What's new in TSG8, 31 July 2019
TSG build 8.0.5.1

This release is mostly about new support in TSG related to mineral unmixing. Custom unmixing has been made more accessible, and chemistry (atomic elements) is starting to show a presence.   Aside from that there are some small improvements / changes.   As always, a log of changes is shown in https://research.csiro.au/static/tsg/tsglog1619.docx.

Custom unmixing

It is now easy to extend one of TSG's built-in unmixing libraries with some[1] mineral spectra of your own and generate unmixing results using the combined library. The CLS, TSA and jCLST[2] unmixing algorithms are available, and control over the minerals active in unmixing is offered by the Domain editor.

Here's the documentation:

https://research.csiro.au/static/tsg/tsg_unmixing_with_custom_libraries.pdf

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[1] Even one or two.
[2] Under the right conditions: for TIR unmixing on a production dataset pair that has a TIR part and a VNIR-SWIR-compatible part.

Chemistry (atomic elements)

TSG's central minerals table now includes standard mineral chemistry[3] (and density), and it's starting to find its way into some parts of TSG. For the time being chemistry just has limited support in plots and utilities but may play an active role in unmixing in the future.

Summary screen

The **Level** selection list has a new item **Element** to supplement Mineral and Group. It is available for all Plot types.
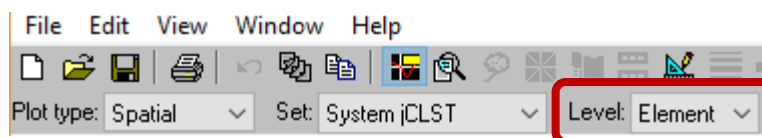
Select it and the unmixing result will be presented in elements. While mineral unmixing weights are relative *volume* fractions[4], relative *mass* fractions are presented for elements.

RD86P016_tsg_tir: Spatial Summary (Bin=3 MaxBin=100% sjCLST 7.07, Mineral Subset)
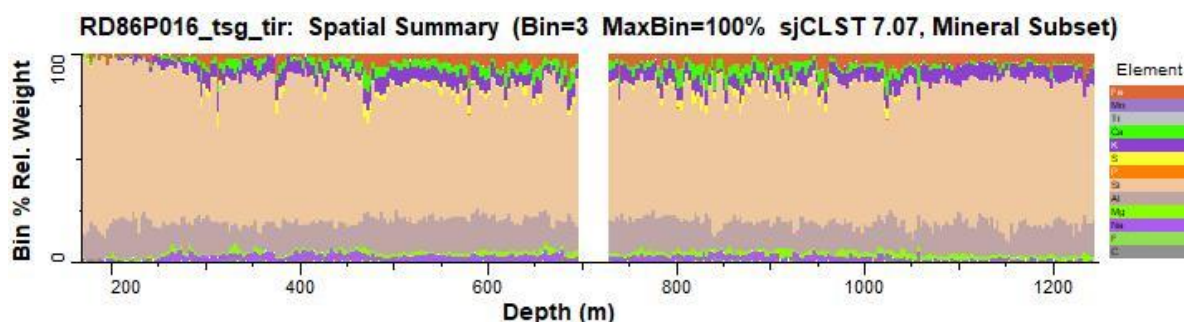
Currently the colour scheme used for elemental Spatial and Difference plots is compatible with JMOL.

Element-level plots work much like mineral and group ones but there are a few things worth noting.

- I recommend that you just stick with Histogram total = **Weight** (menu option). Summary-screen aggregation is convoluted and you won't get much sense out of Count here.
- **Subsetting** controls work for element plots with a couple of differences: The 'NULL item' is never shown and the 'Map junk items to NULL' option hides the display of hydrogen and oxygen.
- **Importantly**, element-level plots are at the mercy of the mineral unmixing results[5] that they are drawn from. They are best suited to **TIR unmixing**. Relatively few minerals are active in SWIR unmixing, and translating just SWIR-active minerals to elements can give a misleading picture.

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[3] TSG currently supports the natural elements from atomic number 1 (hydrogen) to 92 (uranium).

[4] More truthfully, they are relative surface-area fractions at the first level of assumption and relative volume fractions at the second.

[5] And the mineral formulae – currently only standard ones in TSG's central table.

Creating element scalars

Edit -> Scalar sets -> Play out a scalar set into scalars

The Summary screen translates mineral unmixing results to elements on the fly, without making new scalars.

If you would like individual element scalars (one scalar per element) for general use in TSG then there is a new tool that you can use. It is called **Play out a scalar set into scalars** and is launched from the Edit -> Scalar sets menu.

