# **GeoPIXE Change Log**

## GeoPIXE-open-source

Note: For complex changes, tag the source file lines with: ;@month-year (e.g. ;@3-16).

## 5 Aug, 2025

- 1. Pixe fit
  - a. A common problem with fitting SXRF spectra is the effect of the strong scatter peaks. The elastic peak may not be accurate (some beamlines have errors in known beam energy). The Compton peak may be poorly fitted initially until parameters are adjusted. These both skew the fit to the energy Cal parameters and often the Width parameters too (if enabled).
  - b. To avoid the fit to the elastic peak and Compton skewing the fit to the energy cal of a spectrum, 'pixe\_fit' limits 'e\_high' to 85% of e\_beam, if the yield is for SXRF (z1=0,a1=0), a mono beam (beam.continuum=0) and Cal free.
- 2. Fit setup
  - a. Fit setup do fit
    - i. For SXRF (z1=0,a1=0), a mono beam (beam.continuum=0) and Cal free:
      - 1. Calls 'pixe\_fit' as usual first, which will fit the spectrum with 'e\_high' limited (see above) and fit the Cal and Width (if enabled) parameters.
      - 2. Then it calls 'pixe\_fit' again with the Cal and Width parameters fixed, which will fit over the full E range with the Cal and Width preserved.
    - ii. This obviates the need to manually fit it twice (as discussed in the *Worked Examples* for SXRF), first limiting the E range to exclude the scatter peaks, and then again over the full E range with the Cal and Width fixed.
  - b. Fitting SXRF spectra is now (like PIXE) simply a matter of enabling Cal (and possibly Width) and clicking on *Fit*.

## 27 July, 2025

- 1. FalconX device
  - a. Flip\_icr\_raw
    - i. Mislabelled method as a Maia method.
- 2. Standards Wizard
  - a. Add a Device droplist to select the raw data device. Tested for "MAIA\_DEVICE" and "FALCONX MERGE DEVICE".
  - b. Add storage in pstate for the array of available device objects.
  - c. Add event code and an OnRealize routine for the new device droplist.
  - d. Change from using (\*pstate).DevObj to \*(\*pstate).pDevObj throughout.

### 22 July, 2025

- 1. EVT
  - a. evt getcal
    - i. When comparing 'i' index (channel) to list of ADC #s found in file ('n'), needed to add the offset: (\*pp[0]). DevObj->start\_adc()
  - b. Use the test data for the following to sample a range of start-ADC and offsets:
    - i. Sandia-Primecore U48/Grid (Primecore U48)
    - ii. Uppsala-MPA3/Au 3 (MPA3)
    - iii. Madrid MPA4/Aug (MPA4)
    - iv. APS Regolith-82 (APS List)
    - v. Maia Rock3/111163 (CSIRO Maia)
    - vi. Lund/New 8 element (LUND VME MAC)
- 2. Image table eventcb
  - a. Load\_image\_table\_table

- i. Check to see if the filename of the current images match the filename of the images used to create the regions in the image table.
- ii. If not, this means that an "Update: All" has not been done.
- iii. Pop-up warning, advising of the need to do an "Update: All" before adding a new region to the table.

## 10 July, 2025

- 1. Image table eventcb
  - a. Load image table table
    - i. Check to see if the elements in a new region sum (from current image) are present in the columns of the region table, as shown.
    - ii. If not, this means that an "Update: All" has not been done.
    - iii. Pop-up warning, advising of the need to do an "Update: All".

### 30 June, 2025

- 1. File pcm preview
  - a. Preview of PCM file contents for 'file requester' as called from 'fit setup'.
- 2. Fit setup
  - a. Pass "file pcm preview" as preview routine name to 'file requester' for PCM read.
- 3. Experimental\_angles
  - a. Refined tests of sample-beam-detector (array) geometry to detect conditions like (i) detectors looking at back of sample, or (ii) at glancing angle and (iii) beam hitting back of sample.
- 4. Geo\_array\_yield, geo\_yield2
  - a. Handle 'bad' error conditions properly, return error=1 and yield=0.0.
- 5. Blog browser
  - a. Process tag=57 (Report) records, which show blogd statistics.
- 6. Version 8.8x

### 24 June, 2025

- 1. Image routines
  - a. Analyze image
    - i. Use same approach as for "areas" on line profiles (traverse, project, project, Spline8, etc.) to detect non-elemental image planes and great these 'as is' in counts, such as for "Rate" and specials as listed in "special\_elements" function.
    - ii. 'misc\_special' is list of specials. 'nqell' is non-zero for these in 'where' statements testing 'el[i]' against 'misc\_special'. In this case, use simple pixel-count version of 'hcharge' vector (called 'hcharge0').
    - iii. Now the traverse plot shows a sensible count rate versus distance.
- 2. Special elements
  - a. Add "c/s" as a special element as alternative to "Rate".
- 3. File lcm preview
  - a. Preview of LCM file contents for 'file\_requester' as called from 'Layer\_setup'.
- 4. Layer setup
  - a. Pass "file lcm preview" as preview routine name to 'file requester' for LCM read/write.
  - b. Add "file yield preview" for preview of output file too.
- 5. File\_yield\_preview
  - a. Add display of Alpha, Beta.

