What's new in TSG8, 12 March 2018

Scalar batch scripts

Built-in system scripts

TSG's built-in collection of batch scripts has received some attention. All scripts with a claim to mineral interpretation have been removed and only rudimentary scripts remain. One reason for this is that some people may be tempted to run a built-in script on *any* dataset, and running a specialist scalar like this can lead to confusion. A specialist script that claims to calculate something like "white mica abundance" or "kaolinite crystallinity" will only work properly in certain cases.

In addition, the built-in collection has been bolstered by Carsten Laukamp's "Base" scripts. Some documentation for these is included.

The system scripts that were removed have been gathered together in a user script library.

User script libraries

TSG's support for these has moved forward. A few libraries (including a sub-collection of Carsten Laukamp's "MFEM" scripts along with documentation) are now included in the TSG distribution. Further information can be found here: ftp://ftp.csiro.au/MMTG/tsg_user_script_libraries.pdf

Import / export

- The ASCII XY import has a new preset "**Agilent**" for importing ASCII **.ASP** spectrum files from the Agilent 4300 handheld FTIR spectrometer (which covers [2, 15] um approximately).
- The dynamic import system now supports Agilent **.ASP** and PIMA **.DSP** files.

Note: When converting from wavenumbers to wavelengths (as with Agilent spectra), the recommended resampling method in TSG is "DYNA L3".   "Plain L3" and "Gaussian bandpass" are not recommended.   The other methods are okay.

Agilent wavelength correction

The Agilent 4300 handheld FTIR spectrometer presents its spectrum files with a constant channel spacing (in the measurement's wavenumber domain). In practice the spacing is believed to vary slightly.   A correction has been found for one instrument to-date and it results in a change that reaches about 10nm at the spectrum's long-wavelength (15000nm) end.   That's not much of a change, admittedly, but the correction is available if you want it.   In the normal import, click the **Agilent options** button that becomes visible once you select the **Agilent ,ASP** type.   In the dynamic import, click the **Configure** button.

Currently the one known instrument's correction parameters are set as TSG's defaults. They may not be optimal for all instruments.   If you are interested in correction parameters for your instrument then contact peter.mason@csiro.au to investigate options.

Generic de-stepper module

There is a new module for correcting inter-detector steps. It works in much the same way as the de-stepping correction that's built into the ASD binary import but can be used (*as necessary*) at any time on spectra from any instrument. Here is some documentation: ftp://ftp.csiro.au/MMTG/tsg_general_destepper.pdf

Various

- TSG now saves its global settings in ASCII XML format. The settings file is called `tsgeol8settings.xml` and can be found alongside the installed executable.
- There's a new option in the **Floater's Spectrum mode** that allows you to overlay the previous and next spectra.
- The View -> Plot layouts menu now includes all layouts from the primary *and* associated datasets. Note that selecting an associated-dataset layout will also switch to that dataset.
- The **mineral selection lists** in File->Settings[TSA], the Domain editor and Floater CLS mode have a new right-click menu sub-tree called **Preset selection**. Currently it has only one item: **Sedimentary basin (not metamorphosed)**. In addition, the File->Settings[TSA] list (the Global Active Minerals list) auto-saves a versioned text export every time the list is brought up and some edits are made.
- With a dataset open in TSG, you can drag & drop an .ini (plot layout) file from another dataset onto a main TSG screen to have that layout copied.
- A couple of depth-logging tweaks: The right-click menu includes an option to toggle the current sample's final_mask value, and the linescan magnification loupe works in depth-logging mode (middle mouse button with wheel scroll).
- The log and tray screen class browse / edit dialogs have a new option in the sub-tool for selection / deselection by scalar match: **HAS**. It performs a lexical substring match on the tool's (class) scalar.
- Log screen, class-scalar column: If the class-item text includes an http or https link then a double-click will open a browser on it.
- Here's a document that describes TSG's "headless" mode: ftp://ftp.csiro.au/MMTG/tsg_headless_reference.pdf
- Here's a document that summarises TSG's drag & drop support: ftp://ftp.csiro.au/MMTG/tsg8_drag_drop.pdf

Change log

As usual the change log is here: ftp://ftp.csiro.au/MMTG/`tsglog1617.docx`