Tripoli: New Cyberinfrastructure for Mass Spectrometry

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Abstract

Modern mass spectrometers use digital detection systems and software controls to produce large volumes of digital data – ion beam intensities, isotope ratios, and instrumental parameters. For thermal ionization and solution multi-collector inductively-coupled plasma mass spectrometry (TIMS and MC-ICPMS), analyses are often long, and the large amount of data requires some basic manipulation, like outlier rejection and corrections for baselines, isobaric interferences, and/or internal mass bias correction. The output results are summarized with average values and uncertainties, which themselves become input parameters into further geochemical or geochronological calculations, like estimating nucleosynthetic isotope anomalies or radioisotopic dates.

The software supplied with commercial mass spectrometers is effective at both operating the mass spectrometer itself and providing an initial examination of the data. However, commercial mass spectrometer software does not provide a mechanism for users to interact with the data or save subjective data rejection choices alongside corrections, and it does not adopt newer statistical tools, like compositional data analysis or Bayesian methods.

Tripoli is new open-source cyberinfrastructure built to fit into mass spectrometer laboratory workflows and fill the gaps identified above. It replaces a previous software package of the same name, providing updates to both the graphical user interface, cross-platform compatibility, and integration with new mass spectrometers. Tripoli was designed with community input and developed and tested collaboratively on the GitHub platform.

Recent developments in Tripoli include improvements to LiveWorkflow, where data are streamed to Tripoli immediately as they are measured on the mass spectrometer, producing real-time summary statistics, as well as new Markov Chain Monte Carlo methods applied to Bayesian models of beam growth and decay for both static and multi-dynamic or single-collector measurements. We have also developed native session-based data aggregation and interpretation workflows, which link the data interpretations for a larger project across files that may be stored in distributed locations. Future effort will concentrate on improving ways to visualize and interact with the most sophisticated Bayesian models, which are based on both the measured ion beam intensity data and models for mass spectrometer behavior and noise.



This poster presents decades of collaborative work with Jim Bowring and the CIRDLES lab at CofC.

Mass Spectrometer Software



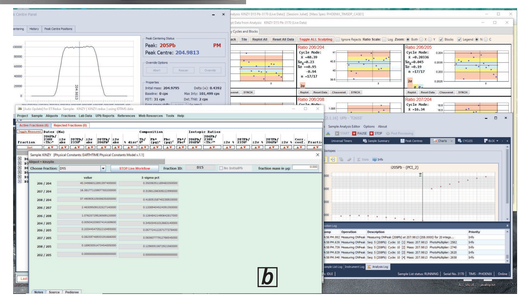
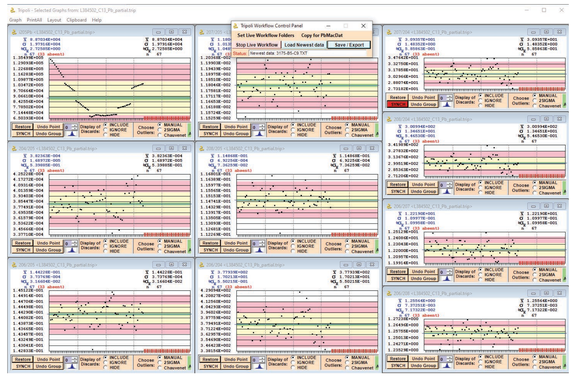


Figure 1.
(a) Older mass spectrometer software documentation for the VG Sector 54 TIMS, including Version 1 and 2 manuals from 1988-1992. The dot matrix printout contained more data than the ASCII files. (b) Modern mass spectrometer workflow, where measured data is immediately reduced to determine whether and how long to run the sample. Manufacturer-provided software (bottom right) is not interactive and has limited data rejection, compilation, and export options.

"OG" Tripoli





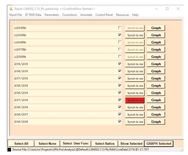
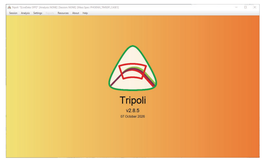


Figure 2. Screenshots of the original Tripoli software, released first as shareware in the late 1990s. Innovations included reading data from Sector54, Triton, and Isoprobe mass spectrometers, automatic isobaric interference corrections and internal normalization, a LiveWorkflow mode that read in data as soon as it was written to the hard drive, and export options that included copy/pasting summary stats to the clipboard or exporting xml files for ET_Redux (U-Pb geochronology software). "OG" Tripoli has U-Pb specific features, but worked for any and all isotope systems. However, it is limited to Windows, uses an outdated Microsoft .NET framework, and is no longer sustainable.

