).

```
import os,glob
PathWrap = lambda fil: os.path.join(
    "/Users/toby/wp/Active/MultidistanceCalibration/multimg",
    fil)

gpx = G2sc.G2Project(newgpx='/tmp/calib.gpx')
for f in glob.glob(PathWrap('*.tif')):
    im = gpx.add_image(f,fmthint="TIF")
# starting image parameter settings
defImgVals = {'wavelength': 0.240, 'center': [206., 205.],
  'pixLimit': 2,  'cutoff': 5.0, 'DetDepth': 0.03,'calibdmin': 0.5,}
# set controls and vary options, then initial fit
for img in gpx.images():
    img.setCalibrant('Si    SRM640c')
    img.setVary('*',False)
    img.setVary(['det-X', 'det-Y', 'phi', 'tilt', 'wave'], True)
    img.setControls(defImgVals)
    if img.getControl('setdist') > 900:
        img.setControls({'calibdmin': 1.,})
    img.Recalibrate()
G2sc.SetPrintLevel('warn') # cut down on output
result,covData = gpx.imageMultiDistCalib()
```

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```
print('1st global fit: initial ring picks',covData['obs'])
print({i:result[i] for i in result if '-' not in i})
# add parameter to all images & refit multiple times
for img in gpx.images(): img.setVary('dep',True)
ringpicks = covData['obs']
delta = ringpicks
while delta > ringpicks/10:
    result,covData = gpx.imageMultiDistCalib(verbose=False)
    delta = covData['obs'] - ringpicks
    print('ring picks went from',ringpicks,'to',covData['obs'])
    print({i:result[i] for i in result if '-' not in i})
    ringpicks = covData['obs']
# once more for good measure & printout
result,covData = gpx.imageMultiDistCalib(verbose=True)
# create image control files
for img in gpx.images():
    img.saveControls(os.path.splitext(img.name)[0]+'.imctrl')
gpx.save()
```

1.8.9 Optimized Image Integration

This example shows how image integration, including pixel masking of outliers, can be accomplished for a series of images where the calibration and other masking (Frame, Spots, etc) are the same for all images. This code has been optimized significantly so that computations are cached and are not repeated where possible. For one set of test data, processing of the first image takes ~5 seconds, but processing of subsequent takes on the order of 0.7 sec.

To simplify use of this script, it is assumed that the script will be placed in the same directory as where the data files will be collected. Other customization is done in variables at the beginning of the code. Note that the beamline where these data are collected opens the output .tif files before the data collection for that image is complete. Once the .metadata file has been created, the image may be read.

Processing progresses as follows:

- Once a set of images are found, a project is created. This is never written and will be deleted after the images are processed.
- For each image file, routine *add_image()* is used to add image(s) from that file to the project. The .tif format can only hold one image, but others can have more than one.
- When the first image is processed, calibration and mask info is read; a number of computations are performed and cached.
- For subsequent images cached information is used.
- Pixel masking is performed in *GeneratePixelMask()* and the mask is saved into the image.
- Image integration is performed in *Integrate()*.
- Note that multiple powder patterns could be created from one image, so creation of data files is done in a loop with *Export()*.
- To reduce memory demands, cached versions of the Pixel map and the Image are deleted and the image file is moved to a separate directory so note that it has been processed.
- The project (.gpx file) is deleted and recreated periodically so that the memory footprint for this script does not grow.

The speed of this code will depend on many things, but the number of pixels in the image is primary, as well as CPU speed. With ~9 Mb images, I have seen average times in the range of 0.7 to 0.9 sec/image, after the first image is processed and the cached arrays are computed. With the Apple M1 chip the time is closer to 0.6 sec/image. There is also a possible tuning parameter that may change speed based on the speed of the CPU vs. memory constraints in variable *GSASIIscriptable.blkSize*. This value should be a power of two and defaults to 128. You might find that a larger or smaller value will improve performance for you.

```
import os,glob,time,shutil
G2sc.blkSize = 2**8  # computer-dependent tuning parameter
G2sc.SetPrintLevel('warn')    # reduces output

cache = {}  # place to save intermediate computations
# define location & names of files
dataLoc = os.path.abspath(os.path.split(__file__)[0]) # data in location of this file
PathWrap = lambda fil: os.path.join(dataLoc,fil) # convenience function for file paths
imgctrl = PathWrap('Si_ch3_d700-00000.imctrl')
imgmask = PathWrap('Si_ch3_d700-00000.immask')
globPattern = PathWrap("*_d700-*.tif")

def wait_for_metadata(tifname):
    '''A .tif file is created before it can be read. Wait for the
    metadata file to be created before trying to read both.
    '''
    while not os.path.exists(tifname + '.metadata'):
        time.sleep(0.05)

# make a subfolder to store integrated images & integrated patterns
pathImg = os.path.join(dataLoc,'img')
if not os.path.exists(pathImg): os.mkdir(pathImg)
pathxye = os.path.join(dataLoc,'xye')
if not os.path.exists(pathxye): os.mkdir(pathxye)

while True:  # Loop will never end, stop with ctrl+C
    tiflist = sorted(glob.glob(globPattern),key=lambda x: os.path.getctime(x)) # get␣
↪images sorted by creation time, oldest 1st
    if not tiflist:
        time.sleep(0.1)
        continue
    gpx = G2sc.G2Project(newgpx=PathWrap('integration.gpx')) # temporary use
    for tifname in tiflist:
        starttime = time.time()
        wait_for_metadata(tifname)
        for img in gpx.add_image(tifname,fmthint="TIF",cacheImage=True):  # loop␣
↪unneeded for TIF (1 image/file)
            if not cache: # load & compute controls & 2theta values once
                img.loadControls(imgctrl)    # set controls/calibrations/masks
                img.loadMasks(imgmask)
                cache['Image Controls'] = img.getControls() # save controls & masks␣
↪contents for quick reload
                cache['Masks'] = img.getMasks()
                cache['intMaskMap'] = img.IntMaskMap() # calc mask & TA arrays to␣
↪save for integrations
                cache['intTAmap'] = img.IntThetaAzMap()
```

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```
                cache['FrameMask'] = img.MaskFrameMask() # calc Frame mask & T array␣
↪to save for Pixel masking
                cache['maskTmap'] = img.MaskThetaMap()
            else:
                img.setControls(cache['Image Controls'])
                img.setMasks(cache['Masks'],True)  # True: reset threshold masks
            img.GeneratePixelMask(esdMul=3,ThetaMap=cache['maskTmap'],FrameMask=cache[
↪'FrameMask'])
            for pwdr in img.Integrate(MaskMap=cache['intMaskMap'],ThetaAzimMap=cache[
↪'intTAmap']):
                pwdr.Export(os.path.join(pathxye,os.path.split(tifname)[1]),'.xye')
↪# '.tif in name ignored
            img.clearImageCache()  # save some space
            img.clearPixelMask()
        shutil.move(tifname, pathImg)       # move file after integration so that it␣
↪is not searchable
        shutil.move(tifname + '.metadata', pathImg)
        print('*=== processing complete, time=',time.time()-starttime,'sec\n')
    del gpx
```

1.8.10 Multicore Image Integration

The previous example (*Optimized Image Integration*) can be accelerated even further on a multicore computer using the following script. In this example, the image integration is moved to a function, *integrate_tif*, that accepts a filename to integrate. Note that with the multiprocessing module is used, the script will be read on each core that will be used, but only on the primary (controller) process will this `__name__ == '__main__'` be True. Thus the code following the if statement runs on the primary process. The primary process uses the mp.Pool() statement to create a set of secondary (worker) processes that are intended to run on other cores. The primary process locates .tif files, if the corresponding .tif.metadata is also found, both are moved to a separate directory where they will be processed in a secondary process. When the secondary process starts, the script is imported and then *integrate_tif* is called with the name of the image file from the primary process. The *integrate_tif* routine will initially have an empty cache and thus the code preceded by "load & compute controls & 2theta values" will be computed once for every secondary process, which should be on an independent core. The size of the pool determines how many images will be processed simultaneously.

The script as given below uses the first argument on the command line to specify the number of cores to be used, where 0 is used to mean run *integrate_tif* directly rather than through a pool. This facilitates timing comparisons. This code seems to have a maximum speed using slightly less than the total number of available cores and does benefit partially from hyper-threading. A two- to three-fold speedup is seen with four cores and a six-fold speedup has been seen with 16 cores.

```
import os,sys,glob,time,shutil
scriptstart = time.time()

if len(sys.argv) >= 2:
    nodes = int(sys.argv[1])
else:
    nodes = 4

if nodes == 0:
    print('no multiprocessing')
else:
    print(f'multiprocessing with {nodes} cores')
```

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```
G2sc.blkSize = 2**8  # computer-dependent tuning parameter
#G2sc.SetPrintLevel('warn')

cache = {}  # place to save intermediate computations

# define location & names of files
dataLoc = '/dataserv/inttest'  # images found here
globPattern = os.path.join(dataLoc,"*_d700-*.tif")
calibLoc = os.path.abspath(os.path.split(__file__)[0]) # calib in location of this␣
↪file
imgctrl = os.path.join(calibLoc,'Si_ch3_d700-00000.imctrl')
imgmask = os.path.join(calibLoc,'Si_ch3_d700-00000.immask')
# locations to put processed files
pathImg = os.path.join(dataLoc,'img')
pathxye = os.path.join(dataLoc,'xye')

def integrate_tif(tifname):
    starttime = time.time()
    gpx = G2sc.G2Project(newgpx='integration.gpx') # temporary use, not written
    for img in gpx.add_image(tifname,fmthint="TIF",cacheImage=True):  # loop unneeded␣
↪for TIF (1 image/file)
        img.setControl('pixelSize',[150,150])
        if not cache: # load & compute controls & 2theta values once
            print('Initializing cache for',tifname)
            img.loadControls(imgctrl)       # set controls/calibrations/masks
            img.loadMasks(imgmask)
            cache['Image Controls'] = img.getControls() # save file contents for␣
↪quick reload
            cache['Masks'] = img.getMasks()
            cache['intMaskMap'] = img.IntMaskMap() # calc mask & TA arrays to save␣
↪for integrations
            cache['intTAmap'] = img.IntThetaAzMap()
            cache['FrameMask'] = img.MaskFrameMask() # calc Frame mask & T array to␣
↪save for Pixel masking
            cache['maskTmap'] = img.MaskThetaMap()
        else:
            img.setControls(cache['Image Controls'])
            img.setMasks(cache['Masks'],True)  # not using threshold masks
        img.GeneratePixelMask(esdMul=3,ThetaMap=cache['maskTmap'],FrameMask=cache[
↪'FrameMask'])
        for pwdr in img.Integrate(MaskMap=cache['intMaskMap'],ThetaAzimMap=cache[
↪'intTAmap']):
            pwdr.Export(os.path.join(pathxye,os.path.split(tifname)[1]),'.xye')  # '.
↪tif in name ignored
        img.clearImageCache()  # save some space
        img.clearPixelMask()

    print(f'*=== image processed, time={time.time()-starttime:.3f} sec\n')
    del gpx

if __name__ == '__main__':
```

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```
    if nodes > 0: import multiprocessing as mp

    # make folder to store integrated images & integrated patterns if needed
    if not os.path.exists(pathImg): os.mkdir(pathImg)
    if not os.path.exists(pathxye): os.mkdir(pathxye)

    if nodes > 0: pool = mp.Pool(nodes)

    while True:       # Loop will never end, stop with ctrl+C
        tiflist = sorted(glob.glob(globPattern),key=lambda x: os.path.getctime(x)) #␣
↪get images sorted by creation time, oldest 1st
        if not tiflist:
            time.sleep(0.1)
            continue
        intlist = []  # list of images read to process
        for tifname in tiflist:
            if not os.path.exists(tifname + '.metadata'): continue
            shutil.move(tifname, pathImg)   # move file before integration so that it␣
↪is not found in another search
            shutil.move(tifname + '.metadata', pathImg)
            intlist.append(os.path.join(pathImg,os.path.split(tifname)[1]))
        if nodes == 0:
            for newtifname in intlist: integrate_tif(newtifname)
        else:
            pool.map(integrate_tif,intlist)

    if nodes > 0: pool.close()
    print(f'Total elapsed time={time.time()-scriptstart:.3f} sec')
```

1.8.11 Access the Image Pixel-Mask

In this example, a pixel mask has already been computed and has been saved with the image in a .gpx file. This example then reads the .gpx file, locates an image and then pulls the spot mask (an array of True and False values for every pixel) from the data structure. As an extra check (and demo) the image is reread and the dimensions of the image are confirmed to match those of the image. Note that the *GeneratePixelMask()* routine could also have been used to compute the mask.

This also provides an example showing how a result that is not made directly available from the GSASIIscriptable API can still be accessed from the GSAS-II data structures, but this requires some care to determine where values are stored.

```
import os
import G2script as G2sc
datadir = os.path.expanduser("~/Scratch/MPE_H5")
PathWrap = lambda fil: os.path.join(datadir,fil)
gpx = G2sc.G2Project(PathWrap('pixelMask.gpx'))
img0 = gpx.image(0) # access 1st image
spotMask = img0.data['Masks']['SpotMask'].get('spotMask')
if spotMask is not None:
    assert spotMask.shape == img0.getImage().shape   # diagnostic to confirm sizes␣
↪match
```

1.8.12 Histogram Export

This example shows how to export a series of histograms from a collection of .gpx (project) files. The Python `glob()` function is used to find all files matching a wildcard in the specified directory (`dataloc`). For each file there is a loop over histograms in that project and for each histogram *`Export()`* is called to write out the contents of that histogram as CSV (comma-separated variable) file that contains data positions, observed, computed and background intensities as well as weighting for each point and Q. Note that for the Export call, there is more than one choice of exporter that can write `.csv` extension files, so the export hint must be specified.

```
import os,glob
dataloc = "/Users/toby/Scratch/"                  # where to find data
PathWrap = lambda fil: os.path.join(dataloc,fil) # EZ way 2 add dir to filename

for f in glob.glob(PathWrap('bkg*.gpx')):  # put filename prefix here
    print(f)
    gpx = G2sc.G2Project(f)
    for i,h in enumerate(gpx.histograms()):
        hfil = os.path.splitext(f)[0]+'_'+str(i) # file to write
        print('\t',h.name,hfil+'.csv')
        h.Export(hfil,'.csv','histogram CSV')
```

1.8.13 Automatic Background

This example shows how to use the automatic background feature in GSAS-II to compute an approximate background and set fixed background points from that background. This approximately example follows that of the Autobackground Tutorial. In this example, a new project is created and the data files from the tutorial are read. Note that scripting is not able to read files from inside a zip archive or use defaulted instrument parameters. The histograms are then processed in turn. The first step is to use *calc_autobkg* to compute the fixed background points. The refinement flag is then set for the Chebyschev polynomial terms and three background peaks are added with the width flag set for refinement. The first call to *fit_fixed_points()* will refine the three Chebyschev terms and the intensities of the three background peaks to fit the fixed background points. The refinement flags for the widths of the three background peaks are then set as well and the refinement is repeated. The location of the third background peaks is added and the refinement is repeated. Finally, the number of Chebyschev polynomial terms is increased to six and the refinement is repeated.

```
import os,glob
PathWrap = lambda fil: os.path.join('/tmp',fil)
gpx = G2sc.G2Project(newgpx=PathWrap('autobkg.gpx'))
for i in glob.glob(PathWrap('test_RampDown-*.xye')):
    hist = gpx.add_powder_histogram(i,PathWrap('testData.instprm'))
for hist in gpx.histograms('PWDR'):
    hist.calc_autobkg(logLam=3.5)
    hist.set_refinements({"Background": {"no. coeffs": 3, "refine": True}})
    for pk in [2.4,3.1,4.75]:
        hist.add_back_peak(pk,1000,1000,0,[False,True,False,False])
    hist.fit_fixed_points()
    for i in [0,1,2]: hist.ref_back_peak(i,[False,True,True,False])
    hist.fit_fixed_points()
    hist.ref_back_peak(2,[True,True,True,False])
    hist.fit_fixed_points()
    hist.set_refinements({"Background": {"no. coeffs": 6, "refine": True}})
    hist.fit_fixed_points()
    gpx.save()
```

1.8.14 Specify Instrument Parameters Directly

Rather than read instrument parameters from a file, it is also possible to specify them directly in a script. See the documentation on instrument parameter file contents, *CW Instrument Parameters* and *TOF Instrument Parameters* for more information on the parameters supplied here.

```
import G2script as G2sc
import os
datadir = os.path.expanduser("~/Scratch/peakfit")
PathWrap = lambda fil: os.path.join(datadir,fil)
gpx = G2sc.G2Project(newgpx=PathWrap('pkfit.gpx'))
# specify instrmental parameters dictionaries
inst_params = [
    {
        "Type": ["PXC", "PXC", 0],
        "Lam": [1.5405, 1.5405, 0],
        "Zero": [0.0, 0.0, 0],
        "Polariz.": [0.7, 0.7, 0],
        "U": [2.0, 2.0, 0],
        "V": [-2.0, -2.0, 0],
        "W": [5.0, 5.0, 0],
        "X": [0.0, 0.0, 0],
        "Y": [0.0, 0.0, 0],
        "Z": [0.0, 0.0, 0],
        "SH/L": [0.002, 0.002, 0],
        "Azimuth": [0.0, 0.0, 0],
        "Bank": [1, 1, 0],
    },
    {},
]
hist = gpx.add_powder_histogram(PathWrap('FAP.XRA'), fmthint='GSAS powder',
                                iparams=inst_params)
```

1.8.15 Use Bilboa Website to Clean up Symmetry

Periodically I come across CIFs that are in weird settings that GSAS-II cannot read directly, but fortunately the Bilbao "CIF to Standard Setting" (strtidy) is much more tolerant. Here is some code that reads in a CIF, calling strtidy if needed and then the transformed coordinates are written out. Note that the BCS_API_KEY needs to be supplied. See the "Setup Access to the Bilbao Crystallographic Server" tutorial for information on how to obtain this. Note that you do not want to run this script on a very large number of files over a very short time and overload the BCS server.

```
import os
import G2script as G2sc
os.environ.update({"BCS_API_KEY":"BCS_API_KEY_..."})
PathWrap = lambda fil: os.path.join('/Users/toby/Scratch/CIF_problems',fil)
files = [
    'data_104906-ICSD_original.cif',
    'data_260095-ICSD_original.cif',
for f in files:
    gpx = G2sc.G2Project(newgpx='Junk.gpx') # create a new project
    newname = f.replace('.cif','_rev.cif')
    phase0 = gpx.add_phase(PathWrap(f),
        phasename=os.path.split(f)[1],fmthint='CIF',
        useNet=True,
```

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```
        )
    phase0.export_CIF(newname)
    print(f'file {newname} written')
    del gpx  # gets written anyway, alas
```

1.9 GSASIIscriptable Command-line Interface

The routines described above are intended to be called from a Python script, but an alternate way to access some of the same functionality is to invoke the `GSASIIscriptable.py` script from the command line usually from within a shell script or batch file. This mode of accessing GSAS-II scripting does not appear to get much use and is no longer being developed. Please do communicate to the developers if keeping this mode of access would be of value in your work.

To use the command-line mode is done with a command like this:

```
python <path/>GSASIIscriptable.py <subcommand> <file.gpx> <options>
```

The following subcommands are defined:

- create, see *create()*
- add, see *add()*
- dump, see *dump()*
- refine, see *refine()*
- export, *export()*
- browse, see *IPyBrowse()*

Run:

```
python GSASIIscriptable.py --help
```

to show the available subcommands, and inspect each subcommand with *python GSASIIscriptable.py <subcommand> –help* or see the documentation for each of the above routines.

1.9.1 Parameters in JSON files

The refine command requires two inputs: an existing GSAS-II project (.gpx) file and a JSON format file (see Introducing JSON) that contains a single dict. This dict may have two keys:

refinements:
: This defines the a set of refinement steps in a JSON representation of a *Refinement recipe* list.

code:
: This optionally defines Python code that will be executed after the project is loaded, but before the refinement is started. This can be used to execute Python code to change parameters that are not accessible via a *Refinement recipe* dict (note that the project object is accessed with variable `proj`) or to define code that will be called later (see key `call` in the *Refinement recipe* section.)

JSON website: Introducing JSON.

1.10 API: Complete Documentation

Classes and routines defined in *GSASIIscriptable* follow. A script will create one or more *G2Project* objects by reading a GSAS-II project (.gpx) file or creating a new one and will then perform actions such as adding a histogram (method *G2Project.add_powder_histogram()*), adding a phase (method *G2Project.add_phase()*), or setting parameters and performing a refinement (method *G2Project.do_refinements()*).

To change settings within histograms, images and phases, one usually needs to use methods inside *G2PwdrData*, *G2Image* or *G2Phase*.

class GSASII.GSASIIscriptable.**G2AtomRecord**(*data*, *indices*, *proj*)

Wrapper for an atom record. Allows many atom properties to be access and changed. See the *Atom Records description* for the details on what information is contained in an atom record.

Scripts should not try to create a *G2AtomRecord* object directly as these objects are created via access from a *G2Phase* object.

Example showing some uses of *G2AtomRecord* methods:

```
>>> atom = some_phase.atom("O3")
>>> # We can access the underlying data structure (a list):
>>> atom.data
['O3', 'O-2', '', ... ]
>>> # We can also use wrapper accessors to get or change atom info:
>>> atom.coordinates
(0.33, 0.15, 0.5)
>>> atom.coordinates = [1/3, .1, 1/2]
>>> atom.coordinates
(0.3333333333333333, 0.1, 0.5)
>>> atom.refinement_flags
'FX'
>>> atom.ranId
4615973324315876477
>>> atom.occupancy
1.0
```

property ADP

Get or set the associated atom's Uiso or Uaniso value(s). Use as `x = atom.ADP` to obtain the value(s) and `atom.ADP = x` to set the value(s). For isotropic atoms a single float value is returned (or used to set). For anisotropic atoms a list of six values is used.

See also

adp_flag() uiso()

property adp_flag

Get the associated atom's iso/aniso setting. The value will be 'I' or 'A'. No API provision is offered to change this.

property coordinates

Get or set the associated atom's coordinates. Use as `x = atom.coordinates` to obtain a tuple with the three (x,y,z) values and `atom.coordinates = (x,y,z)` to set the values.

Changes needed to adapt for changes in site symmetry have not yet been implemented:

property element

Parses element symbol from the atom type symbol for the atom associated with the current object.

> **See also**
>
> *type()*

property label

Get the associated atom's label. Use as `x = atom.label` to obtain the value and `atom.label = x` to set the value.

property mult

Get the associated atom's multiplicity value. Should not be changed by user.

property occupancy

Get or set the associated atom's site fraction. Use as `x = atom.occupancy` to obtain the value and `atom.occupancy = x` to set the value.

property ranId

Get the associated atom's Random Id number. Don't change this.

property refinement_flags

Get or set refinement flags for the associated atom. Use as `x = atom.refinement_flags` to obtain the flags and `atom.refinement_flags = "XU"` (etc) to set the value.

property type

Get or set the associated atom's type. Call as a variable (`x = atom.type`) to obtain the value or use `atom.type = x` to change the type. It is the user's responsibility to make sure that the atom type is valid; no checking is done here.

> **See also**
>
> *element()*

property uiso

A synonym for *ADP()* to be used for Isotropic atoms. Get or set the associated atom's Uiso value. Use as `x = atom.uiso` to obtain the value and `atom.uiso = x` to set the value. A single float value is returned or used to set.

> **See also**
>
> *adp_flag() ADP()*

class GSASII.GSASIIscriptable.**G2Image**(*data*, *name*, *proj*, *image=None*)

Wrapper for an IMG tree entry, containing an image and associated metadata.

Note that in a GSASIIscriptable script, instances of G2Image will be created by calls to *G2Project.add_image()* or *G2Project.images()*. Scripts should not try to create a *G2Image* object directly as `G2Image.__init__()` should be invoked from inside *G2Project*.

The object contains these class variables:

- G2Image.proj: contains a reference to the *G2Project* object that contains this image

- G2Image.name: contains the name of the image
- G2Image.data: contains the image's associated data in a dict, as documented for the *Image Data Structure*.
- G2Image.image: optionally contains a cached the image to save time in reloading. This is saved only when cacheImage=True is specified when *G2Project.add_image()* is called.

Example use of G2Image:

```
>>> gpx = G2sc.G2Project(newgpx='itest.gpx')
>>> imlst = gpx.add_image(idata,fmthint="TIF")
>>> imlst[0].loadControls('stdSettings.imctrl')
>>> imlst[0].setCalibrant('Si    SRM640c')
>>> imlst[0].loadMasks('stdMasks.immask')
>>> imlst[0].Recalibrate()
>>> imlst[0].setControl('outAzimuths',3)
>>> pwdrList = imlst[0].Integrate()
```

More detailed image processing examples are shown in the *Image Processing* section of this chapter.

ControlList = {'bool': ['setRings', 'setDefault', 'centerAzm', 'fullIntegrate', 'DetDepthRef', 'showLines'], 'dict': ['varyList'], 'float': ['cutoff', 'setdist', 'wavelength', 'Flat Bkg', 'azmthOff', 'tilt', 'calibdmin', 'rotation', 'distance', 'DetDepth'], 'int': ['calibskip', 'pixLimit', 'edgemin', 'outChannels', 'outAzimuths'], 'list': ['GonioAngles', 'IOtth', 'LRazimuth', 'Oblique', 'PolaVal', 'SampleAbs', 'center', 'ellipses', 'linescan', 'pixelSize', 'range', 'ring', 'rings', 'size'], 'str': ['SampleShape', 'binType', 'formatName', 'color', 'type']}

Defines the items known to exist in the Image Controls tree section and the item's data types. A few are not included here ('background image', 'dark image', 'Gain map', and 'calibrant') because these items have special set routines, where references to entries are checked to make sure their values are correct.

GeneratePixelMask(*esdMul=3.0*, *ttmin=0.0*, *ttmax=180.0*, *FrameMask=None*, *ThetaMap=None*, *fastmode=True*, *combineMasks=False*)

Generate a Pixel mask with True at the location of pixels that are statistical outliers (in comparison with others with the same 2theta value.) The process for this is that a median is computed for pixels within a small 2theta window and then the median difference is computed from magnitude of the difference for those pixels from that median. The medians are used for this rather than a standard deviation as the computation used here is less sensitive to outliers. The image must be properly calibrated so that radial averaging is possible. (See `GSASIIimage.AutoPixelMask()` and `scipy.stats.median_abs_deviation()` for more details.)

The mask is placed into the G2image object, where it will be accessed during integration. Note that this increases the .gpx file size significantly; use *clearPixelMask()* to delete this, if it need not be retained if the .gpx file is to be saved.

This code is based on `GSASIIimage.FastAutoPixelMask()`, but has been modified to recycle expensive computations where possible.

Parameters

- **esdMul** (*float*) – Significance threshold applied to remove outliers. Default is 3. The larger this number, the fewer "glitches" that will be removed.
- **ttmin** (*float*) – A lower 2theta limit to be used for pixel searching. Pixels outside this region may be considered for establishing the medians, but only pixels with 2theta >= `ttmin` are masked. Default is 0.
- **ttmax** (*float*) – An upper 2theta limit to be used for pixel searching. Pixels outside this region may be considered for establishing the medians, but only pixels with 2theta < `ttmax`

are masked. Default is 180.

- **FrameMask** (*np.array*) – An optional precomputed Frame mask (from *MaskFrameMask()*). Compute this once for a series of similar images to reduce computational time.
- **ThetaMap** (*np.array*) – An optional precomputed array that defines 2theta for each pixel, computed in *MaskThetaMap()*. Compute this once for a series of similar images to reduce computational time.
- **fastmode** (*bool*) – If True (default) fast Pixel map searching is done if the C module is available. If the module is not available or this is False, the pure Python implementatruion is used. It is not clear why False is ever needed.
- **combineMasks** (*bool*) – When True, the current Pixel mask will be combined with any previous Pixel map. If False (the default), the Pixel map from the current search will replace any previous ones. The reason for use of this as True would be where different `esdMul` values are used for different regions of the image (by setting `ttmin` & `ttmax`) so that the outlier level can be tuned by combining different searches.

IntMaskMap()

Computes a series of masking arrays for the current image (based on mask input, but not calibration parameters or the image intensities). See `GSASIIimage.MakeMaskMap()` for more details. The output from this is optionally supplied as input to *Integrate()*).

Note this is not the same as pixel mask searching (*GeneratePixelMask()*).

IntThetaAzMap()

Computes the set of blocked arrays for 2theta-azimuth mapping from the controls settings of the current image for image integration. The output from this is optionally supplied as input to *Integrate()*. Note that if not supplied, image integration will compute this information as it is needed, but this is a relatively slow computation so time can be saved by caching and reusing this computation for other images that have the same calibration parameters as the current image.

Integrate(*name=None*, *MaskMap=None*, *ThetaAzimMap=None*)

Invokes an image integration (same as Image Controls/Integration/Integrate menu command). All parameters will have previously been set with Image Controls so no input is needed here. However, the optional parameters MaskMap and ThetaAzimMap may be supplied to save computing these items more than once, speeding integration of multiple images with the same image/mask parameters.

Note that if integration is performed on an image more than once, histogram entries may be overwritten. Use the name parameter to prevent this if desired.

Parameters

- **name** (*str*) – base name for created histogram(s). If None (default), the histogram name is taken from the image name.
- **MaskMap** (*list*) – from *IntMaskMap()*
- **ThetaAzimMap** (*list*) – from *G2Image.IntThetaAzMap()*

Returns

a list of created histogram (*G2PwdrData* or *G2SmallAngle*) objects.

MaskFrameMask()

Computes a Frame mask from map input for the current image to be used for a pixel mask computation in *GeneratePixelMask()*. This is optional, as if not supplied, mask computation will compute this, but this is a relatively slow computation and the results computed here can be reused for other images that have the same calibration parameters.

MaskThetaMap()

Computes the theta mapping matrix from the controls settings of the current image to be used for pixel mask computation in *GeneratePixelMask()*. This is optional, as if not supplied, mask computation will compute this, but this is a relatively slow computation and the results computed here can be reused for other images that have the same calibration parameters.

Recalibrate()

Invokes a recalibration fit (same as Image Controls/Calibration/Recalibrate menu command). Note that for this to work properly, the calibration coefficients (center, wavelength, distance & tilts) must be fairly close. This may produce a better result if run more than once.

TestFastPixelMask()

Tests to see if the fast (C) code for pixel masking is installed.

Returns

A value of True is returned if fast pixel masking is available. Otherwise False is returned.

clearImageCache()

Clears a cached image, if one is present

clearPixelMask()

Removes a pixel map from an image, to reduce the .gpx file size & memory use

findControl(*arg=''*)

Finds the Image Controls parameter(s) in the current image that match the string in arg. Default is '' which returns all parameters.

Example:

```
>>> findControl('calib')
[['calibskip', 'int'], ['calibdmin', 'float'], ['calibrant', 'str']]
```

Parameters

arg (*str*) – a string containing part of the name of a parameter (dict entry) in the image's Image Controls.

Returns

a list of matching entries in form [['item','type'], ['item','type'],...] where each 'item' string contains the sting in arg.

getControl(*arg*)

Return an Image Controls parameter in the current image. If the parameter is not found an exception is raised.

Parameters

arg (*str*) – the name of a parameter (dict entry) in the image.

Returns

the value as a int, float, list,...

getControls(*clean=False*)

returns current Image Controls as a dict

Parameters

clean (*bool*) – causes the calbration information to be deleted

getImage()

Returns the image, even if not already cached

getMasks()

load masks from an IMG tree entry

getVary(**args*)

Return the refinement flag(s) for calibration of Image Controls parameter(s) in the current image. If the parameter is not found, an exception is raised.

Parameters

- **arg** (*str*) – the name of a refinement parameter in the varyList for the image. The name should be one of 'dep', 'det-X', 'det-Y', 'dist', 'phi', 'tilt', or 'wave'
- **arg1** (*str*) – the name of a parameter (dict entry) as before, optional

Returns

a list of bool value(s)

initMasks()

Initialize Masks, including resetting the Thresholds values

loadControls(*filename=None*, *imgDict=None*)

load controls from a .imctrl file

Parameters

- **filename** (*str*) – specifies a file to be read, which should end with .imctrl (defaults to None, meaning parameters are input with imgDict.)
- **imgDict** (*dict*) – contains a set of image parameters (defaults to None, meaning parameters are input with filename.)

loadMasks(*filename*, *ignoreThreshold=False*)

load masks from a .immask file

Parameters

- **filename** (*str*) – specifies a file to be read, which should end with .immask
- **ignoreThreshold** (*bool*) – If True, masks are loaded with threshold masks. Default is False which means any Thresholds in the file are ignored.

loadPixelMask(*mask*, *tag='loaded in G2sc.loadPixelMask'*)

Loads a pixel map from an array supplied by the user

Parameters

- **mask** (*np.array*) – An array that has a True or False value for each pixel. True means that the pixel should be masked. The array dimensions must match the current image.
- **tag** (*str*) – provides a name that is saved to indicate the source of the mask. At present this name is not used.

saveControls(*filename*)

write current controls values to a .imctrl file

Parameters

filename (*str*) – specifies a file to write, which should end with .imctrl

setCalibrant(*calib*)

Set a calibrant for the current image

Parameters
calib (*str*) – specifies a calibrant name which must be one of the entries in file ImageCalibrants.py. This is validated and an error provides a list of valid choices.

setControl(*arg*, *value*)

Set an Image Controls parameter in the current image. If the parameter is not found an exception is raised.

Parameters

- **arg** (*str*) – the name of a parameter (dict entry) in the image. The parameter must be found in *ControlList* or an exception is raised.
- **value** – the value to set the parameter. The value is cast as the appropriate type from *ControlList*.

setControlFile(*typ*, *imageRef*, *mult=None*)

Set a image to be used as a background/dark/gain map image

Parameters

- **typ** (*str*) – specifies image type, which must be one of: 'background image', 'dark image', 'gain map'; N.B. only the first four characters must be specified and case is ignored.
- **imageRef** – A reference to the desired image. Either the Image tree name (str), the image's index (int) or a image object (*G2Image*)
- **mult** (*float*) – a multiplier to be applied to the image (not used for 'Gain map'; required for 'background image', 'dark image'

setControls(*controlsDict*)

uses dict from *getControls()* to set Image Controls for current image

setMasks(*maskDict*, *resetThresholds=False*)

load masks dict (from *getMasks()*) into current IMG record

Parameters

- **maskDict** (*dict*) – specifies a dict with image parameters, from *getMasks()*
- **resetThresholds** (*bool*) – If True, Threshold Masks in the dict are ignored. The default is False which means Threshold Masks are retained.

setVary(*arg*, *value*)

Set a refinement flag for Image Controls parameter in the current image that is used for fitting calibration parameters. If the parameter is not '*' or found, an exception is raised.

Parameters

- **arg** (*str*) – the name of a refinement parameter in the varyList for the image. The name should be one of 'dep', 'det-X', 'det-Y', 'dist', 'phi', 'tilt', or 'wave', or it may be a list or tuple of names, or it may be '*' in which all parameters are set accordingly.
- **value** – the value to set the parameter. The value is cast as bool.

exception GSASII.GSASIIscriptable.**G2ImportException**

class GSASII.GSASIIscriptable.**G2ObjectWrapper**(*datadict*)

Base class for all GSAS-II object wrappers.

The underlying GSAS-II format can be accessed as *wrapper.data*. A number of overrides are implemented so that the wrapper behaves like a dictionary.

Author: Jackson O'Donnell (jacksonhodonnell .at. gmail.com)

class GSASII.GSASIIscriptable.**G2PDF**(*data*, *name*, *proj*)

Wrapper for a PDF tree entry, containing the information needed to compute a PDF and the S(Q), G(r) etc. after the computation is done. Note that in a GSASIIscriptable script, instances of G2PDF will be created by calls to *G2Project.add_PDF()* or *G2Project.pdf()*. Scripts should not try to create a *G2PDF* object directly.

Example use of *G2PDF*:

```
gpx.add_PDF('250umSiO2.pdfprm',0)
pdf.set_formula(['Si',1],['O',2])
pdf.set_background('Container',1,-0.21)
for i in range(5):
    if pdf.optimize(): break
pdf.calculate()
pdf.export(gpx.filename,'S(Q), pdfGUI')
gpx.save('pdfcalc.gpx')
```

See also

G2Project.pdf() G2Project.pdfs()

calculate(*xydata=None*, *limits=None*, *inst=None*)

Compute the PDF using the current parameters. Results are set in the PDF object arrays (self.data['PDF Controls']['G(R)'] etc.). Note that if `xydata`, is specified, the background histograms(s) will not be accessed from the project file associated with the current PDF entry. If `limits` and `inst` are both specified, no histograms need be in the current project. However, the self.data['PDF Controls'] sections ('Sample', 'Sample Bkg.','Container Bkg.') must be non-blank for the corresponding items to be used from``xydata``.

Parameters

- **xydata** (*dict*) – an array containing the Sample's I vs Q, and any or none of the Sample Background, the Container scattering and the Container Background. If xydata is None (default), the values are taken from histograms, as named in the PDF's self.data['PDF Controls'] entries with keys 'Sample', 'Sample Bkg.','Container Bkg.' & 'Container'.
- **limits** (*list*) – upper and lower Q values to be used for PDF computation. If None (default), the values are taken from the Sample histogram's .data['Limits'][1] values.
- **inst** (*dict*) – The Sample histogram's instrument parameters to be used for PDF computation. If None (default), the values are taken from the Sample histogram's .data['Instrument Parameters'][0] values.

export(*fileroot*, *formats*)

Write out the PDF-related data (G(r), S(Q),…) into files

Parameters

- **fileroot** (*str*) – name of file(s) to be written. The extension will be ignored and set to .iq, .sq, .fq or .gr depending on the formats selected.
- **formats** (*str*) – string specifying the file format(s) to be written, should contain at least one of the following keywords: I(Q), S(Q), F(Q), G(r) and/or PDFgui (capitalization and punctuation is ignored). Note that G(r) and PDFgui should not be specifed together.

optimize(*showFit=True*, *maxCycles=5*, *xydata=None*, *limits=None*, *inst=None*)

Optimize the low R portion of G(R) to minimize selected parameters. Note that this updates the parameters in the settings (self.data['PDF Controls']) but does not update the PDF object arrays (self.data['PDF Controls']['G(R)'] etc.) with the computed values, use *calculate()* after a fit to do that.

Parameters

- **showFit** (*bool*) – if True (default) the optimized parameters are shown before and after the fit, as well as the RMS value in the minimized region.
- **maxCycles** (*int*) – the maximum number of least-squares cycles; defaults to 5.
- **xydata** (*dict*) – an array containing the Sample's I vs Q, and any or none of the Sample Background, the Container scattering and the Container Background. If xydata is None (default), the values are taken from histograms, as named in the PDF's self.data['PDF Controls'] entries with keys 'Sample', 'Sample Bkg.','Container Bkg.' & 'Container'.
- **limits** (*list*) – upper and lower Q values to be used for PDF computation. If None (default), the values are taken from the Sample histogram's .data['Limits'][1] values.
- **inst** (*dict*) – The Sample histogram's instrument parameters to be used for PDF computation. If None (default), the values are taken from the Sample histogram's .data['Instrument Parameters'][0] values.

Returns

the result from the optimizer as True or False, depending on if the refinement converged.

set_background(*btype*, *histogram*, *mult=-1.0*, *refine=False*)

Sets a histogram to be used as the 'Sample Background', the 'Container' or the 'Container Background.'

Parameters

- **btype** (*str*) – Type of background to set, must contain the string 'samp' for Sample Background', 'cont' and 'back' for the 'Container Background' or only 'cont' for the 'Container'. Note that capitalization and extra characters are ignored, so the full strings (such as 'Sample Background' & 'Container Background') can be used.
- **histogram** – A reference to a histogram, which can be reference by object, name, or number.
- **mult** (*float*) – a multiplier for the histogram; defaults to -1.0
- **refine** (*bool*) – a flag to enable refinement (only implemented for 'Sample Background'); defaults to False

set_formula(**args*)

Set the chemical formula for the PDF computation. Use pdf.set_formula(['Si',1],['O',2]) for SiO2.

Parameters

- **item1** (*list*) – The element symbol and number of atoms in formula for first element
- **item2** (*list*) – The element symbol and number of atoms in formula for second element,…

repeat parameters as needed for all elements in the formula.

class GSASII.GSASIIscriptable.**G2Phase**(*data*, *name*, *proj*)

A wrapper object around a given phase. The object contains these class variables:

- G2Phase.proj: contains a reference to the *G2Project* object that contains this phase
- G2Phase.name: contains the name of the phase
- G2Phase.data: contains the phases's associated data in a dict, as documented for the *Phase Tree items*.

Scripts should not try to create a *G2Phase* object directly as `G2Phase.__init__()` should be invoked from inside *G2Project*.

Author: Jackson O'Donnell (jacksonhodonnell .at. gmail.com)

HAPvalue (*param=None*, *newValue=None*, *targethistlist='all'*)

Retrieves or sets individual HAP parameters for one histogram or multiple histograms.

Parameters

- **param** (*str*) – is a parameter name, which can be 'Scale' or 'PhaseFraction' (either can be used for phase fraction), 'Use', 'Extinction', 'LeBail', 'PO' (for Preferred Orientation). If not specified or invalid an exception is generated showing the list of valid parameters. At present, only these HAP parameters cannot be accessed with this function: 'Size', 'Mustrain', 'HStrain', 'Babinet'. This might be addressed in the future. Some of these values can be set via *G2Phase.set_HAP_refinements()*.
- **newValue** – the value to use when setting the HAP parameter for the appropriate histogram(s). Will be converted to the proper type or an exception will be generated if not possible. If not specified, and only one histogram is selected, the value is retrieved and returned. When param='PO' then this value is interpreted as the following:

  if the value is 0 or an even integer, then the preferred orientation model is set to "Spherical harmonics". If the value is 1, then "March-Dollase" is used. Any other value generates an error.
- **targethistlist** (*list*) – a list of histograms where each item in the list can be a histogram object (*G2PwdrData*), a histogram name or the index number of the histogram. The index number is relative to all histograms in the tree, not to those in the phase. If the string 'all' (default), then all histograms in the phase are used.

  targethistlist must correspond to a single histogram if a value is to be returned (i.e. when argument newValue is not specified).

Returns

the value of the parameter, when argument newValue is not specified.

See also

set_HAP_refinements()

Example:

```
val = ph0.HAPvalue('Scale')
val = ph0.HAPvalue('PhaseFraction',targethistlist=[0])
ph0.HAPvalue('Scale',2.5)
```

The first command returns the phase fraction if only one histogram is associated with the current phase, or raises an exception. The second command returns the phase fraction from the first histogram associated with the current phase. The third command sets the phase fraction for all histograms associated with the current phase.

InitDisAgl (*useAll=True*)

Create the default controls used for distance and angle searching. Perform distance and angle searching by passing the results from this to `GSASIIstrMain.RetDistAngle()` or `GSASIIstrMain.PrintDistAngle()` At present, this does not populate the values needed for uncertainty computations.

Parameters

useAll (*bool*) – when True (default) all atoms are included in the origin atom list. When False, only atoms with full occupancy are included. All atoms are included in the target atom list.

Returns
DisAglCtls, DisAglData. See the *Distance/Angle controls documentation* for a description of these.

Origin1to2Shift()

Applies an Origin 1 to Origin 2 shift to the selected phase, if defined. Note that GSAS-II only uses Origin 2 settings when both are offered in the International Tables. (These are space groups where the centre of symmetry is not at the highest symmetry site in the cell.) If the structure is not in the Origin 1 setting, this routine will create garbage.

A copy of the phase is made where the new phase name has the string "_shifted" added to it. The routine returns a reference to the new *G2Phase* object for the new phase.

If the phase is not one of the space groups that has Origin 1 & Origin 2 settings, None is returned.

Returns
the newly created phase object or None

ShortDistances(*useAll=False*)

Looks for unrealistic distances in a structure, which are atom-atom distances < 1.1 A for non-H(D) atoms. To reduce the likelihood of distances between disordered fragments being noted, set useAll=False (the default) so that disordered atoms are ignored.

addDistRestraint(*origin*, *target*, *bond*, *factor=1.1*, *ESD=0.01*)

Adds bond distance restraint(s) for the selected phase

This works by search for interatomic distances between atoms in the origin list and the target list (the two lists may be the same but most frequently will not) with a length between bond/factor and bond*factor. If a distance is found in that range, it is added to the restraints if it was not already found.

Parameters

- **origin** (*list*) – a list of atoms, each atom may be an atom object, an index or an atom label
- **target** (*list*) – a list of atoms, each atom may be an atom object, an index or an atom label
- **bond** (*float*) – the target bond length in A for the located atom
- **factor** (*float*) – a tolerance factor used when searching for bonds (defaults to 1.1)
- **ESD** (*float*) – the uncertainty for the bond (defaults to 0.01)

Returns
returns the number of new restraints that are found

As an example:

```
gpx = G2sc.G2Project('restr.gpx')
ph = gpx.phases()[0]
ph.clearDistRestraint()
origin = [a for a in ph.atoms() if a.element == 'Si']
target = [i for i,a in enumerate(ph.atoms()) if a.element == 'O']
c = ph.addDistRestraint(origin, target, 1.64)
print(c,'new restraints found')
ph.setDistRestraintWeight(1000)
gpx.save('restr-mod.gpx')
```

This example locates the first phase in a project file, clears any previous restraints. Then it places restraints on bonds between Si and O atoms at 1.64 A. Each restraint is weighted 1000 times in comparison to (obs-calc)/sigma for a data point. To show how atom selection can work, the origin atoms are identified here by atom object while the target atoms are identified by atom index. The methods are interchangeable. If atom labels are unique, then:

```
origin = [a.label for a in ph.atoms() if a.element == 'Si']
```

would also work identically.

add_atom(*x*, *y*, *z*, *element*, *lbl*, *occ=1.0*, *uiso=0.01*)

Adds an atom to the current phase

Parameters

- **x** (*float*) – atom fractional x coordinate
- **y** (*float*) – atom fractional y coordinate
- **z** (*float*) – atom fractional z coordinate
- **element** (*str*) – an element symbol (capitalization is ignored). Optionally add a valence (as in Ba+2)
- **lbl** (*str*) – A label for this atom
- **occ** (*float*) – A fractional occupancy for this atom (defaults to 1).
- **uiso** (*float*) – A Uiso value for this atom (defaults to 0.01).

Returns
the G2AtomRecord atom object for the new atom

atom(*atomlabel*)

Returns the atom specified by atomlabel, or None if it does not exist.

Parameters
atomlabel (*str*) – The name of the atom (e.g. “O2”)

Returns
A *G2AtomRecord* object representing the atom.

atoms()

Returns a list of atoms present in the current phase.

Returns
A list of *G2AtomRecord* objects.

See also

atom() G2AtomRecord

clearDistRestraint()

Deletes any previously defined bond distance restraint(s) for the selected phase

See also

G2Phase.addDistRestraint()

clear_HAP_refinements(*refs*, *histograms='all'*)

Clears the given HAP refinement parameters between this phase and the given histograms.

Parameters

- **refs** (*dict*) – A dictionary of the parameters to be cleared. See the the *Histogram-and-phase parameters* table for what can be specified.
- **histograms** – Either 'all' (default) or a list of the histograms by index, name or object. The index number is relative to all histograms in the tree, not to those in the phase. Histograms not associated with the current phase will be ignored. whose HAP parameters will be set with this phase. Histogram and phase must already be associated

Returns

None

clear_refinements(*refs*)

Clears a given set of parameters.

Parameters

refs (*dict*) – The parameters to clear. See the *Phase parameters* table for what can be specified.

property composition

Provides a dict where keys are atom types and values are the number of atoms of that type in cell (such as {'H': 2.0, 'O': 1.0})

copyHAPvalues(*sourcehist*, *targethistlist='all'*, *skip=[]*, *use=None*)

Copies HAP parameters for one histogram to a list of other histograms. Use skip or use to select specific entries to be copied or not used.

Parameters

- **sourcehist** – is a histogram object (*G2PwdrData*) or a histogram name or the index number of the histogram to copy parameters from. The index number is relative to all histograms in the tree, not to those in the phase.
- **targethistlist** (*list*) – a list of histograms where each item in the list can be a histogram object (*G2PwdrData*), a histogram name or the index number of the histogram. If the string 'all' (default), then all histograms in the phase are used.
- **skip** (*list*) – items in the HAP dict that should not be copied. The default is an empty list, which causes all items to be copied. To see a list of items in the dict, use *getHAPvalues()*. Don't use with `use`.
- **use** (*list*) – specifies the items in the HAP dict should be copied. The default is None, which causes all items to be copied. Don't use with `skip`.

examples:

```
ph0.copyHAPvalues(0,[1,2,3])
ph0.copyHAPvalues(0,use=['HStrain','Size'])
```

The first example copies all HAP parameters from the first histogram to the second, third and fourth histograms (as listed in the project tree). The second example copies only the 'HStrain' (Dij parameters and refinement flags) and the 'Size' (crystallite size settings, parameters and refinement flags) from the first histogram to all histograms.

property density

Provides a scalar with the density of the phase. In case of a powder this assumes a 100% packing fraction.

export_CIF (*outputname*, *quickmode=True*)

Write this phase to a .cif file named outputname

Parameters

- **outputname** (*str*) – The name of the .cif file to write to
- **quickmode** (*bool*) – Currently ignored. Carryover from exports.G2export_CIF

getHAPentryList (*histname=None*, *keyname=''*)

Returns a dict with HAP values. Optionally a histogram may be selected.

Parameters

- **histname** – is a histogram object (*G2PwdrData*) or a histogram name or the index number of the histogram. The index number is relative to all histograms in the tree, not to those in the phase. If no histogram is specified, all histograms are selected.
- **keyname** (*str*) – an optional string. When supplied only entries where at least one key contains the specified string are reported. Case is ignored, so 'sg' will find entries where one of the keys is 'SGdata', etc.

Returns

a set of HAP dict keys.

Example:

```
>>> p.getHAPentryList(0,'Scale')
[(['PWDR test Bank 1', 'Scale'], list, [1.0, False])]
```

See also

getHAPentryValue() setHAPentryValue()

getHAPentryValue (*keylist*)

Returns the HAP value associated with a list of keys. Where the value returned is a list, it may be used as the target of an assignment (as in `getHAPentryValue(...)[...] = val`) to set a value inside a list.

Parameters

keylist (*list*) – a list of dict keys, typically as returned by *getHAPentryList()*. Note the first entry is a histogram name. Example: `['PWDR hist1.fxye Bank 1', 'Scale']`

Returns

HAP value

Example:

```
>>> sclEnt = p.getHAPentryList(0,'Scale')[0]
>>> sclEnt
(['PWDR test Bank 1', 'Scale'], list, [1.0, False])]
>>> p.getHAPentryValue(sclEnt[0])
[1.0, False]
>>> p.getHAPentryValue(sclEnt[0])[1] = True
>>> p.getHAPentryValue(sclEnt[0])
[1.0, True]
```

getHAPvalues (*histname*)

Returns a dict with HAP values for the selected histogram

Parameters
histogram – is a histogram object (*G2PwdrData*) or a histogram name or the index number of the histogram. The index number is relative to all histograms in the tree, not to those in the phase.

Returns
HAP value dict

getPhaseEntryList(*keyname=''*)

Returns a dict with control values.

Parameters
keyname (*str*) – an optional string. When supplied only entries where at least one key contains the specified string are reported. Case is ignored, so 'sg' will find entries where one of the keys is 'SGdata', etc.

Returns
a set of phase dict keys. Note that HAP items, while technically part of the phase entries, are not included.

See *getHAPentryList()* for a related example.

See also
getPhaseEntryValue() setPhaseEntryValue()

getPhaseEntryValue(*keylist*)

Returns the value associated with a list of keys. Where the value returned is a list, it may be used as the target of an assignment (as in `getPhaseEntryValue(...)[...] = val`) to set a value inside a list.

Parameters
keylist (*list*) – a list of dict keys, typically as returned by *getPhaseEntryList()*.

Returns
a phase setting; may be a int, float, bool, list,…

See *getHAPentryValue()* for a related example.

get_cell()

Returns a dictionary of the cell parameters, with keys:
'length_a', 'length_b', 'length_c', 'angle_alpha', 'angle_beta', 'angle_gamma', 'volume'

Returns
a dict

See also
get_cell_and_esd()

get_cell_and_esd()

Returns a pair of dictionaries, the first representing the unit cell, the second representing the estimated standard deviations of the unit cell.

Returns
a tuple of two dictionaries

> **See also**
>
> *get_cell()*

histograms()

Returns a list of histogram names associated with the current phase ordered as they appear in the tree (see *G2Project.histograms()*).

mu(*wave*)

Provides mu values for a phase at the supplied wavelength in A. Uses GSASIImath.XScattDen which seems to be off by an order of magnitude, which has been corrected here.

setDistRestraintWeight(*factor=1*)

Sets the weight for the bond distance restraint(s) to factor

Parameters

factor (*float*) – the weighting factor for this phase's restraints. Defaults to 1 but this value is typically much larger (10**2 to 10**4)

> **See also**
>
> *G2Phase.addDistRestraint()*

setHAPentryValue(*keylist*, *newvalue*)

Sets an HAP value associated with a list of keys.

Parameters

- **keylist** (*list*) – a list of dict keys, typically as returned by *getHAPentryList()*. Note the first entry is a histogram name. Example: `['PWDR hist1.fxye Bank 1', 'Scale']`
- **newvalue** – a new value for the HAP setting. The type must be the same as the initial value, but if the value is a container (list, tuple, np.array,…) the elements inside are not checked.

Example:

```
>>> sclEnt = p.getHAPentryList(0,'Scale')[0]
>>> p.getHAPentryValue(sclEnt[0])
[1.0, False]
>>> p.setHAPentryValue(sclEnt[0], (1, True))
GSASIIscriptable.G2ScriptException: setHAPentryValue error: types do not␣
↪agree for keys ['PWDR test.fxye Bank 1', 'Scale']
>>> p.setHAPentryValue(sclEnt[0], [1, True])
>>> p.getHAPentryValue(sclEnt[0])
[1, True]
```

setHAPvalues(*HAPdict*, *targethistlist='all'*, *skip=[]*, *use=None*)

Copies HAP parameters for one histogram to a list of other histograms. Use skip or use to select specific entries to be copied or not used. Note that `HStrain` and sometimes `Mustrain` values can be specific to a Laue class and should be copied with care between phases of different symmetry. A "sanity check" on the number of Dij terms is made if `HStrain` values are copied.

Parameters

- **HAPdict** (*dict*) – is a dict returned by *getHAPvalues()* containing HAP parameters.

- **targethistlist** (*list*) – a list of histograms where each item in the list can be a histogram object (*G2PwdrData*), a histogram name or the index number of the histogram. The index number is relative to all histograms in the tree, not to those in the phase. If the string 'all' (default), then all histograms in the phase are used.
- **skip** (*list*) – items in the HAP dict that should not be copied. The default is an empty list, which causes all items to be copied. To see a list of items in the dict, use *getHAPvalues()*. Don't use with `use`.
- **use** (*list*) – specifies the items in the HAP dict should be copied. The default is None, which causes all items to be copied. Don't use with `skip`.

Example:

```
HAPdict = ph0.getHAPvalues(0)
ph1.setHAPvalues(HAPdict,use=['HStrain','Size'])
```

This copies the Dij (hydrostatic strain) HAP parameters and the crystallite size broadening terms from the first histogram in phase `ph0` to all histograms in phase `ph1`.

setPhaseEntryValue(*keylist*, *newvalue*)

Sets a phase control value associated with a list of keys.

Parameters

- **keylist** (*list*) – a list of dict keys, typically as returned by *getPhaseEntryList()*.
- **newvalue** – a new value for the phase setting. The type must be the same as the initial value, but if the value is a container (list, tuple, np.array,…) the elements inside are not checked.

See *setHAPentryValue()* for a related example.

setSampleProfile(*histname*, *parmType*, *mode*, *val1*, *val2=None*, *axis=None*, *LGmix=None*)

Sets sample broadening parameters for a histogram associated with the current phase. This currently supports isotropic and uniaxial broadening modes only.

Parameters

- **histogram** – is a histogram object (*G2PwdrData*) or a histogram name or the index number of the histogram. The index number is relative to all histograms in the tree, not to those in the phase.
- **parmType** (*str*) – should be 'size' or 'microstrain' (can be abbreviated to 's' or 'm')
- **mode** (*str*) – should be 'isotropic' or 'uniaxial' (can be abbreviated to 'i' or 'u')
- **val1** (*float*) – value for isotropic size (in μm) or microstrain (unitless, $\Delta Q/Q \times 10^6$) or the equatorial value in the uniaxial case
- **val2** (*float*) – value for axial size (in μm) or axial microstrain (unitless, $\Delta Q/Q \times 10^6$) in uniaxial case; not used for isotropic
- **axis** (*list*) – tuple or list with three values indicating the preferred direction for uniaxial broadening; not used for isotropic
- **LGmix** (*float*) – value for broadening type (1=Lorentzian, 0=Gaussian or a value between 0 and 1. Default value (None) is ignored.

Examples:

```
phase0.setSampleProfile(0,'size','iso',1.2)
phase0.setSampleProfile(0,'micro','isotropic',1234)
phase0.setSampleProfile(0,'m','u',1234,4567,[1,1,1],.5)
phase0.setSampleProfile(0,'s','uni',1.2,2.3,[0,0,1])
```

set_HAP_refinements(*refs*, *histograms='all'*)

Sets the given HAP refinement parameters between the current phase and the specified histograms.

Parameters

- **refs** (*dict*) – A dictionary of the parameters to be set. See the *Histogram-and-phase parameters* table for a description of this dictionary.
- **histograms** – Either 'all' (default) or a list of the histograms by index, name or object. The index number is relative to all histograms in the tree, not to those in the phase. Histograms not associated with the current phase will be ignored. whose HAP parameters will be set with this phase. Histogram and phase must already be associated.

Returns

None

Example for Size and Mustrain with LG_mix:

```
phase.set_HAP_refinements({
    'Size': {'type':'isotropic', 'refine': True,
             'LGmix': {'value': 0.5, 'refine': False}},
    'Mustrain': {'type':'uniaxial',
                 'LGmix': {'value': 0.8, 'refine': True}}
})
```

set_refinements(*refs*)

Sets the phase refinement parameter 'key' to the specification 'value'

Parameters

refs (*dict*) – A dictionary of the parameters to be set. See the *Phase parameters* table for a description of this dictionary.

Returns

None

class GSASII.GSASIIscriptable.**G2Project**(*gpxfile=None*, *author=None*, *filename=None*, *newgpx=None*)

Represents an entire GSAS-II project. The object contains these class variables:

- G2Project.filename: contains the .gpx filename
- G2Project.names: contains the contents of the project "tree" as a list of lists. Each top-level entry in the tree is an item in the list. The name of the top-level item is the first item in the inner list. Children of that item, if any, are subsequent entries in that list.
- G2Project.data: contains the entire project as a dict. The keys for the dict are the top-level names in the project tree (initial items in the G2Project.names inner lists) and each top-level item is stored as a dict.
  - The contents of Top-level entries will be found in the item named 'data', as an example, `G2Project.data['Notebook']['data']`
  - The contents of child entries will be found in the item using the names of the and child, for example `G2Project.data['Phases']['NaCl']`

Parameters

- **gpxfile** (*str*) – Existing .gpx file to be loaded. If nonexistent, creates an empty project.
- **author** (*str*) – Author's name (not yet implemented)
- **newgpx** (*str*) – The filename the project should be saved to in the future. If both newgpx and gpxfile are present, the project is loaded from the file named by gpxfile and then when saved will be written to the file named by newgpx.
- **filename** (*str*) – To be deprecated. Serves the same function as newgpx, which has a somewhat more clear name. (Do not specify both newgpx and filename).

There are two ways to initialize this object:

```
>>> # Load an existing project file
>>> proj = G2Project('filename.gpx')
```

```
>>> # Create a new project
>>> proj = G2Project(newgpx='new_file.gpx')
```

Histograms can be accessed easily.

```
>>> # By name
>>> hist = proj.histogram('PWDR my-histogram-name')
```

```
>>> # Or by index
>>> hist = proj.histogram(0)
>>> assert hist.id == 0
```

```
>>> # Or by random id
>>> assert hist == proj.histogram(hist.ranId)
```

Phases can be accessed the same way.

```
>>> phase = proj.phase('name of phase')
```

New data can also be loaded via *add_phase()* and *add_powder_histogram()*.

