OneGeochemistry

a Proposed International Framework to Enable Online Interchange of Globally Distributed Geochemical Data.

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OneGeochemistry

Land Acknowledgement

We acknowledge and celebrate the
First Australians on whose traditional lands we meet, and we pay our respect to the elders past, present and future.

OneGeochemistry

Abstract

Geochemical data are fundamental to understanding processes in natural systems and have been collected for more than a century. They are a vital input into many of the UN Sustainable Development Goals (SDG), in particular SDG#6 (Clean Water and Sanitation); SDG#7 (Affordable and Clean Energy); SDG#8 (Decent Work and Economic Growth); SDG#9 (Industry, Innovation and Infrastructure); SDG#13 (Climate Action) and SDG#15 (Life on Land).

Unfortunately, it is near impossible to reuse the vast amounts of geochemical data as they are currently fragmented over thousands of geochemical databases located in either personal, institutional or national silos. Very little is accessible online and where it is, lack of agreed international standards for metadata/data make it impossible to reuse without considerable human effort in data wrangling and cleaning.

A mapping of the global landscape identified some major national geochemical data ‘Systems’ (GeoRoc, EarthChem, Deep-time Digital Earth, AuScope Geochemistry Network, EPOS): each deals with various parts of the geochemical ecosystem ranging from collection /description of samples in the field, through laboratory analysis, to publication of the results and their long term accessibility in online databases.

Although each ‘System’ has a different driver, funding and context, there are common elements within each that can be leveraged into a OneGeochemistry ‘Framework’ (eg, target analytes are based on the Periodic Table; all require standard units of measure; many use rock or mineral names). The overall goal is to create a FAIR global network of interoperable distributed geochemical databases and data systems.

Source:
https://conference.eresearch.edu.au/events/onegeochemistry-a-proposed-international-framework-to-enable-online-interchange-of-globally-distributed-geochemical-data/

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Geochemistry has Scientific and Societal Relevance

- Acquisition and analysis of geochemical data is pervasive in the Earth, environmental, and planetary sciences, and has been since the mid-19th century.
- Geochemistry is fundamental to the **scientific** understanding past, present, and future processes in natural systems including the evolution of the Earth system, solar system, and universe.
- Geochemistry is **societally** relevant to many domains including environment, resources (minerals, energy, groundwater), geohealth, oceans and agriculture.

SUSTAINABLE DEVELOPMENT GOALS

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Geochemistry is highly relevant the UN SDGs

- Highly relevant to the 17 UN Sustainable Development Goals set in 2015 by the UN General Assembly as a universal call to action to end poverty, protect the planet, and ensure that by 2030 all people enjoy peace and prosperity.
- Geochemistry has a potential role in all 17 SDGs - in particular:
  i. SDG#6 (Clean Water and Sanitation);
  ii. SDG#7 (Affordable and Clean Energy);
  iii. SDG#8 (Decent Work and Economic Growth);
  iv. SDG#9 (Industry, Innovation and Infrastructure);
  v. SDG#13 (Climate Action);
  vi. SDG#15 (Life on Land).

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Action is needed for Geochemical Data to be able to contribute to these ambitions

- Data volumes are rapidly growing due to advancements in analytical instrumentation.
- Researchers need access to comprehensive, global data stores to solve the ‘Grand Challenges’ in science and for society.
- In response to Open Access policies and science demands, even more geochemical database systems are emerging at the national, programmatic, and subdomain levels.
- But there is little collaboration between individual systems and sometimes there is competition for the portal with the best visualisations and tools to process the data, as opposed to machine-to-machine access to geochemical data from multiple distributed repositories.

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Geochemistry Research is Diverse and Complex

- Bringing multiple systems together is not easy.
- Geochemistry research is **diverse**:
  - Data can come from multiple groups - many of which compete, do not talk to each other and will not share data.
  - Funding sources vary radically in requirements, size, longevity and IP/licensing conditions.
- Geochemistry research is **complex**:
  - There is an incredible medley of data types and techniques to measure each of those data types;
  - There are few standards for formats and metadata to enable interoperability and describe provenance.

