
GSAS-II Developers Documentation

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GSAS-II MAIN MODULE

Main routines for the GSAS-II program

class GSASII.**GSASII** (*parent*)

Define the main GSAS-II frame and its associated menu items

CheckNotebook ()

Make sure the data tree has the minimally expected controls. (BHT) correct?

class **ConstraintDialog** (*parent, title, text, data, separator='*'*)

Window to edit Constraint values

class GSASII.**CopyDialog** (*parent, title, text, data*)

Creates a dialog for copying control settings between data tree items

GSASII.**ErrorDialog** (*title, message, parent=None, wtype=4*)

Display an error message

GSASII.**ExitMain** (*event*)

Called if the main window is closed

GSASII.**FillMainMenu** (*menubar*)

Define contents of the main GSAS-II menu for the (main) data tree window in the mac, used also for the data item windows as well.

GSASII.**GetFileList** (*fileType, skip=None*)

Appears unused. Note routine of same name in GSASIIpwdGUI

GSASII.**GetHKLFdatafromTree** (*HKLFname*)

Returns single crystal data from GSASII tree

Parameters **HKLFname** (*str*) – a single crystal histogram name as obtained from
GSASIIstruct.GetHistogramNames

Returns HKLFdata = single crystal data list of reflections

GSASII.**GetPWDRdatafromTree** (*PWDRname*)

Returns powder data from GSASII tree

Parameters **PWDRname** (*str*) – a powder histogram name as obtained from
GSASIIstruct.GetHistogramNames

Returns PWDRdata = powder data dictionary with Powder data arrays, Limits, Instrument Parameters, Sample Parameters

GSASII.**GetPhaseData** ()

Returns a list of defined phases. Used only in GSASIIgrid Note routine
GSASIIstruct.GetPhaseData also exists.

GSASII.GetPowderIparm (*rd, prevIparm, lastIparmfile, lastdatafile*)

Open and read an instrument parameter file for a data file Returns the list of parameters used in the data tree

Parameters

- **rd** (*obj*) – the raw data (histogram) data object.
- **prevIparm** (*str*) – not used
- **lastIparmfile** (*str*) – Name of last instrument parameter file that was read, or a empty string.
- **lastdatafile** (*str*) – Name of last data file that was read.

GSASII.GetUsedHistogramsAndPhasesfromTree ()

Returns all histograms that are found in any phase and any phase that uses a histogram :returns: two dicts:

- Histograms = dictionary of histograms as {name:data,...}
- Phases = dictionary of phases that use histograms

GSASII.OnAddPhase (*event*)

Add a new, empty phase to the tree. Called by Data/Add Phase menu

GSASII.OnDataDelete (*event*)

Delete one or more histograms from data tree. Called by the Data/DeleteData menu

GSASII.OnDeletePhase (*event*)

Delete a phase from the tree. Called by Data/Delete Phase menu

GSASII.OnFileClose (*event*)

Clears the data tree in response to the File/Close Project menu button. User is given option to save the project.

GSASII.OnFileExit (*event*)

Called in response to the File/Quit menu button

GSASII.OnFileOpen (*event*)

Reads in a GSAS-II .gpx project file in response to the File/Open Project menu button

GSASII.OnFileSave (*event*)

Save the current project in response to the File/Save Project menu button

GSASII.OnFileSaveas (*event*)

Save the current project in response to the File/Save as menu button

GSASII.OnImageRead (*event*)

Called to read in an image in any known format

GSASII.OnImageSum (*event*)

Sum together image data(?)

GSASII.OnImportGeneric (*reader, readerlist, label, multiple=False*)

Used to import Phases, powder dataset or single crystal datasets (structure factor tables) using reader objects subclassed from GSASIIIO.ImportPhase, GSASIIIO.ImportStructFactor or GSASIIIO.ImportPowderData. If a reader is specified, only that will be attempted, but if no reader is specified, every one that is potentially compatible (by file extension) will be tried on the selected file(s).

Parameters

- **reader** (*readerobject*) – This will be a reference to a particular object to be used to read a file or None, if every appropriate reader should be used.

- **readerlist** (*list*) – a list of reader objects appropriate for the current read attempt. At present, this will be either `self.ImportPhaseReaderlist`, `self.ImportSfactReaderlist` or `self.ImportPowderReaderlist` (defined in `_init_Imports` from the files found in the path), but in theory this list could be tailored. Used only when reader is `None`.
- **label** (*str*) – string to place on the open file dialog: Open *label* input file
- **multiple** (*bool*) – True if multiple files can be selected in the file dialog. False is default. At present True is used only for reading of powder data.

Returns a list of reader objects (`rd_list`) that were able to read the specified file(s). This list may be empty.

GSASII.OnImportPhase (*event*)

Called in response to an Import/Phase/... menu item to read phase information. dict `self.ImportMenuId` is used to look up the specific reader item associated with the menu item, which will be `None` for the last menu item, which is the “guess” option where all appropriate formats will be tried.