The top 2/3 of the dialog has a selection list of the dataset's[6] scalar sets. Scalars will be created from the one that you select here.
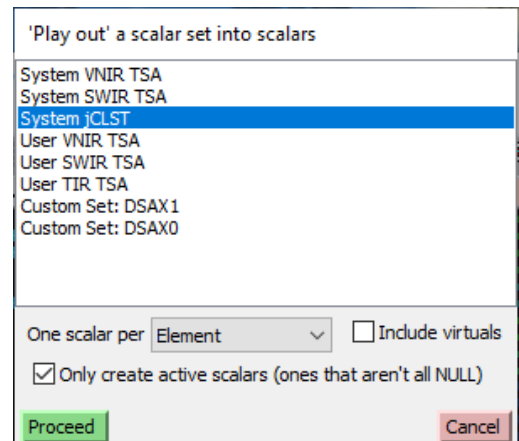
Side trip - not just element scalars

I introduced this tool in the context of elements but there's more to it. It can also 'play out' an unmixing result into individual group, *subgroup* or mineral scalars. As part of their workflow, some analysts have been 'playing out' unmixing results into individual mineral scalars – the hard way. They have had to run copy-processing with a template containing a squad of class-extraction scalars. Hopefully this task will be easier now. Also, subgroup-level unmixing results have not been exposed in TSG until now.

Continuing

- The list labelled '**One scalar per**' lets you select what level of result to play out. The choices are **Mineral**, **Subgroup**, **Group** and **Element**.
- The '**Include virtuals**' checkbox controls whether *non-mineral* items like 'Aspectral' also get played out. (It has no effect when playing out elements.)
- The '**Only create active scalars**' checkbox governs what happens with items that have no valid (non-NULL results)[7]. Some analysts just want active scalars while others want the complete set for all datasets.
  - If you turn this option off then you'll most probably get some empty (all NULL) scalars.
  - 'The complete set' is defined by the selected scalar set's full unmixing library.

This tool will create a squad of numeric import-type scalars in the same display folder as the source set's scalars. For example, if you play out the System jCLST set then you will find the scalars in the System TIR display folder.

If a dataset sample has a valid unmixing result then its scalar values will sum to 1. For minerals, subgroups and groups the scalar fractions are assumed to be relative volume fractions. For elements the scalar fractions are (converted) relative mass fractions.

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[6] Both datasets in the case of a dataset pair.

[7] For example, if you are playing out mineral scalars and the dataset has no valid alunite results, do you still want (all-NULL) alunite scalars? Or if elements and the dataset has nothing with calcium, do you still want a (NULL) calcium scalar?

Re-runs

If you play out a set more than once to the same sort of output (e.g., to mineral scalars) then any existing scalars get re-used.   In other words you *can* update played-out scalars if something about the original TSA result set is modified, but you have to be quite deliberate about it.

Other changes to unmixing support

Floater in TSA mode

Background

In the last release (April 2019), new support was added for spinning off a copy of a normal unmixing result set like 'system SWIR TSA' or 'domained TIR TSA'.   It gives a set of scalars that look like normal imports and do not get updated by TSA / CLS recalculations.   April's release notes had a dot point: 'Soon to come: to reassign individual samples' unmixing results using a TSA Floater in 'multiple result' sub-mode.'   Somehow this has turned out to be true.

The TSA unmixing algorithm computes several unmixing results for a dataset sample. The one that's judged to be the best is taken and saved to scalars.   You never get to see any of the alternative results anywhere in TSG except in a Floater.   If you have a TSA-mode Floater and enable its '**Multiple result (overlay) mode**' menu item then you can browse the best alternatives.   Up to three results are kept at each mixture level.

Looking at the alternative results, an analyst might sometimes feel that the best one wasn't chosen.   TSA / TSG will have selected one according to the numbers but there might be another result (with a higher fit error for example) that makes more geological sense.

The new functionality allows an alternative Floater result to be selected and saved to a spun-off scalar set, overwriting the result there.

What to do

1. Use the **Edit -> Scalar Sets -> Copy a scalar set** tool to make a copy of the unmixing result set (e.g., user SWIR TSA) that you would like to fine-tune.
2. Bring up a Floater, put it in TSA mode, and select 'a compatible' TSA set for it (first items in the floater TSA menu).
   a. TSA sets based on the same library are compatible.   E.g., 'System SWIR' and 'user SWIR' are compatible.
3. Turn on the Floater's **Multiple result (overlay) mode** menu item.
4. Browse the dataset.   Alternative results for a sample are shown in the Floater's Candidate TSA results list.   The one chosen by TSA / TSG has an asterisk on the left.   If you think another result is better:
   a. Select the result you prefer.

b. You will find that the Floater has a new menu item called '**Replace result in user set**'. Use it to select the copy that you made in step 1.

Small changes

Downsampler

There has been a small change that can fall under the banner of unmixing support.

Background

In page 2 of the Downsampler wizard there is a checkbox called **Consolidate scalar sets**. If you leave it on then a special thing happens in the Scalars page (which is usually page 4). For a scalar set like System SWIR TSA for example, the list of 'scalars' gets *two* special entries S_SWIR_TSA705_Mineral and S_SWIR_TSA705_Group instead of the *sixteen* scalars in the set. These entries enable the Downsampler to handle the set's scalars collectively. Some tasks should access all mixture levels in a set, and this is how it's done.