#### 10 June, 2025

- 1. Image table eventcb
  - a. OnCellSelect Image Table
    - i. Try to fix error when doing regions for STIM and ion scattering, where el[2] index becomes illegal.
- 2. file source preview
  - a. Preview for file requester for lab .source and .pink beam files.

- b. Now called from layer\_setup, source\_setup, pink\_setup, compare\_soure, compare\_pink, etc. in 'file requester' args.
- 3. file yield preview
  - a. Preview for file requester for yield calc .yield files.
  - b. Now called from fit setup, layer setup, compare yields, etc. in 'file requester' args.
- 4. Version 8.8w

### 3 June, 2025

- 1. Swap bytes
  - a. Add recursive handling of Lists, Hashes, Ordered Hashes and Dictionaries.
  - b. Use 'var type(t)' function for more detailed types.
- 2. Image DA preview
  - a. Used by 'file\_requester' to provide preview data from a selected DA matrix file during file selection. This data (element list) is shown in the preview field of the requester.
- 3. Evt
  - a. File\_requster called from the DA 'file\_button' event now uses the preview routine option to select "image DA preview" as the preview routine.
- 4. Spectrum DA load
  - a. Uses the File\_requster preview routine option to select "image\_DA\_preview" as the DA preview routine.
  - b. Set /image option on file\_requester to make preview of spectrum "image" shown by default. This option ("image") is a bit ambiguous.
- 5. Select periodic
  - a. Correct "n states" (was "n state") before 'periodic table'.
- 6. Version 8.8v

### 28 Apr, 2025

- 1. Add "Plot ALL regions" option to "Export→Image Plot" to draw ALL regions on export image plot.
  - a. Define
    - i. Add 'ShowALLregions' to /plot options.
  - b. Save\_plot\_options
    - i. Increment to version -6 for extra plot options data.
  - c. Load plot options
    - i. Handle version -5 as an old struct and add version -6 using define(/plot options).
  - d. Plot image select
    - i. Add checkbox for "Plot ALL regions".
  - e. Plot images
    - i. Detect 'options. Show ALL regions' true and loop through all regions (if found) and use 'plot mark' for each.
- 2. Version 8.8u

#### 8 Apr., 2025

- 1. Fix case sensitive filenames and dirs used in database build on Linux.
  - a. Fix filenames on PC to match case in routines:
    - i. alpha.txt, element.txt, isotope.txt, mass.txt, proton.txt
  - b. Fix case in routines:
    - i. build ebel data, init xsect.
  - c. Fix case of some projects:
    - i. GUI plugins
- 2. Builder
  - a. Build project
    - i. If search returns "then return.

## 1 Apr, 2025

1. Bug in device name shown in *Spectrum History* window for old files (pre about 2012).

- a. Would display as Mpsys device, when not so.
- b. Read spec
  - i. Type of old 'device' not declared properly (appears as Float). Now fixed as Integer. Seems default behaviour in IDL has changed at some time.
- 2. Bug with the selection of a ADC # in the *Energy Cal* window for a "Get" of that selected energy calibration.
  - a. Read\_spec
    - Now form 'find\_offset' for use in call to 'get\_spec' to retrieve selected ADC # spectrum:
      - 1. find offset = find 1 adc offset device(obj), clipped at zero,
        - a. where 'find' is the *Cal* Get droplist index (e.g. 0 for "any", 1 for "0", 2 for "1", etc.).
        - b. The 'adc\_offset\_device(obj)' function returns 0 for devices where the ADC # start at 1, -1 for devices where the ADC # start at 0 and 2 for devices where the ADC # start at 3, etc. (i.e. "start ADC" -1).
    - ii. Tested OK for a range of device spec files with different Start ADC and offsets.
    - iii. Note that some old spec files have inconsistent ADC # shown in the "label" field.
- 3. Version 8.8t

### 27 Mar, 2025

- 1. Revisit Linux IDL display/resize bug
  - a. Background
    - i. In the main *gImage* window, when resized (either by dragging the window size or using the "+", "-" buttons) it sometimes displays the image offset in Y, with grey beneath and the top of the image truncated. This only happens when the whole image is visible and hence (normally) the scroll bars disappear.
    - ii. This only happens under Linux, and has persisted through IDL 8.8 to 9.1.
    - iii. And only if the Y scroll bar disappears.
    - iv. Attempts to use the viewport position controls fail to fix this.
    - v. Tests manually using the "tv" command, to draw an image into the Draw widget's wid also show this offset, but not on a fresh window (using the "window" command).
  - b. Work-around
    - i. The previous work-around simply prevented the scroll bars from disappearing.
    - ii. The new work-around allows the X scroll bars to disappear, but not Y.
    - iii. It also adjusts this to the pixel level, to minimize the area of image hidden in Y.
- 2. Set image view
  - a. Add new offsets 'scr\_xtrim' and 'scr\_ytrim' to prevent Y scroll bars going in setting 'new.w', 'new.h'. These are zero except for Linux.
- 3. OnSize image
  - a. Add new offsets 'scr\_xtrim' and 'scr\_ytrim' to prevent Y scroll bars going in setting 'w', 'h'. These are zero except for Linux.