GSASII.OnImportPowder (*event*)

Called in response to an Import/Powder Data/... menu item to read a powder diffraction data set. dict `self.ImportMenuId` is used to look up the specific reader item associated with the menu item, which will be `None` for the last menu item, which is the “guess” option where all appropriate formats will be tried.

Also reads an instrument parameter file for each dataset.

GSASII.OnImportSfact (*event*)

Called in response to an Import/Structure Factor/... menu item to read single crystal datasets. dict `self.ImportMenuId` is used to look up the specific reader item associated with the menu item, which will be `None` for the last menu item, which is the “guess” option where all appropriate formats will be tried.

GSASII.OnMakePDFs (*event*)

Calculates PDFs

GSASII.OnPatternTreeItemActivated (*event*)

Called when a tree item is activated

GSASII.OnPatternTreeItemCollapsed (*event*)

Called when a tree item is collapsed

GSASII.OnPatternTreeItemDelete (*event*)

Called when a tree item is deleted – not sure what this does

GSASII.OnPatternTreeItemExpanded (*event*)

Called when a tree item is expanded

GSASII.OnPatternTreeKeyDown (*event*)

Not sure what this does

GSASII.OnPatternTreeSelChanged (*event*)

Called when a data tree item is selected

GSASII.OnPwdrSum (*event*)

Sum together powder data(?)

GSASII.OnReadPowderPeaks (*event*)

Bound to menu Data/Read Powder Peaks – still needed?

GSASII.OnRefine (*event*)

Perform a refinement. Called from the Calculate/Refine menu.

GSASII.OnRenameData (*event*)

Renames an existing phase. Called by Data/Rename Phase menu

GSASII.OnSeqRefine (*event*)

Perform a sequential refinement. Called from the Calculate/Sequential refine menu.

GSASII.OnSize (*event*)

Called when the main window is resized. Not sure why

GSASII.OnViewLSParms (*event*)

Displays a window showing all parameters in the refinement. Called from the Calculate/View LS Params menu.

GSASII.ReadPowderInstprm (*instfile*)

Read a GSAS-II (new) instrument parameter file

Parameters *instfile* (*str*) – name of instrument parameter file

GSASII.ReadPowderIparm (*instfile*, *bank*, *databanks*, *rd*)

Read a GSAS (old) instrument parameter file

Parameters

- **instfile** (*str*) – name of instrument parameter file
- **bank** (*int*) – the bank number read in the raw data file
- **databanks** (*int*) – the number of banks in the raw data file. If the number of banks in the data and instrument parameter files agree, then the sets of banks are assumed to match up and bank is used to select the instrument parameter file. If not, the user is asked to make a selection.
- **rd** (*obj*) – the raw data (histogram) data object. This sets rd.instbank.

class GSASII.SumDialog (*parent*, *title*, *text*, *dataType*, *data*)

Allows user to supply scale factor(s) when summing data

class GSASII.ViewParmDialog (*parent*, *title*, *parmDict*)

Window to show all parameters in the refinement. Called from OnViewLSParms

class GSASII.GSASIImain (*redirect=True*, *filename=None*, *useBestVisual=False*, *clearSigInt=True*)

Defines a wxApp for GSAS-II

Creates a wx frame (self.main) which contains the display of the data tree.

OnInit ()

Called automatically when the app is created.

GSASII.main ()

Start up the GSAS-II application

GSASIIMAPVARS: PARAMETER CONSTRAINTS

Module to implements algebraic constraints, parameter redefinition and parameter simplification constraints.

Parameter redefinition (new vars) is done by creating one or more relationships between a set of parameters

```
Mx1 * Px + My1 * Py + ...  
Mx2 * Px + Mz2 * Pz + ...
```

where P_j is a parameter name and M_{jk} is a constant.

Constant constraint Relations can also be supplied in the form of an equation:

```
nx1 * Px + ny1 * Py + ... = C1
```

where C_n is a constant. These equations define an algebraic constraint.

Parameters can also be “fixed” (held), which prevents them from being refined.

All of the above three cases are input using routines GroupConstraints and GenerateConstraints. The input consists of a list of relationship dictionaries:

```
constrDict = [  
    {'0:12:Scale': 2.0, '0:14:Scale': 4.0, '0:13:Scale': 3.0, '0:0:Scale': 0.5},  
    {'2::C(10,6,1)': 1.0, '1::C(10,6,1)': 1.0},  
    {'0::A0': 0.0}]  
fixedList = ['5.0', None, '0']
```

Where the dictionary defines the first part of an expression and the corresponding fixedList item is either None (for parameter redefinition) or the constant value, for a constant constraint equation. A dictionary that contains a single term defines a variable that will be fixed (held). The multiplier and the fixedList value in this case are ignored.