One such task is '**expansion**'. The Downsampler can take a special set entry (or an ordinary class scalar) and write 'expanded' output for it. When generating CSV output you get one column per class *item* (one column per mineral for example). It's a useful tabular report for an unmixing result set. Analysts with large depth-registered datasets often generate 1-metre-binned reports like this.

Expansion can be set individually for each set item or class scalar: Select an entry in the **Scalar** list in the middle of the dialog and then turn on **Expanded**.

### The change (absolute expanded)

Until now the Downsampler would always normalise a row of expanded outputs to sum to 1. Although the **Absolute** button was shown, it changed nothing in expansion. It works now. If you have both Expanded and Absolute on then you will get a **raw (not normalised) output table**. This gives a clearer picture of mineral content in a 1-metre-binned output for example.

jCLST

There have been a couple of small changes to SWIR moderation:
- SWIR now overrides TIR on Pyrophyllite.
- SWIR now overrides TIR on alunites *at the mineral level*.

Miscellaneous
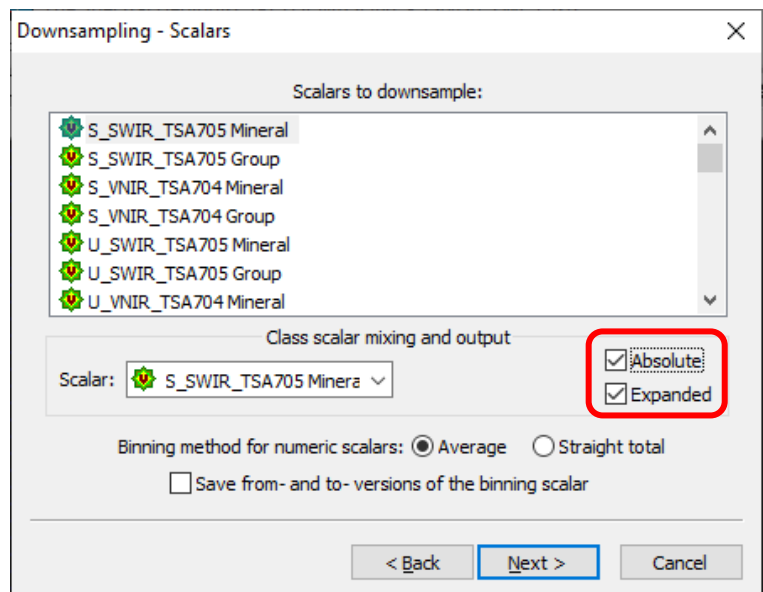
Summary screen

Aside from the new element-level plots, the Summary screen has received some enhancements.

- The **Spatial** plot now has **sample-level tracking** and **current-sample markers**.
- You can now do '**colourbar highlighting**' in Spatial and Difference plots. Left-mouse down over a colourbar block will highlight its samples in the plot.
- The **Subset** sub-dialog has a new checkbox '**Maximum col %**' and accompanying value field. It's best for Spatial and Difference plots. You can use it to exclude 'big' things from the plot so that any patterns in the surviving 'small' things are more evident.
- The coloured tiles in an Overview plot are rendered more faithfully (tile height).

Scatter screen

This one's *big*.

You can now rotate a histogram subscreen clockwise! **<Right-click> -> Hist extras -> rotated clockwise**. Yes! Depth going vertically down the screen like it's supposed to do.

Tray screen

An unpleasant glitch has been fixed in the tray-picture-generation tool, which could fail unexpectedly for no good reason. It should be more stable now.

Headless mode

- The **CLIMPORT** task has received a major update. It can now do HyLogger SDS and SDF imports in addition to Corescan imports.
- The **UPLOAD** task now supports including a dataset's (presumably modified) linescan raster on subsequent uploads, not just the first.

Documentation has been updated.

https://research.csiro.au/static/tsg/tsg_headless_reference.pdf

Feature extraction

- The 'MinMax' algorithm has a new parameter in File -> Settings [FeatEx]. You can now select the spectral layer that drives it. In the past it was always driven by the Reflectance layer but now you can drive it from the second derivative layer (for example) if you like.
- The floater's FFC (feature frequency chart) mode continues to evolve. There have been some subtle changes to automatic range handling.

Log screen

There is a new standard layout option. **<right-click> -> Standard setup -> VNIR, SWIR and TIR TSA**. It sets up the Log screen with 'the best'[8] TSA / jCLST result it can find for each wavelength interval. It is active for VNIR-SWIR + TIR dataset pairs.

Stragglers

- **File -> Dataset Info [Description]** can now handle both datasets in a pair. It has two radio buttons along the top.
- When running **PLS prediction** where some 'input-side' scalars were used in the calibration, some NULLS are allowed in these scalars in the target dataset.
- **Layout copying** – **Summary screen X ranges** are handled a bit more intelligently.
- The main toolbar has a **refresh (⟳) button**. It triggers a thorough refresh.
- The **daily licence check** can offer to **download a new TSG build** (if relevant).

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[8] Domained / User TSA / jCLST if present, otherwise System.