## 24 Mar, 2025

- 1. Layer setup
  - a. Problem arose if manual enter parameters into layer setup (not restore from LCM).
    - i. Then 'beam' not defined.
  - b. 'calculate-button' event:
    - i. Only assign beam.continuum and beam.energy if 'beam' is defined.
- 2. Geo yield2
  - a. Move 'beam2' spectrum code inside the contuuum==true if block.
- 3. Compare tests:
  - a. Tested (i) simple PIXE yield calc (single detector) donuts2, and (ii) MM continuum yield calculation with Maia detector rock-slab-poly2.
  - b. Used 'compare yield' test: Results equal to reference yields.

### 24 Mar, 2025

- 1. Geopixe default
  - a. Tests for valid "path data" and "path config" in '.geopixe/geopixe.conf' file only happen once now, reducing annoying popups.

#### 14 Mar. 2025

- 1. Geopixe default
  - a. Tests for valid "path data" and "path config" in '.geopixe/geopixe.conf' file.
  - b. Pops up a warning if these are not setup, suggests Edit of "geopixe.conf" file.
- 2. Strip non alphanumeric, strip non print
  - a. Extended to vector string arguments.

#### 5 Mar, 2025

- 1. Maia launch
  - a. maia launch version2
    - i. Add set *antialias.enable*, once and for all to enable antialiasing in the Maia FPGA pipeline to prevent aliasing using Linearization and Gain-trimming.
  - b. Version 8.8s
- 2. GeoPIXE
  - a. Version 8.8s

#### 4 Mar, 2025

- 1. Plot maia paarameters
  - a. This calls 'file\_requester', which may use 'file\_search2', which uses the 'progress' bar. The 'progress' bar will set a new window to draw the progress bar in.
  - b. Hence, in 'plot\_maia\_parameters', do not call 'file\_requester' between opening a new window and plotting to it.
- 2. Pulser FWHM map spectrum plugin
  - a. Don't need to open window with 'window,0' as this is done in 'plot maia parameters'.

#### 17 Feb, 2025

- 1. Petra P06 H5 Nexus device object (draft)
  - a. Reads P06 tree of NXS files into spectra.
  - b. Get flux and dwell working, but no gain scales.
- 2. Scan list
  - a. Updated tests of python and IDL versions in scan list.
  - b. Fixed errors in bin/scripts for this.
  - c. Changed it to make settings from 'geopixe.conf' take precedence, it found.
- 3. Maia launch
  - a. Fixed bug in LED[3] used to flag all background processes running.

#### 12 Feb, 2025

- 1. Petra P06 H5 Nexus device object (draft)
  - a. Added adding 'adc\_\*/value1, value2, ...', 'qbpm\_\*/value1, value2, ...' as PVs.
  - b. Added reading this PV in 'read setup' for each data file.

### 4 Feb, 2025

- 1. Python valid
  - a. Check python version against IDL for compatibility.

	Python version									
IDL version	2.7	3.4	3.5	3.6	3.7	3.8	3.9	3.10	3.11	3.12
8.5	~	<b>✓</b>								
8.5.1	~	<b>✓</b>								
8.5.2	~	<b>✓</b>	<b>/</b>							
8.6	<b>~</b>	<b>✓</b>	<b>/</b>							
8.6.1	~	~	~	~						
8.7	~	<b>✓</b>	~	<b>/</b>						
8.7.1	~		<b>~</b>	<b>✓</b>						
8.7.2	~		~	~						
8.7.3	~		<b>/</b>	<b>/</b>						
8.8				<b>✓</b>	<b>✓</b>	<b>✓</b>				
8.8.1				<b>~</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>			
8.8.2					<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>		
8.8.3					<b>/</b>	~	~	<b>✓</b>		
8.9						~	~	<b>✓</b>		
9.0						~	~	<b>✓</b>	<b>✓</b>	
9.1							<b>✓</b>	<u> </u>	<b>✓</b>	<u> </u>

NOTE: IDL versions prior to 8.5 do not support Python bridge functionality.

This fixes an error in doing these tests in Maia-Control.

#### 2. Maia control

a. Check python against IDL using 'python\_valid()'.

### 27 Jan, 2025

- 1. File requester
  - a. 'updir' was stopping one level short. Fixed.
- 2. Detector\_update
  - a. If a detector is not found on path1 (geopixe\_root), path2 (prefs.path.config) or the detector file's path, then popup file\_requester (with updir=3 from local dir) to prompt for it, and append it to the list (at end, not alphabetically sorted).
- 3. Fit setup
  - a. Only read detector once: pending after normal detector entry and done after yield detector entry.
  - b. As detector file is saved in PCM with no path, use the path for the PCM as a start (as well as config/detectors in 'detector update').
  - c. Make detector Layout behave similarly, inheriting the path for the detector file.