Parameters can also be equivalenced or “slaved” to another parameter, such that one (independent) parameter is equated to several (now dependent) parameters. In algebraic form this is:

```
P0 = M1 * P1 = M2 * P2 = ...
```

Thus parameters P_0, P_1 and P_2, \dots are linearly equivalent. Routine StoreEquivalence is used to specify these equivalences.

Parameter redefinition (new vars) describes a new, independent, parameter, which is defined in terms of dependent parameters that are defined in the Model, while fixed constrained relations effectively reduce the complexity of the Model by removing a degree of freedom. It is possible for a parameter to appear in both a parameter redefinition expression and a fixed constraint equation, but a parameter cannot be used a parameter equivalence cannot be used elsewhere (not fixed, constrained or redefined). Likewise a fixed parameter cannot be used elsewhere (not equivalenced, constrained or redefined).

Relationships are grouped so that a set of dependent parameters appear in only one group (done in routine GroupConstraints.) Note that if a group contains relationships/equations that involve N dependent parameters, there must exist $N-C$ new parameters, where C is the number of constraint equations in the group. Routine GenerateConstraints takes the output from GroupConstraints and generates the “missing” relationships and saves that information in the module’s global variables. Each generated parameter is named sequentially using paramPrefix.

A list of parameters that will be varied is specified as input to GenerateConstraints (varyList). A fixed parameter will simply be removed from this list preventing that parameter from being varied. Note that all parameters in a relationship must specified as varied (appear in varyList) or none can be varied. This is checked in GenerateConstraints (as well as for generated relationships in SetVaryFlags).

- If all parameters in a parameter redefinition (new var) relationship are varied, the parameter assigned to this expression (::constr:n, see paramPrefix) newly generated parameter is varied. Note that any generated “missing” relations are not varied. Only the input relations are varied.
- If all parameters in a fixed constraint equation are varied, the generated “missing” relations in the group are all varied. This provides the $N-C$ degrees of freedom.

2.1 External Routines

To define a set of constrained and unconstrained relations, one defines a list of dictionary defining constraint parameters and their values, a list of fixed values for each constraint and a list of parameters to be varied. In addition, one uses StoreEquivalence() to define parameters that are equivalent. One can then use CheckConstraints() to check that the input is internally consistent and finally GroupConstraints() and GenerateConstraints() to generate the internally used tables. Routines Map2Dict() is used to initialize the parameter dictionary and Dict2Map(), Dict2Deriv(), and ComputeDepESD() are used to apply constraints. Routine VarRemapShow() is used to print out the constraint information, as stored by GenerateConstraints().

InitVars() This is optionally used to clear out all defined previously defined constraint information

StoreEquivalence() To implement parameter redefinition, one calls StoreEquivalence. This should be called for every set of equivalence relationships. There is no harm in using StoreEquivalence with the same independent variable:

```
StoreEquivalence('x', ('y',))  
StoreEquivalence('x', ('z',))
```

or equivalently

```
StoreEquivalence('x', ('y', 'z'))
```

The latter will run more efficiently. Note that mixing independent and dependent variables is problematic. This is not allowed:

```
StoreEquivalence('x', ('y',))  
StoreEquivalence('y', ('z',))
```

Use StoreEquivalence before calling GenerateConstraints or CheckConstraints

CheckConstraints() To check that input is internally consistent, use CheckConstraints

Map2Dict() To determine values for the parameters created in this module, one calls Map2Dict. This will not apply constraints.

Dict2Map() To take values from the new independent parameters and constraints, one calls Dict2Map. This will apply constraints.

Dict2Deriv() Use Dict2Deriv to determine derivatives on independent parameters from those on dependent ones

ComputeDepESD () Use ComputeDepESD to compute uncertainties on dependent variables

VarRemapShow () To show a summary of the parameter remapping, one calls VarRemapShow

2.2 Global Variables

dependentParmList: contains a list by group of lists of parameters used in the group. Note that parameters listed in dependentParmList should not be refined as they will not affect the model

indParmList: a list of groups of Independent parameters defined in each group. This contains both parameters used in parameter redefinitions as well as names of generated new parameters.

fixedVarList: a list of variables that have been ‘fixed’ by defining them as equal to a constant (`::var: = 0`). Note that the constant value is ignored at present. These variables are later removed from varyList which prevents them from being refined. Unlikely to be used externally.

arrayList: a list by group of relationship matrices to relate parameters in dependentParmList to those in indParmList. Unlikely to be used externally.

invarrayList: a list by group of relationship matrices to relate parameters in indParmList to those in dependentParmList. Unlikely to be used externally.

fixedDict: a dictionary containing the fixed values corresponding to parameter equations. The dict key is an ascii string, but the dict value is a float. Unlikely to be used externally.

2.3 Routines

Note that parameter names in GSAS-II are strings of form `<ph>:<hst>:<nam>`

`GSASIImapvars.CheckConstraints (varyList, constrDict, fixedList)`

Takes a list of relationship entries comprising a group of constraints and checks for inconsistencies such as conflicts in parameter/variable definitions and or inconsistently varied parameters.