‘Long Tail’ First raised by Heidorn[1] in 2008

- “While the data volumes are small when viewed individually, in total they represent a very significant portion of the country’s scientific output.”
- “There may only be a few scientists world-wide that want to see a particular boutique dataset, but there are many thousands of these datasets”.
- “The long tail is a breeding ground for new ideas and never before attempted science”.

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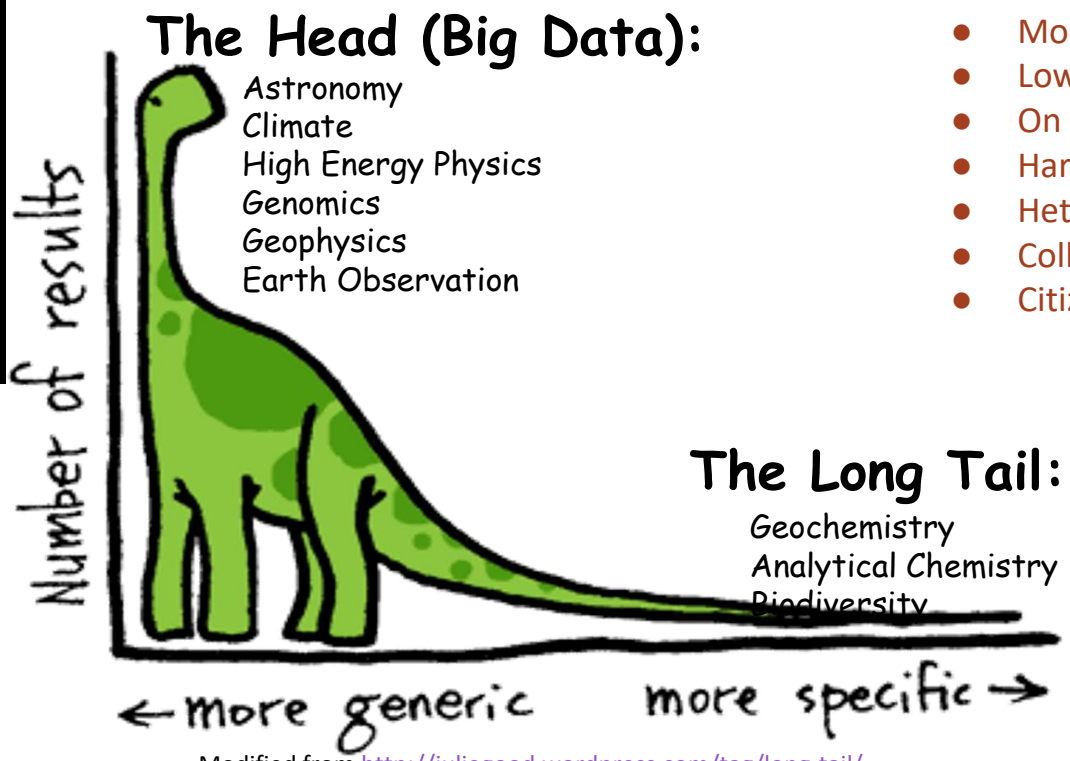
Above all Geochemistry is classic ‘Long Tail’



Modified from http://juliegood.wordpress.com/tag/long-tail/

Long Tail Characteristics

- More specialised
- Low volume
- On C drives
- Hard to find
- Heterogeneous
- Collected by large numbers of people
- Citizen science

[1] Heidorn, P.B. 2008, Shedding Light on the Dark Data in the Long Tail of Science. Library Trends 57(2):280-299 DOI: 10.1353/lib.0.0036

