

Tripoli, U-Pb_Redux, Dzdatabase, and EarthChem: components of an integrated system for archiving, analyzing, and portraying U-Th-Pb geochronologic data

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Introduction

This is an initiative to develop a set of tools for :

- analyzing U-Th-Pb data collected by ID-TIMS, SIMS, or LA-ICPMS
- calculating robust ages and uncertainties,
- gathering all information necessary to fully characterize the age data,
- archiving and sharing the age information,
- integrating age data with other data sets available through EarthChem & related databases, and
- portraying the ages on geologic maps and paleogeographic/paleocontinental reconstructions.

Initial efforts have focused on development of separate modules for each of the above tasks. Future efforts will be directed toward integration of these modules, modification based on community feedback, and enhancement of the system as new techniques and data sets become available. It is hoped that laboratories will be able to operate within this integrated system in such a way that analyzing/reducing/plotting U-Pb data, exporting data into the EarthChem database, and integrating with other existing geologic and geochronologic information will be a seamless and user-friendly procedure.

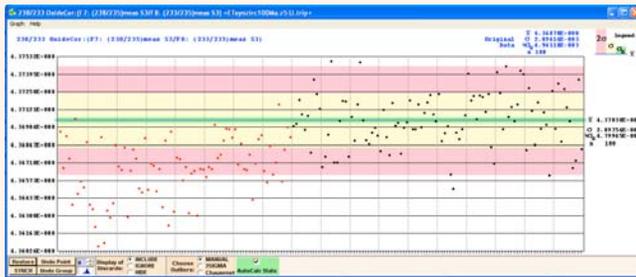
Engineered Software for Data Reduction

EARTHTIME is a community-based effort focused on the calibration of at least the last 800 million years of Earth history. A major goal of EARTHTIME is to assess and improve inter-laboratory agreement, enabling geologists, stratigraphers, and paleontologists to make detailed comparisons between published geochronological datasets. A universal approach to the treatment and reduction of isotopic data is imperative; for U-Pb geochronology, this means free, publicly accessible software that transparently and quickly navigates from inputs to outputs.

Tripoli

Data processing begins with *Tripoli*, which imports raw mass spectrometer data files and supports interactive review of the isotopic data. This new tool facilitates visualization of temporal trends and scatter during measurement, statistically rigorous filtering of data, and calculation of statistical parameters. *Tripoli* recognizes and reads data files generated by the Sector 54, Isoprobe, and Triton mass spectrometers. In addition, *Tripoli* permits ratio-by-ratio U and Pb fractionation correction using a double spike, as well as automatic U oxide correction. Each lab may customize their copy of *Tripoli* by entry of tracer and oxygen isotopic compositions, and certified EARTHTIME tracer data are provided online.

Tripoli is designed to export this user-reviewed isotopic data to data reduction software, recording the oxide and fractionation corrections applied. *Tripoli* also provides for the creation, import and export of utilized tracers as XML files. At present it can export to PbMacDat, but within the next few months *Tripoli* will export data to a forthcoming U-Pb data reduction program called *U-Pb_Redux*.



Engineered Software for Data Reduction (cont'd)

U-Pb_Redux

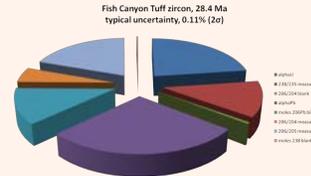
U-Pb_Redux is an open-source Java-based application being developed for the EarthChem and EARTHTIME communities for full U-Pb data reduction and error propagation for any U-bearing phase. The program will provide sophisticated graphical and statistical tools for data analysis and compilation, and produce publication-ready data tables, concordia, and weighted-mean plots. U-Pb_Redux also produces a standardized output detailing analysis results—as an aliquot XML file—that it can export to the NSF-sponsored community EarthChem database. It can also import one or several aliquots from EarthChem for compilation, visualization, and detailed analysis. U-Pb_Redux is compatible with a variety of platforms, including Windows, MacOs, Linux, and Unix.