Parameters

- **varyList** (*list*) – a list of parameters names that will be varied
- **constrDict** (*dict*) – a list of dicts defining relationships/constraints (as defined in `GroupConstraints()`)
- **fixedList** (*list*) – a list of values specifying a fixed value for each dict in constrDict. Values are either strings that can be converted to floats or None if the constraint defines a new parameter rather than a constant.

Returns

two strings:

- the first lists conflicts internal to the specified constraints
- the second lists conflicts where the varyList specifies some parameters in a constraint, but not all

If there are no errors, both strings will be empty

`GSASIImapvars.ComputeDepESD (covMatrix, varyList, parmDict)`

Compute uncertainties for dependent parameters from independent ones returns a dictionary containing the esd values for dependent parameters

`GSASIImapvars.Dict2Deriv (varyList, derivDict, dMdv)`

Compute derivatives for Independent Parameters from the derivatives for the original parameters

Parameters

- **varyList** (*list*) – a list of parameters names that will be varied
- **derivDict** (*dict*) – a dict containing derivatives for parameter values keyed by the parameter names.
- **dMdv** (*dict*) – a dict containing derivatives for dependent parameter computed from deriv-Dict

`GSASIImapvars.Dict2Map (parmDict, varyList)`

Applies the constraints defined using `StoreEquivalence()`, `GroupConstraints()` and `GenerateConstraints()` by changing values in a dict containing the parameters. This should be done before the parameters are used for any computations

Parameters

- **parmDict** (*dict*) – a dict containing parameter values keyed by the parameter names. This will contain updated values for both dependent and independent parameters after Dict2Map is called. It will also contain some unexpected entries of every constant value `{‘0’:0.0}` & `{‘1.0’:1.0}`, which do not cause any problems.
- **varyList** (*list*) – a list of parameters names that will be varied

`GSASIImapvars.GenerateConstraints (groups, parmList, varyList, constrDict, fixedList)`

Takes a list of relationship entries comprising a group of constraints and builds the relationship lists and their inverse and stores them in global variables Also checks for internal conflicts or inconsistencies in parameter/variable definitions.

Parameters

- **groups** (*list*) – a list of grouped constraints where each constraint grouped contains a list of indices for constraint constrDict entries, created in `GroupConstraints()` (returned as 1st value)
- **parmList** (*list*) – a list containing lists of parameter names contained in each group, created in `GroupConstraints()` (returned as 1st value)
- **varyList** (*list*) – a list of parameters names (strings of form `<ph>:<hst>:<nam>`) that will be varied
- **constrDict** (*dict*) – a list of dicts defining relationships/constraints (as defined in `GroupConstraints()`)
- **fixedList** (*list*) – a list of values specifying a fixed value for each dict in constrDict. Values are either strings that can be converted to floats, float values or None if the constraint defines a new parameter
- **constrDict** – a list of dicts defining relationships/constraints

`GSASIImapvars.GetDependentVars ()`

Return a list of dependent variables: e.g. variables that are constrained in terms of other variables

Returns a list of variable names

`GSASIImapvars.GetIndependentVars ()`

Return a list of independent variables: e.g. variables that are created by constraints of other variables

Returns a list of variable names

`GSASIImapvars.GramSchmidtOrtho(a, nkeep=0)`

Use the Gram-Schmidt process (<http://en.wikipedia.org/wiki/Gram-Schmidt>) to find orthonormal unit vectors relative to first row.

If nkeep is non-zero, the first nkeep rows in the array are not changed

input: arrayin: a 2-D non-singular square array

returns: a orthonormal set of unit vectors as a square array

`GSASIImapvars.GroupConstraints(constrDict)`

divide the constraints into groups that share no parameters.

Parameters `constrDict` (*dict*) – a list of dicts defining relationships/constraints

`constrDict = [{<constr1>}, {<constr2>}, ...]`

where {<constr1>} is {‘param1’: mult1, ‘param2’: mult2,...}

Returns

two lists of lists:

- a list of grouped constraints where each constraint grouped contains a list of indices for constraint `constrDict` entries
- a list containing lists of parameter names contained in each group

`GSASIImapvars.InitVars()`

Initializes all constraint information

`GSASIImapvars.Map2Dict(parmDict, varyList)`

Create (or update) the Independent Parameters from the original set of Parameters

Removes dependent variables from the `varyList`

This should be done once, after the constraints have been defined using `StoreEquivalence()`, `GroupConstraints()` and `GenerateConstraints()` and before any variable refinement is done to complete the parameter dictionary by defining independent parameters and satisfying the constraint equations.

