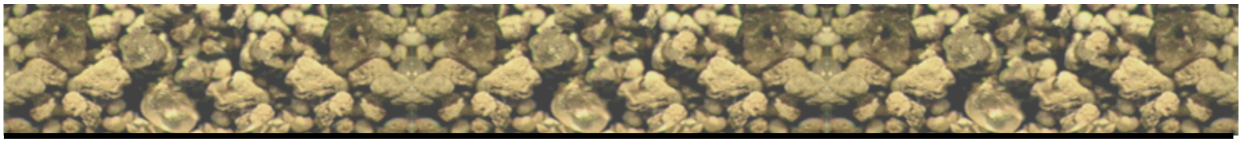

Linking Information Systems in Marine and Terrestrial Geosciences:

Sediment Geochemistry

Workshop Report

Washington, DC
June 3 – 4, 2004

supported by the National Science Foundation

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Workshop Summary

The Workshop "Linking Information Systems in Marine and Terrestrial Geosciences: Sediment Geochemistry" was convened in order to bring together researchers and information technologists to discuss options, requirements, and specifications for the design of digital information systems that will support and maximize the application of geochemical data on continental and marine sediments to a wide range of research topics, from the chemical evolution of the Earth's crust and mantle to paleoclimate reconstruction. Special emphasis was placed on identifying the advantages, requirements, and challenges of linking and integrating geochemical data and other data types from marine and terrestrial environments. The goal was to generate a set of recommendations on how to move forward with the development of digital information systems including databases as well as analysis and visualization tools that will fundamentally impact the way in which geochemical data of sediments are used for research and education.

The workshop was attended by 34 participants who met for 2 days at the Joint Oceanographic Institutions in Washington, DC. The agenda included (a) presentations that provided participants with an overview of ongoing efforts within the marine and terrestrial community and within the information technology community that are relevant to the development of a comprehensive information system for the geochemistry of sediments and to issues such as interoperability, data integration, and visualization, (b) breakout sessions during which participants were able to focus in small discussion groups on various aspects of system design, and (c) plenary discussions to evaluate recommendations from the breakout groups with the entire audience.

Participants placed a high priority on the development of a database system as soon as possible, for all geochemical and taxonomic data of all sample types such as whole rock, mineral, leachate, residue, and size fractions. The database should include sufficient metadata, to be both comprehensive and practical to use, and that allow for data evaluation and possible re-evaluation. A key objective would be the seamless integration of datasets from multiple data repositories to make them accessible through a common interface as part of a networked distributed information system. Implementation of unique sample identification was strongly recommended as a fundamental requirement for such data integration.

Rationale

The Geoscience community is increasingly taking advantage of the exciting opportunities that state-of-the-art and cutting edge information technologies (IT) offer to efficiently apply a rapidly growing quantity of observational, measured, and computed data to science and education. Projects are being developed on various scales to improve the preservation and management of the data, to provide easy access to these data for all interested audiences from researchers and educators to students and the general public. There are increasing attempts to link and integrate related data types in order to facilitate their analysis and to support new cross-disciplinary approaches to scientific questions. The development of digital information systems that make use of rigorous data management technologies, interchange tools such as markup languages and web services, knowledge networking, data mining, and sophisticated visualization tools can have a major impact on the application of geochemical data in research and Earth science education, as shown by systems developed over the last decade for geochemical data for igneous rocks.

Sediments are the fundamental record of the history of the Earth, and a primary paleoclimate record on the Earth. Scientific investigations of sediments have important implications for the understanding of the way the Earth works now and in the past. Greater accessibility of geochemical data of sediments will enhance integration of diverse types of data in order to better understand the Earth system. For example, such accessibility will facilitate comparison of global circulation models with climate data, and will aid in determining the possible effects of human actions on global climate change. Such understanding will form the basis of government policy decisions.

Sediment data have potentially a large educational audience, and can be applied to many fields associated with Earth history, tectonics, the atmosphere, life, and climate. By making scientific data easily accessible to students, they are being used in courses, and giving Earth science students new appreciation for manipulation and interpretation of data.