```
>>> hist = proj.add_powder_histogram('some_data_file.chi',
                                     'instrument_parameters.prm')
>>> phase = proj.add_phase('my_phase.cif', histograms=[hist])
```

Parameters for Rietveld refinement can be turned on and off at the project level as well as described in *set_refinement()*, *iter_refinements()* and *do_refinements()*.

ComputeWorstFit()

Computes the worst-fit parameters in a model.

Returns

(keys, derivCalcs, varyList) where:

- keys is a list of parameter names where the names are ordered such that first entry in the list will produce the largest change in the fit if refined and the last entry will have the smallest change;
- derivCalcs is a dict where the key is a variable name and the value is a list with three partial derivative values for d(Chi**2)/d(var) where the derivatives are computed for values v-d to

v; v-d to v+d; v to v+d where v is the current value for the variable and d is a small delta value chosen for that variable type;

- varyList is a list of the parameters that are currently set to be varied.

SAS (*sasRef*)

Gives an object representing the specified SAS entry in this project.

Parameters

sasRef – A reference to the desired SASD entry. Either the SASD tree name (str), the SASD's index (int) or a SASD object (*G2SmallAngle*)

Returns

A *G2SmallAngle* object

Raises

KeyError

See also

SASs() G2PDF

SASs ()

Returns a list of all the Small Angle histograms in the project.

Returns

A list of *G2SmallAngle* objects

add_EqnConstr (*total*, *varlist*, *multlist=[]*, *reloadIdx=True*, *override=False*)

Set a constraint equation on a list of variables.

Note that this will cause the project to be saved if not already done so. It will always save the .gpx file before creating a constraint if reloadIdx is True.

Parameters

- **total** (*float*) – A value that the constraint must equal
- **varlist** (*list*) – A list of variables to use in the equation. Each value in the list may be one of the following three items: (A) a `GSASIIobj.G2VarObj` object, (B) a variable name (str), or (C) a list/tuple of arguments for *make_var_obj()*.
- **multlist** (*list*) – a list of multipliers for each variable in varlist. If there are fewer values than supplied for varlist then missing values will be set to 1. The default is [] which means that all multipliers are 1.
- **reloadIdx** (*bool*) – If True (default) the .gpx file will be saved and indexed prior to use. This is essential if atoms, phases or histograms have been added to the project.
- **override** (*bool*) – This routine looks up variables using `GSASIIobj.getDescr()` (which is not comprehensive). If not found, the routine will throw an exception, unless override=True is specified.

Example:

```
gpx.add_EqnConstr(1.0,('0::Ax:0','0::Ax:1'),[1,1])
```

add_EquivConstr (*varlist*, *multlist=[]*, *reloadIdx=True*, *override=False*)

Set a equivalence on a list of variables.

Note that this will cause the project to be saved if not already done so. It will always save the .gpx file before creating a constraint if reloadIdx is True.

Parameters

- **varlist** (*list*) – A list of variables to make equivalent to the first item in the list. Each value in the list may be one of the following three items: (A) a `GSASIIobj.G2VarObj` object, (B) a variable name (str), or (C) a list/tuple of arguments for *make_var_obj()*.
- **multlist** (*list*) – a list of multipliers for each variable in varlist. If there are fewer values than supplied for varlist then missing values will be set to 1. The default is [] which means that all multipliers are 1.
- **reloadIdx** (*bool*) – If True (default) the .gpx file will be saved and indexed prior to use. This is essential if atoms, phases or histograms have been added to the project.
- **override** (*bool*) – This routine looks up variables using `GSASIIobj.getDescr()` (which is not comprehensive). If not found, the routine will throw an exception, unless override=True is specified.

Examples:

```
gpx.add_EquivConstr(('0::AUiso:0','0::AUiso:1','0::AUiso:2'))
gpx.add_EquivConstr(('0::dAx:0','0::dAx:1'),[1,-1])
```

add_HoldConstr(*varlist*, *reloadIdx=True*, *override=False*)

Set a hold constraint on a list of variables.

Note that this will cause the project to be saved if not already done so. It will always save the .gpx file before creating constraint(s) if reloadIdx is True.

Parameters

- **varlist** (*list*) – A list of variables to hold. Each value in the list may be one of the following three items: (A) a `GSASIIobj.G2VarObj` object, (B) a variable name (str), or (C) a list/tuple of arguments for *make_var_obj()*.
- **reloadIdx** (*bool*) – If True (default) the .gpx file will be saved and indexed prior to use. This is essential if atoms, phases or histograms have been added to the project.
- **override** (*bool*) – This routine looks up variables using `GSASIIobj.getDescr()` (which is not comprehensive). If not found, the routine will throw an exception, unless override=True is specified.

Example:

```
gpx.add_HoldConstr(('0::A4','0:1:D12',':0:Lam'))
```

add_NewVarConstr(*varlist*, *multlist=[]*, *name=None*, *vary=False*, *reloadIdx=True*, *override=False*)

Set a new-variable constraint from a list of variables to create a new parameter from two or more predefined parameters.

Note that this will cause the project to be saved, if not already done so. It will always save the .gpx file before creating a constraint if reloadIdx is True.

Parameters

- **varlist** (*list*) – A list of variables to use in the expression. Each value in the list may be one of the following three items: (A) a `GSASIIobj.G2VarObj` object, (B) a variable name (str), or (C) a list/tuple of arguments for *make_var_obj()*.

- **multlist** (*list*) – a list of multipliers for each variable in varlist. If there are fewer values than supplied for varlist then missing values will be set to 1. The default is [] which means that all multipliers are 1.
- **name** (*str*) – An optional string to be supplied as a name for this new parameter.
- **vary** (*bool*) – Determines if the new variable should be flagged to be refined.
- **reloadIdx** (*bool*) – If True (default) the .gpx file will be saved and indexed prior to use. This is essential if atoms, phases or histograms have been added to the project.
- **override** (*bool*) – This routine looks up variables using `GSASIIobj.getDescr()` (which is not comprehensive). If not found, the routine will throw an exception, unless override=True is specified.

Examples:

```
gpx.add_NewVarConstr(('0::AFrac:0','0::AFrac:1'),[0.5,0.5],'avg',True)
gpx.add_NewVarConstr(('0::AFrac:0','0::AFrac:1'),[1,-1],'diff',False,False)
```

The example above is a way to treat two variables that are closely correlated. The first variable, labeled as avg, allows the two variables to refine in tandem while the second variable (diff) tracks their difference. In the initial stages of refinement only avg would be refined, but in the final stages, it might be possible to refine diff. The second False value in the second example prevents the .gpx file from being saved.

add_PDF(*prmfile*, *histogram*)

Creates a PDF entry that can be used to compute a PDF. Note that this command places an entry in the project, but *G2PDF.calculate()* must be used to actually perform the computation.

Parameters

- **datafile** (*str*) – The powder data file to read, a filename.
- **histogram** – A reference to a histogram, which can be reference by object, name, or number.

Returns

A *G2PDF* object for the PDF entry

add_SmallAngle(*datafile*)

Placeholder for an eventual routine that will read a small angle dataset from a file.

Parameters

datafile (*str*) – The SASD data file to read, a filename.

Returns

A *G2SmallAngle* object for the SASD entry

add_constraint_raw(*cons_scope*, *constr*)

Adds a constraint to the project.

Parameters

- **cons_scope** (*str*) – should be one of “Hist”, “Phase”, “HAP”, or “Global”.
- **constr** (*list*) – a constraint coded with `GSASIIobj.G2VarObj` objects as described in the *constraint definition descriptions*.

WARNING this function does not check the constraint is well-constructed. Please use *G2Project.add_HoldConstr()* or *G2Project.add_EquivConstr()* (etc.) instead, unless you are really certain you know what you are doing.

add_image(*imagefile*, *fmthint=None*, *defaultImage=None*, *indexList=None*, *cacheImage=False*, *URL=False*, *download_loc=None*, *imageKey=None*)

Load an image into a project

Parameters

- **imagefile** (*str*) – The image file to read, a filename.
- **fmthint** (*str*) – If specified, only importers where the format name (reader.formatName, as shown in Import menu) contains the supplied string will be tried as importers. If not specified, all importers consistent with the file extension will be tried (equivalent to "guess format" in menu).
- **defaultImage** (*str*) – The name of an image to use as a default for setting parameters for the image file to read.
- **indexList** (*list*) – specifies the image numbers (counting from zero) to be used from the file when a file has multiple images. A value of `[0,2,3]` will cause the only first, third and fourth images in the file to be included in the project. Note that with this option, all images are read from the file, but only the specified image(s) are retained. Do not use imageKey and indexList together.
- **cacheImage** (*bool*) – When True, the image is cached to save in rereading it later. Default is False (no caching).
- **URL** (*bool*) – if True, the contents of imagefile is a URL and the file will be downloaded and saved. The file will be written in the specified directory (see *download_loc*) or a temporary location, if not specified. Note that if a temporary location, if the proiject (.gpx) file is saved, the image may not be accessible if the .gpx file is later reopened. Default is False. If URL is specified and the Python requests package is not installed, a *ModuleNotFoundError* Exception will occur. will occur.
- **download_loc** (*str*) – a location or file name where the image will be saved. Note that for almost all image types, the image cannot be read if the file extension does not match what is expected for the format. (This can be determined by looking at the importer code; if *strictExtension=True*, the extension must be in the *extensionlist* list.) If only a directory is specified, the file name will be taken from the URL, which will likely cause problems if it does not match the needed extension. If URL is specified and the default download_loc value is used (None), the image will be saved in a temporary location that will persist until the OS removes it.
- **imageKey** – This can be a single image number (int) to read a specific image (numbered starting with 1) or for files that have images in named sections, (right now this is only HDF5), it can be a tuple of form ('section',0) where 'section' is the section name (such as '/exchange/data') and 0 is the image number in that section. If imageKey is specified, only one image is read. Do not use imageKey and indexList together.

Returns

a list of *G2Image* object(s) for the added image(s)

add_phase(*phasefile=None*, *phasename=None*, *histograms=[]*, *fmthint=None*, *mag=False*, *spacegroup='P 1'*, *cell=None*, *URL=False*, *useNet=False*, *PhaseRef=None*)

Loads a phase into the project, usually from a .cif file

Parameters

- **phasefile** (*str*) – The CIF file (or other file type, see fmthint) that the phase will be read from. May be left as None (the default) if the phase will be constructed a step at a time.

- **phasename** (*str*) – The name of the new phase, or None for the default. A phasename must be specified when a phasefile is not.
- **histograms** (*list*) – The names of the histograms to associate with this phase. Use proj.histograms() to add to all histograms.
- **fmthint** (*str*) – If specified, only importers where the format name (reader.formatName, as shown in Import menu) contains the supplied string will be tried as importers. If not specified, all importers consistent with the file extension will be tried (equivalent to "guess format" in menu). Specifying this is optional but is strongly encouraged.
- **mag** (*bool*) – Set to True to read a magCIF
- **spacegroup** (*str*) – The space group name as a string. The space group must follow the naming rules used in `GSASIIspc.SpcGroup()`. Defaults to 'P 1'. Note that this is only used when phasefile is None.
- **cell** (*list*) – a list with six unit cell constants (a, b, c, alpha, beta and gamma in Angstrom/degrees).
- **URL** (*bool*) – if True, the contents of phasefile is a URL and the file will be downloaded to a temporary location and read. The downloaded file will not be saved. If URL is specified and the Python requests package is not installed, a *ModuleNotFoundError* Exception will occur. will occur.
- **useNet** (*bool*) – if True, when an incompatible space group setting is detected (at present this is only tested with CIFs, where symmetry operators are supplied), which is most likely to occur with origin-1 settings, where allowed, the importer will call Bilbao "CIF to Standard Setting" web service. (Default is False).
- **PhaseRef** – Used for magnetic phases only, a reference to the (aka chemical/nuclear) phase. This can be the phase name (str), the phase's ranId, the phase's index (both int) or a phase object (*G2Phase*)

Returns

A *G2Phase* object representing the new phase.

add_powder_histogram(*datafile*, *iparams=None*, *phases=[]*, *fmthint=None*, *databank=None*, *instbank=None*, *multiple=False*, *URL=False*)

Loads a powder data histogram or multiple powder histograms into the project.

Note that the data type (x-ray/CW neutron/TOF) for the histogram will be set from the instrument parameter file. The instrument geometry is assumed to be Debye-Scherrer except for dual-wavelength x-ray, where Bragg-Brentano is assumed.

Parameters

- **datafile** (*str*) – A filename with the powder data file to read. Note that in unix fashion, "~" can be used to indicate the home directory (e.g. ~/G2data/data.fxye).
- **iparams** (*str*) – A filename for an instrument parameters file, or a pair of instrument parameter dicts from *load_iprms()*. This may be omitted for readers that provide the instrument parameters in the file. (Only a few importers do this.)
- **phases** (*list*) – A list of phases to link to the new histogram, phases can be references by object, name, rId or number. Alternately, use 'all' to link to all phases in the project.
- **fmthint** (*str*) – If specified, only importers where the format name (reader.formatName, as shown in Import menu) contains the supplied string will be tried as importers. If not specified, all importers consistent with the file extension will be tried (equivalent to "guess format" in menu).

- **databank** (*int*) – Specifies a dataset number to read, if file contains more than set of data. This should be 1 to read the first bank in the file (etc.) regardless of the number on the Bank line, etc. Default is None which means the first dataset in the file is read. When multiple is True, optionally a list of dataset numbers can be supplied here.
- **instbank** (*int*) – Specifies an instrument parameter set to read, if the instrument parameter file contains more than set of parameters. This will match the INS # in an GSAS type file so it will typically be 1 to read the first parameter set in the file (etc.) Default is None which means there should only be one parameter set in the file.
- **multiple** (*bool*) – If False (default) only one dataset is read, but if specified as True, all selected banks of data (see databank) are read in.
- **URL** (*bool*) – if True, the contents of datafile is a URL and if not a dict, the contents of iparams is also a URL. both files will be downloaded to a temporary location and read. The downloaded files will not be saved. If URL is specified and the Python requests package is not installed, a *ModuleNotFoundError* Exception will occur. will occur.

Returns

A *G2PwdrData* object representing the histogram, or if multiple is True, a list of *G2PwdrData* objects is returned.

add_simulated_powder_histogram(*histname*, *iparams*, *Tmin*, *Tmax*, *Tstep=None*, *wavelength=None*, *scale=None*, *phases=[]*, *ibank=None*, *Npoints=None*)

Create a simulated powder data histogram for the project.

Requires an instrument parameter file. Note that in unix fashion, "~" can be used to indicate the home directory (e.g. ~/G2data/data.prm). The instrument parameter file will determine if the histogram is x-ray, CW neutron, TOF, etc. as well as the instrument type.

Parameters

- **histname** (*str*) – A name for the histogram to be created.
- **iparams** (*str*) – The instrument parameters file, a filename.
- **Tmin** (*float*) – Minimum 2theta or TOF (millisec) for dataset to be simulated
- **Tmax** (*float*) – Maximum 2theta or TOF (millisec) for dataset to be simulated
- **Tstep** (*float*) – Step size in 2theta or deltaT/T (TOF) for simulated dataset. Default is to compute this from Npoints.
- **wavelength** (*float*) – Wavelength for CW instruments, overriding the value in the instrument parameters file if specified. For single-wavelength histograms, this should be a single float value, for K alpha 1,2 histograms, this should be a list or tuple with two values.
- **scale** (*float*) – Histogram scale factor which multiplies the pattern. Note that simulated noise is added to the pattern, so that if the maximum intensity is small, the noise will mask the computed pattern. The scale needs to be a large number for neutrons. The default, None, provides a scale of 1 for x-rays, 10,000 for CW neutrons and 100,000 for TOF.
- **phases** (*list*) – Phases to link to the new histogram. Use proj.phases() to link to all defined phases.
- **ibank** (*int*) – provides a bank number for the instrument parameter file. The default is None, corresponding to load the first bank.
- **Npoints** (*int*) – the number of data points to be used for computing the diffraction pattern. Defaults as None, which sets this to 2500. Do not specify both Npoints and Tstep. Due to roundoff the actual number of points used may differ by +-1 from Npoints. Must be below 25,000.

Returns
A *G2PwdrData* object representing the histogram

add_single_histogram(*datafile*, *phase=None*, *fmthint=None*)

Loads a powder data histogram or multiple powder histograms into the project.

Parameters

- **datafile** (*str*) – A filename with the single crystal data file to read. Note that in unix fashion, "~" can be used to indicate the home directory (e.g. ~/G2data/data.hkl).
- **phases** – A phase to link to the new histogram. A phase can be referenced by object, name, rId or number. If not specified, no phase will be linked.
- **fmthint** (*str*) – If specified, only importers where the format name (reader.formatName, as shown in Import menu) contains the supplied string will be tried as importers. If not specified, an error will be generated, as the file format will not distinguish well between different data types.

Returns
A *G2Single* object representing the histogram

clone_powder_histogram(*histref*, *newname*, *Y*, *Yerr=None*)

Creates a copy of a powder diffraction histogram with new Y values. The X values are not changed. The number of Y values must match the number of X values.

Parameters

- **histref** – The histogram object, the name of the histogram (str), or ranId or histogram index.
- **newname** (*str*) – The name to be assigned to the new histogram
- **Y** (*list*) – A set of intensity values
- **Yerr** (*list*) – A set of uncertainties for the intensity values (may be None, sets all weights to unity)

Returns
the new histogram object (type G2PwdrData)

copyHistParms(*sourcehist*, *targethistlist='all'*, *modelist='all'*)

Copy histogram information from one histogram to others

Parameters

- **sourcehist** – is a histogram object (*G2PwdrData*) or a histogram name or the index number of the histogram
- **targethistlist** (*list*) – a list of histograms where each item in the list can be a histogram object (*G2PwdrData*), a histogram name or the index number of the histogram. if the string 'all' (default value), then all histograms in the project are used.
- **modelist** (*list*) – May be a list of sections to copy, which may include 'Background', 'Instrument Parameters', 'Limits' and 'Sample Parameters' (items may be shortened to uniqueness and capitalization is ignored, so ['b','i','L','s'] will work.) The default value, 'all' causes the listed sections to

copy_PDF(*PDFobj*, *histogram*)

Creates a PDF entry that can be used to compute a PDF as a copy of settings in an existing PDF (*G2PDF*) object. This places an entry in the project but *G2PDF.calculate()* must be used to actually perform the PDF computation.

Parameters

- **PDFobj** – A *G2PDF* object which may be in a separate project or the dict associated with the PDF object (G2PDF.data).
- **histogram** – A reference to a histogram, which can be reference by object, name, or number.

Returns

A *G2PDF* object for the PDF entry

do_refinements(*refinements=[{}]*, *histogram='all'*, *phase='all'*, *outputnames=None*, *makeBack=False*)

Conducts one or a series of refinements according to the
input provided in parameter refinements. This is a wrapper around *iter_refinements()*

Parameters

- **refinements** (*list*) – A list of dictionaries specifiying changes to be made to parameters before refinements are conducted. See the *Refinement recipe* section for how this is defined. If not specified, the default value is `[{}]`, which performs a single refinement step is performed with the current refinement settings.
- **histogram** (*str*) – Name of histogram for refinements to be applied to, or 'all'; note that this can be overridden for each refinement step via a "histograms" entry in the dict.
- **phase** (*str*) – Name of phase for refinements to be applied to, or 'all'; note that this can be overridden for each refinement step via a "phases" entry in the dict.
- **outputnames** (*list*) – Provides a list of project (.gpx) file names to use for each refinement step (specifying None skips the save step). See *save()*. Note that this can be overridden using an "output" entry in the dict.
- **makeBack** (*bool*) – determines if a backup).bckX.gpx) file is made before a refinement is performed. The default is False.

To perform a single refinement without changing any parameters, use this call:

```
my_project.do_refinements([])
```

classmethod from_dict_and_names(*gpxdict*, *names*, *filename=None*)

Creates a *G2Project* directly from a dictionary and a list of names. If in doubt, do not use this.

Returns

a *G2Project*

get_Constraints(*ctype*)

Returns a list of constraints of the type selected.

Parameters

ctype (*str*) – one of the following keywords: 'Hist', 'HAP', 'Phase', 'Global'

Returns

a list of constraints, see the *constraint definition descriptions*. Note that if this list is changed (for example by deleting elements or by changing them) the constraints in the project are changed.

get_Controls(*control*, *variable=None*)

Return project controls settings

Parameters

- **control** (*str*) – the item to be returned. See below for allowed values.

- **variable** (*str*) – a variable name as a str or (as a `GSASIIobj.G2VarObj` object). Used only with control set to "parmMin" or "parmMax".

Returns
The value for the control.

Allowed values for parameter control:

- cycles: the maximum number of cycles (returns int)
- sequential: the histograms used for a sequential refinement as a list of histogram names or an empty list when in non-sequential mode.
- Reverse Seq: returns True or False. True indicates that fitting of the sequence of histograms proceeds in reversed order.
- seqCopy: returns True or False. True indicates that results from each sequential fit are used as the starting point for the next histogram.
- parmMin & parmMax: retrieves a maximum or minimum value for a refined parameter. Note that variable will be a GSAS-II variable name, optionally with * specified for a histogram or atom number. Return value will be a float. (See *Parameter Limits* description.)
- Anything else returns the value in the Controls dict, if present. An exception is raised if the control value is not present.

See also

set_Controls()

get_Covariance(*varList*)

Returns the values and covariance matrix for a series of variable parameters. as defined in the last refinement cycle

Parameters
varList (*tuple*) – a list of variable names of form '<p>:<h>:<name>'

Returns
(valueList,CovMatrix) where valueList contains the (n) values in the same order as varList (also length n) and CovMatrix is a (n x n) matrix. If any variable name is not found in the varyList then None is returned.

Use this code, where sig provides standard uncertainties for parameters and where covArray provides the correlation between off-diagonal terms:

```
sig = np.sqrt(np.diag(covMatrix))
xvar = np.outer(sig,np.ones_like(sig))
covArray = np.divide(np.divide(covMatrix,xvar),xvar.T)
```

get_Frozen(*histogram=None*)

Gets a list of Frozen variables, where parameters are frozen after refining outside the range where their values are allowed due to parameter limits, when these limits are set. (See *Parameter Limits* description.) Note that use of this will cause the project to be saved if not already done so.

Parameters
histogram – A reference to a histogram, which can be reference by object, name, or number. Used for sequential fits only. If left as the default (None) for a sequential fit, all Frozen variables in all histograms are returned.

Returns
a list containing variable names, as str values

get_LastFitResults()

Returns the shifts on refined variables and their uncertainties in the last refinement cycle

Returns
a dict with the last least-squares shifts and a dict of sigma values.

get_ParmList()

Returns a list of all the parameters defined in the last refinement cycle

Returns
a list of parameters or None if no refinement has been performed.

get_Variable(*var*)

Returns the value and standard uncertainty (esd) for a variable parameters, as defined in the last refinement cycle

Parameters
var (*str*) – a variable name of form '<p>:<h>:<name>', such as ':0:Scale'

Returns
(value,esd) if the parameter is refined or (value, None) if the variable is in a constraint or is not refined or None if the parameter is not found.

get_VaryList()

Returns a list of the refined variables in the last refinement cycle

Returns
a list of variables or None if no refinement has been performed.

histType(*histname*)

Returns the type for histogram object associated with histname, or None if it does not exist.

Parameters
histname – The name of the histogram (str), or ranId or (for powder) the histogram index.

Returns
'PWDR' for a Powder histogram, 'HKLF' for a single crystal histogram, or None if the histogram does not exist

See also

histogram()

histogram(*histname*)

Returns the histogram object associated with histname, or None if it does not exist.

Parameters
histname – The name of the histogram (str), or ranId or (for powder) the histogram index.

Returns
A *G2PwdrData* object, or *G2Single* object, or None if the histogram does not exist

See also

histograms() phase() phases()

histograms(*typ=None*)

Return a list of all histograms, as *G2PwdrData* objects

For now this only finds Powder/Single Xtal histograms, since that is all that is currently implemented in this module.

Parameters

typ (*ste*) – The prefix (type) the histogram such as 'PWDR ' for powder or 'HKLF ' for single crystal. If None (the default) all known histograms types are found.

Returns

a list of objects

See also

histogram() phase() phases()

hold_many(*vars*, *ctype*)

Apply holds for all the variables in vars, for constraint of a given type. This routine has been superceeded by `add_Hold()`

Parameters

- **vars** (*list*) – A list of variables to hold. Each may be a `GSASIIobj.G2VarObj` object, a variable name (str), or a list/tuple of arguments for *make_var_obj()*.
- **ctype** (*str*) – A string constraint type specifier, passed directly to *add_constraint_raw()* as consType. Should be one of "Hist", "Phase", or "HAP" ("Global" not implemented).

image(*imageRef*)

Gives an object representing the specified image in this project.

Parameters

imageRef (*str*) – A reference to the desired image. Either the Image tree name (str), the image's index (int) or a image object (*G2Image*)

Returns

A *G2Image* object

Raises

KeyError

See also

images()

imageMultiDistCalib(*imageList=None*, *verbose=False*)

Invokes a global calibration fit (same as Image Controls/Calibration/Multi-distance Recalibrate menu command) with images as multiple distance settings. Note that for this to work properly, the initial calibration parameters (center, wavelength, distance & tilts) must be close enough to converge. This may produce a better result if run more than once.

See *Image Calibration* for example code.

Parameters

imageList (*str*) – the images to include in the fit, if not specified all images in the project will be included.

Returns
parmDict,covData where parmDict has the refined parameters and their values and covData is a dict containing the covariance matrix ('covMatrix'), the number of ring picks ('obs') the reduced Chi-squared ('chisq'), the names of the variables ('varyList') and their values ('variables')

images()

Returns a list of all the images in the project.

Returns
A list of *G2Image* objects

iter_refinements(*refinements*, *histogram='all'*, *phase='all'*, *outputnames=None*, *makeBack=False*)

Conducts a series of refinements, iteratively. Stops after every refinement and yields this project, to allow error checking or logging of intermediate results. Parameter use is the same as for *do_refinements()* (which calls this method).

```
>>> def checked_refinements(proj):
...     for p in proj.iter_refinements(refs):
...         # Track intermediate results
...         log(p.histogram('0').residuals)
...         log(p.phase('0').get_cell())
...         # Check if parameter diverged, nonsense answer, or whatever
...         if is_something_wrong(p):
...             raise Exception("I need a human!")
```

link_histogram_phase(*histogram*, *phase*)

Associates a given histogram and phase.

See also
histogram() phase()

make_var_obj(*phase=None*, *hist=None*, *varname=None*, *atomId=None*, *reloadIdx=True*)

Wrapper to create a G2VarObj. Takes either a string representation ("p:h:name:a") or individual names of phase, histogram, varname, and atomId.

Automatically converts string phase, hist, or atom names into the ID required by G2VarObj.

Note that this will cause the project to be saved if not already done so.

pdf(*pdfRef*)

Gives an object representing the specified PDF entry in this project.

Parameters
pdfRef – A reference to the desired image. Either the PDF tree name (str), the pdf's index (int) or a PDF object (*G2PDF*)

Returns
A *G2PDF* object

Raises
KeyError

See also
pdfs() G2PDF

pdfs()

Returns a list of all the PDFs in the project.

Returns
A list of *G2PDF* objects

phase(*phasename*)

Gives an object representing the specified phase in this project.

Parameters
phasename (*str*) – A reference to the desired phase. Either the phase name (str), the phase's ranId, the phase's index (both int) or a phase object (*G2Phase*)

Returns
A *G2Phase* object

Raises
KeyError

See also

histograms() phase() phases()

phases()

Returns a list of all the phases in the project.

Returns
A list of *G2Phase* objects

See also

histogram() histograms() phase()

refine(*newfile=None*, *printFile=None*, *makeBack=False*)

Invoke a refinement for the project. The project is written to the currently selected gpx file and then either a single or sequential refinement is performed depending on the setting of 'Seq Data' in Controls (set in *get_Controls()*).

reload()

Reload self from self.filename

save(*filename=None*)

Saves the project, either to the current filename, or to a new file.

Updates self.filename if a new filename provided

seqref()

Returns a sequential refinement results object, if present

Returns
A *G2SeqRefRes* object or None if not present

set_Controls(*control*, *value*, *variable=None*)

Set project controls.

Controls determine how refinements are performed, including setting lower (parmMin) or upper limits (parmMax) values for parameters where you choose to set refinement limits. Note that use of this with to set to parmMin or parmMax will cause the project to be saved, if not already done so.

Parameters

- **control** (*str*) – the item to be set. See below for allowed values.
- **value** – the value to be set.
- **variable** (*str*) – used only with control set to "parmMin" or "parmMax"

Allowed values for *control* parameter:

- `'cycles'`: sets the maximum number of cycles (value must be int)
- `'sequential'`: sets the histograms to be used for a sequential refinement. Use an empty list to turn off sequential fitting. The values in the list may be the name of the histogram (a str), or a ranId or index (int values), see *histogram()*.
- `'seqCopy'`: when True, the results from each sequential fit are used as the starting point for the next. After each fit is is set to False. Ignored for non-sequential fits.
- `'Reverse Seq'`: when True, sequential refinement is performed on the reversed list of histograms.
- `'parmMin'` & `'parmMax'`: set a minimum or maximum value for a refined parameter. Note that *variable* will be a GSAS-II variable name, optionally with * specified for a histogram or atom number and value must be a float. (See *Parameter Limits* description.)

See also

get_Controls()

set_Frozen(*variable=None*, *histogram=None*, *mode='remove'*)

Removes one or more Frozen variables (or adds one), where parameters are frozen after refining outside the range where their values are allowed due to parameter limits, when these limits are set. (See *Parameter Limits* description and *G2Project.set_Controls()* for setting limits.) Note that use of this will cause the project to be saved if not already done so.

Parameters

- **variable** (*str*) – a variable name as a str or (as a `GSASIIobj.G2VarObj` object). Should not contain wildcards. If None (default), all frozen variables are deleted from the project, unless a sequential fit and a histogram is specified.
- **histogram** – A reference to a histogram, which can be reference by object, name, or number. Used for sequential fits only.
- **mode** (*str*) – The default mode is to remove variables from the appropriate Frozen list, but if the mode is specified as 'add', the variable is added to the list.

Returns

True if the variable was added or removed, False otherwise. Exceptions are generated with invalid requests.

set_refinement(*refinement*, *histogram='all'*, *phase='all'*)

Set refinment flags at the project level to specified histogram(s) or phase(s).

Parameters

- **refinement** (*dict*) – The refinements to be conducted

- **histogram** – Specifies either 'all' (default), a single histogram or a list of histograms. Histograms may be specified as histogram objects (see *G2PwdrData*), the histogram name (str) or the index number (int) of the histogram in the project, numbered starting from 0. Omitting the parameter or the string 'all' indicates that parameters in all histograms should be set.
- **phase** – Specifies either 'all' (default), a single phase or a list of phases. Phases may be specified as phase objects (see *G2Phase*), the phase name (str) or the index number (int) of the phase in the project, numbered starting from 0. Omitting the parameter or the string 'all' indicates that parameters in all phases should be set.

Note that refinement parameters are categorized as one of three types:

1. Histogram parameters
2. Phase parameters
3. Histogram-and-Phase (HAP) parameters

See also

G2PwdrData.set_refinements() *G2PwdrData.clear_refinements()* *G2Phase.set_refinements()* *G2Phase.clear_refinements()* *G2Phase.set_HAP_refinements()* *G2Phase.clear_HAP_refinements()* *G2Single.set_refinements()*

update_ids()

Makes sure all phases and histograms have proper hId and pId

class GSASII.GSASIIscriptable.**G2PwdrData**(*data*, *proj*, *name*)

Wraps a Powder Data Histogram. The object contains these class variables:

- G2PwdrData.proj: contains a reference to the *G2Project* object that contains this histogram
- G2PwdrData.name: contains the name of the histogram
- G2PwdrData.data: contains the histogram's associated data in a dict, as documented for the *Powder Diffraction Tree*. The actual histogram values are contained in the 'data' dict item, as documented for Data.

Scripts should not try to create a *G2PwdrData* object directly as `G2PwdrData.__init__()` should be invoked from inside *G2Project*.

property Background

Provides a list with with the Background parameters for this histogram.

Note that the returned list is a reference to the actual list as stored in the .gpx file; use care not to modify this unless intended.

Returns

list containing a list and dict with background values

ComputeMassFracs()

Computes the mass fractions (or equivalently the weight fractions) for the phases linked to the current histogram with uncertainties from the results of the last refinement, if the phase fractions were refined.

Returns

a dict where the keys are phase names and the values associated with is a tuple where the first value is the phase's mass fraction and the second value is the s.u. on that value.

EditSimulated(*Tmin*, *Tmax*, *Tstep=None*, *Npoints=None*)

Change the parameters for an existing simulated powder histogram. This will reset the previously computed "observed" pattern.

Parameters

- **Tmin** (*float*) – Minimum 2theta or TOF (microsec) for dataset to be simulated
- **Tmax** (*float*) – Maximum 2theta or TOF (usec) for dataset to be simulated
- **Tstep** (*float*) – Step size in 2theta or TOF (usec) for dataset to be simulated Default is to compute this from Npoints.
- **Npoints** (*int*) – the number of data points to be used for computing the diffraction pattern. Defaults as None, which sets this to 2500. Do not specify both Npoints and Tstep. Due to roundoff the actual nuber of points used may differ by +-1 from Npoints. Must be below 25,000.

Excluded(*value=None*)

Used to obtain or set the excluded regions for a histogram. When a value is specified, the excluded regions are set. Otherwise, the list of excluded region pairs is returned. Note that excluded regions may be an empty list or a list of regions to be excluded, where each region is provided as pair of numbers, where the lower limit comes first. Some sample excluded region lists are:

```
[[4.5, 5.5], [8.0, 9.0]]

[[130000.0, 140000.0], [160000.0, 170000.0]]

[]
```

The first above describes two excluded regions from 4.5-5.5 and 8-9 degrees 2-theta. The second is for a TOF pattern and also describes two excluded regions, for 130-140 and 160-170 milliseconds. The third line would be the case where there are no excluded regions.

Parameters

value (*list*) – A list of pairs of excluded region numbers (as two-element lists). Some error checking/reformatting is done, but users are expected to get this right. Use the GUI to create examples or check input. Numbers in the list are in units of degrees or TOF (microsec.).

If a value is not specified, the command returns the list of excluded regions.

Returns

The list of excluded regions (when `value=None`). Units are 2-theta (degrees) or TOF (microsec).

Example 1:

```
h = gpx.histogram(0)  # adds an excluded region (11-13 degrees)
h.Excluded(h.Excluded() + [[11,13]])
```

Example 2:

```
h = gpx.histogram(0) # changes the range of the first excluded region
excl = h.Excluded()
excl[0] = [120000.0, 160000.0]  # microsec
h.Excluded(excl)
```

Example 3:

```
h = gpx.histogram(0)  # deletes all excluded regions
h.Excluded([])
```

Export (*fileroot*, *extension*, *fmthint=None*)

Write the histogram into a file. The path is specified by fileroot and extension.

Parameters

- **fileroot** (*str*) – name of the file, optionally with a path (extension is ignored)
- **extension** (*str*) – includes '.', must match an extension in global exportersByExtension['powder'] or a Exception is raised.
- **fmthint** (*str*) – If specified, the first exporter where the format name (obj.formatName, as shown in Export menu) contains the supplied string will be used. If not specified, an error will be generated showing the possible choices.

Returns

name of file that was written

Export_peaks (*filename*)

Write the peaks file. The path is specified by filename extension.

Parameters

filename (*str*) – name of the file, optionally with a path, includes an extension

Returns

name of file that was written

property InstrumentParameters

Provides a dictionary with with the Instrument Parameters for this histogram.

Note that the returned dict is a reference to the actual dict as stored in the .gpx file; use care not to modify this unless intended.

Limits (*typ*, *value=None*)

Used to obtain or set the histogram limits. When a value is specified, the appropriate limit is set. Otherwise, the value is returned. Note that this provides an alternative to setting histogram limits with the `G2Project:do_refinements()` or *G2PwdrData.set_refinements()* methods.

Parameters

- **typ** (*str*) – a string which must be either 'lower' (for 2-theta min or TOF min) or 'upper' (for 2theta max or TOF max). Anything else produces an error.
- **value** (*float*) – the number to set the limit (in units of degrees or TOF (microsec.). If not specified, the command returns the selected limit value rather than setting it.

Returns

The current value of the requested limit (when `value=None`). Units are 2-theta (degrees) or TOF (microsec).

Examples:

```
h = gpx.histogram(0)
val = h.Limits('lower')
h.Limits('upper',75)
```

LoadProfile (*filename*, *bank=0*)

Reads a GSAS-II (new style) .instprm file and overwrites the current parameters

Parameters

- **filename** (*str*) – instrument parameter file name, extension ignored if not .instprm
- **bank** (*int*) – bank number to read, defaults to zero

property PeakList

Provides a list of peaks parameters for this histogram.

Returns

a list of peaks, where each peak is a list containing [pos,area,sig,gam] (position, peak area, Gaussian width, Lorentzian width)

property Peaks

Provides a dict with the Peak List parameters for this histogram.

Returns

dict with two elements where item 'peaks' is a list of peaks where each element is [pos,pos-ref,area,area-ref,sig,sig-ref,gam,gam-ref], where the -ref items are refinement flags and item 'sigDict' is a dict with possible items 'Back;#', 'pos#', 'int#', 'sig#', 'gam#'

property SampleParameters

Provides a dictionary with with the Sample Parameters for this histogram.

Note that the returned dict is a reference to the actual dict as stored in the .gpx file; use care not to modify this unless intended.

SaveProfile(*filename*)

Writes a GSAS-II (new style) .instprm file

add_back_peak(*pos*, *int*, *sig*, *gam*, *refflags=[]*)

Adds a background peak to the Background parameters

Background in diffraction patterns is usually fit with a slowly varying smooth function, such as a Chebyschev polynomial, but when the background contains broad peaks (for example from a Kapton sample container) those peaks are usually better fit by adding extra peaks to the smooth background function rather that providing enough parameters to the smooth function in order fit the peak(s). Note that background peaks are typically treated as Gaussian only (`gam``=0) with very large ``sig` values (>1000). Normally one should refine `int` and then `sig` and only after the background peak is well fit can one refine the `pos` value.

Parameters

- **pos** (*float*) – position of peak, a 2theta or TOF value
- **int** (*float*) – integrated intensity of background peak, usually large
- **sig** (*float*) – Gaussian width of background peak, usually large
- **gam** (*float*) – Lorentzian width of background peak, usually not used (small)
- **refflags** (*list*) – a list of 1 to 4 boolean refinement flags for pos,int,sig & gam, respectively (e.g. use [0,1] to refine int only). Defaults to [] which means nothing is refined.

add_peak(*area*, *dspace=None*, *Q=None*, *ttheta=None*)

Adds a single peak to the peak list

Parameters

- **area** (*float*) – peak area
- **dspace** (*float*) – peak position as d-space (A)
- **Q** (*float*) – peak position as Q (A-1)

- **ttheta** (*float*) – peak position as 2Theta (deg)

Note: only one of the parameters: dspace, Q or ttheta may be specified. See *Peak Fitting* for an example.

calc_autobkg(*opt=0*, *logLam=None*)

Sets fixed background points using the pybaselines Whittaker algorithm.

Parameters

- **opt** (*int*) – 0 for 'arpls' or 1 for 'iarpls'. Default is 0.
- **logLam** (*float*) – log_10 of the Lambda value used in the pybaselines.whittaker.arpls/.iarpls computation. If None (default) is provided, a guess is taken for an appropriate value based on the number of points.

Returns

the array of computed background points

clear_refinements(*refs*)

Clears the PWDR refinement parameter 'key' and its associated value.

Parameters

refs (*dict*) – A dictionary of parameters to clear. See the *Histogram parameters* table for what can be specified.

del_back_peak(*peaknum*)

Removes a background peak from the Background parameters

Parameters

peaknum (*int*) – the number of the peak (starting from 0)

fit_fixed_points()

Attempts to apply a background fit to the fixed points currently specified.

getHistEntryList(*keyname=''*)

Returns a dict with histogram setting values.

Parameters

keyname (*str*) – an optional string. When supplied only entries where at least one key contains the specified string are reported. Case is ignored, so 'sg' will find entries where one of the keys is 'SGdata', etc.

Returns

a set of histogram dict keys.

See *G2Phase.getHAPentryList()* for a related example.

See also

getHistEntryValue() setHistEntryValue()

getHistEntryValue(*keylist*)

Returns the histogram control value associated with a list of keys. Where the value returned is a list, it may be used as the target of an assignment (as in `getHistEntryValue(...)[...] = val`) to set a value inside a list.

Parameters
keylist (*list*) – a list of dict keys, typically as returned by *getHistEntryList()*.

Returns
a histogram setting; may be a int, float, bool, list,…

See *G2Phase.getHAPentryValue()* for a related example.

get_wR()

returns the overall weighted profile R factor for a histogram

Returns
a wR value as a percentage or None if not defined

getdata(*datatype*)

Provides access to the histogram data of the selected data type.

It should be noted that for TOF data, GSAS-II expects input where the TOF value is the minimum for the bin, but does computations using the TOF value for the center of each bin. The values reported using the 'X' option here are the values used in computation, while the 'X-orig' option reverses the shift applied when TOF values are read in.

Parameters
datatype (*str*) – must be one of the following values (case is ignored):

- 'X': the 2theta or TOF values for the pattern
- **'X-orig': for TOF, time values for the pattern shifted**
  as used as input for GSAS-II. For everything else, the values are the same as with the 'X' option (see above.)
- 'Q': the 2theta or TOF values for the pattern transformed to Q
- 'd': the 2theta or TOF values for the pattern transformed to d-space
- 'Yobs': the observed intensity values
- 'Yweight': the weights for each data point (1/sigma**2)
- 'Ycalc': the computed intensity values
- 'Background': the computed background values
- 'Residual': the difference between Yobs and Ycalc (obs-calc)

Returns
a numpy MaskedArray with data values of the requested type. Note that the returned values are a copy of the GSAS-II histogram array, not a reference to the actual data as stored in the .gpx file.

ref_back_peak(*peaknum*, *refflags=[]*)

Sets refinement flag for a background peak

Parameters

- **peaknum** (*int*) – the number of the peak (starting from 0)
- **refflags** (*list*) – a list of 1 to 4 boolean refinement flags for pos,int,sig & gam, respectively. If a flag is not specified it defaults to False (use [0,1] to refine int only). Defaults to [] which means nothing is refined.

refine_peaks(*mode='useIP'*)

Causes a refinement of peak position, background and instrument parameters

Parameters

mode (*str*) – this determines how peak widths are determined. If the value is 'useIP' (the default) then the width parameter values (sigma, gamma, alpha,…) are computed from the histogram's instrument parameters. If the value is 'hold', then peak width parameters are not overridden. In this case, it is not possible to refine the instrument parameters associated with the peak widths and an attempt to do so will result in an error.

Returns

a list of dicts with refinement results. Element 0 has uncertainties on refined values (also placed in self.data['Peak List']['sigDict']) element 1 has the peak fit result, element 2 has the peak fit uncertainties and element 3 has r-factors from the fit. (These are generated in `GSASIIpwd.DoPeakFit()`).

reflections()

Returns a dict with an entry for every phase in the current histogram. Within each entry is a dict with keys 'RefList' (reflection list, see *Powder Reflections*), 'Type' (histogram type), 'FF' (form factor information), 'Super' (True if this is superspace group).

Note that the returned array is a reference to the actual data as stored in the .gpx file; use care not to modify this.

property residuals

Provides a dictionary with with the R-factors for this histogram. Includes the weighted and unweighted profile terms (R, Rb, wR, wRb, wRmin) as well as the Bragg R-values for each phase (ph:H:Rf and ph:H:Rf^2).

setHistEntryValue(*keylist*, *newvalue*)

Sets a histogram control value associated with a list of keys.

See *G2Phase.setHAPentryValue()* for a related example.

Parameters

keylist (*list*) –

a list of dict keys, typically as returned by *getHistEntryList()*.

param newvalue

a new value for the hist setting. The type must be the same as the initial value, but if the value is a container (list, tuple, np.array,…) the elements inside are not checked.

set_background(*key*, *value*)

Set background parameters (this serves a similar function as in *set_refinements()*, but with a simplified interface).

Parameters

- **key** (*str*) – a string that defines the background parameter that will be changed. Must appear in the table below.

key name	type of value	meaning of value
fixed-Hist	int, str, None or G2PwdrData	reference to a histogram in the current project or None to remove the reference.
fixed-File-Mult	float	multiplier applied to intensities in the background histogram where a value of -1.0 means full subtraction of the background histogram.

- **value** – a value to set the selected background parameter. The meaning and type for this parameter is listed in the table above.

set_peakFlags(*peaklist=None*, *area=None*, *pos=None*, *sig=None*, *gam=None*, *alp=None*, *bet=None*)

Set refinement flags for peaks

Parameters

- **peaklist** (*list*) – a list of peaks to change flags. If None (default), changes are made to all peaks.
- **area** (*bool*) – Sets or clears the refinement flag for the peak area value. If None (the default), no change is made.
- **pos** (*bool*) – Sets or clears the refinement flag for the peak position value. If None (the default), no change is made.
- **sig** (*bool*) – Sets or clears the refinement flag for the peak sigma (Gaussian width) value. If None (the default), no change is made.
- **gam** (*bool*) – Sets or clears the refinement flag for the peak gamma (Lorentzian width) value. If None (the default), no change is made.
- **alp** (*bool*) – Sets or clears the refinement flag for the peak alpha (TOF width) value. If None (the default), no change is made.
- **bet** (*bool*) – Sets or clears the refinement flag for the peak beta (TOF width) value. If None (the default), no change is made.

Note that when peaks are first created the area flag is on and the other flags are initially off.

Example:

```
set_peakFlags(sig=False,gam=True)
```

causes the sig refinement flag to be cleared and the gam flag to be set, in both cases for all peaks. The position and area flags are not changed from their previous values.

set_refinements(*refs*)

Sets the PWDR histogram refinement parameter 'key' to the specification 'value'.

Parameters

refs (*dict*) – A dictionary of the parameters to be set. See the *Histogram parameters* table for a description of what these dictionaries should be.

Returns

None

y_calc()

Returns the calculated intensity values; better to use *getdata()*.

Note that the returned array is a reference to the actual data as stored in the .gpx file; use care not to modify this.

exception GSASII.GSASIIscriptable.**G2ScriptException**

class GSASII.GSASIIscriptable.**G2SeqRefRes**(*data*, *proj*)

Wrapper for a Sequential Refinement Results tree entry, containing the results for a refinement

Scripts should not try to create a *G2SeqRefRes* object directly as this object will be created when a .gpx project file is read.

As an example:

```
import os
PathWrap = lambda fil: os.path.join('/Users/toby/Scratch/SeqTut2019Mar',fil)
gpx = G2sc.G2Project(PathWrap('scr4.gpx'))
seq = gpx.seqref()
lbl = ('a','b','c','alpha','beta','gamma','Volume')
for j,h in enumerate(seq.histograms()):
    cell,cellU,uniq = seq.get_cell_and_esd(1,h)
    print(h)
    print([cell[i] for i in list(uniq)+[6]])
    print([cellU[i] for i in list(uniq)+[6]])
    print('')
print('printed',[lbl[i] for i in list(uniq)+[6]])
```

See also

G2Project.seqref()

RefData (*hist*)

Provides access to the output from a particular histogram

Parameters

hist – Specify a histogram or using the histogram name (str) or the index number (int) of the histogram in the sequential refinement (not the project), numbered as in the project tree starting from 0.

Returns

a list of dicts where the first element has sequential refinement results and the second element has the contents of the histogram tree items.

get_Covariance (*hist*, *varList*)

Returns the values and covariance matrix for a series of variable parameters, as defined for the selected histogram in the last sequential refinement cycle

Parameters

- **hist** – Specify a histogram or using the histogram name (str) or the index number (int) of the histogram in the sequential refinement (not the project), numbered as in the project tree starting from 0.
- **varList** (*tuple*) – a list of variable names of form '<p>:<h>:<name>'

Returns

(valueList,CovMatrix) where valueList contains the (n) values in the same order as varList (also length n) and CovMatrix is a (n x n) matrix. If any variable name is not found in the varyList then None is returned.

Use this code, where sig provides standard uncertainties for parameters and where covArray provides the correlation between off-diagonal terms:

```
sig = np.sqrt(np.diag(covMatrix))
xvar = np.outer(sig,np.ones_like(sig))
covArray = np.divide(np.divide(covMatrix,xvar),xvar.T)
```

get_ParmList (*hist*)

Returns a list of all the parameters defined in the last refinement cycle for the selected histogram

Parameters
hist – Specify a histogram or using the histogram name (str) or the index number (int) of the histogram in the sequential refinement (not the project), numbered as in the project tree starting from 0.

Returns
a list of parameters or None if no refinement has been performed.

get_Variable(*hist*, *var*)

Returns the value and standard uncertainty (esd) for a variable parameters, as defined for the selected histogram in the last sequential refinement cycle

Parameters

- **hist** – Specify a histogram or using the histogram name (str) or the index number (int) of the histogram in the sequential refinement (not the project), numbered as in the project tree starting from 0.
- **var** (*str*) – a variable name of form '<p>:<h>:<name>', such as ':0:Scale'

Returns
(value,esd) if the parameter is refined or (value, None) if the variable is in a constraint or is not refined or None if the parameter is not found.

get_VaryList(*hist*)

Returns a list of the refined variables in the last refinement cycle for the selected histogram

Parameters
hist – Specify a histogram or using the histogram name (str) or the index number (int) of the histogram in the sequential refinement (not the project), numbered starting from 0.

Returns
a list of variables or None if no refinement has been performed.

get_cell_and_esd(*phase*, *hist*)

Returns a vector of cell lengths and esd values

Parameters

- **phase** – A phase, which may be specified as a phase object (see *G2Phase*), the phase name (str) or the index number (int) of the phase in the project, numbered starting from 0.
- **hist** – Specify a histogram or using the histogram name (str) or the index number (int) of the histogram in the sequential refinement (not the project), numbered as in in the project tree starting from 0.

Returns
cell,cellESD,uniqCellIndx where cell (list) with the unit cell parameters (a,b,c,alpha,beta,gamma,Volume); cellESD are the standard uncertainties on the 7 unit cell parameters; and uniqCellIndx is a tuple with indicies for the unique (non-symmetry determined) unit parameters (e.g. [0,2] for a,c in a tetragonal cell)

histograms()

returns a list of histograms in the squential fit

class GSASII.GSASIIscriptable.**G2Single**(*data*, *proj*, *name*)

Wrapper for a HKLF tree entry, containing a single crystal histogram Note that in a GSASIIscriptable script, instances of G2Single will be created by calls to *G2Project.histogram()*, *G2Project.histograms()*, or *G2Project.add_single_histogram()*. Scripts should not try to create a *G2Single* object directly.

This object contains these class variables:

- G2Single.proj: contains a reference to the *G2Project* object that contains this histogram
- G2Single.name: contains the name of the histogram
- G2Single.data: contains the histogram's associated data in a dict, as documented for the *Single Crystal Tree Item*. This contains the actual histogram values, as documented for Data.

Example use of *G2Single*:

```
gpx0 = G2sc.G2Project('HTO_base.gpx')
gpx0.add_single_histogram('HTO_xray/xtal1/xs2555a.hkl',0,fmthint='Shelx HKLF 4')
gpx0.save('HTO_scripted.gpx')
```

This opens an existing GSAS-II project file and adds a single crystal dataset that is linked to the first phase and saves it under a new name.

See also

add_single_histogram() histogram() histograms() link_histogram_phase()

Export (*fileroot*, *extension*, *fmthint=None*)

Write the HKLF histogram into a file. The path is specified by fileroot and extension.

Parameters

- **fileroot** (*str*) – name of the file, optionally with a path (extension is ignored)
- **extension** (*str*) – includes '.', must match an extension in global exportersByExtension['single'] or a Exception is raised.
- **fmthint** (*str*) – If specified, the first exporter where the format name (obj.formatName, as shown in Export menu) contains the supplied string will be used. If not specified, an error will be generated showing the possible choices.

Returns

name of file that was written

clear_refinements (*refs*)

Clears the HKLF refinement parameter 'key' and its associated value.

Parameters

refs (*dict*) – A dictionary of parameters to clear. See the *Histogram parameters* table for what can be specified.

Example:

```
hist.clear_refinements(['Scale','Es','Flack'])
hist.clear_refinements({'Scale':True,'Es':False,'Flack':True})
```

Note that the two above commands are equivalent: the values specified in the dict in the second command are ignored.

set_refinements (*refs*)

Sets the HKLF histogram refinement parameter 'key' to the specification 'value'.

Parameters

refs (*dict*) – A dictionary of the parameters to be set. See the *Histogram parameters* table for a description of what these dictionaries should be.

Example:

```
hist.set_refinements({'Scale':True,'Es':False,'Flack':True})
```

class GSASII.GSASIIscriptable.**G2SmallAngle**(*data*, *proj*, *name*)

Wrapper for SASD histograms (and hopefully, in the future, other small angle histogram types).

Note that in a GSASIIscriptable script, instances of G2SmallAngle will be created by calls to *SAS()*, *SASs()*, or by `G2Project.Integrate()`. Also, someday `G2Project.add_SAS()`. Scripts should not try to create a *G2SmallAngle* object directly.

This object contains these class variables:

- G2SmallAngle.proj: contains a reference to the *G2Project* object that contains this histogram
- G2SmallAngle.name: contains the name of the histogram
- G2SmallAngle.data: contains the histogram's associated data in a dict with keys 'Comments', 'Limits', 'Instrument Parameters', 'Substances', 'Sample Parameters' and 'Models'. Further documentation on SASD entries needs to be written.

See also

`add_SAS()` *SAS()* *SASs()* `Integrate()`

GSASII.GSASIIscriptable.**GenerateReflections**(*spcGrp*, *cell*, *Qmax=None*, *dmin=None*, *TTmax=None*, *wave=None*)

Generates the crystallographically unique powder diffraction reflections for a lattice and space group (see `GSASIIlattice.GenHLaue()`).

Parameters

- **spcGrp** (*str*) – A GSAS-II formatted space group (with spaces between axial fields, e.g. 'P 21 21 21' or 'P 42/m m c'). Note that non-standard space groups, such as 'P 21/n' or 'F -1' are allowed (see `GSASIIspc.SpcGroup()`).
- **cell** (*list*) – A list/tuple with six unit cell constants, (a, b, c, alpha, beta, gamma) with values in Angstroms/degrees. Note that the cell constants are not checked for consistency with the space group.
- **Qmax** (*float*) – Reflections up to this Q value are computed (do not use with dmin or TTmax)
- **dmin** (*float*) – Reflections with d-space above this value are computed (do not use with Qmax or TTmax)
- **TTmax** (*float*) – Reflections up to this 2-theta value are computed (do not use with dmin or Qmax, use of wave is required.)
- **wave** (*float*) – wavelength in Angstroms for use with TTmax (ignored otherwise.)

Returns

a list of reflections, where each reflection contains four items: h, k, l, d, where d is the d-space (Angstroms)

Example:

```
>>> refs = G2sc.GenerateReflections('P 1',
...                     (5.,6.,7.,90.,90.,90),
...                     TTmax=20,wave=1)
>>> for r in refs: print(r)
```

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```
...
[0, 0, 1, 7.0]
[0, 1, 0, 6.0]
[1, 0, 0, 5.0]
[0, 1, 1, 4.55553961419178]
[0, 1, -1, 4.55553961419178]
[1, 0, 1, 4.068667356033675]
[1, 0, -1, 4.068667356033674]
[1, 1, 0, 3.8411063979868794]
[1, -1, 0, 3.8411063979868794]
```

GSASII.GSASIIscriptable.**IPyBrowse**(*args*)

Load a .gpx file and then open a IPython shell to browse it:

```
usage: GSASIIscriptable.py browse [-h] files [files ...]
```

positional arguments:

```
files       list of files to browse
```

optional arguments:

```
-h, --help  show this help message and exit
```

GSASII.GSASIIscriptable.**LoadDictFromProjFile**(*ProjFile*)

Read a GSAS-II project file and load items to dictionary

Parameters

ProjFile (*str*) – GSAS-II project (name.gpx) full file name

Returns

Project,nameList, where

- Project (dict) is a representation of gpx file following the GSAS-II tree structure for each item: key = tree name (e.g. 'Controls','Restraints',etc.), data is dict data dict = {'data':item data whch may be list, dict or None,'subitems':subdata (if any)}
- nameList (list) has names of main tree entries & subentries used to reconstruct project file

Example for fap.gpx:

```
Project = {                 #NB:dict order is not tree order
  'Phases':{'data':None,'fap':{phase dict}},
  'PWDR FAP.XRA Bank 1':{'data':[histogram data list],'Comments':comments,'Limits
↪':limits, etc},
  'Rigid bodies':{'data': {rigid body dict}},
  'Covariance':{'data':{covariance data dict}},
  'Controls':{'data':{controls data dict}},
  'Notebook':{'data':[notebook list]},
  'Restraints':{'data':{restraint data dict}},
  'Constraints':{'data':{constraint data dict}}]
  }
nameList = [                #NB: reproduces tree order
  ['Notebook',],
```

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```
  ['Controls',],
  ['Covariance',],
  ['Constraints',],
  ['Restraints',],
  ['Rigid bodies',],
  ['PWDR FAP.XRA Bank 1',
       'Comments',
       'Limits',
       'Background',
       'Instrument Parameters',
       'Sample Parameters',
       'Peak List',
       'Index Peak List',
       'Unit Cells List',
       'Reflection Lists'],
  ['Phases', 'fap']
  ]
```

GSASII.GSASIIscriptable.**LoadG2fil**()

Setup GSAS-II importers. Delay importing this module when possible, it is slow. Multiple calls are not. Only the first does anything.

GSASII.GSASIIscriptable.**PreSetup**(*data*)

Create part of an initial (empty) phase dictionary

from GSASIIphsGUI.py, near end of UpdatePhaseData

Author: Jackson O'Donnell (jacksonhodonnell .at. gmail.com)

GSASII.GSASIIscriptable.**Readers = {'Image': [], 'Phase': [], 'Pwdr': [], 'importErrpkgs': []}**

Readers by reader type

GSASII.GSASIIscriptable.**SaveDictToProjFile**(*Project*, *nameList*, *ProjFile*)

Save a GSAS-II project file from dictionary/nameList created by LoadDictFromProjFile

Parameters

- **Project** (*dict*) – representation of gpx file following the GSAS-II tree structure as described for LoadDictFromProjFile
- **nameList** (*list*) – names of main tree entries & subentries used to reconstruct project file
- **ProjFile** (*str*) – full file name for output project.gpx file (including extension)

GSASII.GSASIIscriptable.**SetDebugMode**(*mode*)

Set the debug configuration mode on (mode=True) or off (mode=False). This will provide some additional output that may help with tracking down problems in the code.

GSASII.GSASIIscriptable.**SetPrintLevel**(*level*)

Set the level of output from calls to `GSASIIfiles.G2Print()`, which should be used in place of print() where possible. This is a wrapper for `GSASIIfiles.G2SetPrintLevel()` so that this routine is documented here.

Parameters

level (*str*) – a string used to set the print level, which may be 'all', 'warn', 'error' or 'none'. Note that capitalization and extra letters in level are ignored, so 'Warn', 'warnings', etc. will all set the mode to 'warn'

GSASII.GSASIIscriptable.**SetupGeneral**(*data*, *dirname*)

Initialize phase data.

GSASII.GSASIIscriptable.**ShowVersions**()

Show the versions all of required Python packages, etc.

GSASII.GSASIIscriptable.**add**(*args*)

Implements the add command-line subcommand. This adds histograms and/or phases to GSAS-II project:

```
usage: GSASIIscriptable.py add [-h] [-d HISTOGRAMS [HISTOGRAMS ...]]
                               [-i IPARAMS [IPARAMS ...]]
                               [-hf HISTOGRAMFORMAT] [-p PHASES [PHASES ...]]
                               [-pf PHASEFORMAT] [-l HISTLIST [HISTLIST ...]]
                               filename
```

positional arguments:

```
filename              the project file to open. Should end in .gpx
```

optional arguments:

```
-h, --help            show this help message and exit
-d HISTOGRAMS [HISTOGRAMS ...], --histograms HISTOGRAMS [HISTOGRAMS ...]
                      list of datafiles to add as histograms
-i IPARAMS [IPARAMS ...], --iparams IPARAMS [IPARAMS ...]
                      instrument parameter file, must be one for every
                      histogram
-hf HISTOGRAMFORMAT, --histogramformat HISTOGRAMFORMAT
                      format hint for histogram import. Applies to all
                      histograms
-p PHASES [PHASES ...], --phases PHASES [PHASES ...]
                      list of phases to add. phases are automatically
                      associated with all histograms given.
-pf PHASEFORMAT, --phaseformat PHASEFORMAT
                      format hint for phase import. Applies to all phases.
                      Example: -pf CIF
-l HISTLIST [HISTLIST ...], --histlist HISTLIST [HISTLIST ...]
                      list of histgram indices to associate with added
                      phases. If not specified, phases are associated with
                      all previously loaded histograms. Example: -l 2 3 4
```

GSASII.GSASIIscriptable.**blkSize = 128**

Integration block size; 128 or 256 seems to be optimal for CPU use, but 128 uses less memory, must be <=1024 (for histogram3d)

GSASII.GSASIIscriptable.**calcMaskMap**(*imgprms*, *mskprms*)

Computes a set of blocked mask arrays for a set of image controls and mask parameters. This capability is also provided with *G2Image.IntMaskMap()*.

GSASII.GSASIIscriptable.**calcThetaAzimMap**(*imgprms*)

Computes the set of blocked arrays for theta-azimuth mapping from a set of image controls, which can be cached and reused for integration of multiple images with the same calibration parameters. This capability is also provided with *G2Image.IntThetaAzMap()*.

GSASII.GSASIIscriptable.**create**(*args*)

Implements the create command-line subcommand. This creates a GSAS-II project, optionally adding histograms and/or phases:

```
usage: GSASIIscriptable.py create [-h] [-d HISTOGRAMS [HISTOGRAMS ...]]
                                  [-i IPARAMS [IPARAMS ...]]
                                  [-p PHASES [PHASES ...]]
                                  filename
```

positional arguments:

```
filename              the project file to create. should end in .gpx
```

optional arguments:

```
-h, --help            show this help message and exit
-d HISTOGRAMS [HISTOGRAMS ...], --histograms HISTOGRAMS [HISTOGRAMS ...]
                      list of datafiles to add as histograms
-i IPARAMS [IPARAMS ...], --iparams IPARAMS [IPARAMS ...]
                      instrument parameter file, must be one for every
                      histogram
-p PHASES [PHASES ...], --phases PHASES [PHASES ...]
                      list of phases to add. phases are automatically
                      associated with all histograms given.
```

GSASII.GSASIIscriptable.**dictDive**(*d*, *search=''*, *keylist=[]*, *firstcall=True*, *l=None*)

Recursive routine to scan a nested dict. Reports a list of keys and the associated type and value for that key.

Parameters

- **d** (*dict*) – a dict that will be scanned
- **search** (*str*) – an optional search string. If non-blank, only entries where one of the keys constains search (case ignored)
- **keylist** (*list*) – a list of keys to apply to the dict.
- **firstcall** (*bool*) – do not specify
- **l** (*list*) – do not specify

Returns

a list of keys located by this routine in form [([keylist], type, value),…] where if keylist is [‘a’,’b’,’c’] then d[[‘a’][‘b’][‘c’] will have the value.

This routine can be called in a number of ways, as are shown in a few examples:

```
>>> for i in G2sc.dictDive(p.data['General'],'paw'): print(i)
...
(['Pawley dmin'], <class 'float'>, 1.0)
(['doPawley'], <class 'bool'>, False)
(['Pawley dmax'], <class 'float'>, 100.0)
(['Pawley neg wt'], <class 'float'>, 0.0)
>>>
>>> for i in G2sc.dictDive(p.data,'paw',['General']): print(i)
...
(['General', 'Pawley dmin'], <class 'float'>, 1.0)
```

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```
(['General', 'doPawley'], <class 'bool'>, False)
(['General', 'Pawley dmax'], <class 'float'>, 100.0)
(['General', 'Pawley neg wt'], <class 'float'>, 0.0)
>>>
>>> for i in G2sc.dictDive(p.data,'',['General','doPawley']): print(i)
...
(['General', 'doPawley'], <class 'bool'>, False)
```

GSASII.GSASIIscriptable.**downloadFile**(*URL*, *download_loc=None*)

Download the URL

GSASII.GSASIIscriptable.**dump**(*args*)

Implements the dump command-line subcommand, which shows the contents of a GSAS-II project:

```
usage: GSASIIscriptable.py dump [-h] [-d] [-p] [-r] files [files ...]
```

positional arguments:

```
files
```

optional arguments:

```
-h, --help        show this help message and exit
-d, --histograms  list histograms in files, overrides --raw
-p, --phases      list phases in files, overrides --raw
-r, --raw         dump raw file contents, default
```

GSASII.GSASIIscriptable.**export**(*args*)

Implements the export command-line subcommand: Exports phase as CIF:

```
usage: GSASIIscriptable.py export [-h] gpxfile phase exportfile
```

positional arguments:

```
gpxfile     the project file from which to export
phase       identifier of phase to export
exportfile  the .cif file to export to
```

optional arguments:

```
-h, --help  show this help message and exit
```

GSASII.GSASIIscriptable.**exportersByExtension = {}**

Specifies the list of extensions that are supported for Powder data export

GSASII.GSASIIscriptable.**import_generic**(*filename*, *readerlist*, *fmthint=None*, *bank=None*, *URL=False*, *download_loc=None*, *useNet=True*, *buffer=None*, *imageKey=None*)

Attempt to import a filename, using a list of reader objects.