#### 4. Deleted rogue SAV file

- a. A plugin (FWHM map) had been compiled into the local project dir.
  - i. This SAV file then gets included in the next compile in that project (a nasty habit of IDL).
  - ii. It included 'resolve\_all', which means it included ALL GeoPIXE routines into the plugin's SAV file.
  - iii. On running GeoPIXE, these SAV files get loaded and write over newer versions of many routines that have been compiled (into GeoPIXE.sav) since the plugin. This of course a really bad thing, and confusing for debugging.
- b. Deleted the offending SAV file.
  - i. There should be NO SAV files in any plugin dir, only in the "geopixe" Runtime dir.
- 5. Version 8.8r.

#### 20 Jan, 2025

- 1. maia launch
  - a. Instead of just reporting an over-leakage event, it now takes action to set the bias back to minimum.
- 2. maia launch read\_da\_info
  - a. Removed illegal ref to \*pl.

### 10 Jan, 2025

- 1. maia launch
  - a. Corrected code to check compatibility between python and IDL.
  - b. Maia Version 8.8r
- 2. Idl query
  - a. Added code to check compatibility between python and IDL.

### 8 Jan, 2025

- 1. maia launch
  - a. The frame=0 option on widget text used to have this behavior:
    - i. Ignored under Windows, frame drawn anyway.
    - ii. Seemed to draw a frame under Linux as well.
  - b. Now in v9.1 IDL
    - i. Windows does not draw a frame.
    - ii. Linux still does, weird.
  - c. Fixed by explicitly using frame=1 for widget text
    - i. Status field, help field, blog number field.
    - ii. Under Linux, frame seems a bit wider now.
- 2. Idl\_query
  - a. Lmgr2
    - i. Can't spawn "activate" in IDL v9, as it does not exist; skip.
- 3. Version 8.8q

### 7 Jan, 2025

- 1. Plot maia parameters
  - a. Add a call to "file\_requester( /read, /skip\_if\_exists, updir=2, ...) to find the default layout file 'Maia 384C.csv" on a neighbouring path in the runtime distribution.
  - b. This is used in: 'Pulser\_FWHM\_map\_spectrum\_plugin', 'Peak\_Stats\_spectrum\_plugin', 'Peak\_Fit\_Stats\_spectrum\_plugin' and compiled in main 'GeoPIXE.sav'. The latter ('Peak\_Fit\_Stats\_spectrum\_plugin') does supply an explicit filename.
  - c. Only need to recompile main GeoPIXE.
- 2. Merged develop branch, which had conflicts to fix:
  - a. Firstly, I forgot I was in "develop" when upgrading the Workspace in IDL 9.1.
  - b. No way to fix this except merging "develop" into main.
  - c. There were duplicates: bat file to run IDLDE, GeoPIXE.sav.
  - d. Deleted the sav files and fix bat, git Add and Commit.
  - e. Did not fix new "No explicit project encoding" project warnings.

#### 3 Dec, 2024

- 1. Plot corr
  - a. Add options for /PNG (bit mapped) and /JPEG (true) plots for *Association* window following prescription in 'plot\_images'.
- 2. Plot corr select
  - a. Add options for /PNG and /JPEG plots for Association window.
- 3. Corr\_export
  - a. Add options for /PNG and /JPEG plots for Association window.
- 4. Corr event
  - a. Make /JPEG plot the default for call to 'corr export'.
- 5. Gimage
  - a. Add Test menu item to test Pink Beam sources, calling 'compare pink'.
- 6. Export da2
  - a. Added more notes in software organization doc for binary export for DA real-time imaging.

### 20 Nov, 2024

- 1. Compare yield
  - a. Test for New and Ref both array detectors, else flag error in output file.

### 11 Nov, 2024

- 1. Compare\_fit
  - b. Add ability to deal with a PFR file with multiple rows (e.g. for ROI or individual array detectors).
  - c. Shows any models that differ by more than 0.1 % generally and 3% for fitted areas/concs.
  - d. Veto "Compton", "elastic" and "sum" in comparisons.
- 2. Compare source
  - a. Add 'tol' argument, defaults to 0.001.
- 3. Compare pink
  - a. Add 'tol' argument, defaults to 0.001.
- 4. Compare yields
  - a. Add 'tol' argument, defaults to 0.001.
- 5. Builder
  - a. Make sure !path is not cumulative as projects are processed.
  - b. Output 'build.spro' always to "main" dir.
- 6. Gimage
  - a. Add a "tests" menu for the 'compare' routines.