Within the Geosciences, data management systems are frequently built with limited scope and objectives defined to satisfy the immediate needs of specific disciplines, communities, and programs. While this clearly is the preferred approach to maximize the usefulness of the systems and encourage participation and support of the community, it may lead to redundant development efforts and divergent data standards. Such “artificial” separation of equivalent types of data can make the application of the full data set to broader and global questions more cumbersome. One such separation has occurred along the ‘waterline’ into systems for marine data on the one hand and terrestrial data on the other. An example is the division of geochemical data for igneous rocks in three separate databases – PetDB for the oceanic crust, NAVDAT for the Western North American continent, and GEOROC for ocean islands and convergent margins. All three databases handle identical data and metadata, and they all use the same database schema developed by PetDB and GEOROC (LEHNERT et al. 2000), but the data sets are isolated from each other and there is currently no way to explore the complete data set at once.

First steps to work across the waterline are taken by CHRONOS (www.chronos.org) with respect to paleontologic data. CHRONOS is partnering with PaleoStrat (www.paleostrat.com) to build chronostratigraphic and sedimentary geologic databases for the Earth sciences. However, neither of these efforts have developed modules for geochemistry, petrology, etc. that target both marine and terrestrial data. In addition, there is the JANUS database and various smaller ones hosted at Scripps, Woods Hole, and Lamont that neither cross the waterline nor are interoperable.

Due to the success of the igneous databases, which have become important tools in that research community, the organizers decided that an intensive debate on the needs surrounding relational databases that would serve the sediment research community was overdue. This workshop was organized in order to initiate an open and broad-based discussion with the purpose of identifying the needs of the community working with sediments. It was hoped that such a meeting would generate support for the development of information systems to enhance access to geochemical data for marine and terrestrial samples, and to integrate the geochemistry with other essential data such as stratigraphic information and geochronology.

Workshop Objectives

The goals for the workshop were identified as threefold:

1) Educate participants:
   a) Educate scientists about ongoing projects in sediment and igneous data and geochemical data management, and about IT options and requirements to build interoperable and integrated systems;
   b) Educate IT experts about the needs of the science community.
2) Define requirements for a data system such as:
   a) What data/metadata need to be included?
   b) How far do we need to integrate marine and terrestrial data?
   c) What is needed for integration and interoperability (data standards, ontologies)?
   d) What tools for map interfaces, visualization, and data analysis need to be integrated?
3) Community building: Begin the process of developing a community consensus on how to approach a truly integrated marine and terrestrial information system:
   a) Should it be a centralized or a distributed system?
   b) How do we agree on and implement policies for data sharing, data publication, data reporting?

The ultimate goal for this workshop was to agree on a set of recommendations on how to move forward with the development of digital information systems, including databases as well as analysis and visualization tools that will fundamentally impact the way in which geochemical data of sediments are used for research and education

Workshop Structure

Location

The workshop was held at the offices of the Joint Oceanographic Institutions in Washington, DC. We are grateful to JOI for generously providing the meeting facilities.

Participants

The Workshop was attended by 34 participants, which included researchers from 18 universities and research institutions, the US Geological Survey, NOAA, the Kansas Geological Survey, and the Japanese Agency for Marine Earth Science and Technology, as well as 5 representatives from the NSF Division of Geosciences (both EAR and OCE were represented). The workshop included researchers currently involved in active and developing geochemistry and sediment database efforts that include:

- PetDB (Petrological Database of the Ocean Floor)
- NAVDAT (Western North American Volcanic and Intrusive Rock Database)
- CHRONOS (Interactive Network of Data and Tools for Earth System History)
- JANUS (Database for the Ocean Drilling Program)
- J-CORES (Shipboard science database for the Japanese Ocean Drilling ship CHIKYU)
- Marine Geoscience Data Management System (including the MARGINS Data Management System)
- PaleoStrat (Paleontologic and Stratigraphic Information System)
- dbSEABED (Database for Coastal-marine Substrates on Global Scales)

The Workshop also included information technology (IT) experts from organizations involved in IT development in the geosciences, including representatives from

- GEON (Cyberinfrastructure for the Geosciences)
- CIESIN (Center for International Earth Science Information Network)
- KGS (Kansas Geological Survey)
- SDSC (San Diego Supercomputing Center)
- Information Technology & Systems Center, University of Alabama at Huntsville
- National Geophysical Data Center, NOAA

A large number of attendees were researchers in igneous geochemistry that use the igneous databases, and researchers in paleoclimate who have no access to equivalent databases. A list of all participants can be found in Appendix 2.