Parameters

- **parmDict** (*dict*) – a dict containing parameter values keyed by the parameter names. This will contain updated values for both dependent and independent parameters after `Dict2Map` is called. It will also contain some unexpected entries of every constant value {‘0’:0.0} & {‘1.0’:1.0}, which do not cause any problems.
- **varyList** (*list*) – a list of parameters names that will be varied

`GSASIImapvars.PrintIndependentVars(parmDict, varyList, sigDict, PrintAll=False, pFile=None)`

Print the values and uncertainties on the independent variables

`GSASIImapvars.StoreEquivalence(independentVar, dependentList)`

Takes a list of dependent parameter(s) and stores their relationship to a single independent parameter (`independentVar`)

Parameters

- **independentVar** (*str*) – name of master parameter that will be used to determine the value to set the dependent variables
- **dependentList** (*list*) – a list of parameters that will set from `independentVar`. Each item in the list can be a string with the parameter name or a tuple containing a name and multiplier: `['parm1', ('parm2', .5),]`

`GSASIImapvars.VarRemapShow` (*varyList*)

List out the saved relationships. This should be done after the constraints have been defined using `StoreEquivalence()`, `GroupConstraints()` and `GenerateConstraints()`.

Returns a string containing the details of the constraint relationships

GSAS-II GUI ROUTINES

3.1 GSASIIgrid: Basic GUI routines

class GSASIIgrid.**AddHelp** (*frame, helpType, helpLbl=None, title=''*)

This class a single entry for the help menu (used on the Mac only): 'Help on <helpType>': where helpType is a reference to an HTML page to be opened

NOTE: the title when appending this menu should be '&Help' so the wx handles it correctly.

OnHelpById (*event*)

Called when Help on... is pressed in a menu. Brings up a web page for documentation.

class GSASIIgrid.**DataFrame** (*parent, frame, data=None, name=None, size=None, pos=None*)

Create the dataframe window and all the entries in menus. The binding is for the menus is not done here, but rather is done where the functions can be accessed (in various GSASII*GUI modules).

Bind (**args, **kwargs*)

Override the Bind() function: on the Mac the binding is to the main window, so that menus operate with any window on top. For other platforms, call the default wx.Frame Bind()

PostfillDataMenu (*empty=False*)

Create the "standard" part of data frame menus. Note that on Linux and Windows, this is the standard help Menu. On Mac, this menu duplicates the tree menu, but adds an extra help command for the data item and a separator.

PrefillDataMenu (*menu, helpType, helpLbl=None, empty=False*)

Create the "standard" part of data frame menus. Note that on Linux and Windows nothing happens here. On Mac, this menu duplicates the tree menu, but adds an extra help command for the data item and a separator.

class GSASIIgrid.**DisAglDialog** (*parent, data, default*)

Distance Angle Controls dialog

class GSASIIgrid.**G2HtmlWindow** (*parent, *args, **kwargs*)

Displays help information in a primitive HTML browser type window

class GSASIIgrid.**GSGrid** (*parent, name=''*)

Basic wx.Grid implementation

class GSASIIgrid.**GSNoteBook** (*parent, name='', size=None*)

Notebook used in various locations; implemented with wx.aui extension

GSASIIgrid.**GetPatternTreeDataNames** (*G2frame, dataTypes*)

Needs a doc string

`GSASIIgrid.GetPatternTreeItemId (G2frame, parentId, itemText)`

Needs a doc string

class `GSASIIgrid.GridFractionEditor (grid)`

A grid cell editor class that allows entry of values as fractions as well as sine and cosine values [as s() and c()]

`GSASIIgrid.HorizontalLine (sizer, parent)`

Draws a horizontal line as wide as the window. This shows up on the Mac as a very thin line, no matter what I do

`GSASIIgrid.MovePatternTreeToGrid (G2frame, item)`

Needs a doc string

class `GSASIIgrid.MyHelp (frame, helpType=None, helpLbl=None, morehelpitems=[], title='')`

A class that creates the contents of a help menu. The menu will start with two entries:

- ‘Help on <helpType>’: where helpType is a reference to an HTML page to be opened
- About: opens an About dialog using OnHelpAbout. N.B. on the Mac this gets moved to the App menu to be consistent with Apple style.

NOTE: for this to work properly with respect to system menus, the title for the menu must be &Help, or it will not be processed properly:

```
menu.Append(menu=MyHelp(self, ...), title="&Help")
```

OnCheckUpdates (event)

Check if the GSAS-II repository has an update for the current source files and perform that update if requested.

OnHelpAbout (event)

Display an ‘About GSAS-II’ box

OnHelpById (event)

Called when Help on... is pressed in a menu. Brings up a web page for documentation.

class `GSASIIgrid.MyHtmlPanel (frame, id)`

Defines a panel to display Help information

class `GSASIIgrid.PickTwoDialog (parent, title, prompt, names, choices)`

This does not seem to be in use

`GSASIIgrid.SetDataMenuBar (G2frame, menu=None)`

Set the menu for the data frame. On the Mac put this menu for the data tree window instead.

Note that data frame items do not have menus, for these (menu=None) display a blank menu or on the Mac display the standard menu for the data tree window.