### 28 Oct, 2024

- 1. Compare fit
  - e. New routine to compare fit results files (.PFR files) as a step towards a unit test.
  - f. Simply prints out any inconsistencies found to the 'output' file.
  - g. Also reports diffs for derived area, conc, MDL, etc.
- 2. Pixe fit
  - a. The order of "state" and "e\_beam" in the 'ryield' struct have been reversed at some stage (2 instances of 'ryield'). But this effects the format in the PFR fit results file. Hence, newer PFR files read back with these switched.
  - b. Fortunately, these parameters do not get used they are for info only. However, the 'compare fit' routine flagged them as inconsistent.
  - c. Hence, they have been switched back, so that new PFR files are consistrent with old ones.
  - d. This will mean some instances of PFR file in between remain switched, which will be flagged harmlessly by 'compare\_fit'.
- 3. Pixe initial
  - a. For negative Z, and Compton line index, name "element", e.g. as "cIn".
  - b. But do these cIn lines inherit normal In rel-ints, rather than from beam lines?
    - i. Rel-ints for Comptons lines <u>do</u> come from beam lines. Good. However, the rel-int of the source lines is coming from normal rel-ints at the moment.
    - ii. Fixed this in 'select element lines'.
- 4. Sum peaks
  - a. Use abs(z) to form el names for lines (to account for -Z used for Comptons).
- 5. Select element lines
  - a. Use -Z for Compton peaks from source lines (mark all changes with ;@10-24).
  - b. Add option (in line) to match lines for any element that is also in source, to source rel-ints.
    - i. Uses 'match source intensity' = 1 in code.
  - c. Do not change Continuum Beam Lines rel int here (done now in 'source calculate').
- 6. Source calculate
  - a. Calculate change to lines rel due to polycapillary (not in 'select element lines' now).
- 7. Version 8.8p

### 16-21 Oct, 2024

- 1. Compare source
  - a. New routine to compare Lab source model results (.source files) as a step towards a unit test for the lab source modelling.
  - b. Checks beam.model should be "1".
  - c. Shows any results that differ by more than 0.1 %.
  - d. Simply prints out any inconsistencies found to the 'output' file.
  - e. Also reports diffs for derived source spectra.
- 2. Sig change
  - a. Shows any results that differ by more than a 'tol' value, defaults to 1 ppm.
- 3. Source\_calculate
  - a. Veto any input or interpolated polycapillary transmission table values less than zero.
- 4. Source setup
  - a. Fix the mapping of polycapillary and monochromator widgets.
- 5. Compare\_pink
  - a. New routine to compare Pink Beam source model results (.pink files) as a step towards a unit test for the pink beam modelling.
  - b. Checks beam.model should be "2".
  - c. Ignores polycapillary, for later.
  - d. Shows any results that differ by more than 0.1 %.
  - e. Simply prints out any inconsistencies found to the 'output' file.
  - f. Also reports diffs for derived pink beam spectra.
- 6. Compare\_yields
  - a. Needs to switch between 'compare source'; and 'compare pink' depending on beam.model.
  - b. Tests for consistent beam.model.

### 7 Oct, 2024

- 1. /sec fl in yield calculation tidy up.
  - a. Geo\_array\_yield
    - i. Argument 'sec fl' not used, remove
  - b. Results properties
    - i. Remove arg 'sec fl' passed to geo array yield.
  - c. Geo\_yield2
    - i. Tidy comments about 'sec fl'.
- 2. Compare yields
  - a. New routine to compare yield calculation results (.yield files) as a step towards a unit test for the yield modelling.
  - b. Shows any results that differ by more than 0.1 %.
  - c. Simply prints out any inconsistencies found to the 'output' file for the time being.
- 3. Geopixe do command
  - a. If first agv[0] is NOT a GCF file name, then assume a simple command execution, with three arguments: "command, files (string vector in stringify format), output".
  - b. This enables the test to be run in a script or workflow.
  - c. See test in BAT script: "Unit test Runtime GeoPIXE.bat".
- 4. Q to xyz
  - a. Routine to convert index vector 'q' into a 3D array to vectors of the indices for x,y,z in the array. Analogous to old 'q to xy' for a 2D array.
- 5. File requester
  - a. Will now call 'startupp' if geopixe root is not defined.

#### 2 Oct, 2024

- 1. Make branch 'develop' for development and beta release.
  - a. This is identical with current 'main' at the moment.
- 2. Recommend to make other branches off 'develop' for feature additions and other fixes.

### 1 Oct, 2024

- 1. Export DA2
  - a. Accepts keywords for pileup, throttle and linear, which can be set from fields in Evt window.
    - i. Linear is not used at present, as we don't have tools for realtime use of the Maia v2 Linearization functions.
  - b. Binary (dmx) mode changed:
    - i. Does not output individual detector E cals to the export file. These are supposed to be set elsewhere and should not be part of the DA matrix.
    - ii. Version now -2.
  - c. iThemba (dmm) mode changed:
    - i. Similar to DMX binary, but limits size of DA matrix (compressed if necessary).
    - ii. Does not output individual detector E cals to the export file. These are supposed to be set elsewhere and should not be part of the DA matrix.
    - iii. Version now -2.
  - d. Further work:
    - i. Does not export the *rGamma* matrix or *Pure* arrays. This is needed(?) to properly integrate contributions across an array (using selected channels) for quantitative estimation from regions/spectra, or at least for the spectra overlays.
- 2. EVT
  - a. Add "Exp" button next to DA matrix file fields to call 'export\_DA2' to export the chosen DA matrix for use in a data acquisition system for realtime imaging and spectra analysis.
- 3. Fit setup
  - a. Used to call 'export\_DA' from "Export" button next to "Generate DA" button to output an expot file for use in a data acquisition system for realtime imaging and spectra analysis.
  - b. Now it calls 'Export\_DA2', which does not include the pointers to spectra and does not output individual detector E cals to the export file. These are supposed to be set elsewhere and should not be part of the DA matrix. These files now have version = -2.