Agenda

An Icebreaker Party sponsored by the Lamont-Doherty Earth Observatory was held the evening before the actual beginning of the Workshop, giving participants the opportunity to introduce themselves and begin discussions in a relaxed atmosphere. The actual Workshop lasted 2 days, ending on the second day at 3 pm. Roughly one third of the time was devoted to short presentations that provided participants with an overview of ongoing database efforts within the marine and terrestrial research communities, and within the IT community. These were relevant to the development of an information system for the geochemistry of sediments, and to issues such as interoperability and data integration (see Table 1). Two-thirds of the workshop were assigned to breakout sessions during which small groups of participants were charged to discuss various aspects of sediment geochemistry data management and recommend draft specifications for a system, and to plenary discussions to summarize and synthesize the results of the work group sessions in a well-defined recommendation for the future of data management for sediment geochemistry.

The agenda of the workshop is given in Appendix 1. Workshop presentations are posted on the workshop web site at http://www.seddb.org/workshop/index.html.

Workshop Results

Breakout discussions

Four different breakout discussions were convened throughout the workshop:

- *What are the needs of the Paleoclimate community? (Data types, metadata, access, QC, etc.)*
- *What are the needs of the Global Fluxes community? (Data types, metadata, access, QC, etc.)*
- *What are the requirements, possibilities, & challenges for integration of marine and terrestrial data systems?*
- *Practical steps for implementing an integrated system for sediment data (two parallel breakout sessions)*

Each one of the breakout groups was chaired by two workshop participants who presented a summary of the discussion in their group during a plenary session.

1. What are the needs of the Paleoclimate community?

The paleoclimate group breakout session had a wide-ranging discussion on what this community would expect from a database, and concluded that an ideal database would include all data archives relevant for paleoclimate, including marine sediments, lake sediments, terrestrial sediments (marine sequences exposed on land as well as paleosols and fossil plant archives), ice-cores, sediment traps, rivers, cave deposits etc. It should include all types of relevant physical and chemical data and metadata that would facilitate scientific interpretation and help to identify opportunities for further work. The group concluded that not all the data has to be administered at one site (location) but links to relevant databases and coordination between databases (identical format and interface) are needed.

2. What are the needs of the Global Fluxes community?

This group was mainly composed of the high temperature petrologists and geochemists, who have been using the currently available igneous geochemistry databases. They noted that the availability of sea floor basalt and peridotite data through PetDB and global volcanic rock data through GEOROC and NAVDAT has had a major impact on this field. Currently, an investigator studying a region of convergent margin volcanism can obtain relevant data on the arc lavas from GEOROC or NAVDAT, and on ridge or back-arc lavas from PetDB. However, data on sediments and fluids associated with subduction zones are currently unavailable through any of the geochemical databases. The group emphasized the need to fill this gap, noting that these data are crucial for interpretation of arc magmatism and on global fluxes from the surface to the deep Earth. They also noted the tie between sediment geochemistry, tectonics, and erosion and suggested the Himalayan margin as a focus zone; emphasized the importance of loess and composite samples (samples that are mixtures of individual samples) because they reflect the average compositions of large areas. They noted that it would be important to include platinum group elements and osmium isotopes to characterize extra-terrestrial vs terrestrial fluxes, and the importance of coal/carbonate inventories over time.

3. What are the requirements, possibilities, & challenges for integration of marine and terrestrial data systems?

This group was composed mainly of IT developers and discussed issues related to the integration of data sets and development of interoperability among systems. The group noted that from a technical point of view the integration of terrestrial and marine dataset does not pose significant problems and that these datasets are comparable. The major challenges for data and system integration are generic to the development of a broad science cyberinfrastructure and encompass formats for linking databases (including metadata standards), consensus with publishers regarding metadata, formal documentation of system interfaces such Interface Control Documents (ICD) as recommended by the Interoperability Challenge Workshop), interfaces with tools and resources, and the data acquisition process.