This is not intended to be called directly in scripting, only by routines like G2Project.add_phase() and G2Project.add_image but this may be used to read CIFs, as is done with OnISODISTORT_kvec in GSASIIpwdGUI.

Returns the first reader object which is read successfully.

GSASII.GSASIIscriptable.**installScriptingShortcut**()

Creates a file named G2script in the current Python site-packages directory. This is equivalent to the "Install GSASIIscriptable shortcut" command in the GUI's File menu. Once this is done, a shortcut for calling GSASIIscriptable is created, where the command:

```
>>> import G2script as G2sc
```

will provide access to GSASIIscriptable without changing the sys.path; also see *Accessing the GSASIIscriptable Module*.

Note that this only affects the current Python installation. If more than one Python installation will be used with GSAS-II (for example because different conda environments are used), this command should be called from within each Python environment.

If more than one GSAS-II installation will be used with a Python installation, this shortcut can only be used with one of them.

GSASII.GSASIIscriptable.**load_iprms**(*instfile*, *reader*, *bank=None*)

Loads instrument parameters from a file, and edits the given reader.

Returns a 2-tuple of (Iparm1, Iparm2) parameters

GSASII.GSASIIscriptable.**load_pwd_from_reader**(*reader*, *instprm*, *existingnames=[]*, *bank=None*)

Loads powder data from a reader object, and assembles it into a GSASII data tree.

Returns
(name, tree) - 2-tuple of the histogram name (str), and data

Author: Jackson O'Donnell (jacksonhodonnell .at. gmail.com)

GSASII.GSASIIscriptable.**main**()

The command-line interface for calling GSASIIscriptable as a shell command, where it is expected to be called as:

```
python GSASIIscriptable.py <subcommand> <file.gpx> <options>
```

The following subcommands are defined:

- create, see *create()*
- add, see *add()*
- dump, see *dump()*
- refine, see *refine()*
- export, *export()*
- browse, see *IPyBrowse()*

See also

create() add() dump() refine() export() IPyBrowse()

GSASII.GSASIIscriptable.**make_empty_project**(*author=None*, *filename=None*)

Creates an dictionary in the style of GSASIIscriptable, for an empty project.

If no author name or filename is supplied, 'no name' and <current dir>/test_output.gpx are used , respectively.

Returns: project dictionary, name list

Author: Jackson O'Donnell (jacksonhodonnell .at. gmail.com)

GSASII.GSASIIscriptable.**refine**(*args*)

Implements the refine command-line subcommand:
conducts refinements on GSAS-II projects according to a JSON refinement dict:

```
usage: GSASIIscriptable.py refine [-h] gpxfile [refinements]
```

positional arguments:

```
gpxfile      the project file to refine
refinements  json file of refinements to apply. if not present refines file
             as-is
```

optional arguments:

```
-h, --help   show this help message and exit
```

CHAPTER

TWO

GSASII DATA OBJECT & VARIABLE ORGANIZATION

This chapter documents how data is organized within the data structures used in GSAS-II.

2.1 *Summary/Contents*

Section Contents

2.2 Parameter names in GSAS-II

Parameters in GSAS-II contain values that are used in diffraction computations. These include atom positions, but also factors that affect peak shapes or compensate for physical effects such as absoption. Many, but not all, can be optimized. The term variables is intended to refer to parameters that are being optimized in GSAS-II, but this usage is not always applied consistently within GSAS-II and in places the term variables may be applied to unvaried parameters.

Parameter in GSAS-II are uniquely named using the following pattern, `p:h:<var>:n`, where `<var>` is a variable name, as shown in the following table. Also, `p` is the phase number, `h` is the histogram number, and `n` is the atom parameter number If a parameter does not depend on a histogram, phase or atom, `h`, `p` and/or `n` will be omitted, so `p::<var>:n`, `:h:<var>` and `p:h:<var>` are all valid names.

Table 1: Naming for GSAS-II parameter names, `p:h:<var>:n`

`<var>`	usage
K (example: `a`)	Lattice parameter, *K*, from Ai and Djk; where *K* is one of the characters a, b or c.
α	Lattice parameter, α, computed from both Ai and Djk.
β	Lattice parameter, β, computed from both Ai and Djk.
γ	Lattice parameter, γ, computed from both Ai and Djk.
Scale	Phase fraction (as p:h:Scale) or Histogram scale factor (as :h:Scale).
A*I* (example: `A0`)	Reciprocal metric tensor component *I*; where *I* is a digit between 0 and 5.
*L*ol (example: `vol`)	Unit cell volume; where *L* is one of the characters v or V.
dA*M* (example: `dAx`)	Refined change to atomic coordinate, *M*; where *M* is one of the characters x, y or z.
A*M* (example: `Ax`)	Fractional atomic coordinate, *M*; where *M* is one of the characters x, y or z.
AUiso	Atomic isotropic displacement parameter.
AUN_0N_1 (example: `AU11`)	Atomic anisotropic displacement parameter UN_0N_1; where N_0 is one of the characters 1, 2 or 3 and N_1 is one of the characters 1, 2 or 3.
Afrac	Atomic site fraction parameter.
Amul	Atomic site multiplicity value.
AM*M* (example: `AMx`)	Atomic magnetic moment parameter, *M*; where *M* is one of the characters x, y or z.
Akappa*O* (example: `Akappa0`)	Atomic orbital softness for valence radial fxn, *O*; where *O* is one of the characters 0, - or 6.
O“ (example: `0"`)	Atomic orbital softness for deformation radial fxn, 1; where *O* is one of the characters 0, - or 6.
ANe*P* (example: `ANe0`)	Atomic <j0> orbital population for orbital, *P*; where *P* is one of the characters 0 or 1.

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Table 1 – continued from previous page

<var>	usage
ADO_0,O_1O_0 (example: `AD0,00`)	Atomic sp. harm. coeff for orbital, 1; where O_0 is one of the characters 0, - or 6 and O_1 is one of the characters 0, - or 6 and O_0 is one of the characters 0, - or 6.
ADO_0,-O_1O_0 (example: `AD0,-00`)	Atomic sp. harm. coeff for orbital, 1; where O_0 is one of the characters 0, - or 6 and O_1 is one of the characters 0, - or 6 and O_0 is one of the characters 0, - or 6.
AUVmat	Atomic orbital orientation matrix, 1.
ARadial	Atomic radial function, 1.
Back$J$ (example: `Back11`)	Background term #J; where J is the background term number.
BkPkint;J (example: `BkPkint;11`)	Background peak #J intensity; where J is the background peak number.
BkPkpos;J (example: `BkPkpos;11`)	Background peak #J position; where J is the background peak number.
BkPksig;J (example: `BkPksig;11`)	Background peak #J Gaussian width; where J is the background peak number.
BkPkgam;J (example: `BkPkgam;11`)	Background peak #J Cauchy width; where J is the background peak number.
BF mult	Background file multiplier.
Bab$Q$ (example: `BabA`)	Babinet solvent scattering coef. Q; where Q is one of the characters A or U.
DN_0N_1 (example: `D11`)	Anisotropic strain coef. N_0N_1; where N_0 is one of the characters 1, 2 or 3 and N_1 is one of the characters 1, 2 or 3.
Extinction	Extinction coef.
MD	March-Dollase coef.
Mustrain;J (example: `Mustrain;11`)	Microstrain coefficient (delta Q/Q x 10**6); where J can be i for isotropic or equatorial and a is axial (uniaxial broadening), a number for generalized (Stephens) broadening or mx for the Gaussian/Lorentzian mixing term (LGmix).
Size;J (example: `Size;11`)	Crystallite size value (in microns); where J can be i for isotropic or equatorial, and a is axial (uniaxial broadening), a number between 0 and 5 for ellipsoidal broadening or mx for the Gaussian/Lorentzian mixing term (LGmix).
eA	Cubic mustrain value.
Ep	Primary extinction.
Es	Secondary type II extinction.
Eg	Secondary type I extinction.
Ma	microED dynamic scattering coeff A.
Mb	microED dynamic scattering coeff B.
Mc	microED dynamic scattering coeff C.
Flack	Flack parameter.
TwinFr	Twin fraction.
Layer Disp	Layer displacement along beam.
Absorption	Absorption coef.
LayerDisp	Bragg-Brentano Layer displacement.
Displace$R$ (example: `DisplaceX`)	Debye-Scherrer sample displacement R; where R is one of the characters X or Y.
Lam	Wavelength.
I(L2)\/I(L1)	Ka2/Ka1 intensity ratio.
Polariz.	Polarization correction.
SH/L	FCJ peak asymmetry correction.
S (example: `U`)	Gaussian instrument broadening S; where S is one of the characters U, V or W.
T (example: `X`)	Cauchy instrument broadening T; where T is one of the characters X, Y or Z.

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Table 1 – continued from previous page

<var>	usage
Zero	Debye-Scherrer zero correction.
Shift	Bragg-Brentano sample displ.
SurfRoughA	Bragg-Brentano surface roughness A.
SurfRoughB	Bragg-Brentano surface roughness B.
Transparency	Bragg-Brentano sample tranparency.
DebyeA	Debye model amplitude.
DebyeR	Debye model radius.
DebyeU	Debye model Uiso.
RBV$_J$ (example: `RBV11`)	Vector rigid body parameter.
RBVO$_U$ (example: `RBVOa`)	Vector rigid body orientation parameter U; where U is one of the characters a, i, j or k.
RBVP$_M$ (example: `RBVPx`)	Vector rigid body M position parameter; where M is one of the characters x, y or z.
RBVf	Vector rigid body site fraction.
RBV$_{V_0W_0W_1}$ (example: `RBVT11`)	Residue rigid body group disp. param.; where V_0 is one of the characters T, L or S and W_0 is one of the characters 1, 2, 3, A or B and W_1 is one of the characters 1, 2, 3, A or B.
RBVU	Residue rigid body group Uiso param.
RBRO$_U$ (example: `RBROa`)	Residue rigid body orientation parameter U; where U is one of the characters a, i, j or k.
RBRP$_M$ (example: `RBRPx`)	Residue rigid body M position parameter; where M is one of the characters x, y or z.
RBRTr;$_J$ (example: `RBRTr;11`)	Residue rigid body torsion parameter.
RBRf	Residue rigid body site fraction.
RBR$_{V_0W_0W_1}$ (example: `RBRT11`)	Residue rigid body group disp. param.; where V_0 is one of the characters T, L or S and W_0 is one of the characters 1, 2, 3, A or B and W_1 is one of the characters 1, 2, 3, A or B.
RBRU	Residue rigid body group Uiso param.
RBSAtNo	Atom number for spinning rigid body.
RBSO$_U$ (example: `RBSOa`)	Spinning rigid body orientation parameter U; where U is one of the characters a, i, j or k.
RBSP$_M$ (example: `RBSPx`)	Spinning rigid body M position parameter; where M is one of the characters x, y or z.
RBSSh;[0-9];R$_J$ (example: `RBSSh;[0-9];R11`)	Spinning rigid body shell radius.
RBSSh;[0-9];C$_J$ (example: `RBSSh;[0-9];C11`)	Spinning rigid body sph. harmonics term.
constr$_G$ (example: `constr10`)	Generated degree of freedom from constraint; where G is one or more digits (0, 1,… 9).
nv-(.+)	New variable assignment with name 1.
mV$_H$ (example: `mV0`)	Modulation vector component H; where H is the digits 0, 1, or 2.
Fsin	Sin site fraction modulation.
Fcos	Cos site fraction modulation.
Fzero	Crenel function offset.
Fwid	Crenel function width.
Tmin	ZigZag/Block min location.
Tmax	ZigZag/Block max location.
$_T$max (example: `Xmax`)	ZigZag/Block max value for T; where T is one of the characters X, Y or Z.
$_T$sin (example: `Xsin`)	Sin position wave for T; where T is one of the characters X, Y or Z.
$_T$cos (example: `Xcos`)	Cos position wave for T; where T is one of the characters X, Y or Z.

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Table 1 – continued from previous page

<var>	usage
UN_0N_1sin (example: `U11sin`)	Sin thermal wave for UN_0N_1; where N_0 is one of the characters 1, 2 or 3 and N_1 is one of the characters 1, 2 or 3.
UN_0N_1cos (example: `U11cos`)	Cos thermal wave for UN_0N_1; where N_0 is one of the characters 1, 2 or 3 and N_1 is one of the characters 1, 2 or 3.
MTsin (example: `MXsin`)	Sin mag. moment wave for T; where T is one of the characters X, Y or Z.
MTcos (example: `MXcos`)	Cos mag. moment wave for T; where T is one of the characters X, Y or Z.
PDFpos	PDF peak position.
PDFmag	PDF peak magnitude.
PDFsig	PDF peak std. dev.
Aspect ratio	Particle aspect ratio.
Length	Cylinder length.
Diameter	Cylinder/disk diameter.
Thickness	Disk thickness.
Shell thickness	Multiplier to get inner(<1) or outer(>1) sphere radius.
Dist	Interparticle distance.
VolFr	Dense scatterer volume fraction.
epis	Sticky sphere epsilon.
Sticky	Stickyness.
Depth	Well depth.
Width	Well width.
Volume	Particle volume.
Radius	Sphere/cylinder/disk radius.
Mean	Particle mean radius.
StdDev	Standard deviation in Mean.
G	Guinier prefactor.
Rg	Guinier radius of gyration.
B	Porod prefactor.
P	Porod power.
Cutoff	Porod cutoff.
PkInt	Bragg peak intensity.
PkPos	Bragg peak position.
PkSig	Bragg peak sigma.
PkGam	Bragg peak gamma.
eX_0X_1 (example: `e11`)	strain tensor eX_0X_1; where X_0 is one of the characters 1 or 2 and X_1 is one of the characters 1 or 2.
Dcalc	Calc. d-spacing.
Back	background parameter.
pos	peak position.
int	peak intensity.
WgtFrac	phase weight fraction.
alpha	TOF profile term.
alpha-P (example: `alpha-0`)	Pink profile term; where P is one of the characters 0 or 1.
beta-Y (example: `beta-0`)	TOF/Pink profile term; where Y is one of the characters 0, 1 or q.
sig-Z (example: `sig-0`)	TOF profile term; where Z is one of the characters 0, 1, 2 or q.
dif$a$ (example: `difA`)	TOF to d-space calibration; where a is one of the characters A, B or C.
CG_0,G_1 (example: `C10,10`)	spherical harmonics preferred orientation coef.; where G_0 is one or more digits (0, 1,… 9) and G_1 is one or more digits (0, 1,… 9).
Pressure	Pressure level for measurement in MPa.
Temperature	T value for measurement, K.

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<var>	usage
FreePrm*N* (example: FreePrm1)	User defined measurement parameter *N*; where *N* is one of the characters 1, 2 or 3.
Gonio. radius	Distance from sample to detector, mm.

2.3 GSAS-II Data Tree

A GSAS-II project is stored in a data file and is loaded into a wxPython data tree (wx.TreeCtrl) defined by GSASIIctrlGUI.G2TreeCtrl. Each entry in the tree has a text label and a data object associated with it. Note that all information used in a GSAS-II project is stored in the data tree, with the exception of images (which are too large). For images, a reference to the file location is saved and images are loaded from the file when needed.

To save a GSAS-II project, routine GSASIImiscGUI.ProjFileSave() is used to convert the tree contents to a "flat" format and write it to a file. The tree is transversed, and for each first-level tree item, a list is created, where the first item in that list is a two-element list containing the label of the tree item and the data object associated with the label. If there are second-level tree items that are children of that first-level tree item, additional items are added to the outermost list with pairs of text labels and data objects. Finally the outermost list is converted to a binary representation and written to disk with the Python pickle function. Note that GSAS-II does not use any data tree items other than first-level and second-level. Routine GSASIImiscGUI.ProjFileOpen() is used to read a GSAS-II project file and populate the data tree. GSAS-II project files are written with the .gpx extension.

Two pointers are kept for a selected tree entry in the GSAS-II data tree, saved as class variables in GSASIIdataGUI.GSASII (often referenced as G2frame). These are G2frame.PickId, which points to the selected data tree item, and G2frame.PatternId, which points to the parent of the data tree item, when G2frame.PickId points to a histogram. The two pointer may be the same when the first-level tree item for a histogram is selected.

2.3.1 Constraints Tree Item

Constraints are stored in a dict, separated into groups. Note that parameter are named in the following pattern, p:h:<var>:n, where p is the phase number, h is the histogram number <var> is a variable name and n is the parameter number. If a parameter does not depend on a histogram or phase or is unnumbered, that number is omitted. Note that the contents of each dict item is a List where each element in the list is a *constraint definition objects*. The constraints in this form are converted in GSASIImapvars.ProcessConstraints() to the form used in GSASIImapvars

The keys in the Constraints dict are:

key	explanation
Hist	This specifies a list of constraints on histogram-related parameters, which will be of form :h:<var>:n.
HAP	This specifies a list of constraints on parameters that are defined for every histogram in each phase and are of form p:h:<var>:n.
Phase	This specifies a list of constraints on phase parameters, which will be of form p::<var>:n.
Global	This specifies a list of constraints on parameters that are not tied to a histogram or phase and are of form ::<var>:n

Each constraint is defined as an item in a list. Each constraint is of form:

```
[[<mult1>, <var1>], [<mult2>, <var2>],..., <fixedval>, <varyflag>, <constype>]
```

Where the variable pair list item containing two values [<mult>, <var>], where:

- <mult> is a multiplier for the constraint (float)
- <var> a `G2VarObj` object. (Note that in very old .gpx files this might be a str with a variable name of form 'p:h:name[:at]')

Note that the last three items in the list play a special role:

- <fixedval> is the fixed value for a *constant equation* (`constype=c`) constraint or is None. For a *New variable* (`constype=f`) constraint, a variable name can be specified as a str (used for externally generated constraints)
- <varyflag> is True or False for *New variable* (`constype=f`) constraints or is None. This indicates if this variable should be refined.
- <constype> is one of four letters, 'e', 'c', 'h', 'f' that determines the type of constraint:
  - 'e' defines a set of equivalent variables. Only the first variable is refined (if the appropriate refine flag is set) and and all other equivalent variables in the list are generated from that variable, using the appropriate multipliers.
  - 'c' defines a constraint equation of form, $m_1 \times var_1 + m_2 \times var_2 + ... = c$
  - 'h' defines a variable to hold (not vary). Any variable on this list is not varied, even if its refinement flag is set. Only one [mult,var] pair is allowed in a hold constraint and the mult value is ignored. This is of particular value when needing to hold one or more variables where a single flag controls a set of variables such as, coordinates, the reciprocal metric tensor or anisotropic displacement parameter.
  - 'f' defines a new variable (function) according to relationship $newvar = m_1 \times var_1 + m_2 \times var_2 + ...$

2.3.2 Covariance Tree Item

The Covariance tree item has results from the last least-squares run. They are stored in a dict with these keys:

key	sub-key	explanation
newCellDict		(dict) lattice parameters computed by `GSASIIstrMath.GetNewCellParms()`
title		(str) Name of gpx file
variables		(list) Values for refined variables (list of float values, length N, ordered to match varyList)
sig		(list) Standard uncertainty values for refined variables (list of float values, length N, ordered to match varyList)
varyList		(list of str values, length N) List of directly refined variables
varyListStart		(list) initial refined variables before dependent vars are removed
newAtomDict		(dict) atom position values computed in `GSASIIstrMath.ApplyXYZshifts()`
Lastshft		(list) The shifts applied to each variable in the last refinement run. (list of float values, length N, ordered to match varyList)
depSigDict		(dict) Values along with standard uncertainty values for dependent variables
covMatrix		(np.array) The (NxN) covVariance matrix
freshCOV		(bool) indicates if the covMatrix has been freshly computed
msg		Warning/error messages from the last refinement run
Rvals		(dict) R-factors, GOF, Marquardt value for last refinement cycle
	Nobs	(int) Number of observed data points
	Nvars	(int) Number of refined parameters
	Rwp	(float) overall weighted profile R-factor (%)
	chisq	(float) $\sum w * (I_{obs} - I_{calc})^2$ for all data. Note: this is what GSAS-II calls χ^2, which is not the same thing as the reduced χ^2.
	lamMax	(float) Marquardt value applied to Hessian diagonal
	GOF	(float) The goodness-of-fit, aka square root of the reduced χ^2 squared, after refinement.
	GOF0	(float) The goodness-of-fit, aka square root of the reduced χ^2 square, before refinement.
	lastShifts	(dict) values of the shifts applied in the last refinement cycle (note: differs from *Lastshft*, which has values from the last run).
	SVD0	(int) number of singular value decomposition (SVD) singularities
	converged	(bool) True if last refinement run converged
	DelChi2	(float) change in χ^2 in last refinement cycle
	RestraintSum	(float) sum of restraints
	RestraintTerms	(float) total number of restraints
	Max shft/sig	(float) maximum shift/s.u. for shifts applied in last refinement run

2.3.3 Phase Tree Items

Phase information is stored in the GSAS-II data tree as children of the Phases item in a dict with keys:

key	sub-key	explanation
General		(dict) Overall information for the phase
	3Dproj	(list of str) projections for 3D pole distribution plots
	AngleRadii	(list of floats) Default radius for each atom used to compute interatomic angles
	AtomMass	(list of floats) Masses for atoms

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key	sub-key	explanation
	AtomPtrs	(list of int) four locations (cx,ct,cs & cu) to use to pull info from the atom records
	AtomTypes	(llist of str) Atom types
	BondRadii	(list of floats) Default radius for each atom used to compute interatomic distances
	Cell	Unit cell parameters & ref. flag (list with 8 items. All but first item are float.) 0: cell refinement flag (True/False), 1-3: a, b, c, (Å) 4-6: alpha, beta & gamma, (degrees) 7: volume (Å^3)
	Color	(list of (r,b,g) triplets) Colors for atoms
	Compare	(dict) Polygon comparison parameters
	Data plot type	(str) data plot type ('Mustrain', 'Size' or 'Preferred orientation') for powder data
	DisAglCtls	(dict) with distance/angle search controls, see *Controls used for Distance/Angle computation*.
	F000X	(float) x-ray F(000) intensity
	F000N	(float) neutron F(000) intensity
	Flip	(dict) Charge flip controls
	HydIds	(dict) geometrically generated hydrogen atoms
	Isotope	(dict) Isotopes for each atom type
	Isotopes	(dict) Scattering lengths for each isotope combination for each element in phase
	MCSA controls	(dict) Monte Carlo-Simulated Annealing controls
	Map	(dict) Map parameters
	Mass	(float) Mass of unit cell contents in g/mol
	Modulated	(bool) True if phase modulated
	Mydir	(str) Directory of current .gpx file
	Name	(str) Phase name
	NoAtoms	(dict) Number of atoms per unit cell of each type
	POhkl	(list) March-Dollase preferred orientation direction
	Pawley dmin	(float) maximum Q (as d-space) to use for Pawley extraction
	Pawley dmax	(float) minimum Q (as d-space) to use for Pawley extraction
	Pawley neg wt	(float) Restraint value for negative Pawley intensities
	SGData	(object) Space group details as a *space group (SGData)* object, as defined in `GSASIIspc.SpcGroup()`.
	SH Texture	(dict) Spherical harmonic preferred orientation parameters
	Super	(int) dimension of super group (0,1 only)
	Type	(str) phase type (e.g. 'nuclear')
	Z	(dict) Atomic numbers for each atom type
	doDysnomia	(bool) flag for max ent map modification via Dysnomia
	doPawley	(bool) Flag for Pawley intensity extraction
	vdWRadii	(dict) Van der Waals radii for each atom type
ranId		(int) unique random number Id for phase
pId		(int) Phase Id number for current project.
Atoms		(list of lists) Atoms in phase as a list of lists. The outer list is for each atom, the inner list contains varying items depending on the type of phase, see the *Atom Records* description.

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key	sub-key	explanation
Drawing		(dict) Display parameters
	Atoms	(list of lists) with an entry for each atom that is drawn
	Plane	(list) Controls for contour density plane display
	Quaternion	(4 element np.array) Viewing quaternion
	Zclip	(float) clipping distance in Å
	Zstep	(float) Step to de/increase Z-clip
	atomPtrs	(list) positions of x, type, site sym, ADP flag in Draw Atoms
	backColor	(list) background for plot as and R,G,B triplet (default = [0, 0, 0], black).
	ballScale	(float) Radius of spheres in ball-and-stick display
	bondList	(dict) Bonds
	bondRadius	(float) Radius of binds in Å
	cameraPos	(float) Viewing position in Å for plot
	contourLevel	(float) map contour level in $e/Å^3$
	contourMax	(float) map contour maximum
	depthFog	(bool) True if use depthFog on plot - set currently as False
	ellipseProb	(float) Probability limit for display of thermal ellipsoids in % .
	magMult	(float) multiplier for magnetic moment arrows
	mapSize	(float) x & y dimensions of contourmap (fixed internally)
	modelView	(4,4 array) from openGL drawing transofmation matrix
	oldxy	(list with two floats) previous view point
	radiusFactor	(float) Distance ratio for searching for bonds. Bonds are located that are within r(Ra+Rb) and (Ra+Rb)/r where Ra and Rb are the atomic radii.
	selectedAtoms	(list of int values) List of selected atoms
	showABC	(bool) Flag to show view point triplet. True=show.
	showHydrogen	(bool) Flag to control plotting of H atoms.
	showRigidBodies	(bool) Flag to highlight rigid body placement
	showSlice	(bool) flag to show contour map
	sizeH	(float) Size ratio for H atoms
	unitCellBox	(bool) Flag to control display of the unit cell.
	vdwScale	(float) Multiplier of van der Waals radius for display of vdW spheres.
	viewDir	(np.array with three floats) cartesian viewing direction
	viewPoint	(list of lists) First item in list is [x,y,z] in fractional coordinates for the center of the plot. Second item list of previous & current atom number viewed (may be [0,0])
ISODISTORT		(dict) contains controls for running ISODISTORT and results from it
	ISOmethod	(int) ISODISTORT method (currently 1 or 4; 2 & 3 not implemented in GSAS-II)
	ParentCIF	(str) parent cif file name for ISODISTORT method 4
	ChildCIF	(str) child cif file name for ISODISTORT method 4
	SGselect	(dict) selection list for lattice types in radio result from ISODISTORT method 1
	selection	(int) chosen selection from radio
	radio	(list) results from ISODISTORT method 1
	ChildMatrix	(3x3 array) transformation matrix for method 3 (not currently used)
	ChildSprGp	(str) child space group for method 3 (not currently used)
	ChildCell	(str) cell ordering for nonstandard orthorhombic ChildSprGrp in method 3 (not currently used)
	G2ModeList	(list) ISODISTORT mode names
	modeDispl	(list) distortion mode values; refinable parameters
	ISOmodeDispl	(list) distortion mode values as determined in method 4 by ISODISTORT

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key	sub-key	explanation
	NormList	(list) ISODISTORT normalization values; to convert mode value to fractional coordinate dsplacement
	G2parentCoords	(list) full set of parent structure coordinates transformed to child structure; starting basis for mode displacements
	G2VarList	(list)
	IsoVarList	(list)
	G2coordOffset	(list) only adjustible set of parent structure coordinates
	G2OccVarList	(list)
	Var2ModeMatrix	(array) atom variable to distortion mode transformation
	Mode2VarMatrix	(array) distortion mode to atom variable transformation
	rundata	(dict) saved input information for use by ISODISTORT method 1
RBModels		Rigid body assignments (note Rigid body definitions are stored in their own main top-level tree entry.)
RMC		(dict) RMCProfile, PDFfit & fullrmc controls
Pawley ref		(list) Pawley reflections
Histograms		(dict of dicts) The key for the outer dict is the histograms tied to this phase. The inner dict contains the combined phase/histogram parameters for items such as scale factors, size and strain parameters. The following are the keys to the inner dict. (dict)
	Babinet	(dict) For protein crystallography. Dictionary with two entries, 'BabA', 'BabU'
	Extinction	(list of float, bool) Extinction parameter
	Flack	(list of [float, bool]) Flack parameter & refine flag
	HStrain	(list of two lists) Hydrostatic strain. The first is a list of the HStrain parameters (1, 2, 3, 4, or 6 depending on unit cell), the second is a list of boolean refinement parameters (same length)
	Histogram	(str) The name of the associated histogram
	Layer Disp	(list of [float, bool]) Layer displacement in beam direction & refine flag
	LeBail	(bool) Flag for LeBail extraction
	Mustrain	(list) Microstrain parameters, in order: 0. Type, one of 'isotropic', 'uniaxial', 'generalized' 1. Isotropic/uniaxial parameters - list of 3 floats 2. Refinement flags - list of 3 bools 3. Microstrain axis - list of 3 ints, [h, k, l] 4. Generalized mustrain parameters - list of 2-6 floats, depending on space group 5. Generalized refinement flags - list of bools, corresponding to the parameters of (4)
	Pref.Ori.	(list) Preferred Orientation. List of eight parameters. Items marked SH are only used for Spherical Harmonics. 0. (str) Type, 'MD' for March-Dollase or 'SH' for Spherical Harmonics 1. (float) Value 2. (bool) Refinement flag 3. (list) Preferred direction, list of ints, [h, k, l] 4. (int) SH - number of terms 5. (dict) SH - 6. (list) SH 7. (float) SH