## 4 June, 2024

- 1. spectrum display eventcb
  - a. Spectrum Menu Clear Cal
    - i. Only check second string in label for "/X" and "/Y", not whole label, which may include path components with these sub-strings. Only want to test the post-fix tags.
- 2. wizard standards
  - a. Allow "serial" to be blank, and match with a blank in "standards.csv" table.
  - b. Do not set "On" zero if serial is blank.
- 3. NSLS MARS Ge device
  - a. Swapped to big endian byte order for read in device.
- 4. Version 8.8n

### 3 June, 2024

- 1. Maia device
  - a. Added an options widget to adjust/correct a skew in X values, expressed as "correct X by one for every 'n' Y rows", with this set via a droplist.
  - b. Read/write options now version -7 to cater for skew.x
    - i. This will require this new version Maia device to read DAI file.
  - c. 'Read\_buffer' corrects x1 by y1 (i.e. x1 = x1 long( y1 / float(self.sort\_options.skew.x) ). This is done before any xoffset, so should work fine in cluster mode. Also done before any flip axis options, so applies to raw X1,Y1.
- 2. GUI Image Table XFM AS plugin
  - a. image table xfm as gui plugin
    - i. Renamed this plugin from "image\_table\_xfm\_as\_gui\_plugin" for the XFM beamline of the Australian Synchrotron.
    - ii. Writes a CSV table with region details to be loaded into the online run spreadsheet.
- 3. GUI Image Table XFM NSLS plugin

- a. image table xfm nsls gui plugin
  - i. Adapted this plugin from the AS version for the XFM beamline of the NSLS-II synchrotron, BNL, NY.
  - ii. Writes a CSV table with region details to be loaded into the online run spreadsheet.

## 31 May, 2024

- 1. Builder issue
  - a. Some plugins are missing routines. These used to be done as IDLDE build options, not supported in new 'builder'.
  - b. Needed to resolve missing routines and save/routines a new SAV file.
  - c. Applies to: linearize\_spectrum\_plugin, linearize\_cuts\_energies\_spectrum\_plugin, linearize\_cuts\_fit\_offset\_spectrum\_plugin, linearize\_cuts\_spectrum\_plugin, linearize\_spectrum\_plugin.
  - d. Need to add: *lmfit*.
  - e. Add a new place for miscellaneous resolves: 'resolve misc'.
- 2. Resolve misc:
  - a. Resolve routines: *lmfit*.
  - b. Users who add plugins can also resolve their own added routines before saving a SAV file. But many basic ones can be added here, as this is not supported yet in builder.

## 19 May, 2024

- 1. Notes about /modal, /floating, blocking (File Requester and Progress)
  - a. Originally, 'file\_requester' was setup as a normal modal widget, which blocks until is closes. It's also floating, which means it sits in front of other windows.
    - i. Blocking is similar, keeping control in xmanager near the end of the main file requester program.
    - ii. We don't want to set no\_block=1 on xmanager, to keep it modal.
    - iii. However, we should never set no block=0 on xmanager
      - 1. This does some weird stuff, like disable debugging.
      - 2. Simply, *omit* the no\_block keyword to xmanager to achieve the same result. See 'file requester' code.
  - b. Then file\_requester was changed to permit a progress bar popup while searching for a file match using "Find".
    - i. i.e. It was found that you could use modal=0, floating=1 on the top base widget and *omit* no block on xmanager.
  - c. However, then file\_requester could not work properly if called from another modal widget (e.g. 'flux\_select').
    - i. In that case, we use another option '/within\_modal' to remind file\_requester to use /modal (and disable the Find).
    - ii. Only use '/within modal' when called from a modal widget.
- 2. File requester
  - a. New '/within modal' option, if called from a modal popup (e.g. 'flux select').
  - b. This means that the file "Find" does not work as the Progress window cannot function properly then.
- 3. Flux select
  - a. As this is a modal popup, all calls from it to 'file\_requester' use /within\_modal.
- 4. Spectrum load prep
  - a. Call 'file\_requester' for pileup, linearize and throttle with 'updir=3' so that it looks in the local neighbourhood for a file match.
- 5. Version 8.8m.

## 15 May, 2024

- 1. Plugin: Cal by centroids
  - a. peak cal cut centroid spectrum plugin
    - i. Use a common to save the 2 energies, so they appear next invocation.

