What's new in TSG8, 5 September 2018

TSG build 8.0.3.2

The main new items are in "headless" mode, supporting HyLogger-3 wavelength-calibration checking and the automated import of ASD field spectra. There have been a number of other changes but only some detail will be given here. Also see the log file (ftp://ftp.csiro.au/MMTG/tsglog1618.docx) if you are interested.

Note: Again, this build of TSG carries a **dataset version bump**. Older TSG8 versions will not be able to read a dataset that has been created or modified by this one, but remember that **updating TSG8 is free**.

"Headless" TSG

Two new modules have been added to support the automated import of ASD field spectra and spawn a general external application. The TPOLYCAL task has been renamed to PUCKWCAL and upgraded to handle Vis-SWIR datasets too (in addition to TIR ones). The script system has been given looping functionality, and there is now an option to load & run a script without having to schedule it.
The script documentation (ftp://ftp.csiro.au/MMTG/tsg_headless_reference.pdf) has been updated and is current.

SPIMPORT module

This module imports spectrum files to a new TSG dataset or appends to an existing dataset. Presently it only supports ASD binary spectrum files. It offers all of the ASD import and resampling options that are to be found in TSG's interactive import wizard, so it has quite a large set of script commands. (See the script documentation.)
It works in a similar manner to TSG's dynamic import. It checks the specified watchdir directory for any files that may be imported. If there are any files there then they are examined for suitability. If enough pass examination then the import goes ahead: Spectra are imported to a new TSG dataset or appended to an existing one (script options) and, if movedir is given, all of the files in watchdir are moved to movedir.
It can optionally use a script mechanism to pass the name of the TSG dataset that it created / modified to subsequent script tasks.
It has its own looping mechanism as it was coded before the general script looping mechanism was introduced. One would rather use the general mechanism for multiple-task scripts.

SHELLEXEC module

This task spawns another process from headless TSG using Windows' ShellExecute command. It was put into the headless system mainly to allow you to pick up where TSG left off, for example to handle (with some other program that you have) a CSV file produced by the DOWNSAMP task.
Optionally, headless TSG can be forced to wait for the spawned process to finish instead of carrying on in parallel.

PUCKWCAL module

This module is an upgraded and renamed version of the TPOLYCAL module. It does an empirical wavelength check by finding calibration-standard spectra in the dataset(s) and reporting the positions (mean and standard deviation) of selected absorptions. The calibration standard for Vis-SWIR is based on the NIST SRM-1920a standard, and the one for TIR on NIST SRM-1921. (These standards will be issued to NVCL HyLogger-3 operators in due course.) The Vis-SWIR check is very specific to its standard but ***the TIR check should work on any reasonable polystyrene spectra***, e.g., those from polystyrene film on an aluminium reflector.
It looks for and reports on 17 Vis-SWIR absorption features, and 8 TIR features. It builds up one CSV report file for Vis-SWIR and another for TIR. It is best run on many datasets at once, using the script language's "multifile" mechanism, giving one row per dataset in the CSV report(s).

Script looping

Script looping can be enabled with an optional "BATCHLOOP" line at the start of the script file:

BATCHLOOP wait_seconds,loops

It is given with two integer parameters, separated by a comma. The first is a wait time in seconds between loops, and the second is the number of loops (0 for infinite). E.g., BATCHLOOP 3600,12 will run the script 12 times with a pause of 1 hour between each run.
The way things are at present, looping is cancelled if a script task returns an error status.

Scheduling "now"

The script scheduler (File -> Special -> Schedule a script for unsupervised TSG) has a new button **Run now!** Click it and your script will be run straight away by a new, headless instance of TSG. You do not have to provide a time, username or password for this. You can exit the TSG that you are using but don't log off or switch off your computer until the run has completed.
Also remember: You can drag & drop a script file onto the main TSG window. TSG will probably recognise it and bring up the scheduler dialog.

General

TSG7 compatibility

TSG8 was opening certain TSG7 Pro datasets read-only for no apparent reason. This has been fixed.

Profile scalar

The profile scalar has a new parameter in the scalar construction wizard and the scalar-script world. It is called **Min. Depth** in the wizard or **minrad** (minimum relative absorption depth) in the script language. It is a **quality-control measure** based on the profile method's "relative absorption depth" calculation. It is offered for all except the SNR profile types **if local continuum removal is enabled**. When this threshold is active (greater than zero), the profile method will calculate relative absorption depth

(along with the main result that you selected in the Profiler type list) and return NULL if this depth is below threshold.
The profile also has a new Profile type result called **Centroid Minimum Wavelength**, or **centwmin** in the script world. It uses a centroid or centre-of-mass algorithm to estimate an absorption's wavelength-at-minimum. Please note that, like the Extrapolated Bisection method (but even more so), it is of limited use with the sorts of reflectance spectra that we commonly encounter in mineral exploration. My personal advice is to try it on an absorption that:

- Is well-defined such that a meaningful FWHM (full-width-at-half-maximum) can be calculated reliably;
- Spans a good number of spectrometer channels (at least a dozen I would say);
- Has a wide, flattish minimum that gives trouble with other methods.

Stats calculation

The stats-calculation dialog (File -> Calculate stats) has a new checkbox called **Zero the mean!** When enabled, a flat zero mean will be used instead of the data mean, in the calculations and subsequent transforms. It is hoped that a transform calculated with this option will not pull apart "arms" of spectra of the same shape but varying intensity.

Binary ASD import

There's a new option to create import-time TSG scalars from the **instrument serial number** and **integration count** in the ASD headers. Also, the Parse filenames control has been changed from a checkbox to a list, and a new option added to it for extracting **sample numbers** from the ASD filenames and saving to an import-time scalar.
The ASD import documentation (ftp://ftp.csiro.au/MMTG/tsg8_importing_ASD.pdf) has been updated.

General spectral import

Given general ASCII XY spectrum files where the wavelengths have a constant step but go "backwards" from large to small, TSG could mess up and import the spectra the wrong way around. A quick fix was to turn on wavelength resampling but this issue should be resolved now.

Other changes

- Depth logging: "Bounds" calculations have been reworked. (They were problematic when section start / end depth markers were involved.)
- Dialog tagging: Each floater has a different-coloured icon at top-left, and the dialogs that a floater brings up are tagged like it. The Domain editor and its sub-dialogs are tagged similarly.
- TSG's recent-files list now goes up to 16 entries.
- Multiple displays: The positioning of TSG's dialogs and pop-up menus has been given further attention.
- Scatter screen: The virtual [Set weight] scalar that accompanies set scope has been reworked to be like a class-extraction scalar. It used to be the largest single weight found for a sample's [Set mineral] but is now the weight total for all occurrences (all mixing levels) of a sample's [Set mineral]. For a group rather than mineral scope there is an option in File->Settings [Sys] to make it a group rather than mineral weight total.