4. Practical steps for implementing an integrated system for sediment data

By the end of the *first* day of the workshop, the overall consensus among the workshop participants was "We need a data management system for sediment geochemistry equivalent to the igneous rock databases. The task is big. **Don't just keep talking, let's get started getting it done**." Responding to this recommendation, on the second day of the workshop we established two breakout groups, which were both given the charge to recommend 3-5 action items related to the implementation of an integrated data management system for sediment geochemistry. Discussions focused on the most important features of the system including specifications for data and metadata as well as organizational issues. Both groups recommended to start with 'a low-hanging fruit' such as ODP data reports in a pilot project, to apply the PetDB schema while at the same time adhering to international and federal metadata standards, to carefully evaluate dependencies on existing data resources, implement data submission capabilities that make community contributions of data easy, and to establish a system for unique sample identification.

General recommendations of the Breakout Groups

The following list is a compilation of all recommendations from the breakout groups. Many of the recommendations were provided more than once from different breakout groups.

- ***Scope of data management system:***
    - The DMS should include data for marine sediments, lake and river sediments, ice cores, speleothems, soils, corals, and soon to be sediments (sediment traps, water column concentration data, aerosol concentrations), as well as pore fluids.
    - A sedimentary database should include unpublished as well as published data, as long as the data are well documented with appropriate metadata and attributed to an investigator.

- ***Data types:***
    - Scientific data includes chemical data, lithological data, physical properties, and taxonomy.
    - Chemical: major, minor and trace elements, stable and radiogenic isotopes, gases, organic compounds.
    - Ages (see below).
    - Lithological: sediment characterization (carbonate, biogenic silica, terrestrial, organic matter, cosmogenic, volcanic ash, etc), grain size, sedimentary association (lamination, bioturbation) etc.
    - Physical properties: dry bulk density, porosity, grape, color, magnetism, etc.
    - Taxonomy: all identifiable species and groups macro and microfossils and trace fossils.
    - Images of the samples and taxa.
    - "Derived data" should be included, such as paleo-temperature, salinity, pCO2, total CO2, pH, paleodepth below sea-level, paleolocation.
- ***Metadata***:
    - Basic metadata such as location, depth below sea level, and the depth of samples in a core should be mandatory
    - Sample type, sample ID, collection date, PI are essential.
    - Samples should have a unique and consistent identifier in order to identify work done in different labs or at different times on the same sample.
    - Images of the samples and taxa should be included whenever possible.
    - With the existence of these databases there is a greater need than ever before to be able to compare data between laboratories. Along with geochemical data, users should be able to access analytical metadata, which should be comprehensive enough to give users the ability to evaluate data quality. This should include PI, lab, analysis date, methods of analyses, instrument, errors, specific description and information about quality of the data.
    - Information about how samples were treated before analysis should be part of the analytical metadata.
    - If there is a way to determine sample availability, it should be included in the database
    - Most importantly, links to published papers where data was produced and used should be included.
- ***Data model:***
    - The igneous databases PetDB, GEOROC, and NAVDAT have served the needs of the igneous community and should be used as a model for a sedimentary database, taking into account the special needs of sediments. A primary consideration is the importance of ages (discussed in more detail below). Output from a sedimentary database should be easy to integrate with that of the igneous databases.Sample definition: The ambiguity of the concept of what is a "sample" needs to be addressed. In association with a single depth in a deep sea core, there may be a large number of

"samples", such as the "bulk", size fractions, leachates, different species, organics, etc. All of these need to be taken into account, and subsamples of larger samples should appropriately linked.