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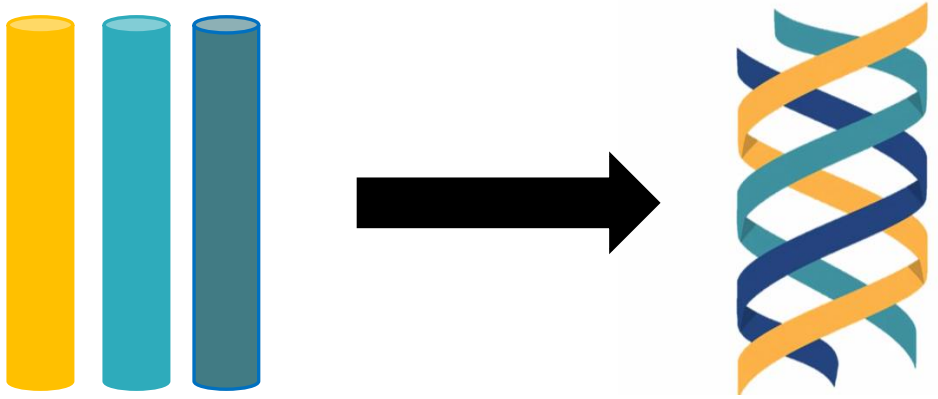
Geochemistry Data is Fragmented and Un-FAIR

- Being LongTail, it is easy to see why the Geochemical data landscape is fragmented.
  - Geochemical data lack common data schemas, formats, vocabularies, which makes it hard to find, access, and reuse them.
  - Geochemical databases tend to be built in thematic, institutional, national, or programmatic silos.
  - Geochemical databases are uncoordinated and analyses can be duplicated within them, making global merging of datasets complex and leading to unnecessary reinvention of the wheel.
- ***We need the silos to seamlessly come together to harness the wealth of geochemical data in support of basic and applied science.***



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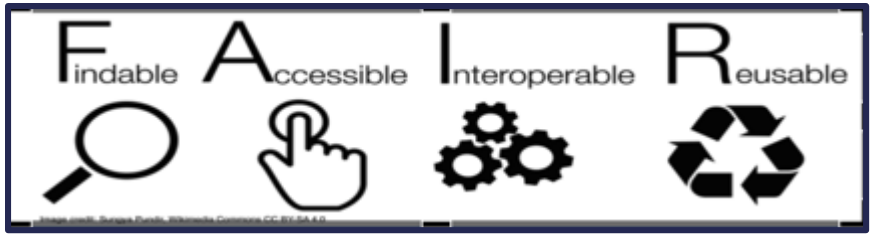
The Vision

- A distributed framework, whereby geochemical data are globally accessible via APIs.
- A coordinated data federation that ensures complementarity of data resources to minimize duplication and maximize comprehensiveness.
- A sustainable data infrastructure that guarantees persistent, programmatic access to a growing global wealth of FAIR geochemical data.
- Note: if a system is not both human- and machine-readable, it is NOT FAIR (Wilkinson et al., 2016)



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Our Vision will be enabled through a Global Infrastructure Framework

- OneGeochemistry is not building:
  - a single database
  - human-readable-only portals, dashboards, etc.
  - a single global geochemistry system
  - a ‘System of Systems’
- OneGeochemistry is building a framework that enables networking of multiple, globally distributed geochemical data systems that can be accessed by machine-to-machine interfaces that are enabled by community agreed:
  - definitions of minimum core variables for each geochemical data type/technique;
  - agreed vocabularies and ontologies
- In essence OneGeochemistry is a Global Infrastructure Framework