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key	sub-key	explanation
	Scale	(list of [float, bool]) Phase fraction & refine flag
	Size	List of crystallite size parameters, in order: 0. (str) Type, one of 'isotropic', 'uniaxial', 'ellipsoidal' 1. (list) Isotropic/uniaxial parameters - list of 3 floats 2. (list) Refinement flags - list of 3 bools 3. (list) Size axis - list of 3 ints, [h, k, l] 4. (list) Ellipsoidal size parameters - list of 6 floats 5. (list) Ellipsoidal refinement flags - list of bools, corresponding to the parameters of (4)
	Use	(bool) True if this histogram is to be used in refinement
MCSA		(dict) Monte-Carlo simulated annealing parameters

2.3.4 Rigid Body Objects

Rigid body descriptions are available for two types of rigid bodies: 'Vector' and 'Residue'. Vector rigid bodies are developed by a sequence of translations each with a refinable magnitude and Residue rigid bodies are described as Cartesian coordinates with defined refinable torsion angles.

key	sub-key	explanation
Vector	RBId	(dict of dict) vector rigid bodies
	AtInfo	(dict) Drad, Color: atom drawing radius & color for each atom type
	RBname	(str) Name assigned by user to rigid body
	VectMag	(list) vector magnitudes in Å
	rbXYZ	(list of 3 float Cartesian coordinates for Vector rigid body)
	rbRef	(list of 3 int & 1 bool) 3 assigned reference atom nos. in rigid body for origin definition, use center of atoms flag
	VectRef	(list of bool refinement flags for VectMag values)
	rbTypes	(list of str) Atom types for each atom in rigid body
	rbVect	(list of lists) Cartesian vectors for each translation used to build rigid body
	useCount	(int) Number of times rigid body is used in any structure
Residue	RBId	(dict of dict) residue rigid bodies
	AtInfo	(dict) Drad, Color: atom drawing radius & color for each atom type
	RBname	(str) Name assigned by user to rigid body
	rbXYZ	(list of 3 float) Cartesian coordinates for Residue rigid body
	rbTypes	(list of str) Atom types for each atom in rigid body
	atNames	(list of str) Names of each atom in rigid body (e.g. C1,N2…)
	rbRef	(list of 3 int & 1 bool) 3 assigned reference atom nos. in rigid body for origin definition, use center of atoms flag
	rbSeq	(list) Orig,Piv,angle,Riding : definition of internal rigid body torsion; origin atom (int), pivot atom (int), torsion angle (float), riding atoms (list of int)
	SelSeq	(int,int) used by SeqSizer to identify objects
	useCount	(int)Number of times rigid body is used in any structure
RBIds		(dict) unique Ids generated upon creation of each rigid body
	Vector	(list) Ids for each Vector rigid body
	Residue	(list) Ids for each Residue rigid body

2.3.5 Space Group Objects

Space groups are interpreted by `GSASIIspc.SpcGroup()` and the information is placed in a SGdata object which is a dict with these keys. Magnetic ones are marked "mag"

key	explanation
BNSlattsym	mag - (str) BNS magnetic space group symbol and centering vector
GenFlg	mag - (list) symmetry generators indices
GenSym	mag - (list) names for each generator
MagMom	mag - (list) "time reversals" for each magnetic operator
MagPtGp	mag - (str) Magnetic point group symbol
MagSpGrp	mag - (str) Magnetic space group symbol
OprNames	mag - (list) names for each space group operation
SGCen	(np.array) Symmetry cell centering vectors. A (n,3) np.array of centers. Will always have at least one row: `np.array([[0, 0, 0]])`
SGFixed	(bool) Only True if phase mported from a magnetic cif file then the space group can not be changed by the user because operator set from cif may be nonstandard
SGGen	(list) generators
SGGray	(bool) True if space group is a gray group (incommensurate magnetic structures)
SGInv	(bool) True if centrosymmetric, False if not
SGLatt	(str)Lattice centering type. Will be one of P, A, B, C, I, F, R
SGLaue	(str) one of the following 14 Laue classes: -1, 2/m, mmm, 4/m, 4/mmm, 3R, 3mR, 3, 3m1, 31m, 6/m, 6/mmm, m3, m3m
SGOps	(list) symmetry operations as a list of form `[[M1,T1], [M2,T2],...]` where M_n is a 3x3 np.array and T_n is a length 3 np.array. Atom coordinates are transformed where the Asymmetric unit coordinates [X is (x,y,z)] are transformed using $X' = M_n * X + T_n$
SGPolax	(str) Axes for space group polarity. Will be one of '', 'x', 'y', 'x y', 'z', 'x z', 'y z', 'xyz'. In the case where axes are arbitrary '111' is used (P 1, and ?).
SGPtGrp	(str) Point group of the space group
SGUniq	unique axis if monoclinic. Will be a, b, or c for monoclinic space groups. Will be blank for non-monoclinic.
SGSpin	mag - (list) of spin flip operatiors (+1 or -1) for the space group operations
SGSys	(str) symmetry unit cell: type one of 'triclinic', 'monoclinic', 'orthorhombic', 'tetragonal', 'rhombohedral', 'trigonal', 'hexagonal', 'cubic'
SSGK1	(list) Superspace multipliers
SpGrp	(str) space group symbol
SpnFlp	mag - (list) Magnetic spin flips for every magnetic space group operator

Superspace groups [3+1] are interpreted by `GSASIIspc.SSpcGroup()` and the information is placed in a SSGdata object which is a dict with these keys:

key	explanation
SSGCen	(list) 4D cell centering vectors [0,0,0,0] at least
SSGK1	(list) Superspace multipliers
SSGOps	(list) 4D symmetry operations as [M,T] so that M*x+T = x'
SSpGrp	(str) superspace group symbol extension to space group symbol, accidental spaces removed
modQ	(list) modulation/propagation vector
modSymb	(list of str) Modulation symbols

2.3.6 Phase Information

Phase information is placed in one of the following keys:

key	explanation
General	Overall information about a phase
Histograms	Information about each histogram linked to the current phase as well as parameters that are defined for each histogram and phase (such as sample peak widths and preferred orientation parameters.
Atoms	Contains a list of atoms, as described in the *Atom Records* description.
Drawing	Parameters that determine how the phase is displayed, including a list of atoms to be included, as described in the *Drawing Atom Records* description
MCSA	Monte-Carlo simulated annealing parameters
pId	The index of each phase in the project, numbered starting at 0
ranId	An int value with a unique value for each phase
RBModels	A list of dicts with parameters for each rigid body inserted into the current phase, as defined in the *Rigid Body Insertions*. Note that the rigid bodies are defined as *Rigid Body Objects*
RMC	PDF modeling parameters
Pawley ref	Pawley refinement parameters

Atom Records

If `phasedict` points to the phase information in the data tree, then atoms are contained in a list of atom records (list) in `phasedict['Atoms']`. Also needed to read atom information are four pointers, `cx,ct,cs,cia = phasedict['General']['AtomPtrs']`, which define locations in the atom record, as shown below. Items shown are always present; additional ones for macromolecular phases are marked 'mm', and those for magnetic structures are marked 'mg'

location	explanation
ct-4	mm - (str) residue number
ct-3	mm - (str) residue name (e.g. ALA)
ct-2	mm - (str) chain label
ct-1	(str) atom label
ct	(str) atom type
ct+1	(str) refinement flags; combination of 'F', 'X', 'U', 'M'
cx,cx+1,cx+2	(3 floats) the x,y and z coordinates
cx+3	(float) site occupancy
cx+4,cx+5,cx+6	mg - (list) atom magnetic moment along a,b,c in Bohr magnetons
cs	(str) site symmetry
cs+1	(int) site multiplicity
cia	(str) ADP flag: Isotropic ('I') or Anisotropic ('A')
cia+1	(float) Uiso
cia+2…cia+7	(6 floats) U11, U22, U33, U12, U13, U23
cia+8, -1	(int) unique atom identifier
-1	(dict) wave info (modulated structures only)

Drawing Atom Records

If `phasedict` points to the phase information in the data tree, then drawing atoms are contained in a list of drawing atom records (list) in `phasedict['Drawing']['Atoms']`. Also needed to read atom information are four pointers, `cx, ct,cs,ci = phasedict['Drawing']['AtomPtrs']`, which define locations in the atom record, as shown below. Items shown are always present; additional ones for macromolecular phases are marked 'mm', and those for magnetic structures are marked 'mg'

location	explanation
ct-4	mm - (str) residue number
ct-3	mm - (str) residue name (e.g. ALA)
ct-2	mm - (str) chain label
ct-1	(str) atom label
ct	(str) atom type
cx,cx+1,cx+2	(3 floats) the x,y and z coordinates
cx+3,cx+4,cx+5	mg - (3 floats) atom magnetic moment along a,b,c in Bohr magnetons
cs-1	(str) Sym Op symbol; sym. op number + unit cell id (e.g. '1,0,-1')
cs	(str) atom drawing style; e.g. 'balls & sticks'
cs+1	(str) atom label style (e.g. 'name')
cs+2	(int) atom color (RBG triplet)
cs+3	(str) ADP flag: Isotropic ('I') or Anisotropic ('A')
cs+4	(float) Uiso
cs+5…cs+11	(6 floats) U11, U22, U33, U12, U13, U23
ci	(int) unique atom identifier; matches source atom Id in Atom Records

Rigid Body Insertions

If `phasedict` points to the phase information in the data tree, then rigid body information is contained in list(s) in `phasedict['RBModels']['Residue']` and/or `phasedict['RBModels']['Vector']` for each rigid body inserted into the current phase.

key	explanation
fixOrig	Should the origin be fixed (when editing, not the refinement flag)
Ids	Ids for assignment of atoms in the rigid body
numChain	Chain number for macromolecular fits
Orient	Orientation of the RB as a quaternion and a refinement flag (' ', 'A' or 'AV')
OrientVec	Orientation of the RB expressed as a vector and azimuthal rotation angle
Orig	Origin of the RB in fractional coordinates and refinement flag (bool)
RBId	References the unique ID of a rigid body in the *Rigid Body Objects*
RBname	The name for the rigid body (str)
AtomFrac	The atom fractions for the rigid body
ThermalMotion	The thermal motion description for the rigid body, which includes a choice for the model and can include TLS parameters or an overall Uiso value.
Torsions	Defines the torsion angle and refinement flag for each torsion defined in the *Rigid Body Object*

2.3.7 Powder Diffraction Tree Items

Every powder diffraction histogram is stored in the GSAS-II data tree with a top-level entry named beginning with the string "PWDR ". The diffraction data for that information are directly associated with that tree item and there are a series of children to that item. The routines `GSASIIdataGUI.GSASII.GetUsedHistogramsAndPhasesfromTree()` and

`GSASIIstrIO.GetUsedHistogramsAndPhases()` will load this information into a dictionary where the child tree name is used as a key, and the information in the main entry is assigned a key of `Data`, as outlined below.

key	sub-key	explanation
Comments		(list of str) Text strings extracted from the original powder data header. These cannot be changed by the user; it may be empty.
Limits		(list) two two element lists, as [[Ld,Hd],[L,H]] where L and Ld are the current and default lowest two-theta value to be used and where H and Hd are the current and default highest two-theta value to be used.
Reflection Lists		(dict of dicts) with an entry for each phase in the histogram. The contents of each dict item is a dict containing reflections, as described in the *Powder Reflections* description.
Instrument Parameters		(dict) The instrument parameters uses different dicts for the constant wavelength (CW) and time-of-flight (TOF) cases. See below for the descriptions of each.
wtFactor		(float) A weighting factor to increase or decrease the leverage of data in the histogram . A value of 1.0 weights the data with their standard uncertainties and a larger value increases the weighting of the data (equivalent to decreasing the uncertainties).
Sample Parameters		(dict) Parameters that describe how the data were collected, as listed below. Refinable parameters are a list containing a float and a bool, where the second value specifies if the value is refined, otherwise the value is a float unless otherwise noted.
	Scale	The histogram scale factor (refinable)
	Absorption	The sample absorption coefficient as μr where r is the radius (refinable). Only valid for Debye-Scherrer geometry.
	SurfaceRoughA	Surface roughness parameter A as defined by Surotti, *J. Appl. Cryst*, **5**, 325-331, 1972. (refinable - only valid for Bragg-Brentano geometry)
	SurfaceRoughB	Surface roughness parameter B (refinable - only valid for Bragg-Brentano geometry)
	DisplaceX, DisplaceY	Sample displacement from goniometer center where Y is along the beam direction and X is perpendicular. Units are μm (refinable).
	Phi, Chi, Omega	Goniometer sample setting angles, in degrees.
	Gonio. radius	Radius of the diffractometer in mm
	InstrName	(str) A name for the instrument, used in preparing a CIF .
	Force, Temperature, Humidity, Pressure, Voltage	Variables that describe how the measurement was performed. Not used directly in any computations.
	ranId	(int) The random-number Id for the histogram (same value as where top-level key is ranId)
	Type	(str) Type of diffraction data, may be 'Debye-Scherrer' or 'Bragg-Brentano' .
hId		(int) The number assigned to the histogram when the project is loaded or edited (can change)
ranId		(int) A random number id for the histogram that does not change
Background		(list) The background is stored as a list with where the first item in the list is list and the second item is a dict. The list contains the background function and its coefficients; the dict contains Debye diffuse terms and background peaks. (TODO: this needs to be expanded.)
Data		(list) The data consist of a list of 6 np.arrays containing in order: 0. the x-postions (two-theta in degrees), 1. the intensity values (Yobs), 2. the weights for each Yobs value 3. the computed intensity values (Ycalc) 4. the background values 5. Yobs-Ycalc

CW Instrument Parameters

Instrument Parameters are placed in a list of two dicts, where the keys in the first dict are listed below. Note that the dict contents are different for constant wavelength (CW) vs. time-of-flight (TOF) histograms. The value for each item is a list containing three values: the initial value, the current value and a refinement flag which can have a value of True, False or 0 where 0 indicates a value that cannot be refined. The first and second values are floats unless otherwise noted. Items not refined are noted as [*]

key	sub-key	explanation
Instrument Parameters[0]	Type [*]	(str) Histogram type: * 'PXC' for constant wavelength x-ray * 'PNC' for constant wavelength neutron
	Bank [*]	(int) Data set number in a multidata file (usually 1)
	Lam	(float) Specifies a wavelength in Å
	Lam1 [*]	(float) Specifies the primary wavelength in Å, used in place of Lam when an α_1, α_2 source is used.
	Lam2 [*]	(float) Specifies the secondary wavelength in Å, used with Lam1
	I(L2)/I(L1)	(float) Ratio of Lam2 to Lam1, used with Lam1
	Zero	(float) Two-theta zero correction in *degrees*
	Azimuth [*]	(float) Azimuthal setting angle for data recorded with differing setting angles
	U, V, W	(float) Cagliotti profile coefficients for Gaussian instrumental broadening, where the FWHM goes as $U \tan^2\theta + V \tan\theta + W$
	X, Y, Z	(float) Cauchy (Lorentzian) instrumental broadening coefficients
	SH/L	(float) Variant of the Finger-Cox-Jephcoat asymmetric peak broadening ratio. Note that this is the sum of S/L and H/L where S is sample height, H is the slit height and L is the goniometer diameter.
	Polariz.	(float) Polarization coefficient.
Instrument Parameters[1]		(empty dict)

TOF Instrument Parameters

Instrument Parameters are also placed in a list of two dicts, where the keys in each dict listed below, but here for time-of-flight (TOF) histograms. The value for each item is a list containing three values: the initial value, the current value and a refinement flag which can have a value of True, False or 0 where 0 indicates a value that cannot be refined. The first and second values are floats unless otherwise noted. Items not refined are noted as [*]

key	sub-key	explanation
Instrument Parameters[0]	Type [*]	(str) Histogram type: * 'PNT' for time of flight neutron
	Bank	(int) Data set number in a multidata file
	2-theta [*]	(float) Nominal scattering angle for the detector
	fltPath [*]	(float) Total flight path source-sample-detector
	Azimuth [*]	(float) Azimuth angle for detector right hand rotation from horizontal away from source
	difC,difA, difB	(float) Diffractometer constants for conversion of d-spacing to TOF in microseconds
	Zero	(float) Zero point offset (microseconds)
	alpha	(float) Exponential rise profile coefficients
	beta-0 beta-1 beta-q	(float) Exponential decay profile coefficients
	sig-0 sig-1 sig-2 sig-q	(float) Gaussian profile coefficients
	X,Y,Z	(float) Lorentzian profile coefficients
Instrument Parameters[1]	Pdabc	(list of 4 float lists) Originally created for use in gsas as optional tables of d, alp, bet, d-true; for a reflection alpha & beta are obtained via interpolation from the d-spacing and these tables. The d-true column is apparently unused.

2.3.8 Powder Reflection Data Structure

The data tree entry for powder diffraction histograms contains an entry labeled `Reflection Lists` containing a dict keyed by phase name, for every phase linked to the histogram. Each entry is itself a dict with four entries, with keys:

key	explanation
RefList	This contains the reflection list, as described below.
FF	Contains a dict with two entries, `El` which contains a list of `n` element types and `FF` which contains a 55 x `n` np.array of of form factor values.
Type	Contains a string specifying the type of histogram, such as 'PXC'
Super	Contains a bool value, which is True when the phase has a superspace spacegroup (3+1 dimension).

one element of which is *'RefList'*, which is a np.array containing reflections. The columns in that array are documented below.

index	explanation
0,1,2	h,k,l
3	multiplicity
4	d-space, Å
5	pos, two-theta
6	sig, Gaussian width
7	gam, Lorenzian width
8	F^2_{obs}
9	F^2_{calc}
10	reflection phase, in degrees
11	intensity correction for reflection, this times F^2_{obs} or F^2_{calc} gives Iobs or Icalc
12	Preferred orientation correction
13	Transmission (absorption correction)
14	Extinction correction

Note that when the `Super` entry in the phase's main dict is True, indicating that the phase is a 3+1 super-space group, the columns are:

index	explanation
0,1,2,3	h,k,l,m
4	multiplicity
5	d-space, Å
6	pos, two-theta
7	sig, Gaussian width
8	gam, Lorenzian width
9	F^2_{obs}
10	F^2_{calc}
11	reflection phase, in degrees
12	intensity correction for reflection, this times F^2_{obs} or F^2_{calc} gives Iobs or Icalc
13	Preferred orientation correction
14	Transmission (absorption correction)
15	Extinction correction

2.3.9 Single Crystal Tree Items

Every single crystal diffraction histogram is stored in the GSAS-II data tree with a top-level entry named beginning with the string "HKLF ". The diffraction data for that information are directly associated with that tree item and there are a series of children to that item. The routines `GSASIIdataGUI.GSASII.GetUsedHistogramsAndPhasesfromTree()` and `GSASIIstrIO.GetUsedHistogramsAndPhases()` will load this information into a dictionary where the child tree name is used as a key, and the information in the main entry is assigned a key of `Data`, as outlined below.

key	sub-key	explanation
Data		(dict) that contains the reflection table, as described in the *Single Crystal Reflections* description.
Instrument Parameters		(list) containing two dicts where the possible keys in each dict are listed below. The value for most items is a list containing two values: the initial value, the current value. The first and second values are floats unless otherwise noted.
	Lam	(two floats) Specifies a wavelength in Å
	Type	(two str values) Histogram type : * 'SXC' for constant wavelength x-ray * 'SNC' for constant wavelength neutron * 'SNT' for time of flight neutron * 'SEC' for constant wavelength electrons (e.g. micro-ED)
	InstrName	(str) A name for the instrument, used in preparing a CIF
wtFactor		(float) A weighting factor to increase or decrease the leverage of data in the histogram. A value of 1.0 weights the data with their standard uncertainties and a larger value increases the weighting of the data (equivalent to decreasing the uncertainties).
hId		(int) The number assigned to the histogram when the project is loaded or edited (can change)
ranId		(int) A random number id for the histogram that does not change

2.3.10 Single Crystal Reflection Data Structure

For every single crystal a histogram, the `'Data'` item contains the structure factors as an np.array in item *'RefList'*. The columns in that array are documented below for non-superspace phases.

index	3+1 index	explanation
0,1,2	0,1,2	reflection indices, h,k,l
	3	3+1 superspace index, m
3	4	flag (0 absent, 1 observed)
4	5	d-space, Å
5	6	F^2_{obs}
6	7	$\sigma(F^2_{obs})$
7	8	F^2_{calc}
8	9	$F^2_{obs}(T)$
9	10	$F^2_{calc}(T)$
10	11	reflection phase, in degrees
11	12	intensity correction for reflection, this times F^2_{obs} or F^2_{calc} gives Iobs or Icalc

Notes:

- The annotation "(T)" in the second set of $F^2(T)$ values stands for "true," where the values are on an absolute scale through application of the scale factor.
- The left-most column gives the entry index for three dimensional spacegroups, the column to the right of that has the index for 3+1 superspace phases, where there are four reflection indices h, k, l, m.

2.3.11 Image Data Structure

Every 2-dimensional image is stored in the GSAS-II data tree with a top-level entry named beginning with the string "IMG ". The image data are directly associated with that tree item and there are a series of children to that item. The routines `GSASIIdataGUI.GSASII.GetUsedHistogramsAndPhasesfromTree()` and `GSASIIstrIO.GetUsedHistogramsAndPhases()` will load this information into a dictionary where the child tree name is used as a key, and the information in the main entry is assigned a key of `Data`, as outlined below.

key	sub-key	explanation
Comments		(list of str) Text strings extracted from the original image data header or a metafile. These cannot be changed by the user; it may be empty.
Image Controls	azmthOff	(float) The offset to be applied to an azimuthal value. Accomodates detector orientations other than with the detector X-axis horizontal.
	background image	(list:str,float) The name of a tree item ("IMG …") that is to be subtracted during image integration multiplied by value. It must have the same size/shape as the integrated image. NB: value < 0 for subtraction.
	calibrant	(str) The material used for determining the position/orientation of the image. The data is obtained from `ImageCalibrants()` and UserCalibrants.py (supplied by user).
	calibdmin	(float) The minimum d-spacing used during the last calibration run.
	calibskip	(int) The number of expected diffraction lines skipped during the last calibration run.
	center	(list:floats) The [X,Y] point in detector coordinates (mm) where the direct beam strikes the detector plane as determined by calibration. This point does not have to be within the limits of the detector boundaries.
	centerAzm	(bool) If True then the azimuth reported for the integrated slice of the image is at the center line otherwise it is at the leading edge.
	color	(str) The name of the colormap used to display the image. Default = 'Paired'.
	cutoff	(float) The minimum value of I/Ib for a point selected in a diffraction ring for calibration calculations. See pixLimit for details as how point is found.
	DetDepth	(float) Coefficient for penetration correction to distance; accounts for diffraction ring offset at higher angles. Optionally determined by calibration.
	DetDepthRef	(bool) If True then refine DetDepth during calibration/recalibration calculation.
	distance	(float) The distance (mm) from sample to detector plane.
	ellipses	(list:lists) Each object in ellipses is a list [center,phi,radii,color] where center (list) is location (mm) of the ellipse center on the detector plane, phi is the rotation of the ellipse minor axis from the x-axis, and radii are the minor & major radii of the ellipse. If radii[0] is negative then parameters describe a hyperbola. Color is the selected drawing color (one of 'b', 'g' ,'r') for the ellipse/hyperbola.
	edgemin	(float) Not used; parameter in EdgeFinder code.
	fullIntegrate	(bool) If True then integrate over full 360 deg azimuthal range.
	GonioAngles	(list:floats) The 'Omega','Chi','Phi' goniometer angles used for this image. Required for texture calculations.
	invert_x	(bool) If True display the image with the x-axis inverted.
	invert_y	(bool) If True display the image with the y-axis inverted.
	IOtth	(list:floats) The minimum and maximum 2-theta values to be used for integration.
	LRazimuth	(list:floats) The minimum and maximum azimuth values to be used for integration.

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Table 3 – continued from previous page

key	sub-key	explanation
	Oblique	(list:float,bool) If True apply a detector absorption correction using the value to the intensities obtained during integration.
	outAzimuths	(int) The number of azimuth pie slices.
	outChannels	(int) The number of 2-theta steps.
	pixelSize	(list:ints) The X,Y dimensions (microns) of each pixel.
	pixLimit	(int) A box in the image with 2*pixLimit+1 edges is searched to find the maximum. This value (I) along with the minimum (Ib) in the box is reported by `GSASIIimage.ImageLocalMax()` and subject to cutoff in `GSASIIimage.makeRing()`. Locations are used to construct rings of points for calibration calcualtions.
	PolaVal	(list:float,bool) If type='SASD' and if True, apply polarization correction to intensities from integration using value.
	rings	(list:lists) Each entry is [X,Y,dsp] where X & Y are lists of x,y coordinates around a diffraction ring with the same d-spacing (dsp)
	ring	(list) The x,y coordinates of the >5 points on an inner ring selected by the user,
	Range	(list) The minimum & maximum values of the image
	rotation	(float) The angle between the x-axis and the vector about which the detector is tilted. Constrained to -180 to 180 deg.
	SampleShape	(str) Currently only 'Cylinder'. Sample shape for Debye-Scherrer experiments; used for absorption calculations.
	SampleAbs	(list: float,bool) Value of absorption coefficient for Debye-Scherrer experimnents, flag if True to cause correction to be applied.
	setDefault	(bool) If True the use the image controls values for all new images to be read. (might be removed)
	setRings	(bool) If True then display all the selected x,y ring positions (vida supra rings) used in the calibration.
	showLines	(bool) If True then isplay the integration limits to be used.
	size	(list:int) The number of pixels on the image x & y axes
	type	(str) One of 'PWDR', 'SASD' or 'REFL' for powder, small angle or reflectometry data, respectively.
	tilt	(float) The angle the detector normal makes with the incident beam; range -90 to 90.
	wavelength	(float) The radiation wavelength (Å) as entered by the user (or someday obtained from the image header).
Masks	Arcs	(list: lists) Each entry [2-theta,[azimuth[0],azimuth[1]],thickness] describes an arc mask to be excluded from integration
	Frames	(list:lists) Each entry describes the x,y points (3 or more - mm) that describe a frame outside of which is excluded from recalibration and integration. Only one frame is allowed.
	Points	(list:lists) Each entry [x,y,radius] (mm) describes an excluded spot on the image to be excluded from integration.
	Polygons	(list:lists) Each entry is a list of 3+ [x,y] points (mm) that describe a polygon on the image to be excluded from integration.
	Rings	(list: lists) Each entry [2-theta,thickness] describes a ring mask to be excluded from integration.
	Thresholds	(list:[tuple,list]) [(Imin,Imax),[Imin,Imax]] This gives lower and upper limits for points on the image to be included in integrsation. The tuple is the image intensity limits and the list are those set by the user.

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Table 3 – continued from previous page

key	sub-key	explanation
	SpotMask	(dict: int & array) 'esdMul'(int) number of standard deviations above mean ring intensity to mask 'spotMask' (bool array) the spot mask for every pixel in image
Stress/Strain	Sample phi	(float) Sample rotation about vertical axis.
	Sample z	(float) Sample translation from the calibration sample position (for Sample phi = 0) These will be restricted by space group symmetry; result of strain fit refinement.
	Type	(str) 'True' or 'Conventional': The strain model used for the calculation.
	d-zero	(list:dict) Each item is for a diffraction ring on the image; all items are from the same phase and are used to determine the strain tensor. The dictionary items are: 'Dset': (float) True d-spacing for the diffraction ring; entered by the user. 'Dcalc': (float) Average calculated d-spacing determined from strain coeff. 'Emat': (list: float) The strain tensor elements e11, e12 & e22 (e21=e12, rest are 0) 'Esig': (list: float) Esds for Emat from fitting. 'pixLimit': (int) Search range to find highest point on ring for each data point 'cutoff': (float) I/Ib cutoff for searching. 'ImxyObs': (list: lists) [[X],[Y]] observed points to be used for strain calculations. 'ImtaObs': (list: lists) [[d],[azm]] transformed via detector calibration from ImxyObs. 'ImtaCalc': (list: lists [[d],[azm]] calculated d-spacing & azimuth from fit.

2.3.12 Controls used for Distance/Angle computation

Two arrays are used as input to `GSASIIstrMain.RetDistAngle()` and `GSASIIstrMain.PrintDistAngle()`, DisAglCtls and DisAglData.

- DisAglCtls is a dict with has keys `Name`, `AtomTypes`, `BondRadii`, `AngleRadii` which are atomic radii to be used in computation of distances. Also contains `Factors`, which is a 2 element list with a multiplier for bond and angle search range [typically (0.85,0.85)]. The maximum search distance is the product of the two radii and the multiplier, so raising the multiplier increases the number of distances or angles that are located. Example:

```
{'Name': 'Example',
'Factors': [0.85, 0.85],
'AtomTypes': ['Co', 'C', 'N', 'O', 'H'],
'BondRadii': [2.2, 1.12, 1.08, 1.09, 0.5],
'AngleRadii': [1.25, 0.92, 0.88, 0.89, 0.98]}
```

- DisAglData is a dict containing phase & refinement data:
  - 'OrigAtoms' and 'TargAtoms' contain the atoms to be used for distance/angle origins and atoms to be used as targets.
  - 'OrigIndx' contains the index numbers for the Origin atoms.
  - 'SGData' has the space group information (see *Space Group object*)
  - 'pId' has the phase id
  - 'Cell' has the unit cell parameters and cell volume
  - 'covData' has the contents of Covariance data tree item

  Added for use with rigid bodies:
  - 'RBlist' has the index numbers for atoms in a rigid body
  - 'rigidbodyDict' the contents of the main Rigid Body data tree item

- 'Phases' has the phase information for all used phases in the data tree. Only the current phase is needed, but this is easy.
- 'parmDict' is the GSAS-II parameter dict

2.4 Parameter Dictionary

The parameter dictionary contains all of the variable parameters for the refinement. The dictionary keys are the name of the parameter (<phase>:<hist>:<name>:<atom>). It is prepared in two ways. When loaded from the tree (in `GSASIIdataGUI.GSASII.MakeLSParmDict()` and `GSASIIfiles.ExportBaseclass.loadParmDict()`), the values are lists with two elements: `[value, refine flag]`

When loaded from the GPX file (in `GSASIIstrMain.Refine()` and `GSASIIstrMain.SeqRefine()`), the value in the dict is the actual parameter value (usually a float, but sometimes a letter or string flag value (such as I or A for iso/anisotropic).

2.5 Texture implementation

There are two different places where texture can be treated in GSAS-II. One is for mitigating the effects of texture in a structural refinement. The other is for texture characterization.

For reducing the effect of texture in a structural refinement there are entries labeled preferred orientation in each phase's data tab. Two different approaches can be used for this, the March-Dollase model and spherical harmonics.

For the March-Dollase model, one axis in reciprocal space is designated as unique (defaulting to the 001 axis) and reflections are corrected according to the angle they make with this axis depending on the March-Dollase ratio. (If unity, no correction is made). The ratio can be greater than one or less than one depending on if crystallites oriented along the designated axis are overrepresented or underrepresented. For most crystal systems there is an obvious choice for the direction of the unique axis and then only a single term needs to be refined. If the number is close to 1, then the correction is not needed.

The second method for reducing the effect of texture in a structural refinement is to create a crystallite orientation probability surface as an expansion in terms spherical harmonic functions. Only functions consistent with cylindrical diffraction suymmetry and having texture symmetry consistent with the Laue class of phase are used and are allowed, so the higher the symmetry the fewer terms that are available for a given spherical harmonics order. To use this correction, select the lowest order that provides refinable terms and perform a refinement. If the texture index remains close to one, then the correction is not needed. If a significant improvement is noted in the profile Rwp, one may wish to see if a higher order expansion gives an even larger improvement.

