Automating U-Pb IDTIMS Data Reduction and Reporting: Cyberinfrastructure Meets Geochronology

James F. Bowring[1], Noah M. McLean[2], J.D. Walker[3], Jason M. Ash[3]. (1) Col of Charleston, Charleston SC 29424, (2) MIT, Cambridge, MA 02139, (3)Univ of Kansas, Lawrence, KS

Tripoli imports raw data files generated by the Sector 54, Isoprobe, and Triton mass spectrometers. *Tripoli* facilitates interactive visualization of temporal trends and scatter during measurement, statistical filtering of data, point-by-point corrections for isobaric interferences, spike stripping, fractionation corrections and calculation of statistical parameters.

Tripoli is an interactive tool (Win OS) that allows the analyst to correct, save and export processed raw isotopic data. *Tripoli* supports live workflow from a mass spectrometer to aid in monitoring data flows. *Tripoli* provides several types of ratio-by-ratio corrections:

- uranium oxide corrections
- fractionation (U & Pb double spike)
- barium phosphate isobaric interferences
- thallium isobaric interferences

For each correction, the analyst can specify parameters, such as a tracer (see below) or a model of the U sample components. *Tripoli* also supports the tracking of long-term trends in standard measurements and faraday gains.

Tripoli exports the processed isotopic data to reduction software, carrying all applied corrections. *Tripoli* supports PbMacDat, but is designed to communicate in realtime with *U-Pb_Redux* using a publish-subscribe protocol that automates data transmission using extensible markup language (XML) schema and documents.

Live Workflow Automation

Tripoli's novel Live Workflow mode automatically detects new mass spectrometer data and refreshes its display. *Tripoli* lets the analyst inspect the data, discard blocks affected by baselines, choose outliers, and calculate statistics in realtime. A button click transmits this data to *U-Pb_Redux*, which provides a variety of analytical tools to monitor data quality (next panel).

Tripoli provides interactive graphs of each ratio, allowing the analyst to discard outliers, blocks of data, or to utilize built-in filters such as 2-sigma or Chauvenet's criterion. The new statistics are displayed live (see below).

U-Pb_Redux is an open-source Java application for full U-Pb data reduction and uncertainty propagation for any U-bearing phase. *U-Pb_Redux* provides sophisticated graphical and statistical tools for data analysis and compilation, and produces publication-ready data tables, concordia, and weighted-mean plots. U-Pb_Redux outputs standardized analysis results—as an aliquot XML file—for export to the Geochron database. It can also import one or several aliquots from Geochron for compilation, visualization, and detailed analysis.

U-Pb_Redux supports the analyst with aliquot-based fast entry of fraction-specific parameters featuring "fill" buttons and keyboard navigation.

U-Pb_Redux produces user-customized data tables. The analyst can choose commonly-used compositional parameters, isotopic ratios (with the option of Th- and Pa-correction), and correlation coefficients, order the columns in any way, and save the data table setup. Uncertainties can be displayed as significant figures or to arbitrary precision, and values may be forced to display the same digits as the uncertainty. The data table automatically adds pertinent footnotes. *U-Pb_Redux* can export this table to Excel or to publication-quality SVG and PDF files.

Date interpretation in *U-Pb_Redux* is streamlined and interactive. Each analysis is organized in a hierarchical structure in a panel on the left. On the right, the analyst can visualize data as a full color concordia or weighted mean plot, with customizable display options. Multiple weighted means and York fits to the data may be calculated for any subset of the data, with parameters dynamically calculated as analyses are included or excluded by the user.

Sensitivity Testing

U-Pb_Redux makes a major contribution to sample analysis with its innovative Sensitivity Testing interface, shown above. The left-hand panel displays value sliders for every input and its uncertainty. When the analyst moves a slider, the data reduction is re-calculated on-the-fly and the other display panels react accordingly:

A **Concordia Panel** displays error ellipses for all fractions in the aliquot with the current fraction highlighted. The concordia plot is navigable by panning and zooming with the mouse.

B **Uncertainty Breakdown Panel** displays $^{206}Pb/^{238}U$, $^{207}Pb/^{235}U$, and $^{207}Pb/^{206}Pb$ dates with a graphical depiction of the contributions of each input's uncertainty to the date's uncertainty. Correlated errors are shown as positive or negative contributions to the variance.

C **Dates Graph Panel** shows each date with its uncertainty as a red bar representing the data, and a green bar representing the changes caused by the input sliders. The user can select which dates to view and the graph re-scales automatically.

Additional Features

D **Uncertainty Selector:** the user can choose only analytical uncertainty, or add in either tracer or tracer plus decay-constant contributions.

Auto-Uranium: when only the Pb portion of a fraction is present, the user can use independent constraints on the $^{206}Pb/^{238}U$ date to assess discordance and uncertainty budgets. *U-Pb_Redux* can generate dummy U data to predict $^{206}Pb/^{238}U$ and $^{207}Pb/^{235}U$ date uncertainties and plot the simulated ellipse on concordia.

The Cyber Infrastructure Research and Development Lab for the Earth Sciences (CIRDLES) collaboratively integrates *Tripoli* and *U-Pb_Redux* with the efforts of EARTHTIME and EarthChem (Geochron). This collaboration between software engineers and geochemists is a model for other cyber infrastructure efforts.

The cyber infrastructure (above) produced in this collaboration successfully integrates an end-to-end system from sample through analysis and date interpretation to archiving and retrieval of results. This process standardization provides a heretofore missing common data reduction protocol, thus promoting the interpretation of precise geochronology and enabling inter-laboratory comparison. This emphasis on precision aids in time-scale calibration, in understanding processes of crustal evolution and early solar system dynamics.

The screen shot below shows how *U-Pb_Redux* interacts with SESAR and Geochron to publish an XML-schema-compliant sample analysis to the EarthChem database.