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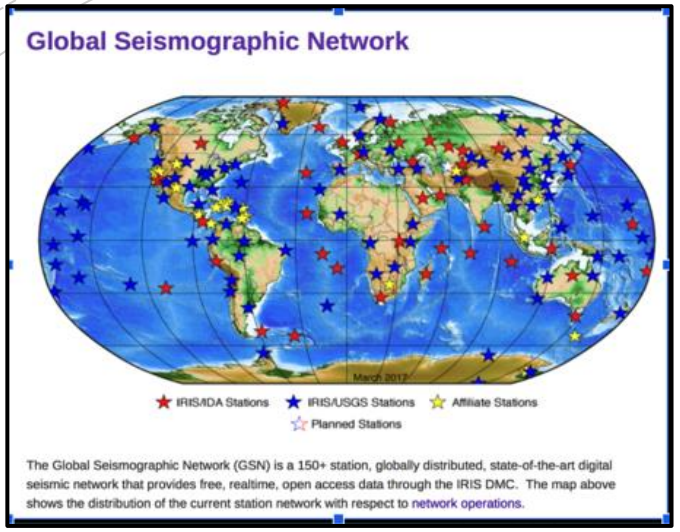
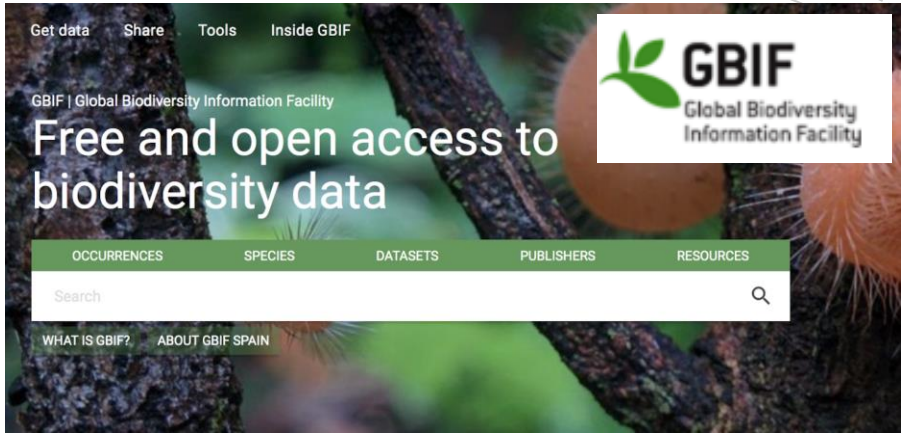
It won't be easy, but it has been done in other disciplines!!

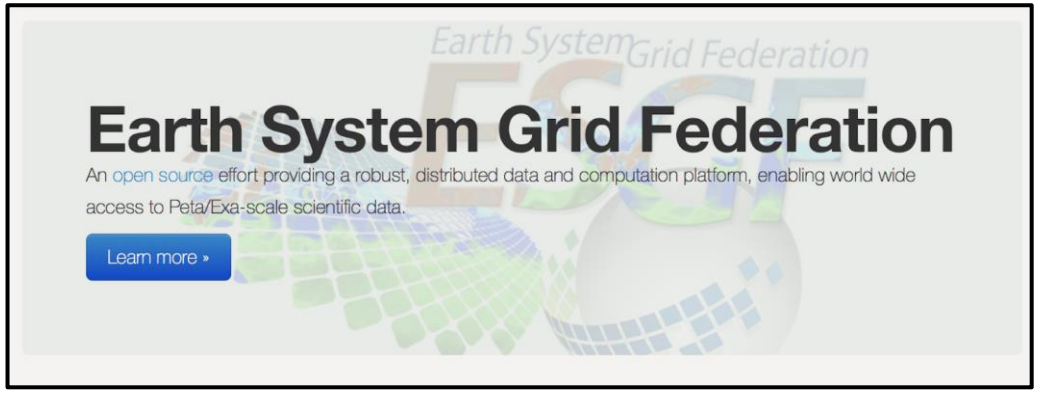


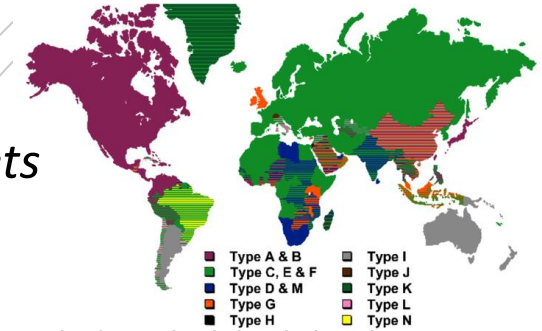


Crystallographic Information Framework

The International Union of Crystallography is the sponsor of the **Crystallographic Information Framework**, a standard for information interchange in crystallography.