`GSASIIgrid.ShowHelp (helpType, frame)`

Called to bring up a web page for documentation.

class `GSASIIgrid.SingleFloatDialog (parent, title, prompt, value, limits=[0.0, 1.0], format='%.5g')`

Dialog to obtain a single float value from user

class `GSASIIgrid.SymOpDialog (parent, SGData, New=True, ForceUnit=False)`

Class to select a symmetry operator

class `GSASIIgrid.Table (data=[], rowLabels=None, colLabels=None, types=None)`

Basic data table for use with GSgrid

`GSASIIgrid.UpdateControls (G2frame, data)`

Edit overall GSAS-II controls in main Controls data tree entry

`GSASIIgrid.UpdateHKLControls (G2frame, data)`

Needs a doc string

`GSASIIgrid.UpdateNotebook (G2frame, data)`

Called when the data tree notebook entry is selected. Allows for editing of the text in that tree entry

`GSASIIgrid.UpdatePWHKPlot (G2frame, kind, item)`

Needs a doc string

`GSASIIgrid.UpdateSeqResults (G2frame, data)`

Called when the Sequential Results data tree entry is selected to show results from a sequential refinement.

Parameters

- **G2frame** (*wx.Frame*) – main GSAS-II data tree windows
- **data** (*dict*) – a dictionary containing the following items:
 - ‘histNames’ - list of histogram names in order as processed by Sequential Refinement
 - ‘varyList’ - list of variables - identical over all refinements in sequence
 - ‘histName’ - dictionaries for all data sets processed, which contains:
 - * ‘variables’ - result[0] from leastsq call
 - * ‘varyList’ - list of variables; same as above
 - * ‘sig’ - esds for variables
 - * ‘covMatrix’ - covariance matrix from individual refinement
 - * ‘title’ - histogram name; same as dict item name
 - * ‘newAtomDict’ - new atom parameters after shifts applied
 - * ‘newCellDict’ - new cell parameters after shifts to A0-A5 applied

3.2 GSASIIIO: Misc I/O routines

Module with miscellaneous routines for input and output. Many are GUI routines to interact with user.

Includes support for image reading.

Also includes base classes for data import routines.

`GSASIIIO.CheckImageFile (G2frame, imagefile)`

Get an new image file name if the specified one does not exist

Parameters

- **G2frame** (*wx.Frame*) – main GSAS-II Frame and data object
- **imagefile** (*str*) – name of image file

Returns imagefile, if it exists, or the name of a file that does exist or False if the user presses Cancel

`GSASIIIO.ExtractFileFromZip (filename, selection=None, confirmread=True, confirmover-
write=True, parent=None, multipleselect=False)`

If the filename is a zip file, extract a file from that archive.

Parameters

- **Selection** (*list*) – used to predefine the name of the file to be extracted. Filename case and zip directory name are ignored in selection; the first matching file is used.

- **confirmread** (*bool*) – if True asks the user to confirm before expanding the only file in a zip
- **confirmoverwrite** (*bool*) – if True asks the user to confirm before overwriting if the extracted file already exists
- **multiplesselect** (*bool*) – if True allows more than one zip file to be extracted, a list of file(s) is returned. If only one file is present, do not ask which one, otherwise offer a list of choices (unless selection is used).

Returns the name of the file that has been created or a list of files (see multiplesselect)

If the file is not a zipfile, return the name of the input file. If the zipfile is empty or no file has been selected, return None

GSASIIIO.**FileDlgFixExt** (*dlg, file*)
this is needed to fix a problem in linux wx.FileDialog

GSASIIIO.**GetEdfData** (*filename, imageOnly=False*)
Read European detector data edf file

GSASIIIO.**GetG2Image** (*filename*)
Read an image as a python pickle

GSASIIIO.**GetGESumData** (*filename, imageOnly=False*)
Read SUM file as produced at 1-ID from G.E. images

GSASIIIO.**GetImageData** (*G2frame, imagefile, imageOnly=False*)
Read an image with the file reader keyed by the file extension

Parameters

- **G2frame** (*wx.Frame*) – main GSAS-II Frame and data object
- **imagefile** (*str*) – name of image file
- **imageOnly** (*bool*) – If True return only the image, otherwise (default) return more (see below)

Returns an image as a numpy array or a list of four items: Comments, Data, Npix and the Image, as selected by imageOnly

GSASIIIO.**GetImgData** (*filename, imageOnly=False*)
Read an ADSC image file

GSASIIIO.**GetMAR345Data** (*filename, imageOnly=False*)
Read a MAR-345 image plate image

GSASIIIO.**GetPowderPeaks** (*fileName*)
Read powder peaks from a file

GSASIIIO.**GetTifData** (*filename, imageOnly=False*)
Read an image in a pseudo-tif format, as produced by a wide variety of software, almost always incorrectly in some way.

class GSASIIIO.**ImportBaseclass** (*formatName, longFormatName=None, extensionlist=[], strictExtension=False*)
Defines a base class for the importing of data files (diffraction data, coordinates,...)