- 2. Write source, write pink, read source, read pink
  - a. Only set 'file' in struct if file opened here, not if 'unit' passed.
- 3. Fit results/save fit resilts
  - a. Write a new version -16 and write 'continuum' first, then 'model'
  - b. Then call either source or pink write.
- 4. Read fit results
  - a. New code for version -16, to read 'continuum' first, then 'model'.
  - b. Then call either source or pink read.
- 5. Pink calculate
  - a. Use file\_requester(/skip\_if\_exists) to search local tree and also along 'path' tree for a file match.

### 6 May, 2024

- 1. Continuum source
  - a. Moved back into 'main/xray' and 'main/' for 'source\_setup'.
  - b. Delete "continuum\_Source" plugin project.
- 2. Pink beam source
  - a. New pink beam routines in 'main/xray' and 'main/' for 'pink setup'.
- 3. Pink setup
  - a. New setup for a pink beam that parallel 'source setup' for lab sources.
  - b. Uses FE beam spectrum and up to 4 mirrors, based on CXRO reflectivity data files.
  - c. Disable inline optics extras for now.
- 4. Define
  - a. New /pink for pink beam
  - b. Set model=1 for lab, model=2 for pink, as was not used before.
- 5. Layer\_setup
  - a. No source plugin load, fixed new droplist options for photon sources.
  - b. (\*p).source is now a pointer to either a lab source or pink beam 'beam' struct
  - c. (\*p).source  $\rightarrow$  \*(\*p).source in most places.
  - d. Cater for 'new-pink' Notify event, similar to new-source.
  - e. 'beam-mode' now just handles lab and pink in "else".
  - f. 'load-source' now handles cases of 6:lab, 7:pink beam.
  - g. 'new-source' launches 'source setup' or 'pink setup' according to beam.mode.
  - h. Add 'ppink' to pstate for notify to pink setup.
- 6. Geo yield2
  - a. At the end, add "rel\_int[1:\*,q] = 0.0" for the zero 'q' array, to avoid NaN 'rel\_int' for elements where the yield drops to zero.
  - b. Some bad elements get through, despite 'zero', so add this to 'q' test:
    - i. Q = where((zero eq 1) or (finite(rel int[1,\*]) eq 0))
  - c. Catch all /0 conditions that affect: branch ratio, ppm, mass yield, total yield, rel int.
- 7. Geo array yield
  - a. Catch all /0 conditions that affect: rIntensity, enhance, rY.
- 8. Select element lines
  - a. Detect lack of "Lines" tag in 'beam' struct and set add lines=0
- 9. Write yield
  - a. Write beam.model before beam, if 'use beam'.
  - b. New version -11
- 10. Read yield
  - a. If version -11, after read 'use beam', read 'model'.
  - b. If 'model = 2 then switch to a pink beam 'beam' struct.
- 11. Read beam
  - a. Read a text file of energy versus beam or CXRO reflectivity data.
  - b. Has a 'skip=' option to skip header of CXRO files.
  - c. Has option 'remap energy=' to remap E,data onto a given energy vector.
  - d. Clip output to >0

#### 12. Pink calculate

- a. Just use FE beam \* mirror and filter reflecitity/transmission, with no solid angle, etc. terms applied. Commented out for now.
- b. Disable inline optics now, as this involves solid-angle considerations also.
- c. Set e beam, which is used to 'init xrf' in 'get lines':
  - i. pink.energy = E[max(where(spec gt 1.0e-10))]
- d. Add pressure and temp args to 'transmit' like in 'source\_tube\_spectrum' called from 'source\_calculate' to cater for spectra with P.T values.

#### 13. Read pink

- a. Read a pink beam file, like read source.
- 14. Write\_pink
  - a. Write a pink beam file, like write source.
- 15. fit recalculate yields
  - a. Add case to either 'source calculate' or 'pink calculate' based on beam.model
  - b. Note for non continuum beam these return passively.
- 16. Version 8.8k.

## 22 Apr, 2024

- 1. Maia Launch
  - a. Maia launch version2
    - i. Cater for 'number' zero for spectra, et2d, roi.
    - ii. Zero means the variable vanishes in Kandinski.
  - b. Maia launch initial, maia launch read enable, maia launch read groups
    - i. Only set spectra parameters if number not zero
  - c. Maia launch
    - i. Only setup groups shared memory is number > 0
    - ii. Catch anywhere shrmem referenced
  - d. Maia\_update\_group\_spectra
    - i. Return if no shared mem
- 2. Spawn\_blog\_parameters
  - a. Pass in region enable, else veto spawn of region spectra
- 3. Maia setup
  - a. Maia setup event, maia setup apply groups
    - i. Only set spectra parameters if number not zero
- 4. Maia client parameters
  - a. Test for (\*pm).number.spectra, roi and skip enable.
- 5. Startupp
  - a. Construct path to 'maia' and 'daq subdirs correctly.
- 6. pixe fit
  - a. Set default value for 'sum\_deficit' to 0.5%
- 7. Version 8.8j

## 8 Apr, 2024

- 1. File-requester
  - a. File\_requester\_preview
    - i. Use \*(\*(\*pstate).p).pfile (array) for files, rather than (\*pstate).file (concatenated list).