The acronym CIF is used both for the *Crystallographic Information File*, the data exchange standard file format of Hall, Allen & Brown (1991) (see Documentation), and for the *Crystallographic Information Framework*, a broader system of exchange protocols based on data dictionaries and relational rules expressible in different machine-readable manifestations, including, but not restricted to, Crystallographic Information File and XML.





Power sockets of the world
(https://www.power-plugs-sockets.com/)

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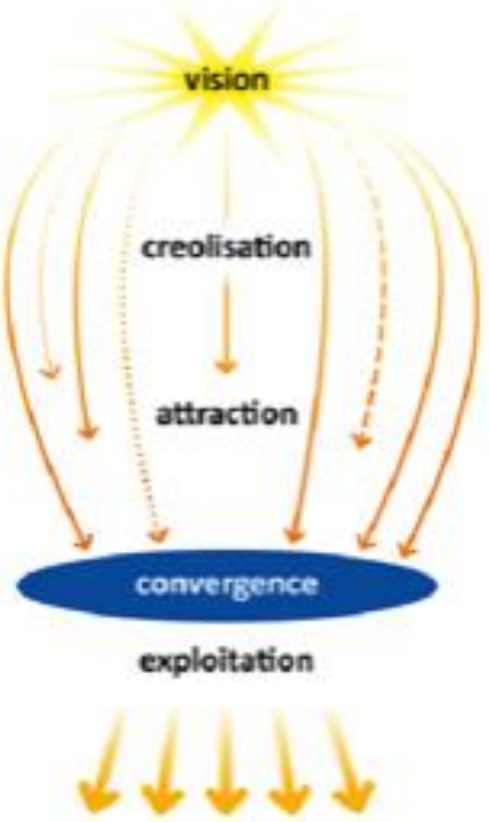
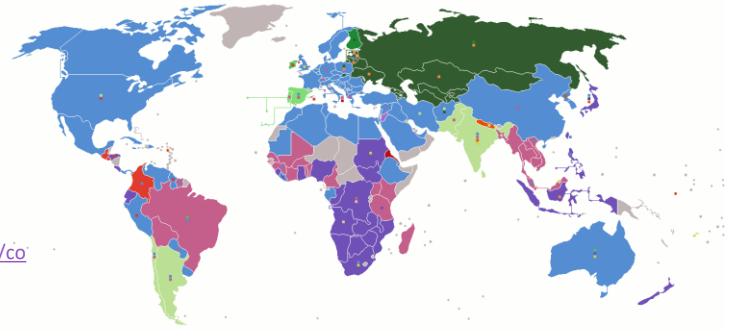
Building Global Infrastructures is NOT NEW!

- Early **visions** about the possibilities of a new technology lead to a phase of **creolization**[1] of approaches.
- A huge 'solutions space' then emerges and fragmentation results.
- **Attraction** begins between similar ideas.
- A transition phase occurs where experts **converge** towards broadly accepted principles, specifications and standards
- **Exploitation** follows!



Wittenburg, P., Strawn, G.: Common patterns in revolutionary infrastructures and data.
Available at: http://doi.org/10.23728/b2share.4e8ac36c0dd343da81fd9e83e72805a0

Railway gauges of the world
(https://upload.wikimedia.org/wikipedia/commons/1/1f/Rail_gauge_world.png)



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[1]Creolization describes a process in which continuously new cultures/languages emerge and mixing resulting in a community agreement