BlockSelector (*ChoiceList, ParentFrame=None, title='Select a block', size=None, header='Block Selector', useCancel=True*)
Provide a wx dialog to select a block if the file contains more than one set of data and one must be selected

ContentsValidator (*filepointer*)
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. Expected to be called via self.Validator()

ExtensionValidator (*filename*)

This methods checks if the file has the correct extension Return False if this filename will not be supported by this reader Return True if the extension matches the list supplied by the reader Return None if the reader allows un-registered extensions

MultipleBlockSelector (*ChoiceList*, *ParentFrame=None*, *title='Select a block'*, *size=None*, *header='Block Selector'*)

Provide a wx dialog to select a block of data if the file contains more than one set of data and one must be selected.

Returns a list of the selected blocks

MultipleChoicesDialog (*choicelist*, *headinglist*, *ParentFrame=None*, ***kwargs*)

A modal dialog that offers a series of choices, each with a title and a wx.Choice widget. Typical input:

•choicelist=[('a','b','c'), ('test1','test2'),('no choice',)]

•headinglist = ['select a, b or c', 'select 1 of 2', 'No option here']

optional keyword parameters are: head (window title) and title returns a list of selected indicies for each choice (or None)

class GSASIIIO.ImportPhase (*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

Defines a base class for the reading of files with coordinates

PhaseSelector (*ChoiceList*, *ParentFrame=None*, *title='Select a phase'*, *size=None*, *header='Phase Selector'*)

Provide a wx dialog to select a phase if the file contains more than one phase

class GSASIIIO.ImportPowderData (*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

Defines a base class for the reading of files with powder data

powderdata = None

A powder data set is a list with items [x,y,w,yc,yb,yd]: np.array(x), # x-axis values np.array(y), # powder pattern intensities np.array(w), # 1/sig(intensity)^2 values (weights) np.array(yc), # calc. intensities (zero) np.array(yb), # calc. background (zero) np.array(yd), # obs-calc profiles

class GSASIIIO.ImportStructFactor (*formatName*, *longFormatName=None*, *extensionlist=[]*, *strictExtension=False*)

Defines a base class for the reading of files with tables of structure factors

UpdateControls (*Type='Fosq'*, *FcalcPresent=False*)

Scan through the reflections to update the Controls dictionary

GSASIIIO.IndexPeakListSave (*G2frame*, *peaks*)

Save powder peaks from the indexing list

class GSASIIIO.MultipleChoicesDialog (*choicelist*, *headinglist*, *head='Select options'*, *title='Please select from options below'*, *parent=None*)

A dialog that offers a series of choices, each with a title and a wx.Choice widget. Intended to be used Modally. typical input:

•choicelist=[('a','b','c'), ('test1','test2'),('no choice',)]

•headinglist = ['select a, b or c', 'select 1 of 2', 'No option here']

selections are placed in self.chosen when OK is pressed

GSASIIIO.PDFSave (*G2frame*, *exports*)

Save a PDF G(r) and S(Q) in column formats

GSASIIIO.PeakListSave (*G2frame, file, peaks*)

Save powder peaks to a data file

GSASIIIO.ProjFileOpen (*G2frame*)

Read a GSAS-II project file

GSASIIIO.ProjFileSave (*G2frame*)

Save a GSAS-II project file

GSASIIIO.PutG2Image (*filename, Comments, Data, Npix, image*)

Write an image as a python pickle

GSASIIIO.ReadEXPPHase (*G2frame, filename*)

Read a phase from a GSAS .EXP file. Called in the GSAS phase import routine (see imports/G2phase.py)

GSASIIIO.ReadPDBPhase (*filename*)

Read a phase from a PDB file. Called in the PDB phase import routine (see imports/G2phase.py)

GSASIIIO.SaveIntegration (*G2frame, PickId, data*)

Save image integration results as powder pattern(s)

SetNewPhase (*Name='New Phase', SGData={'SGCen': array([[0, 0, 0]]), 'SGPolax': 'xyz', 'SGLat' [0., 1., 0.], [0., 0., 1.]], dtype=float32), array([0., 0., 0.], dtype=float32)]]}, cell=[1.0, 1.0, 1.0]*)
Create a new phase

GSASIIIO.powderFxyeSave (*G2frame, exports, powderfile*)

Save a powder histogram as a GSAS FXYE file

GSASIIIO.powderXyeSave (*G2frame, exports, powderfile*)

Save a powder histogram as a Topas XYE file

GSASIIIO.sfloat (*S*)

Convert a string to float. An empty field is treated as zero

GSASIIIO.sint (*S*)

Convert a string to int. An empty field is treated as zero

GSAS-II GUI SUBMODULES

4.1 GSASIIphsGUI: Phase GUI

Module to create the GUI for display of phase information in the data display window when a phase is selected. (pages displayed in response to some phase tabs are done in other modules, such as GSASIIddata.)