To characterize texture in a material, generally one needs data collected with the sample at multiple orientations or, for TOF, with detectors at multiple locations around the sample. In this case the detector orientation is given in each histogram's Sample Parameters and the sample's orientation is described with the Euler angles specifed on the phase's Texture tab, which is also where the texture type (cylindrical, rolling,…) and the spherical harmonic order is selected. This should not be used with a single dataset and should not be used if the preferred orientations corrections are used.

The coordinate system used for texture characterization is defined where the sample coordinates (Psi, gamma) are defined with 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 goniometer eulerian angles (Omega, Chi, Phi) so that Omega and Phi are rotations about K and Chi is a rotation about J when Omega = 0. Finally, as the sample may be mounted so that the sample coordinate system (Is, Js, Ks) does not coincide with the instrument coordinate system (I, J, K), we define three eulerian sample rotation angles (Omega-s, Chi-s, Phi-s) that describe the rotation from (Is, Js, Ks) to (I, J, K). The sample rotation angles are defined so that with the goniometer angles at zero Omega-s and Phi-s are rotations about K and Chi-s is a rotation about J.

Three typical examples:

1) Bragg-Brentano laboratory diffractometer: Chi=0

2) Debye-Scherrer counter detector; sample capillary axis perpendicular to diffraction plane: Chi=90

3) Debye-Scherrer 2D area detector positioned directly behind sample; sample capillary axis horizontal; Chi=0

NB: The area detector azimuthal angle will equal 0 in horizontal plane to right as viewed from x-ray source and will equal 90 at vertical "up" direction.

2.6 ISODISTORT implementation

CIFs prepared with the ISODISTORT web site https://iso.byu.edu/isotropy.php [B. J. Campbell, H. T. Stokes, D. E. Tanner, and D. M. Hatch, "ISODISPLACE: An Internet Tool for Exploring Structural Distortions." J. Appl. Cryst. 39, 607-614 (2006).] can be read into GSAS-II using import CIF. This will cause constraints to be established for structural distortion modes read from the CIF. At present, of the five types of modes only displacive(`_iso_displacivemode`...) and occupancy (`_iso_occupancymode`...) are processed. Not yet processed: `_iso_magneticmode`..., `_iso_rotationalmode`... & `_iso_strainmode`...

The CIF importer `G2phase_CIF` implements class `G2phase_CIF.CIFPhaseReader` which offers two methods associated with ISODISTORT (ID) input. Method `G2phase_CIF.CIFPhaseReader.ISODISTORT_test()` checks to see if a CIF block contains the loops with `_iso_displacivemode_label` or `_iso_occupancymode_label` items. If so, method `G2phase_CIF.CIFPhaseReader.ISODISTORT_proc()` is called to read and interpret them. The results are placed into the reader object's `.Phase` class variable as a dict item with key `'ISODISTORT'`.

Note that each mode ID has a long label with a name such as Pm-3m[1/2,1/2,1/2]R5+(a,a,0)[La:b:dsp]T1u(a). Function `G2phase_CIF.ISODISTORT_shortLbl()` is used to create a short name for this, such as R5_T1u(a) which is made unique by addition of _n if the short name is duplicated. As each mode is processed, a constraint corresponding to that mode is created and is added to list in the reader object's `.Constraints` class variable. Items placed into that list can either be a list, which corresponds to a function (new var) type *constraint definition* entry, or an item can be a dict, which provides help information for each constraint.

2.6.1 Displacive modes

The coordinate variables, as named by ISODISTORT, are placed in `.Phase['ISODISTORT']['IsoVarList']` and the corresponding `GSASIIobj.G2VarObj` objects for each are placed in `.Phase['ISODISTORT']['G2VarList']`. The mode variables, as named by ISODISTORT, are placed in `.Phase['ISODISTORT']['IsoModeList']` and the corresponding `GSASIIobj.G2VarObj` objects for each are placed in `.Phase['ISODISTORT']['G2ModeList']`. [Use `str(G2VarObj)` to get the variable name from the G2VarObj object, but note that the phase number, *n*, for the prefix "*n*::" cannot be determined as the phase number is not yet assigned.]

Displacive modes are a bit complex in that they relate to delta displacements, relative to an offset value for each coordinate, and because the modes are normalized. While GSAS-II also uses displacements, these are added to the coordinates after each refinement cycle and then the delta values are set to zero. ISODISTORT uses fixed offsets (subtracted from the actual position to obtain the delta values) that are taken from the parent structure coordinate and the initial offset value (in `_iso_deltacoordinate_value`) and these are placed in `.Phase['ISODISTORT']['G2coordOffset']` in the same order as `.Phase['ISODISTORT']['G2ModeList']`, `.Phase['ISODISTORT']['IsoVarList']` and ".Phase[ISODISTORT'][‘G2parentCoords']".'

The normalization factors (which the delta values are divided by) are taken from `_iso_displacivemodenorm_value` and are placed in `.Phase['ISODISTORT']['NormList']` in the same order as as `...['IsoModeList']` and `...['G2ModeList']`.

The CIF contains a sparse matrix, from the `loop_` containing `_iso_displacivemodematrix_value` which provides the equations for determining the mode values from the coordinates, that matrix is placed in `.Phase['ISODISTORT']['Mode2VarMatrix']`. The matrix is inverted to produce `.Phase['ISODISTORT']['Var2ModeMatrix']`, which determines how to compute the mode values from the delta coordinate values. These values are used for the in `GSASIIconstrGUI.ShowIsoDistortCalc()`, which shows coordinate and mode values, the latter with s.u. values.

2.6.2 Occupancy modes

The delta occupancy variables, as named by ISODISTORT, are placed in `.Phase['ISODISTORT']['OccVarList']` and the corresponding `GSASIIobj.G2VarObj` objects for each are placed in `.Phase['ISODISTORT']['G2OccVarList']`. The mode variables, as named by ISODISTORT, are placed in `.Phase['ISODISTORT']['OccModeList']` and the corresponding `GSASIIobj.G2VarObj` objects for each are placed in `.Phase['ISODISTORT']['G2OccModeList']`.

Occupancy modes, like Displacive modes, are also refined as delta values. However, GSAS-II directly refines the fractional occupancies. Offset values for each atom, are taken from `_iso_occupancy_formula` and are placed in `.Phase['ISODISTORT']['ParentOcc]`. (Offset values are subtracted from the actual position to obtain the delta values.) Modes are normalized (where the mode values are divided by the normalization factor) are taken from `_iso_occupancymodenorm_value` and are placed in `.Phase['ISODISTORT']['OccNormList']` in the same order as as `...['OccModeList']` and `...['G2OccModeList']`.

The CIF contains a sparse matrix, from the `loop_` containing `_iso_occupancymodematrix_value`, which provides the equations for determining the mode values from the coordinates. That matrix is placed in `.Phase['ISODISTORT']['Occ2VarMatrix']`. The matrix is inverted to produce `.Phase['ISODISTORT']['Var2OccMatrix']`, which determines how to compute the mode values from the delta coordinate values.

2.6.3 Mode Computations

Constraints are processed after the CIF has been read in `GSASIIdataGUI.GSASII.OnImportPhase()` or `GSASIIscriptable.G2Project.add_phase()` by moving them from the reader object's `.Constraints` class variable to the Constraints tree entry's ['Phase'] list (for list items defining constraints) or the Constraints tree entry's ['_Explain'] dict (for dict items defining constraint help information)

The information in `.Phase['ISODISTORT']` is used in `GSASIIconstrGUI.ShowIsoDistortCalc()` which shows coordinate and mode values, the latter with s.u. values. This can be called from the Constraints and Phase/Atoms tree items.

Before each refinement, constraints are processed as *described elsewhere*. After a refinement is complete, `GSASIIstrIO.PrintIndependentVars()` shows the shifts and s.u.'s on the refined modes, using GSAS-II values, but `GSASIIstrIO.PrintISOmodes()` prints the ISODISTORT modes as computed in the web site.

2.7 Parameter Limits

One of the most often requested "enhancements" for GSAS-II would be the inclusion of constraints to force parameters such as occupancies or Uiso values to stay within expected ranges. While it is possible for users to supply their own restraints that would perform this by supplying an appropriate expression with the "General" restraints, the GSAS-II authors do not feel that use of restraints or constraints are a good solution for this common problem where parameters refine to non-physical values. This is because when this occurs, most likely one of the following cases is occurring:

1. there is a significant problem with the model, for example for an x-ray fit if an O atom is placed where a S is actually present, the Uiso will refine artificially small or the occupancy much larger than unity to try to compensate for the missing electrons; or
2. the data are simply insensitive to the parameter or combination of parameters, for example unless very high-Q data are included, the effects of a occupancy and Uiso value can have compensating effects, so an assumption must be made; likewise, with neutron data natural-abundance V atoms are nearly invisible due to weak coherent scattering. No parameters can be fit for a V atom with neutrons.
3. the parameter is non-physical (such as a negative Uiso value) but within two sigma (sigma = standard uncertainty, aka e.s.d.) of a reasonable value, in which case the value is not problematic as it is experimentally indistinguishable from an expected value.
4. there is a systematic problem with the data (experimental error)

In all these cases, this situation needs to be reviewed by a crystallographer to decide how to best determine a structural model for these data. An implementation with a constraint or restraint is likely to simply hide the problem from the user, making it more probable that a poor model choice is obtained.

What GSAS-II does implement is to allow users to specify ranges for parameters that works by disabling refinement of parameters that refine beyond either a lower limit or an upper limit, where either or both may be optionally specified. Parameters limits are specified in the Controls tree entry in dicts named as `Controls['parmMaxDict']` and `Controls['parmMinDict']`, where the keys are `G2VarObj` objects corresponding to standard GSAS-II variable (see `getVarDescr()` and `CompileVarDesc()`) names, where a wildcard ('*') may optionally be used for histogram number or atom number (phase number is intentionally not allowed as a wildcard as it makes little sense to group the same parameter together different phases). Note that `prmLookup()` is used to see if a name matches a wildcard. The upper or lower limit is placed into these dicts as a float value. These values can be edited using the window created by the Calculate/"View LS parms" menu command or in scripting with the `GSASIIscriptable.G2Project.set_Controls()` function. In the GUI, a checkbox labeled "match all histograms/atoms" is used to insert a wildcard into the appropriate part of the variable name.

When a refinement is conducted, routine `GSASIIstrMain.dropOOBvars()` is used to find parameters that have refined to values outside their limits. If this occurs, the parameter is set to the limiting value and the variable name is added to a list of frozen variables (as a `G2VarObj` objects) kept in a list in the `Controls['parmFrozen']` dict. In a sequential refinement, this is kept separate for each histogram as a list in `Controls['parmFrozen'][histogram]` (where the key is the histogram name) or as a list in `Controls['parmFrozen']['FrozenList']` for a non-sequential fit. This allows different variables to be frozen in each section of a sequential fit. Frozen parameters are not included in refinements through removal from the list of parameters to be refined (`varyList`) in `GSASIIstrMain.Refine()` or `GSASIIstrMain.SeqRefine()`. The data window for the Controls tree item shows the number of Frozen variables and the individual variables can be viewed with the Calculate/"View LS parms" menu window or obtained with `GSASIIscriptable.G2Project.get_Frozen()`. Once a variable is frozen, it will not be refined in any future refinements unless the the variable is removed (manually) from the list. This can also be done with the Calculate/"View LS parms" menu window or `GSASIIscriptable.G2Project.set_Frozen()`.

See also

`G2VarObj` `getVarDescr()` `CompileVarDesc()` `prmLookup()` `GSASIIctrlGUI.ShowLSParms` `GSASIIctrlGUI.VirtualVarBox` `GSASIIstrIO.SaveUsedHistogramsAndPhases()` `GSASIIstrIO.SaveUpdatedHistogramsAndPhases()` `GSASIIstrIO.SetSeqResult()` `GSASIIstrMain.dropOOBvars()` `GSASIIscriptable.G2Project.set_Controls()` `GSASIIscriptable.G2Project.get_Frozen()` `GSASIIscriptable.G2Project.set_Frozen()`

CHAPTER

THREE

GSASIIOBJ: DATA OBJECTS & DOCS

This module defines many data structures used in GSAS-II, as well as provides misc. support routines for accessing them.

3.1 GSASIIobj Classes and routines

Classes and routines defined in `GSASIIobj` follow.

`GSASII.GSASIIobj.`**`AddPhase2Index`**(*rdObj*, *filename*)

Add a phase to the index during reading Used where constraints are generated during import (ISODISTORT CIFs)

`GSASII.GSASIIobj.`**`AtomIdLookup = {}`**

dict listing for each phase index as a str, the atom label and atom random Id, keyed by atom sequential index as a str; best to access this using *LookupAtomLabel()*

`GSASII.GSASIIobj.`**`AtomRanIdLookup = {}`**

dict listing for each phase the atom sequential index keyed by atom random Id; best to access this using *LookupAtomId()*

`GSASII.GSASIIobj.`**`CompileVarDesc`**()

Set the values in the variable lookup tables (*reVarDesc* and *reVarStep*). This is called in *getDescr()* and *getVarStep()* so this initialization is always done before use. These variables are also used in script *makeVarTbl.py* which creates the table in section 3.2 of the Sphinx docs (*Parameter names in GSAS-II*).

Note that keys may contain regular expressions, where '[xyz]' matches 'x' 'y' or 'z' (equivalently '[x-z]' describes this as range of values). '.*' matches any string. For example:

```
'AUiso':'Atomic isotropic displacement parameter',
```

will match variable `'p::AUiso:a'`. If parentheses are used in the key, the contents of those parentheses can be used in the value, such as:

```
'AU([123][123])':'Atomic anisotropic displacement parameter U\1',
```

will match `AU11`, `AU23`,... and *U11*, *U23* etc will be displayed in the value when used.

`GSASII.GSASIIobj.`**`CreatePDFitems`**(*G2frame*, *PWDRtree*, *ElList*, *Qlimits*, *numAtm=1*, *FltBkg=0*, *PDFnames=[]*)

Create and initialize a new set of PDF tree entries

Parameters

- **`G2frame`** (*Frame*) – main GSAS-II tree frame object
- **`PWDRtree`** (*str*) – name of PWDR to be used to create PDF item
- **`ElList`** (*dict*) – data structure with composition

- **Qlimits** (*list*) – Q limits to be used for computing the PDF
- **numAtm** (*float*) – no. atom in chemical formula
- **FltBkg** (*float*) – flat background value
- **PDFnames** (*list*) – previously used PDF names

Returns
the Id of the newly created PDF entry

GSASII.GSASIIobj.**DefaultControls = {'Author': 'no name', 'Copy2Next': False, 'F**2': False, 'FreePrm1': 'Sample humidity (%)', 'FreePrm2': 'Sample voltage (V)', 'FreePrm3': 'Applied load (MN)', 'HatomFix': False, 'Reverse Seq': False, 'SVDtol': 1e-06, 'ShowCell': False, 'UsrReject': {'MaxD': 500.0, 'MaxDF/F': 100.0, 'MinD': 0.05, 'MinExt': 0.01, 'minF/sig': 0.0}, 'deriv type': 'analytic Hessian', 'max cyc': 3, 'min dM/M': 0.001, 'newLeBail': False, 'shift factor': 1.0}**

Values to be used as defaults for the initial contents of the `Controls` data tree item.

class GSASII.GSASIIobj.**ExpressionCalcObj**(*exprObj*)

An object used to evaluate an expression from a *ExpressionObj* object.

Parameters
exprObj (ExpressionObj) – a *ExpressionObj* expression object with an expression string and mappings for the parameter labels in that object.

EvalExpression()

Evaluate an expression. Note that the expression and mapping are taken from the *ExpressionObj* expression object and the parameter values were specified in *SetupCalc()*. :returns: a single value for the expression. If parameter values are arrays (for example, from wild-carded variable names), the sum of the resulting expression is returned.

For example, if the expression is `'A*B'`, where A is 2.0 and B maps to `'1::Afrac:*'`, which evaluates to:

```
[0.5, 1, 0.5]
```

then the result will be `4.0`.

SetupCalc(*parmDict*)

Do all preparations to use the expression for computation. Adds the free parameter values to the parameter dict (parmDict).

UpdateDict(*parmDict*)

Update the dict for the expression with values in a dict

Parameters
parmDict (*dict*) – a dict of values, items not in use are ignored

UpdateVars(*varList*, *valList*)

Update the dict for the expression with a set of values

Parameters

- **varList** (*list*) – a list of variable names
- **valList** (*list*) – a list of corresponding values

__init__(*exprObj*)

__weakref__

list of weak references to the object

compiledExpr

The expression as compiled byte-code

eObj

The expression and mappings; a *ExpressionObj* object

exprDict

dict that defines values for labels used in expression and packages referenced by functions

fxnpkgdict

a dict with references to packages needed to find functions referenced in the expression.

lblLookup

Lookup table that specifies the expression label name that is tied to a particular GSAS-II parameters in the parmDict.

parmDict

A copy of the parameter dictionary, for distance and angle computation

su

Standard error evaluation where supplied by the evaluator

varLookup

Lookup table that specifies the GSAS-II variable(s) indexed by the expression label name. (Used for only for diagnostics not evaluation of expression.)

class GSASII.GSASIIobj.**ExpressionObj**

Defines an object with a user-defined expression, to be used for secondary fits or restraints. Object is created null, but is changed using *LoadExpression()*. This contains only the minimum information that needs to be stored to save and load the expression and how it is mapped to GSAS-II variables.

CheckVars()

Check that the expression can be parsed, all functions are defined and that input loaded into the object is internally consistent. If not an Exception is raised.

Returns

a dict with references to packages needed to find functions referenced in the expression.

EditExpression(*exprVarLst*, *varSelect*, *varName*, *varValue*, *varRefflag*)

Load the expression and associated settings from the object into arrays used for editing.

Parameters

- **exprVarLst** (*list*) – parameter labels found in the expression
- **varSelect** (*dict*) – this will be 0 for Free parameters and non-zero for expression labels linked to G2 variables.
- **varName** (*dict*) – Defines a name (str) associated with each free parameter
- **varValue** (*dict*) – Defines a value (float) associated with each free parameter
- **varRefflag** (*dict*) – Defines a refinement flag (bool) associated with each free parameter

Returns

the expression as a str

GetDepVar()

return the dependent variable, or None

GetIndependentVars()

Returns the names of the required independent parameters used in expression

GetVaried()

Returns the names of the free parameters that will be refined

GetVariedVarVal()

Returns the names and values of the free parameters that will be refined

LoadExpression(*expr*, *exprVarLst*, *varSelect*, *varName*, *varValue*, *varRefflag*)

Load the expression and associated settings into the object. Raises an exception if the expression is not parsed, if not all functions are defined or if not all needed parameter labels in the expression are defined.

This will not test if the variable referenced in these definitions are actually in the parameter dictionary. This is checked when the computation for the expression is done in `SetupCalc()`.

Parameters

- **expr** (*str*) – the expression
- **exprVarLst** (*list*) – parameter labels found in the expression
- **varSelect** (*dict*) – this will be 0 for Free parameters and non-zero for expression labels linked to G2 variables.
- **varName** (*dict*) – Defines a name (str) associated with each free parameter
- **varValue** (*dict*) – Defines a value (float) associated with each free parameter
- **varRefflag** (*dict*) – Defines a refinement flag (bool) associated with each free parameter

ParseExpression(*expr*)

Parse an expression and return a dict of called functions and the variables used in the expression. Returns None in case an error is encountered. If packages are referenced in functions, they are loaded and the functions are looked up into the modules global workspace.

Note that no changes are made to the object other than saving an error message, so that this can be used for testing prior to the save.

Returns
a list of used variables

SetDepVar(*var*)

Set the dependent variable, if used

UpdateVariedVars(*varyList*, *values*)

Updates values for the free parameters (after a refinement); only updates refined vars

__init__()

__weakref__

list of weak references to the object

assgnVars

A dict where keys are label names in the expression mapping to a GSAS-II variable. The value a G2 variable name. Note that the G2 variable name may contain a wild-card and correspond to multiple values.

expression

The expression as a text string

freeVars

A dict where keys are label names in the expression mapping to a free parameter. The value is a list with:

- a name assigned to the parameter
- a value for to the parameter and
- a flag to determine if the variable is refined.

lastError

Shows last encountered error in processing expression (list of 1-3 str values)

GSASII.GSASIIobj.**FindFunction**(*f*)

Find the object corresponding to function f

Parameters
f (*str*) – a function name such as 'numpy.exp'

Returns
(pkgdict,pkgobj) where pkgdict contains a dict that defines the package location(s) and where pkgobj defines the object associated with the function. If the function is not found, pkgobj is None.

exception GSASII.GSASIIobj.**G2Exception**(*msg*)

A generic GSAS-II exception class

__init__(*msg*)

__str__()

Return str(self).

__weakref__

list of weak references to the object

exception GSASII.GSASIIobj.**G2RefineCancel**(*msg*)

Raised when Cancel is pressed in a refinement dialog

__init__(*msg*)

__str__()

Return str(self).

__weakref__

list of weak references to the object

class GSASII.GSASIIobj.**G2VarObj**(**args*)

Defines a GSAS-II variable either using the phase/atom/histogram unique Id numbers or using a character string that specifies variables by phase/atom/histogram number (which can change). Note that GSASIIstrIO.GetUsedHistogramsAndPhases(), which calls *IndexAllIds()* (or GSASIIscriptable.G2Project.index_ids()) should be used to (re)load the current Ids before creating or later using the G2VarObj object.

This can store rigid body variables, but does not translate the residue # and body # to/from random Ids

A *G2VarObj* object can be created with a single parameter:

Parameters
varname (*str/tuple*) –

a single value can be used to create a *G2VarObj*
object. If a string, it must be of form "p:h:var" or "p:h:var:a", where

- p is the phase number (which may be left blank or may be '*' to indicate all phases);
- h is the histogram number (which may be left blank or may be '*' to indicate all histograms);
- a is the atom number (which may be left blank in which case the third colon is omitted). The atom number can be specified as '*' if a phase number is specified (not as '*'). For rigid body variables, specify a will be a string of form "residue:body#"

  Alternately a single tuple of form (Phase,Histogram,VarName,AtomID) can be used, where Phase, Histogram, and AtomID are None or are ranId values (or one can be '*') and VarName is a string. Note that if Phase is '*' then the AtomID is an atom number. For a rigid body variables, AtomID is a string of form "residue:body#".

If four positional arguments are supplied, they are:

Parameters

- **phasenum** (*str/int*) – The number for the phase (or None or '*')
- **histnum** (*str/int*) – The number for the histogram (or None or '*')
- **varname** (*str*) – a single value can be used to create a *G2VarObj*
- **atomnum** (*str/int*) – The number for the atom (or None or '*')

__eq__(*other*)

Allow comparison of G2VarObj to other G2VarObj objects or strings. If any field is a wildcard ('*') that field matches.

__hash__()

Allow G2VarObj to be a dict key by implementing hashing

__init__(**args*)

__repr__()

Return the detailed contents of the object

__str__()

Return str(self).

__weakref__

list of weak references to the object

_show()

For testing, shows the current lookup table

fmtVarByMode(*seqmode*, *note*, *warnmsg*)

Format a parameter object for display. Note that these changes are only temporary and are only shown only when the Constraints data tree is selected.

- In a non-sequential refinement or where the mode is 'use-all', the name is converted unchanged to a str
- In a sequential refinement when the mode is 'wildcards-only' the name is converted unchanged to a str but a warning is added for non-wildcarded HAP or Histogram parameters
- In a sequential refinement or where the mode is 'auto-wildcard', a histogram number is converted to a wildcard (*) and then converted to str

Parameters

- **mode** (*str*) – the sequential mode (see above)

- **note** (*str*) – value displayed on the line of the constraint/equiv.
- **warnmsg** (*str*) – a message saying the constraint is not used

Returns

varname, explain, note, warnmsg (all str values) where:

- varname is the parameter expressed as a string,
- explain is blank unless there is a warning explanation about the parameter or blank
- note is the previous value unless overridden
- warnmsg is the previous value unless overridden

varname(*hist=None*)

Formats the GSAS-II variable name as a "traditional" GSAS-II variable string (p:h:<var>:a) or (p:h:<var>)

Parameters

hist (*str/int*) – if specified, overrides the histogram number with the specified value

Returns

the variable name as a str

GSASII.GSASIIobj.**GenWildCard**(*varlist*)

Generate wildcard versions of G2 variables. These introduce '*' for a phase, histogram or atom number (but only for one of these fields) but only when there is more than one matching variable in the input variable list. So if the input is this:

```
varlist = ['0::AUiso:0', '0::AUiso:1', '1::AUiso:0']
```

then the output will be this:

```
wildList = ['*::AUiso:0', '0::AUiso:*']
```

Parameters

varlist (*list*) – an input list of GSAS-II variable names (such as 0::AUiso:0)

Returns

wildList, the generated list of wild card variable names.

GSASII.GSASIIobj.**GetPhaseNames**(*fl*)

Returns a list of phase names found under 'Phases' in GSASII gpx file NB: there is another one of these in GSASIIstrIO.py that uses the gpx filename

Parameters

fl (*file*) – opened .gpx file

Returns

list of phase names

GSASII.GSASIIobj.**HistIdLookup = {}**

dict listing histogram name and random Id, keyed by sequential histogram index as a str; best to access this using *LookupHistName()*

GSASII.GSASIIobj.**HistRanIdLookup = {}**

dict listing histogram sequential index keyed by histogram random Id; best to access this using *LookupHistId()*

GSASII.GSASIIobj.**HowDidIgetHere**(*wherecalledonly=False*)

Show a traceback with calls that brought us to the current location. Used for debugging.

Parameters

wherecalledonly (*bool*) – When True, the entire calling stack is shown. When False (default), only the 2nd to last stack entry (the routine that called the calling routine is shown.

class GSASII.GSASIIobj.**ImportBaseclass**(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

Defines a base class for the reading of input files (diffraction data, coordinates,…). See *Writing a Import Routine* for an explanation on how to use a subclass of this class.

CIFValidator(*filepointer*)

A *ContentsValidator()* for use to validate CIF files.

ContentsValidator(*filename*)

This routine will attempt to determine if the file can be read with the current format. This will typically be overridden with a method that takes a quick scan of [some of] the file contents to do a "sanity" check if the file appears to match the selected format. the file must be opened here with the correct format (binary/text)

ExtensionValidator(*filename*)

This methods checks if the file has the correct extension

Returns

- False if this filename will not be supported by this reader (only when strictExtension is True)
- True if the extension matches the list supplied by the reader
- None if the reader allows un-registered extensions

exception ImportException

Defines an Exception that is used when an import routine hits an expected error, usually in .Reader.

Good practice is that the Reader should define a value in self.errors that tells the user some information about what is wrong with their file.

__weakref__

list of weak references to the object

ReInitialize()

Reinitialize the Reader to initial settings

__init__(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

__weakref__

list of weak references to the object

class GSASII.GSASIIobj.**ImportImage**(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

Defines a base class for the reading of images

Images are read in only these places:

- Initial reading is typically done from a menu item with a call to `GSASIIdataGUI.GSASII.OnImportImage()` which in turn calls `GSASIIdataGUI.GSASII.OnImportGeneric()`. That calls methods `ExtensionValidator()`, `ContentsValidator()` and `Reader()`. This returns a list of reader objects for each read image. Also used in `GSASIIscriptable.import_generic()`.
- Images are read alternatively in `GSASIImiscGUI.ReadImages()`, which puts image info directly into the data tree.

- Unlike all other data types read by GSAS-II, images are only kept in memory as they are used and function `GSASIIfiles.GetImageData()` or `GSASIIfiles.RereadImageData()` is used to reread images if they are reloaded. For quick retrieval of previously read images, it may be useful to save sums of images or save a keyword (see `ImageTag`, below

When reading an image, the `Reader()` routine in the ImportImage class should set:

- `Comments`: a list of strings (str),
- `Npix`: the number of pixels in the image (int),
- `Image`: the actual image as a numpy array (np.array)
- `Data`: a dict defining image parameters (dict). Within this dict the following data items are used:
  - `pixelSize`: size of each pixel (x,y) in microns (such as `[200.,200.]`.
  - `wavelength`: wavelength in Å.
  - `distance`: distance of detector from sample in cm.
  - `center`: uncalibrated center of beam on detector (such as `[204.8,204.8]`, in mm measured from top left corner of the detector
  - `size`: size of image in pixels (x,y) (such as `[2048,2048]`).
  - `ImageTag`: image number or other keyword used to retrieve image from a multi-image data file (defaults to `1` if not specified).
  - `sumfile`: holds sum image file name if a sum was produced from a multi image file
  - `PolaVal`: has two values, the polarization fraction (typically 0.95-0.99 for synchrotrons, 0.5 for lab instruments) and a refinement flag (such as `[0.99, False]`).
  - `setdist`: nominal distance from sample to detector. Note that `distance` may be changed during calibration, but `setdist` will not be, so that calibration may be repeated.

optional data items:

- `repeat`: set to True if there are additional images to read in the file, False otherwise
- `repeatcount`: set to the number of the image.

Note that the above is initialized with *`InitParameters()`*. (Also see *Writing a Import Routine* for an explanation on how to use import classes in general.)

InitParameters()

initialize the instrument parameters structure

LoadImage(*ParentFrame*, *imagefile*, *imagetag=None*)

Optionally, call this after reading in an image to load it into the tree. This saves time by preventing a reread of the same information.

ReInitialize()

Reinitialize the Reader to initial settings – not used at present

__init__(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

class GSASII.GSASIIobj.**ImportPDFData**(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

Defines a base class for the reading of files with PDF G(R) data. See *Writing a Import Routine* for an explanation on how to use this class.

ReInitialize()

Reinitialize the Reader to initial settings

__init__(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

class GSASII.GSASIIobj.**ImportPhase**(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

Defines a base class for the reading of files with coordinates

Objects constructed that subclass this (in import/G2phase_*.py etc.) will be used in `GSASIIdataGUI.GSASII.OnImportPhase()` and in `GSASIIscriptable.import_generic()`. See *Writing a Import Routine* for an explanation on how to use this class.

__init__(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

class GSASII.GSASIIobj.**ImportPowderData**(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

Defines a base class for the reading of files with powder data.

Objects constructed that subclass this (in import/G2pwd_*.py etc.) will be used in `GSASIIdataGUI.GSASII.OnImportPowder()` and in `GSASIIscriptable.import_generic()`. See *Writing a Import Routine* for an explanation on how to use this class.

ReInitialize()

Reinitialize the Reader to initial settings

__init__(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

class GSASII.GSASIIobj.**ImportReflectometryData**(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

Defines a base class for the reading of files with reflectometry data. See *Writing a Import Routine* for an explanation on how to use this class.

ReInitialize()

Reinitialize the Reader to initial settings

__init__(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

class GSASII.GSASIIobj.**ImportSmallAngleData**(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

Defines a base class for the reading of files with small angle data. See *Writing a Import Routine* for an explanation on how to use this class.

ReInitialize()

Reinitialize the Reader to initial settings

__init__(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

class GSASII.GSASIIobj.**ImportStructFactor**(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

Defines a base class for the reading of files with tables of structure factors.