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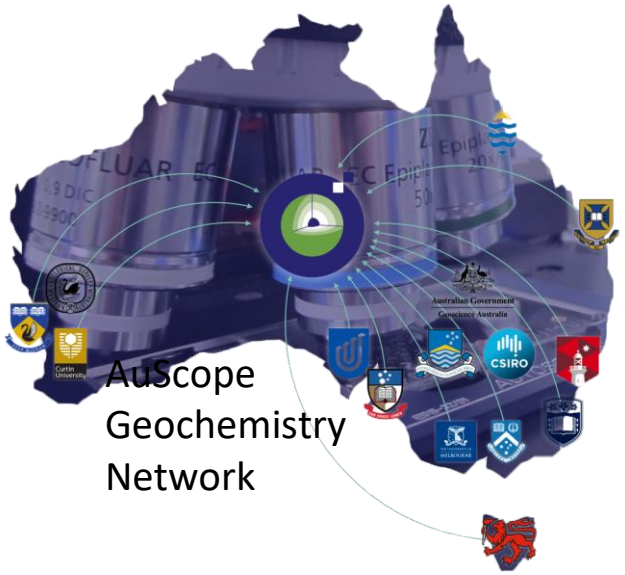
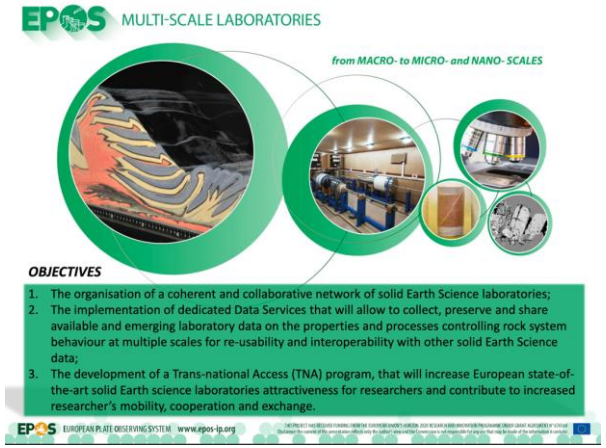
Attraction is starting to happen at National and Regional Scales

Australia: AGN



Germany: DIGIS

Europe: EPOS MSL



United States: EarthChem

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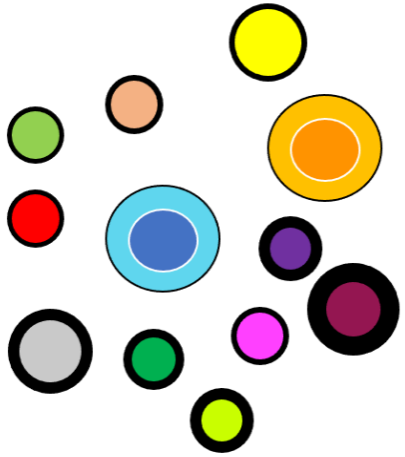
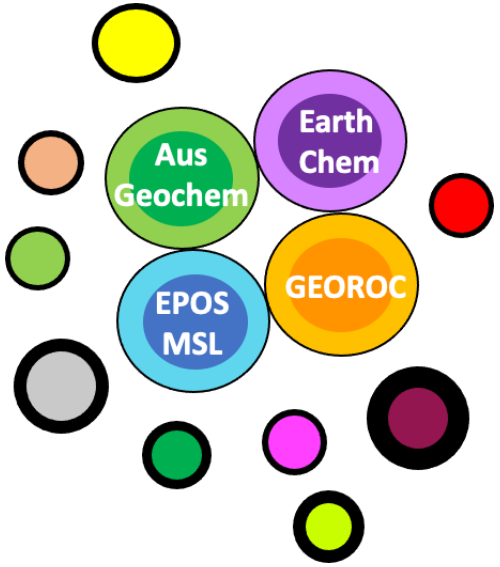
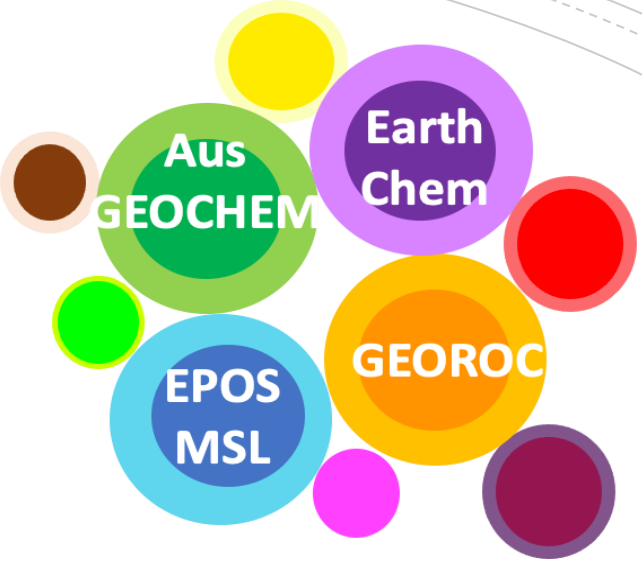
Current, Developing and Future States