`GSASIIphsGUI.UpdatePhaseData (G2frame, Item, data, oldPage)`

Create the data display window contents when a phase is clicked on in the man (data tree) window. Called only from `GSASIIgrid.MovePatternTreeToGrid`, which in turn is called from `GSASII.GSASII.OnPatternTreeSelChanged` when a tree item is selected.

Parameters

- **G2frame** (*wx.frame*) – the main GSAS-II frame object
- **Item** (*wx.TreeItemId*) – the tree item that was selected
- **data** (*dict*) – all the information on the phase in a dictionary
- **oldPage** (*int*) – This sets a tab to select when moving from one phase to another, in which case the same tab is selected to display first. This is set only when the previous data tree selection is a phase, if not the value is None. The default action is to bring up the General tab.

4.2 GSASIIddataGUI: Phase Diffraction Data GUI

Module to create the GUI for display of diffraction data * phase information that is shown in the data display window (when a phase is selected.)

`GSASIIddataGUI.UpdateDDData (G2frame, DData, data)`

Display the Diffraction Data associated with a phase (items where there is a value for each histogram and phase)

Parameters

- **G2frame** (*wx.frame*) – the main GSAS-II frame object
- **DData** (*wx.ScrolledWindow*) – notebook page to be used for the display
- **data** (*dict*) – all the information on the phase in a dictionary

4.3 *GSASIIElemGUI: GUI to select and delete element lists*

Module to select elements from a periodic table and to delete an element from a list of selected elements.

class GSASIIElemGUI.**DeleteElement** (*parent, choice*)

Delete element from selected set widget

ElButton (*id, name, pos*)

Needs a doc string

class GSASIIElemGUI.**PickElement** (*parent, oneOnly=False, ifNone=False*)

Makes periodic table widget for picking element - caller maintains element list

ElButton (*name, pos, tip, color*)

Needs a doc string

4.4 *GSASIIconstrGUI: Constraint GUI routines*

Used to define constraints and rigid bodies.

class GSASIIconstrGUI.**MultiIntegerDialog** (*parent, title, prompts, values*)

Input a series of integers based on prompts

GSASIIconstrGUI.**UpdateConstraints** (*G2frame, data*)

Called when Constraints tree item is selected. Displays the constraints in the data window

GSASIIconstrGUI.**UpdateRigidBodies** (*G2frame, data*)

Called when Rigid bodies tree item is selected. Displays the rigid bodies in the data window

4.5 *GSASIIimgGUI: Image GUI*

Control image display and processing

GSASIIimgGUI.**UpdateImageControls** (*G2frame, data, masks*)

Shows and handles the controls on the “Image Controls” data tree entry

GSASIIimgGUI.**UpdateMasks** (*G2frame, data*)

Shows and handles the controls on the “Masks” data tree entry

GSASIIimgGUI.**UpdateStressStrain** (*G2frame, data*)

Shows and handles the controls on the “Stress/Strain” data tree entry

4.6 *GSASIIpwdGUI: Powder Pattern GUI routines*

Used to define GUI controls for the routines that interact with the powder histogram (PWDR) data tree items.

GSASIIpwdGUI.**IsHistogramInAnyPhase** (*G2frame, histoName*)

Needs a doc string

GSASIIpwdGUI.**SetDefaultSample** ()

Needs a doc string

GSASIIpwdGUI.**UpdateBackground** (*G2frame, data*)

respond to selection of PWDR background data tree item.

`GSASIIpwdGUI.UpdateIndexPeaksGrid(G2frame, data)`
respond to selection of PWDR Index Peak List data tree item.

`GSASIIpwdGUI.UpdateInstrumentGrid(G2frame, data)`
respond to selection of PWDR Instrument Parameters data tree item.

`GSASIIpwdGUI.UpdateLimitsGrid(G2frame, data)`
respond to selection of PWDR Limits data tree item.

`GSASIIpwdGUI.UpdatePDFGrid(G2frame, data)`
respond to selection of PWDR PDF data tree item.

`GSASIIpwdGUI.UpdatePeakGrid(G2frame, data)`
respond to selection of PWDR powder peaks data tree item.

`GSASIIpwdGUI.UpdateReflectionGrid(G2frame, data, HKLF=False, Name='')`
respond to selection of PWDR Reflections data tree item.

`GSASIIpwdGUI.UpdateSampleGrid(G2frame, data)`
respond to selection of PWDR Sample Parameters data tree item.

`GSASIIpwdGUI.UpdateUnitCellsGrid(G2frame, data)`
respond to selection of PWDR Unit Cells data tree item.

4.7 GSASIIrestrGUI: Restraint GUI routines

Used to define restraints.

`GSASIIrestrGUI.UpdateRestraints(G2frame, data, Phases, phaseName)`
Respond to selection of the Restraints item on the data tree

Note that this program requires the Python wxPython, NumPy, SciPy, matplotlib packages, plus the PyOpenGL package (which is installed by GSAS-II if not found).

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