U-Pb data reduction, done transparently:

- U-Pb_Redux is an open-source community program that implements common algorithms and uses common tracer data, so everyone's on the same page

- Eliminates the black box that turns data into dates—all calculations and error propagation are done explicitly, right in front of you

- Results are displayed graphically to guide learning and future efforts toward higher precision



Example output, showing contribution to error in age from different sources. After Schmitz and Schoene, 2007

DZdatabase

Development of a database for archiving and accessing U-Pb ages of detrital zircons is an urgent need within the Earth Sciences community because of the recent explosion of interest in this technique, and because of the development of methods that generate U-Pb ages very efficiently. We are accordingly in the process of developing a module that will allow labs to directly export U-Pb ages into the EarthChem database. Critical input parameters for each analysis are as follows:

- Sample name and metadata (from IGSN)
- Laboratory, analyst, method (SIMS, TIMS, ICP), and reference describing method
- Interpreted sample age, uncertainties (analytic, systematic, total), and MSWD (only for set of cogenetic analyses)
- Decay constants used
- Blank and spike info (for TIMS), primary and secondary standard info (for SIMS & ICP)
- Analysis info (mineral analyzed, abrasion?, leaching?)
- Measured isotope ratios and uncertainties
- Calculated concentrations and uncertainties
- Calculated isotope ratios and uncertainties
- Calculated ages and uncertainties
- Data reduction parameters (common Pb correction method, initial Pb composition and uncertainty, collector type, instrumental fractionation, etc.)
- Comments about the analysis

EarthChem

EarthChem is a community driven project to facilitate the compilation and dissemination of geochemical data of all types. The project is active at building a home for future data contributions by working with authors, societies, and publishers as well as government organizations. In addition, the EarthChem project responds to community needs to facilitate compiling and serving data.

A recently identified community need is in the area of geochronology. At the GeoEarthScope town hall meeting held in association with the 2006 GSA National Meeting in Philadelphia, attendees discussed the necessity of a home for geochronology data collected by that project. Consensus opinion of group attendees and organizers was that EarthChem should be the organization group to provide data management for data collected in association with GeoEarthScope, storing and serving geochronological data submitted by participating facilities. Such a management system would be useful to other workers in geochronology. This emphasis was endorsed by the EarthChem advisory board at its 2006 annual meeting with the caveat that it be designed to facilitate geochronological contributions from the larger Earth Sciences community.

Two workshops were held in 2007, one for the U-Pb community (in conjunction with EARTHTIME) and the other for the (U-Th)/He community. Reports on these workshops are available at: <http://www.earthchem.org/earthchemWeb/workshops.jsp>. Two more workshops were held in 2008 for Ar-Ar geochronology and cosmogenic nuclide dating involving the EARTHTIME and CRONUS groups, respectively. Reports for these workshops are forthcoming. Interestingly, the overall structure for communication and organization has been very similar across the various groups. The main differences has been in the level of documentation and reporting items.

At present, EarthChem and EARTHTIME researchers are developing a seamless Java-based system for release in 2008. Likewise, an Excel-based sheet is under active development for the (U-Th)/He community. The data system for the cosmogenic nuclide group will probably be based on on-line calculators being developed under the CRONUS group. Lastly, the system for Ar-Ar will utilize two existing data reduction programs that are very widely used, and is being done using previous EARTHTIME results.

The main portal for the geochronology system will be hosted by EarthChem. Searches will be flexible in that they can be done by location, age, or method. We anticipate that the searches can return results obtained by multiple methods facilitating geochronological, thermochronological, and provenance analyses.

Potential Applications

U-Pb ages from detrital zircons are providing useful data for a variety of geoscience applications including plate reconstructions, regional tectonic models, paleogeography, paleodrainage evolution, and sandstone composition. Constraints for these applications are provided by the age spectra of the detrital zircon samples and by the ability to relate these spectra to original source terranes. Our goal is to provide data format options for output to standard tools for these kinds of applications.

Following is an example of the type of output that we hope to develop through integration of the database modules. Shown are provenance patterns inferred from ~500 U-Pb age determinations on ~40 samples of Triassic through Cretaceous strata in the western US.