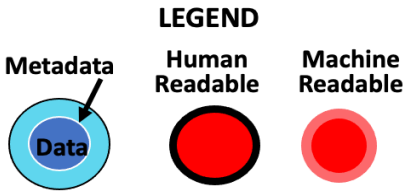
Current State:
Multiple human-readable systems, some with metadata: some are FAIR but only within their system



Developing State:
Some systems attempting to harmonise, but still only human-readable systems: no globally agreed community standards. Data are Findable and Accessible, but not Interoperable or Reusable



Future State:
A global framework made of multiple machine-readable systems, each compliant with globally agreed community standards and **all FAIR and Fully A.I. Ready**



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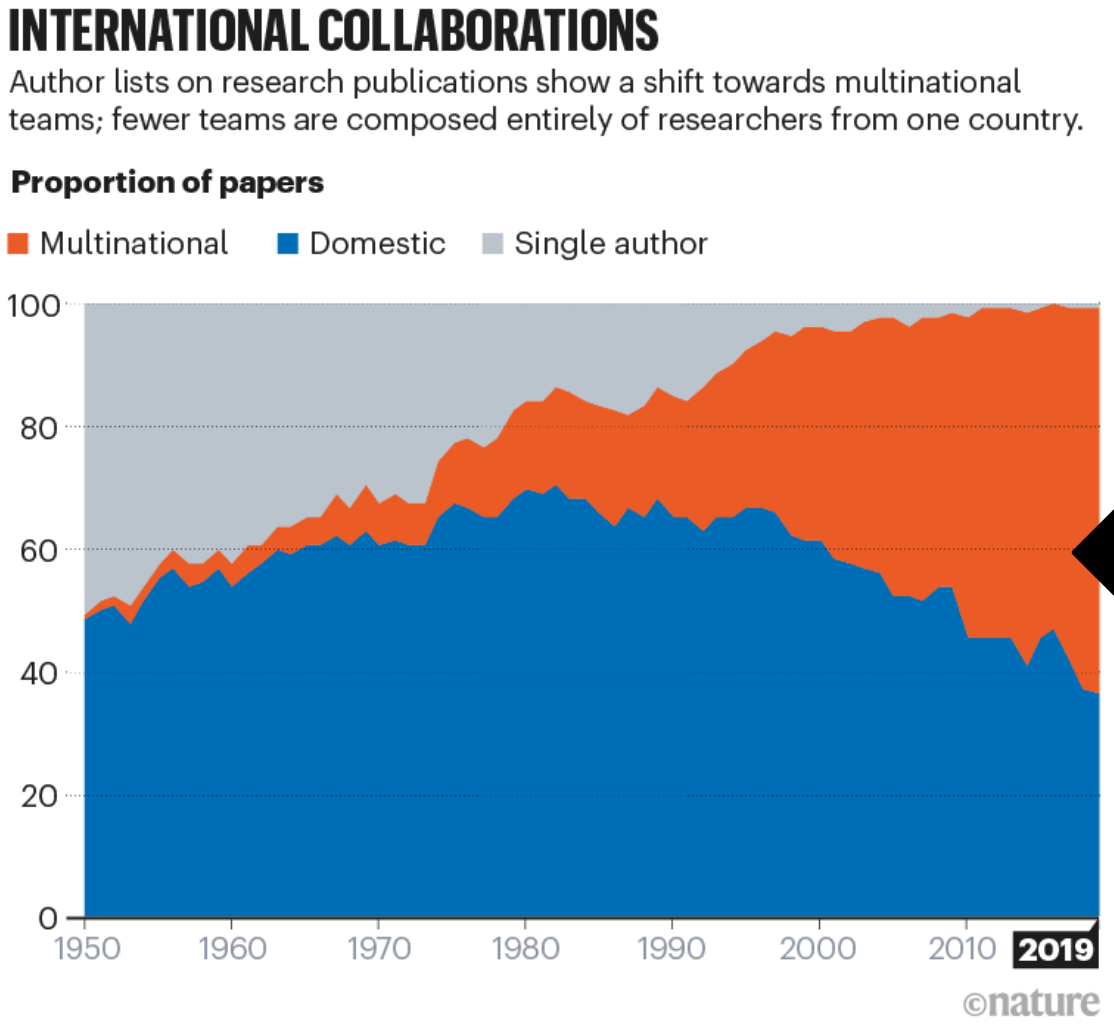
Convergence of geochemistry data standards has to be at an international level