#### 14 Feb, 2024

- 1. Blog browse
  - a. Change format of output to correct a field width.
- 2. GitHub
  - a. Fresh load of GeoPIXE to local Git and to GeoPIXE on GitHub at URL:
  - b. <a href="https://github.com/CSIRO-GeoscienceAnalytics/GeoPIXE">https://github.com/CSIRO-GeoscienceAnalytics/GeoPIXE</a> as branch "main".

#### 27 Nov, 2023

- 1. Use *WinMerge* to view and merge changes across from GeoPIXE-source3 to *Open Source* (between Mar 27 and Nov 27). Take care to:
  - a. Not merge across differences due to licensing.
  - b. Watch for different path constructs, e.g. for Wizards.
- 2. Need to run all tests

#### 24 Nov, 2023

- 1. GeoPIXE
  - a. gImage
    - i. Add menu for Export → Simple Image -> Save as TIFF
    - ii. Call Image Save GIF, Event, /TIFF
  - b. Image Save GIF
    - i. Add /TIFF option
    - ii. For TIFF use 'write tiff' to save as 32-bit float TIFF.

## 8 May, 2023

- 1. GeoPIXE
  - a. Removed modules with non CSIRO code, although the code had been supplied by the laboratories to enable an import object or plugin to be devised for their data and attribution was included.
    - i. These include:
      - 1. Devices:
        - a. "APS LST", "ESRF EDF", "GSE-CARS MCA", "Lund VME", "NSLS MCA", "NSLS NetCDF".
      - 2. Plugins:
        - a. "Image Align", "Image Combine Align", "Image Shear Correct".
      - 3. Background:
        - a. Bayes.
      - 4. These may be added to the GitHub repository by the labs concerned at a later time.
- 1. Builder
  - a. Add build for GUI plugins.
- 2. Eclpse "clean up"
  - a. Move .log and log files to "old/old-files-Open-Source" directory, from:
    - i. .metadata
    - ii. .metadata/.plugins/org.eclipse.ui.workbench
  - b. Move the following dirs with history to "old" as well:
    - i. .metadata/.plugins/org.eclipse.core.resources/.history
    - ii. .metadata/.plugins/org.eclipse.ltk.core.refactoring/.refactorings

#### 21 Dec, 2022

- 1. builder (NEW)
  - a. Build a script "build.spro" to be used (use: "@build.spro") to selectively build the SAV files, by catagories ('all', 'plugin', 'back', 'spectrum', 'image', 'device', 'wizard', 'source', 'maia', 'daq', 'main', 'browse']).
    - i. This avoids issue with poor control of !PATH and using '.compile' by file-name, rather than 'resolve routine'.
  - b. Does full reset session for each project build to clear compiled routines.
    - i. But this makes it very slow if run from IDLDE.
  - c. !PATH built afresh for each project build to include whole "main" tree plus the project.
  - d. Build project:
    - i. Does the fiddly work for builder.
  - e. Build database

- i. Does the database build part.
- f. The following builds do a resolve all:
  - i. Main, IDL Query, GeoPIXE update and Builder.
  - ii. IDL Query now does not need the make routine anymore.
  - iii. GeoPIXE update of a non-GUI version is not done yet.

#### 2. projects:

- a. Needed to enforce consistency in naming:
  - i. SAV file name constructed from project name, with additional options to tag a suffix to SAV filename.
  - ii. Build from Eclipse must match this SAV filename.
  - iii. Deleted some projects not needed for open source, such as junk tests, etc.
- b. image table evt

### 3. Organization

- a. The "builder" imposed some rules that needed to be enforced:
  - i. Plugins must start with "Back", "Spectrum", "Image" and end with "plugin".
  - ii. Except "source" and "Wizards" plugins.
  - iii. Maia projects start with "Blog" or "Maia".
  - iv. All Maia SAV end up in /maia, including maia control.sav and maia scan list.sav.
  - v. All DAQ SAV end up in /daq, including daq\_control.sav.
  - vi. All browsers start with "Browse".
  - vii. Some get renamed: mm\_scan\_list → maia\_scan\_list, GeoPIXE worker → GeoPIXE parallel, "ftp update" → 'GeoPIXE update".
  - viii. 'misc' compiles/builds include 'geopixe index', 'geopixe update', "builder", ...
    - ix. Fake Blogs divided into ET2 and DA2 versions.

#### b. Database build

i. 'make database.pro' has changed, so it gets called from 'builder'.

#### c. Build

- i. Use 'builder' (pops up index selection) to select which classes to build, which creates "build.spro" (note: this will be in "geopixe" for runtime execution and "main" for IDLDE execution). A pop-up reminds the user of "build.spro", its path and the need to run "@build.spro" from the <u>IDL command line</u> after a "cd" to path.
- ii. "@build.spro" from IDL command line to build (after "cd" to the dir). This is much faster than in IDLDE due to long lag after a full reset.

#### 4. Version 8.7o.