A Modern Refresh (but still Tripoli!)



PIs McLean, Bowring, and Burdick received NSF funding in 2022 to refresh and modernize Tripoli, including designing a new app in Java, which
- provides cross-platform (Mac, Windows, Linux) support,
- adds MC-ICPMS data handling,
- updates statistical methods,
- creates new visualizations, and
- provides new export options.

The new and improved Tripoli is available at GitHub:

New Tripoli Capabilities



Figure 3. Time series plots have been updated with modern graphics, but provide the same summary stats and interactive data rejection. Plots are now infinitely customizable (see Fig. 7).

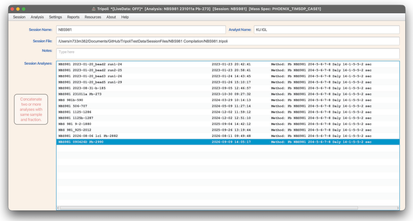


Figure 4. You can now load multiple analyses into a single session, or let them accumulate during LiveData. Export and visualization options work across sessions and facilitate easy navigation. Saved files are now sessions by default.

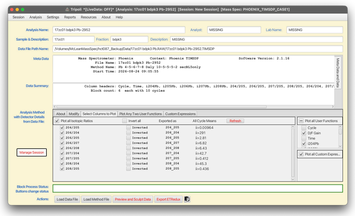


Figure 5. Updated analytical details are more informative and customizable. Select default ratios or intensities to view when plotting, create custom expressions and 2D crossplots of any time series variable vs. another, and record lab metadata. Quick navigation to the session window facilitates rapid inspection of large multi-analysis datasets.

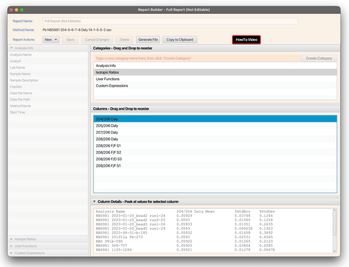


Figure 6. The new, interactive data export builder lets the user choose among all the measured data fields as columns, with rows encompassing any subset of analyses in the session. A report builder lets you drag and drop columns, choose column formats, click and drag to change column ordering, and adjust naming. You can save the report format, and export as a tab-delimited text file.

But Wait, There's More!

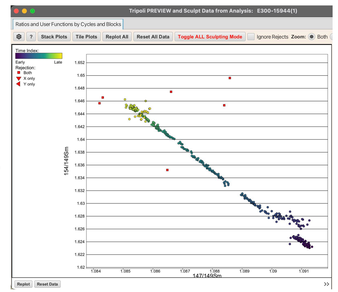


Figure 7. A new "Any 2" plotting feature lets users plot any two time series functions (e.g., intensities or isotope ratios) on x- and y-axes. Each point can be colored by its time index (early to late) and its size scaled by a third variable (e.g., measured intensity, see Figure 3). The same data rejection tools work here, facilitating outlier detection in the presence of expected trends, like the Sm mass-dependent fractionation line shown here. A specific 2D plot can be added by default when every file is loaded from a specified method.

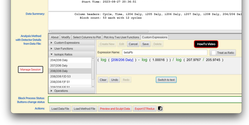
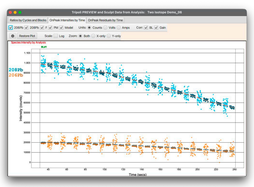


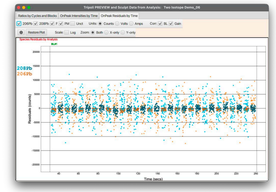
Figure 8. A custom expression builder lets the user build mathematical expressions for important analytical parameters (e.g., internal normalization factors, multidynamic ratios, isobaric interference corrections). The interactive expression builder has drag and drop functionality, and expressions can be saved to load by default for a specified method. Tripoli expressions are editable without reprocessing data in the mass spectrometer software, as for a user function.

Community-Driven Development

Tripoli was developed with input from over a hundred student and professional isotope geochemists, including participants from academic institutions, national laboratories, geologic surveys, and mass spectrometer manufacturers on five continents. Software development efforts involved six undergrad CS majors at CofC.

Conclusions and Future Work





The present:
- A new, updated version of Tripoli is always available!
- Download Tripoli from GitHub, and participate in the ongoing community development process!
- Installation instructions and documentation, including videos, are all online.

The future:
- We are continuing work on development of Markov Chain Monte Carlo methods to model measured intensities (above).
- The goal is to better utilize multiple collectors for more precise beam interpolation and multidynamic measurements.