- Composite samples (mixtures of many samples) should be included

- ***Ages***: The question of how to deal with sample "age" is a fundamental and very complex issue.
  - The basic data to be included in the database should include the original published chronology.
  - Nevertheless, it is fundamentally important to be able to access and apply updated age models. For example, a search should be able to access data for a specific region "between the ages of X to Y", but the chronology should be able to evolve with time. In this context it must include a tool for reevaluating age models and remapping the ages onto the sediment geochemistry data
  - It must include primary chronological control points.
  - Raw data used to determine the ages should be included (micropal, magnetics, isotopes, ^{14}C, $\delta^{18}O$, Sr, U series etc).
  - References to published age models and chronology for each sample.
  - All ^{14}C ages in the database should include the official sample identifier.
  - There should be significant interaction with CHRONOS.
- ***Interface functionality***:
  - *Necessary query types:*
    - Find data by region – coordinates, basin, region.
    - Find data by depositional or paleodepositional environment (grain size, depositional structure).
    - Find data by paleoposition.
    - Find data by depth below sea level.
    - Find data by age – absolute age (years), age range (2-20 myr) or geological time (Miocene).
    - Find data by biostratigraphic age,
    - Find data by section thickness, deposition rate.
    - Find data by provenance (inherited components).
    - Find data by sample type or lithology – bulk sediment, terrigenous fraction, sediment trap, mineralogy, carbonate, corals, ash, macro/micro fossil species, grain size, pore fluid, leachate.
    - Find data by taxonomy (e.g. species abundances, ratios, and derived data)
    - Find data by physical properties (density, porosity, mst parameters)
    - Find data by analysis type – mineralogy, chemistry (e.g. % carbonate, % sulfate, Ti, REE, stable isotopes, Sr isotopes, alkenone, etc.)
    - Find data by ratios of biogenic, detrital, authigenic components
    - Find data by lab, investigator, date of collection, instrument

        - Find data by combinations of the above (e.g. $\delta^{18}O$ on g. sac. from the North Pacific from MIS 2 to MIS 11 from John Doe's lab since 1992).
    - *Analytical tools:*
        - Tools to reconstruct paleo-locations and paleo-environments.
        - Age tools: stable isotope stratigraphy, sedimentation rates, biostratigraphy, sedimentology.
- ***Integration of Marine and Terrestrial Data***
    - Data for marine and terrestrial sediments should be integrated.
    - There are no major differences in metadata requirements for marine and terrestrial data.
    - Start with marine data, but anticipate future correlations with terrestrial data. Build the system in a way that it can accommodate terrestrial data.
- ***Linkages & Interoperability***
    - The sediment database should be linked to underway geophysical data, core location data, repositories, oceanographic and atmospheric climatologies, etc. Thus there should be an emphasis on using available online data through linkages with other databases containing sediment data such as JANUS, NGDC, Paleostrat, MARGINS, CHRONOS, Marine Curator's Database.
    - The sediment database should take advantage of data available through CHRONOS, but should not depend on CHRONOS.
    - The sediment database should mesh with existing metadata standards.
    - Interaction with dif community should be ensured.
    - Interface Control Document (ICD) should be established for the system.
- ***Other recommendations and issues:***
    - Set up a system that would easily input of new data as it becomes available.
    - How can we enforce submission of data by PI's? The use of the power of funding agencies to require submission of data was endorsed.
    - Data that are used in publications but until now have not been included in data tables (including, for example, much of the stable isotope data used for stratigraphy and paleoclimate interpretations) should be submitted to databases.
    - Journals should be encouraged to enforce strict standards for including the appropriate sample and analytical metadata in publications.
    - All papers and all investigators need to be appropriately credited.
    - The global fluxes group maintained that a metasedimentary database is needed, and suggested that until a metamorphic database is available, metasediments should be considered as sediments.

Action Items

Agreement was reached in the final plenary session on the following action items:

- Begin the process of generating a sedimentary database as soon as possible.

- Define the scope for a beginning:
    - Start with a marine database, setting it up to be able to easily incorporate new data.
    - For legacy data, focus on data associated with ODP and DSDP cores, plus a few focus regions.[1]
- Set up a system of unique sample identification so that different types of data measured in different labs at different times on the same samples can be linked.
- Keep the community involved. Town Hall meetings at major meetings such as AGU and GSA, appoint an advisory board.
- Generate of a plan to keep age models updated.

Dissemination of Results

The outcomes of the workshop were presented by K.Lehnert at the following workshops and conferences:

- "CHRONOS Geochemical Cycles" workshop in San Antonio, TX, June 2004,
- GeoSystems Workshop in Arlington, September 2004,
- MARGINS Steering Committee meeting at the Lamont-Doherty Earth Observatory, October 2004,
- AGU Conference Fall 2004 in San Francisco at the MARGINS Town Hall meeting
- EGU General Assembly in Vienna, Austria, April 2005.