Structure factors are read with a call to `GSASIIdataGUI.GSASII.OnImportSfact()` which in turn calls `GSASIIdataGUI.GSASII.OnImportGeneric()`, which calls methods `ExtensionValidator()`, `ContentsValidator()` and `Reader()`.

See *Writing a Import Routine* for an explanation on how to use import classes in general. The specifics for reading a structure factor histogram require that the `Reader()` routine in the import class need to do only a few things: It

should load `RefDict` item `'RefList'` with the reflection list, and set *`Parameters`* with the instrument parameters (initialized with *`InitParameters()`* and set with *`UpdateParameters()`*).

Banks

self.RefDict is a dict containing the reflection information, as read from the file. Item 'RefList' contains the reflection information. See the *Single Crystal Reflection Data Structure* for the contents of each row. Dict element 'FF' contains the form factor values for each element type; if this entry is left as initialized (an empty list) it will be initialized as needed later.

InitParameters()

initialize the instrument parameters structure

Parameters

self.Parameters is a list with two dicts for data parameter settings

ReInitialize()

Reinitialize the Reader to initial settings

UpdateParameters(*Type=None*, *Wave=None*)

Revise the instrument parameters

__init__(*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

GSASII.GSASIIobj.**IndexAllIds**(*Histograms*, *Phases*)

Scan through the used phases & histograms and create an index to the random numbers of phases, histograms and atoms. While doing this, confirm that assigned random numbers are unique – just in case lightning strikes twice in the same place.

Note: this code assumes that the atom random Id (ranId) is the last element each atom record.

This is called when phases & histograms are looked up in these places (only):

- `GSASIIstrIO.GetUsedHistogramsAndPhases()` (which loads the histograms and phases from a GPX file),
- `GetUsedHistogramsAndPhasesfromTree()` (which does the same thing but from the data tree.)
- `OnFileClose()` (clears out an old project)

Note that globals *`PhaseIdLookup`* and *`PhaseRanIdLookup`* are also set in *`AddPhase2Index()`* to temporarily assign a phase number as a phase is being imported.

TODO: do we need a lookup for rigid body variables?

GSASII.GSASIIobj.**LookupAtomId**(*pId*, *ranId*)

Get the atom number from a phase and atom random Id

Parameters

- **pId** (*int/str*) – the sequential number of the phase
- **ranId** (*int*) – the random Id assigned to an atom

Returns

the index number of the atom (str)

GSASII.GSASIIobj.**LookupAtomLabel**(*pId*, *index*)

Get the atom label from a phase and atom index number

Parameters

- **pId** (*int/str*) – the sequential number of the phase

- **index** (*int*) – the index of the atom in the list of atoms

Returns
the label for the atom (str) and the random Id of the atom (int)

GSASII.GSASIIobj.**LookupHistId**(*ranId*)

Get the histogram number and name from a histogram random Id

Parameters
ranId (*int*) – the random Id assigned to a histogram

Returns
the sequential Id (hId) number for the histogram (str)

GSASII.GSASIIobj.**LookupHistName**(*hId*)

Get the histogram number and name from a histogram Id

Parameters
hId (*int/str*) – the sequential assigned to a histogram

Returns
(hist,ranId) where hist is the name of the histogram (str) and ranId is the random # id for the histogram (int)

GSASII.GSASIIobj.**LookupPhaseId**(*ranId*)

Get the phase number and name from a phase random Id

Parameters
ranId (*int*) – the random Id assigned to a phase

Returns
the sequential Id (pId) number for the phase (str)

GSASII.GSASIIobj.**LookupPhaseName**(*pId*)

Get the phase number and name from a phase Id

Parameters
pId (*int/str*) – the sequential assigned to a phase

Returns
(phase,ranId) where phase is the name of the phase (str) and ranId is the random # id for the phase (int)

GSASII.GSASIIobj.**LookupWildCard**(*varname*, *varlist*)

returns a list of variable names from list varname that match wildcard name in varname

Parameters

- **varname** (*str*) – a G2 variable name containing a wildcard (such as *::var)
- **varlist** (*list*) – the list of all variable names used in the current project

Returns
a list of matching GSAS-II variables (may be empty)

GSASII.GSASIIobj.**MakeUniqueLabel**(*lbl*, *labellist*)

Make sure that every a label is unique against a list by adding digits at the end until it is not found in list.

Parameters

- **lbl** (*str*) – the input label
- **labellist** (*list*) – the labels that have already been encountered

Returns
lbl if not found in labellist or lbl with _1-9 (or _10-99, etc.) appended at the end

GSASII.GSASIIobj.**PhaseIdLookup = {}**
dict listing phase name and random Id keyed by sequential phase index as a str; best to access this using *LookupPhaseName()*

GSASII.GSASIIobj.**PhaseRanIdLookup = {}**
dict listing phase sequential index keyed by phase random Id; best to access this using *LookupPhaseId()*

GSASII.GSASIIobj.**ReadCIF**(*URLorFile*)
Open a CIF, which may be specified as a file name or as a URL using PyCifRW (from James Hester). The open routine gets confused with DOS names that begin with a letter and colon "C:dir" so this routine will try to open the passed name as a file and if that fails, try it as a URL.

Used for CIF imports and for reading CIF templates for project CIF exports

Parameters
URLorFile (*str*) – string containing a URL or a file name. Code will try first to open it as a file and then as a URL.

Returns
a PyCifRW CIF object or an empty string if PyCifRW is not accessible

GSASII.GSASIIobj.**SetDefaultSample**()
Fills in default items for the Sample dictionary for Debye-Scherrer & SASD

GSASII.GSASIIobj.**SetNewPhase**(*Name='New Phase'*, *SGData=None*, *cell=None*, *Super=None*)
Create a new phase dict with default values for various parameters

Parameters
- **Name** (*str*) – Name for new Phase
- **SGData** (*dict*) – space group data from GSASIIspc:SpcGroup(); defaults to data for P 1
- **cell** (*list*) – unit cell parameter list; defaults to [1.0,1.0,1.0,90.,90,90.,1.]

GSASII.GSASIIobj.**ShortHistNames = {}**
a dict containing a possibly shortened and when non-unique numbered version of the histogram name. Keyed by the histogram sequential index.

GSASII.GSASIIobj.**ShortPhaseNames = {}**
a dict containing a possibly shortened and when non-unique numbered version of the phase name. Keyed by the phase sequential index.

class GSASII.GSASIIobj.**ShowTiming**
An object to use for timing repeated sections of code.

Create the object with::
tim0 = ShowTiming()

Tag sections of code to be timed with::
tim0.start('start') tim0.start('in section 1') tim0.start('in section 2')

etc. (Note that each section should have a unique label.)

After the last section, end timing with::
tim0.end()

Show timing results with::
tim0.show()

__init__()

__weakref__

list of weak references to the object

GSASII.GSASIIobj.**SortVariables**(*varlist*)

Sorts variable names in a sensible manner

GSASII.GSASIIobj.**StripUnicode**(*string*, *subs='.'*)

Strip non-ASCII characters from strings

Parameters

- **string** (*str*) – string to strip Unicode characters from
- **subs** (*str*) – character(s) to place into string in place of each Unicode character. Defaults to '.'

Returns

a new string with only ASCII characters

GSASII.GSASIIobj.**TestIndexAll**()

Test if *IndexAllIds()* has been called to index all phases and histograms (this is needed before *G2VarObj()* can be used.

Returns

Returns True if indexing is needed.

GSASII.GSASIIobj.**VarDescr**(*varname*)

Return two strings with a more complete description for a GSAS-II variable

Parameters

name (*str*) – A full G2 variable name with 2 or 3 or 4 colons (<p>:<h>:name[:<a>] or <p>::RBname:<r>:<t>])

Returns

(loc,meaning) where loc describes what item the variable is mapped (phase, histogram, etc.) and meaning describes what the variable does.

GSASII.GSASIIobj.**_lookup**(*dic*, *key*)

Lookup a key in a dictionary, where None returns an empty string but an unmatched key returns a question mark. Used in *G2VarObj*

GSASII.GSASIIobj.**fmtVarDescr**(*varname*)

Return a string with a more complete description for a GSAS-II variable

Parameters

varname (*str*) – A full G2 variable name with 2 or 3 or 4 colons (<p>:<h>:name[:<a>] or <p>::RBname:<r>:<t>])

Returns

a string with the description

GSASII.GSASIIobj.**getDescr**(*name*)

Return a short description for a GSAS-II variable

Parameters

name (*str*) – The descriptive part of the variable name without colons (:)

Returns

a short description or None if not found

GSASII.GSASIIobj.**getVarDescr**(*varname*)

Return a short description for a GSAS-II variable

Parameters
name (*str*) – A full G2 variable name with 2 or 3 or 4 colons (<p>:<h>:name[:<a1>][:<a2>])

Returns
a six element list as [*p*,`h`,`name`,`a1`,`a2`,`description`], where *p*, *h*, *a1*, *a2* are str values or *None*, for the phase number, the histogram number and the atom number; *name* will always be a str; and *description* is str or *None*. If the variable name is incorrectly formed (for example, wrong number of colons), *None* is returned instead of a list.

GSASII.GSASIIobj.**getVarStep**(*name*, *parmDict=None*)

Return a step size for computing the derivative of a GSAS-II variable

Parameters

- **name** (*str*) – A complete variable name (with colons, :)
- **parmDict** (*dict*) – A dict with parameter values or None (default)

Returns
a float that should be an appropriate step size, either from the value supplied in *CompileVarDesc()* or based on the value for name in parmDict, if supplied. If not found or the value is zero, a default value of 1e-5 is used. If parmDict is None (default) and no value is provided in *CompileVarDesc()*, then None is returned.

GSASII.GSASIIobj.**patchControls**(*Controls*)

patch routine to convert variable names used in parameter limits to G2VarObj objects (See *Parameter Limits* description.)

GSASII.GSASIIobj.**prmLookup**(*name*, *prmDict*)

Looks for a parameter in a min/max dictionary, optionally considering a wild card for histogram or atom number (use of both will never occur at the same time).

Parameters

- **name** – a GSAS-II parameter name (str, see *getVarDescr()* and *CompileVarDesc()*) or a *G2VarObj* object.
- **prmDict** (*dict*) – a min/max dictionary, (parmMinDict or parmMaxDict in Controls) where keys are *G2VarObj* objects.

Returns

Two values, (**matchname**, **value**), are returned where:

- **matchname** *(str)* is the *G2VarObj* object corresponding to the actual matched name, which could contain a wildcard even if **name** does not; and
- **value** *(float)* which contains the parameter limit.

GSASII.GSASIIobj.**reVarDesc = {}**

This dictionary lists descriptions for GSAS-II variables where keys are compiled regular expressions that will match the name portion of a parameter name. Initialized in *CompileVarDesc()*.

GSASII.GSASIIobj.**reVarStep = {}**

This dictionary lists the preferred step size for numerical derivative computation w/r to a GSAS-II variable. Keys are compiled regular expressions and values are the step size for that parameter. Initialized in *CompileVarDesc()*.

GSASII.GSASIIobj.**removeNonRefined**(*parmList*)

Remove items from variable list that are not refined and should not appear as options for constraints

Parameters

parmList (*list*) – a list of strings of form "p:h:VAR:a" where VAR is the variable name

Returns

a list after removing variables where VAR matches a entry in local variable NonRefinedList

GSASII.GSASIIobj.**restraintNames = [['Bond', 'Bonds'], ['Angle', 'Angles'], ['Plane', 'Planes'], ['Chiral', 'Volumes'], ['Torsion', 'Torsions'], ['Rama', 'Ramas'], ['ChemComp', 'Sites'], ['Texture', 'HKLs'], ['Moments', 'Moments'], ['General', 'General'], ['SpinRB', 'SpinRBs']]**

Names of restraint keys for the restraint dict and the location of the restraints in each dict

GSASII.GSASIIobj.**validateAtomDrawType**(*typ*, *generalData={}*)

Confirm that the selected Atom drawing type is valid for the current phase. If not, use 'vdW balls'. This is currently used only for setting a default when atoms are added to the atoms draw list.

CHAPTER

FOUR

GSAS-II EXECUTION ENVIRONMENT

4.1 Supported Platforms

It should be possible to run GSAS-II on any computer where Python 3.7+ and the appropriate required packages are available, as discussed below, but GSAS-II also requires that some code must be compiled. For the following platforms, binary images for this compiled code are currently provided:

- Windows-10: 64-bit Intel-compatible processors
- MacOS: Intel processors
- MacOS: ARM processors, aka Apple Silicon (M1, etc)
- Linux: 64-bit Intel-compatible processors
- Linux: ARM processors (64-bit Raspberry Pi OS only)

Details for GSAS-II use on these specific platforms follows below:

- **Windows**: self-Installation kits are provided for 64-bit Windows-10 and -11 here. Less testing has been done with Windows-11, but both appear to working interchangeably with respect to GSAS-II.

  In theory it should be possible to run GSAS-II on older versions of Windows, including 32-bit OS versions, but no current installation kit can be provided. Installing GSAS-II will require locating a compatible version (or compiling) Python and the required packages. It may be necessary to recompile the GSAS-II binaries.

- **MacOS**: GSAS-II can run natively on Intel (or ARM ("M1"-"M3" aka "Apple Silicon") processors with relatively current versions of MacOS, with self-installers that can be run from the command-line available for download here. The Intel version will run on both types of Mac processors, but the native ARM versions offer the highest GSAS-II performance we see on any platform.

  It appears that this installer can be used with MacOS versions 11.0 and later. Macs older than Catalina (10.15) will likely require older distributions of Python.

- **Intel Linux**: Note that GSAS-II does not get a lot of testing in Linux by us, but is used fairly widely on this platform nonetheless. We provide an installer here that includes Python and needed packages for Intel-compatible Linuxes, but compatibility with older and very new versions of Linux can sometimes be tricky as compatibility libraries may be needed – not always easy to do. It may be better to use your Linux distribution's versions of Python and packages (typically done with a software tool such as apt or yum or pip. See https://advancedphotonsource.github.io/GSAS-II-tutorials/install-pip.html for more information.

- **Non-Intel Linux**: Will GSAS-II run on Linux with other types of CPUs? That will mostly depend on support for Python and wxPython on that CPU. If those can be used, you can likely build the GSAS-II binaries with gcc & gfortran. Expect to need to modify the meson files.

  Raspberry Pi (ARM) Linux: GSAS-II has been installed on both 32-bit and the 64-bit version of the Raspberry Pi OS (formerly called Raspbian) and some older compiled binaries are provided at present for both, but 32-bit support may not continue. It is expected that these binaries will also function on Ubuntu Linux for Raspberry Pi,

but this has not been tried. The performance of GSAS-II on a Raspberry Pi is not blindingly fast, but one can indeed run GSAS-II on a motherboard that costs only $15 (perhaps even one that costs $5) and uses <5 Watts!

Note that the 64-bit OS is preferred on the models where it can be run (currently including models 3A+, 3B, 3B+, 4, 400, CM3, CM3+, CM4, and Zero 2 W) . With the 32-bit Raspberry Pi OS, which does run on all Raspberry Pi models, it is necessary to use the OS distribution's versions of Python and its packages, see here for more information. With 64-bit Pi OS it may be possible for us to provide a GSAS2MAIN installer (which will need to include a custom-supplied wxPython wheel, since that is not available in conda-forge) or else pip must be used to download and build wxpython (quite slow). Please let Brian know if you are intending to use GSAS-II on a Raspberry Pi for a classroom, etc and would need help with this.

4.2 Source Code Management

The master version of the source code for GSAS-II resides on GitHub at URL (in branch main) and the git version control system (VCS) is usually used to install the files needed by GSAS-II. When GSAS-II is installed in this manner, the software can be easily updated, as git commands can download only the changed sections of files that need to be updated. It is likewise possible to use git to regress to an older version of GSAS-II, though there are some limitations on how far back older versions of GSAS-II will be with current versions of Python and associated packages. While git is not required for use of GSAS-II, special procedures must be used to install GSAS-II without it and once installed without git, updates of GSAS-II must be done manually.

4.3 Python Requirements

GSAS-II requires a standard Python interpreter to be installed, as well as several separately-developed packages that are not supplied with Python, as are described below. While for some packages, we have not seen much dependence on versions, for others we do find significant differences; this is also discussed further below. The GSAS-II GUI will warn about Python and packages versions that are believed to be problematic, as defined in variable `GSASIIdataGUI.versionDict`, but for new installations we are currently recommending the following interpreter/package versions:

- Python 3.11, 3.12 or 3.13 is recommended. No testing has yet been done with Python 3.14, but no problems are expected. GSAS-II should run with any Python version from 3.7 or later, but we do not create binaries for all versions of Python and numpy. You will need to locate (from the old subversion server) older binaries to match older Python versions or compile them yourself.
- wxPython 4.2 or later is recommended, but with Python <=3.9 any wx4.x version should be OK. Problems with newer sections of the GUI are expected for wx <4.0.
- NumPy 1.26 recommended with Python 3.11 and 2.2 with 3.12 or 3.13, but anything from 1.17 on is likely fine, but if you do not match the supplied GSAS-II binaries you will need to build them yourself.
- matplotlib-base Note that matplotlib-base is preferred over matplotlib unless matplotlib will be used outside GSAS-II. 3.10 is recommended, but anything later than 3.4 should be fine.
- pyOpenGL: no version-related problems have been seen.
- SciPy: no version-related problems have been seen, but in at least one case multiple imports are tried to account for where function names have changed.
- PyCifRW: no version issues are known. We had been using an older version for a long time, but in 2025 switched to the latest version and did not see any problems.
- pybaselines: no version issues are known.

For more details on problems noted with specific versions of Python and Python packages, see comments below and details here: `GSASIIdataGUI.versionDict`,

Note that GSAS-II is currently being developed using Python 3.11 through 3.13. We are no longer supporting Python 2.7 and <=3.6, and strongly encourage that systems running GSAS-II under these older Python versions reinstall Python. Typically this is done by reinstalling GSAS-II from a current self-installer.

There are a number of ways to install Python plus the packages needed by GSAS-II. See https://advancedphotonsource.github.io/GSAS-II-tutorials/install.html and links therein for a discussion of installation.

Python package requirements depend on how GSAS-II will be run, as will be discussed in the next section. In order to run the GUI for GSAS-II, a much larger number of packages are required. Several more packages are optional, but some functionally will not be available without those optional packages. Far fewer packages are required to run GSAS-II on a compute server via the scripting interface and without a GUI.

4.3.1 GUI Requirements

When using the GSAS-II graphical user interface (GUI), the following Python extension packages are required:

- wxPython (http://wxpython.org/docs/api/). Note that GSAS-II has been tested with various wxPython versions over the years. We encourage use of 4.x with Python 3.x, but with Py>=3.10 you must use wxPython 4.2.0 or later.
- NumPy (http://docs.scipy.org/doc/numpy/reference/),
- SciPy (http://docs.scipy.org/doc/scipy/reference/),
- matplotlib (http://matplotlib.org/contents.html) and
- PyOpenGL (http://pyopengl.sourceforge.net/documentation).
- PyCifRW: (https://github.com/jamesrhester/pycifrw)

GSAS-II will not start or will start but will not be able to do much if the above packages are not available.

4.3.2 Recommended Packages for GUI Use

In addition to the previous required packages, several Python packages are utilized in limited sections of the GUI code, but are not required. If these packages are not present, warning messages may be generated if they would be needed, or menu items may be omitted, but the vast bulk of GSAS-II will function normally. These optional packages are:

- gitpython: (https://gitpython.readthedocs.io and https://github.com/gitpython-developers/GitPython). This this package provides a bridge between the git version control system and Python. It is required for the standard GSAS-II installation process and for GSAS-II to update itself from GitHub. If your computer does not already have git in the path, also include the git package to obtain that binary (if you are not sure, it does not hurt to do this anyway).
- requests: this package simplifies http access (https://requests.readthedocs.io/). It is used for access to webpages such as ISODISTORT and for some internal software downloads. It is required for support of git updating and installation.
- Pillow (https://pillow.readthedocs.org) or PIL (http://www.pythonware.com/products/pil/). This is used to read and save certain types of images.
- h5py and hdf5: h5py is the HDF5 interface and hdf5 is the support package. These packages are (not surprisingly) required to import images from HDF5 files. If these libraries are not present, the HDF5 importers will not appear in the import menu and a warning message appears on GSAS-II startup.
- imageio is used to make movies. This is optional and is utilized for plotting superspace (modulated) structures.
- seekpath is used for magnetic lattice (k-vector) searches (https://seekpath.readthedocs.io)
- conda: the conda package allows access to package installation, etc. features from inside Python. It is not required but is helpful to have, as it allows GSAS-II to install some packages that are not supplied initially. The conda package is included by default in the base miniconda and anaconda installations, but if you create an environment

for GSAS-II (*conda create -n <env> package-list…*), it will not be added to that environment unless you request it specifically.

- pybaselines: Determines a background for a powder pattern in the "autobackground" option. See https://pybaselines.readthedocs.io and https://github.com/derb12/pybaselines for more information.
- xmltodict: Needed to read Bruker BRML files. The BRML importer will not appear in the importer menu if this package is not installed.
- win32com (windows only): this module is used to install GSAS-II on windows machines. GSAS-II can be used on Windows without this, but the installation will offer less integration into Windows. Conda provides this under the name pywin32.
- zarr: The zarr package is used to read and write compressed hierarchical files. It is used by the APS MIDAS program to produce files of integrated powder diffraction patterns.
- sympy: This package performs symbolic computations and is used for k-vector searching with ISODISTORT.

***Conda command*:**

Should you wish to install Python and the desired packages yourself, this is certainly possible. For Linux, `apt` or `yum` is an option, as is homebrew. Homebrew is a good option on MacOS. However, we recommend use of the miniforge self-installers from conda-forge. Here is a typical conda command used to install a GSAS-II compatible Python interpreter after miniforge has been installed:

```
conda install python=3.13  numpy=2.2 wxpython scipy matplotlib-base pyopengl␣
↪pillow h5py imageio requests git gitpython pycifrw pybaselines -c conda-forge
```

for development environments, it is useful to have build and debugging tools available, so here is a more extensive list of useful packages:

```
conda create -n py311 python=3.11 numpy=1.26 matplotlib-base scipy wxpython ␣
↪pyopengl imageio h5py hdf5 pillow requests pycifrw pybaselines ipython conda␣
↪spyder-kernels meson sphinx sphinx-rtd-theme jupyter git gitpython -c conda-
↪forge
```

To find out what packages have been directly installed in a conda environment this command can be used:

```
conda env export --from-history -n <env>
```

Note that binaries for Python 3.12 and 3.13 using numpy 2.2 are also now supplied.

4.3.3 Scripting Requirements

The GSAS-II scripting interface (`GSASIIscriptable`) will not run without the NumPy Python extension package:

- NumPy (http://docs.scipy.org/doc/numpy/reference/),

In theory, GSAS-II should start without access to the CIF read/write library, PyCifRW, but in practice, almost everything one wants to do with GSAS-II needs CIF access at some point and I have never tested without this package, so I will consider this also as mandatory for scripting:

- PyCifRW: (https://github.com/jamesrhester/pycifrw)

While not required, and not used very much in GSAS-II scripting, installing the SciPy is recommended:

- SciPy (http://docs.scipy.org/doc/scipy/reference/).

These packages fortunately are common and are easy to install.

4.3.4 Recommended Packages for Scripting

There are some relatively minor scripting capabilities that will only run when a few additional packages are installed:

- requests: for web access
- matplotlib (http://matplotlib.org/contents.html),
- Pillow (https://pillow.readthedocs.org) and/or
- h5py (requires hdf5). Used to read HDF5 files.
- pybaselines: for auto-background (https://github.com/derb12/pybaselines)
- xmltodict: for reading Bruker BRML files.
- zarr: reading powder data files produced MIDAS (APS)
- seekpath: for k-vector searching

but none of these are required to run scripts and the vast majority of scripts will not need these packages.

4.3.5 Optional Python Packages

- Sphinx (https://www.sphinx-doc.org) is used to generate the documentation you are currently reading. Generation of this documentation is not generally something needed by users or even most code developers, since the prepared documentation on https://gsas-ii.readthedocs.io is usually reasonably up to date.
- The sphinx-rtd-theme is required to build the documentation in standard the format (though this can be changed with minor editing.)

4.3.6 Compilation Requirements

Most users on Windows and Mac will not need to compile GSAS-II. Binaries are supplied as part of the gsas2main self-installer. Linux users may need to install the software in a manner that allows for local compilation. Developers may wish to perform all installation steps for themselves. These are the requirements:

- The gfortran complier is required. There has been some work done with glang, and I think this passes the self-tests but it is unknown if there are other problems. This can be installed in a number of ways. For Windows and Mac, conda-forge is a good choice. (For MacOS, Apple's XCode must also be installed). For Linux, dist-supplied versions are probably a better choice.
- gcc or other c compiler is required to build one binary for image processing. For Windows use Microsoft Visual C/C++. On Mac, use of conda-forge to install gcc is a good installation choice (again XCode is required). For Linux, dist-supplied versions are probably a better choice.
- meson (https://mesonbuild.com/meson-python/) is used to compile the relatively small amount of Fortran, C and Cython code that is included with GSAS-II. This is a Python package typically installed with conda or pip. On Linux, a dist-supplied version (Debian, RedHat, etc.) is likely available too.
- Cython is needed to build one binary used for magnetism (k-vector searching). Install this typically with conda or pip.

4.3.7 Installation Notes for Minimal Python configuration

There are many ways to install a minimal Python configuration. Below, I show some example commands used to install using the the free miniconda installer from Anaconda, Inc., but I now tend to use the Conda-Forge miniforge distributions instead. However, there are also plenty of other ways to install Python, Numpy and Scipy, depending on if they will be used on Linux, Windows and MacOS. For Linux, the standard Linux distributions provide these using `yum` or `apt-get` etc., but these often supply package versions that are so new that they probably have not been tested with GSAS-II.

```
bash ~/Downloads/Miniconda3-latest-<platform>-x86_64.sh -b -p /loc/pyg2script
source /loc/pyg2script/bin/activate
conda install numpy scipy pycifrw matplotlib-base pillow h5py hdf5
```

Some discussion on these commands follows:

- the 1st command (bash) assumes that the appropriate version of Miniconda has been downloaded from https://docs.conda.io/en/latest/miniconda.html and `/loc/pyg2script` is where I have selected for python to be installed. You might want to use something like `~/pyg2script`.
- the 2nd command (source) is needed to access Python with miniconda.
- the 3rd command (conda) installs all possible packages that might be used by scripting, but note that matplotlib, pillow, h5py and hdf5 are not commonly needed and could be omitted.

Once Python has been installed and is in the path, use these commands to install GSAS-II:

```
git clone https://github.com/AdvancedPhotonSource/GSAS-II.git /loc/GSAS-II
python /loc/GSAS-II/GSASII/GSASIIscriptable.py
```

Notes on these commands:

- the 1st command (git) is used to download the GSAS-II software. `/loc/GSASII` is the location where I decided to install the software. You can select something different.
- the 2nd command (python) is used to invoke GSAS-II scriptable for the first time, which is needed to load the binary files from the server.

4.4 Required Binary Files

As noted before, GSAS-II also requires that some code be compiled. For the following platforms:

- Windows-10: 64-bit Intel-compatible processors.
- MacOS: Intel processors.
- MacOS: ARM processors, aka Apple Silicon (M1, etc).
- Linux: 64-bit Intel-compatible processors.

Some binaries are also supplied for Raspberry Pi, but may not be up-to-date. Please ask for newer if needed:

- Linux: ARM processors (64-bit and 32-bit Raspberry Pi OS and Ubuntu for Raspberry Pi).

Binary images are provided at https://github.com/AdvancedPhotonSource/GSAS-II-buildtools/releases/latest. At present binaries are supplied for the following versions:

- Python 3.11 and NumPy 1.26
- Python 3.12 and NumPy 2.2
- Python 3.13 and NumPy 2.2

Note that these binaries must match the major and minor version of both Python. Usually if the minor version is close to the numpy version (1.25.x and 1.27.x for 1.26) the binaries will still work.

Should one wish to run GSAS-II where binary files are not supplied (such as 32-bit Windows or Linux) or with other combinations of Python/NumPy, compilation will be need to be done by the user. See the compilation information for more information. The build process was recently updated to use meson (in place of scons).

4.5 Supported Externally-Developed Software

GSAS-II provides interfaces to use a number of programs developed by others. Some are included with GSAS-II and others must be installed separately. When these programs are accessed, citation information is provided as we hope that users will recognize the contribution made by the authors of these programs and will honor those efforts by citing that work in addition to GSAS-II.

GSAS-II includes copies of the following programs. No additional steps beyond a standard installation are needed to access their functionality.

DIFFaX
: Simulate layered structures with faulting. https://www.public.asu.edu/~mtreacy/DIFFaX.html

Shapes
: Derives the shapes of particles from small angle scattering data.

NIST FPA
: Use Fundamental Parameters to determine GSAS-II profile function

NIST*LATTICE
: Searches for higher symmetry unit cells and possible relationships between unit cells. An API has been written and this will be integrated into the GSAS-II GUI.

The following web services can also be accessed from computers that have internet access. All software needed for this access is included with GSAS-II.

Bilbao Crystallographic Server (http://cryst.ehu.es/):
: GSAS-II can directly access the Bilbao Crystallographic Server to utilize the k-SUBGROUPSMAG, k-SUBGROUPS and PseudoLattice web utilities for computation of space group subgroups, color (magnetic) subgroups & lattice search.

BYU ISOTROPY Software Suite (https://iso.byu.edu/isotropy.php):
: GSAS-II directly accesses capabilities in the ISOTROPY Software Suite from Brigham Young University for representational analysis and magnetism analysis.

At the request of the program authors, other programs that can be accessed within GSAS-II are not included as part of the GSAS-II distribution. These are listed below. See the web installation instructions for details on how they are installed.

Dysnomia
: Computes enhanced Fourier maps with Maximum Entropy estimated extension of the reflection sphere. See https://jp-minerals.org/dysnomia/en/.

RMCProfile
: Provides large-box PDF & S(Q) fitting. The GSAS-II interface was originally written for use with release 6.7.7 of RMCProfile, but updates have been made for compatible with 6.7.9 as well. RMCProfile must be downloaded by the user from http://rmcprofile.org/Downloads or https://rmcprofile.pages.ornl.gov/nav_pages/download/

fullrmc
: A modern software framework for large-box PDF & S(Q) fitting. Note that the GSAS-II implementation is not compatible with the last open-source version of fullrmc, but rather the version 5.0 must be used, which is distributed only as compiled versions and only for 64-bit Intel-compatible processors running Windows, Linux and MacOS.

PDFfit2
: For small-box fitting of PDFs; see https://github.com/diffpy/diffpy.pdffit2?tab=readme-ov-file#-diffpypdffit2. This software is no longer developed, but it is being maintained with respect to new Python versions.

CHAPTER

FIVE

REFERENCES TO THE GSAS-II DEVELOPER'S DOCUMENTATION

Constraints_processing: See the Constraints Processing from `GSASIImapvars`.

CHAPTER

SIX

REFERENCES TO THE GSAS-II DEVELOPER'S DOCUMENTATION

Imports: See the Import models documentation for information on reading data files.

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