EarthChem/IEDA Workshop on Geochronology for Ion Microprobe

Stanford University, Stanford CA
September 9 2011, 8:30am to 5:00 pm

Report compiled by Doug Walker,

Participants:
Doug Walker, Joe Wooden, John Aleinikoff, Bill Davis, Rita Economos, Ken Ludwig, and Jorge Vazquez.

Background
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 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 and thermochronology data collected by that project. Consensus opinion of attendees and organizers was that EarthChem should be the group to provide 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. EARTHTIME, for example, strongly endorses EarthChem's leadership in this regard and will work to encourage members to contribute data. This emphasis was endorsed by the EarthChem advisory board at its 2006 annual meeting.

Goals
Goals of the meeting were to address important issues for creating a home for data related to Ion Microprobe dating.

a. Establish reporting requirements including metadata and classes of measured values.
b. Identify and evaluate methods of data entry and output that will work for the community.
c. List the important requirements of a geochronology website.
d. Plan approaches and actions for moving forward with the effort.

Workshop Summary

The workshop group focused most of its effort on identifying the important items that must be reported for Ion Microprobe geochronology. This is a relatively mature community with only two major NSF funded laboratories in the US (UCLA and Stanford) involved in geochronology by this method. Both laboratories were represented at the meeting along with lab users and software provider.

The group addressed the need for an easy path for data entry. Although contributors to a database can enter parameters directly into a spreadsheet or web-based form, the group considered that the most appropriate route would be to take output directly from data reduction programs/spreadsheets. The community uses essentially two data reduction programs to compute dates and interpret ages. One is the SQUID package written and support by Ken Ludwig at the Berkeley Geochronology Center. This package is used in the Stanford Lab. The other is ZIPS used at the UCLA lab. Both programs provides most of the information for both data and metadata that should be reported.

The group considered that with some additional metadata and documentation of age interpretations that the path for data entry into a geochronology database is relatively straightforward. The main path for entry would be entering some information either in a web form or in a file and then uploading files associated with the data reduction program and the data collection program.

Approaches

A basic recommendation of data reporting is that there should be an IGSN for each sample. To this end, the data entry system will ask for the IGSN identifier. This can be done with a link to the SESAR site during data entry/upload if the IGSN is not present. If present, the IGSN will be verified against the database. It is important that users be able to establish their own IGSN for host samples in the field. The group endorsed having users come to the laboratories with the identifiers in hand.

The database itself will be built on XML using a schema that preserves the critical data and metadata. This will allow other parties to access the data through the XML if needed; the creation of the XML schema is critical to maintaining interoperability. Upon upload, the user/contributor will be asked to give age interpretations, the purpose(s) of the analysis, and upload files. These files will consist of either the SQUID reduced data and session file from the machine, or the ZIPS (UCLA output) data age file and the ascii files recording data for each spot. In this way the data will be archived and available for users to examine in more detail. Images of individual grains and/ spots can be uploaded as well.

The group understands that the Ion Microprobe geochronology database will be one of several component data types to the Geochron system. The use of an IGSN identifier will ensure that samples analyzed by different methods can be tied together in the future. For example, the participants considered the potential value in comparing high- and low-temperature chronometer ages especially appealing, in light of the potential to make powerful new interpretations of locations and regions.

Lastly, the user interface needs to allow complex queries and tailor the output of such queries to the need of the user. For this reason, the interface must allow for simple display and download for casual/non-geochronologist users (probably the vast majority) and complete and rich interactions for experts.

Next Steps

Considering the approaches listed above, the participants recommended the following next steps to move the process of creating a geochronology database. We anticipate that these steps will be done over the next 6 to 24 months.

1) Prepare and circulate the report of this workshop. The report will be posted on the EarthChem/IEDA and EARTHTIME websites as well as being emailed to a list of critical data providers. This will allow for community comments on the critical reporting items included in the attached table.

2) Start developing the XML schema. This will be done by taking the list of critical items combined with some sample data to create a structure. The schema should allow for efficient search and retrieval. The schema will be normalized to the extent needed by the amount and complexity of potential data. Exploration of existing schemas (such as OGC and GeoSciML) will be done to further foster interoperability. Jason Ash (EarthChem programmer) will work on this effort in conjunction with Ken Ludwig and Rita Economos, who will provide reduction program output.

3) Test data upload and refine user interface as needed. Establish the best formats for output. Work on the search interface options.

EarthChem Workshop on Geochronology – Ion Microprobe

Green Earth Sciences Building, Stanford University – September 9, 2011

Agenda

8:30	Overview of Geoinformatics, data reporting, and examples. Demonstration of EarthChem and Geochron systems. Putting archiving into the workflow.
9:30	Discussion of reporting requirements for U-Pb data. What are the critical items that must be reported? What about unique identifiers?
11:00	Demonstration of Geochron data entry using U-Pb_Redux.
11:15	Discussion of how data entry and submission should work for Ion Probe methods. How much do current reduction programs capture? How do legacy data and new data differ? Do data reduction programs contain enough metadata? What level/depth of data documentation is needed or desirable? Are other elements important?

Lunch (12:00 – 1:00)

1:00	Continue discussion
2:00	Demonstration of EarthChem plotting and maps Demonstration of Geochron.
2:15	Nature of U-Pb geochronology website and geochronology websites in general. What ways do providers and users want to interact with the data? Is it critical to allow reprocessing of data at some level? What sorts of age calculation utilities are needed?
4:00	Discussion of how the website should link to the rest of geoinformatics. What links are needed? What other groups should be involved? How integrated must this be with the main site? How should data be searched?
4:30	Wrap up and listing of goals. Identify next steps and key providers/users to move the effort forward.
6:00	Group dinner at a local restaurant