Together with the organizers of the 'CHRONOS Geochemical Cycles' workshop we published a joint meeting report "Joint Discussion of Sedimentary Geochemistry Data Management Systems That Cross the Waterline" in EOS in November 2004 (Cervato et al., 2004).

Information about the workshop including all powerpoint presentations, and workshop outcomes are accessible at the SedDB web site at http://www.seddb.org.

[1] The Paleoclimate Group recommended to begin by putting together a comprehensive database on ODP cores and in a couple of "test-bed" regions. The Global Fluxes Group emphasized the need for subduction zone inventories and recommended that priority should be given to the MARGINS Subduction Factory focus regions, but that data associated with all convergent margins should be entered as soon as possible; requests were made for the Himalayan margin as a focus zone that ties into tectonics and erosion and for loess and composite samples, as these reflect averages of large areas.

Linking Information Systems in Marine and Terrestrial Geosciences: Sediment Geochemistry Workshop

Agenda

June 3 – 4, 2004

Joint Oceanographic Institutions, Inc., 1201 New York Ave, NW, Suite 400 Washington, DC 20005

supported by the National Science Foundation

June 2, 2004

06:30 pm – 07:30 pm	***Icebreaker*** (sponsored by the Lamont-Doherty Earth Observatory) Lobby, Four Point Sheraton 1201 K Street, NW, Washington, D.C. 20005

June 3, 2004

08:15 am – 08:30 am	***Welcome*** (Organizers, NSF)
08:30 am – 08:45 am	*Steve Goldstein:* Why Do We Need Sedimentary Geochemistry Relational Databases?
08:45 am – 09:05 am	*Lee Allison:* The Hitchhiker's Guide to Geoinformatics: Life, the Universe, and Everything
09:05 am – 09:25 am	*Kerstin Lehnert*: Data Management in Rock Geochemistry
09:25 am – 10:25 am	***Large Integrative Projects*** Doug Fils: CHRONOS IT Structure and Status Rick Carlson: ISES-CI: Cyberinfrastructure for the Solid Earth Sciences Suzanne Carbotte: An integrated data management system for the Margins program
10:25 am – 10:45 am	***Break***
10:45 am – 12:40 pm	***Information Systems for Sediment Data*** Bruce Wardlaw: TBA (PaleoStrat) Rakesh Mithal: Overview of the Janus Database Rick Murray: Proposed IODP Data Management Goals Kyoma Takahashi: J-CORES, CHIKYU shipboard science database system Chris Jenkins: An Information Processing Style of Database for Coastal-Marine Substrates on Global Scales - dbSEABED Carla Moore: Marine Geology Data Systems at NGDC and the collocated World Data Center for Marine Geology and Geophysics, Boulder

12:40 pm – 01:30 pm ***Lunch***

01:30 pm – 04:30 pm ***Breakout sessions***

1. What are the needs of the Paleoclimate community? – Data types, metadata, access, QC, etc. (Curry, Payton)

2. What are the needs of the Global Fluxes community? – Data types, metadata, access, QC, etc. (Carlson)

3. What are the requirements, possibilities, & challenges for integration of marine and terrestrial data systems? (Helly, Lenhardt)

04:30 pm – 06:00 pm ***Plenary session***

Presentation of breakout session results, discussion

June 4, 2004

08:00 am – 10:15 am ***Interoperability of Data Systems, and Integration with Tools for Analysis and Visualization***

Chaitan Baru: Data Integration in GEON (Geosciences Network) *(cancelled)*

John Helly: Interoperability in Scientific Data Systems

Ken Keiser: ESML: Interchange Technology for Data and Tool Interoperability

Ted Haberman: Geospatial Databases: A Foundation for Data Access and Mapping

Jason Leigh: Advanced Technologies for Geoscience Visualization and Collaboration

10:15 am – 10:45 am ***Break***

10:45 am – 12:30 pm ***Breakout Sessions***

"Practical steps for implementing an integrated system for sediment data" (2 parallel breakout seesions)

12:30 pm – 01:00 pm ***Lunch***

01:00 pm – 03:00 pm ***Plenary***

Presentation of Breakout session results

Where do we go from here

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