Modern research papers increasingly result from International collaborations

Monastersky, R., and Van Noorden, R., 2019. 150 years of *Nature*: a data graphic charts our evolution. Nature, 575(7781):22-23. doi: 10.1038/d41586-019-03305.

Geochron Workshop reports sponsored by EarthChem and EARTHTIME

Walker, Douglas J.; Condon, Daniel; Thompson, William; Renne, Paul; Koppers, Anthony; Hodges, Kip; Reiners, Peter; Stockli, Daniel; Schmitz, Mark; Bowring, Samuel; Gehrels, George

This report compilation describes the outcomes of a series of workshops sponsored by EarthChem and EARTHTIME. The goal of the workshops was to establish community requirements regarding data reporting and the approach employed for getting data into the database are used with the Geochron database. The reports are grouped by technique, and include: Ar-Ar, (U-Th)/He, U-Pb, U-series, and Ion Microprobe.

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And Convergence on standards is starting to happen Internationally!

"Reporting and Interpretation of Geochronologic Data": Invitation for special papers in the *Geological Society of America Bulletin*

The science editors of the *Geological Society of America Bulletin* are encouraging a series of invited special papers to be published during the next 3+ years that highlight current best practices in the reporting and interpretation of geochronologic data and metadata.

The need for such reviews has become acute as the number of manuscripts submitted to *GSA Bulletin* (and other journals) whose conclusions are founded on radioisotopic dating of minerals, rocks, and organic materials has grown explosively during the past decade. Justification includes the following. (1) Many radioisotopic dating methods are in use, including some relatively new methods. (2) Data and metadata sets are commonly large and often contain dozens to thousands of isotopic measurements. (3) With increasing precision of many dating methods, the interpretation of large complex data sets is not always straightforward. It is becoming a challenge for many readers of *GSA Bulletin* to appreciate how a large set of isotopic dates is used to determine a geologically meaningful age for a rock or process. (4) Standardization of many methods has been greatly improved, but a plethora of standard values often requires re-calibration of published data sets.

The papers will be written by specialists, but the aim is that they will be presented in a form that is readily accessible to the broad readership of *GSA Bulletin*. Ideally, each paper would: (1) present a brief overview of the chronometer including the fundamental underlying assumptions and sources of uncertainty; (2) discuss what materials are most suited for analysis

GSA Bulletin

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RESEARCH ARTICLE | JULY 01, 2020

Interpreting and reporting $^{40}Ar/^{39}Ar$ geochronologic data

Allen J. Schaen; Brian R. Jicha; Kip V. Hodges; Pieter Vermeesch; Mark E. Stelten; Cameron M. Mercer; David Phillips; Tiffany A. Rivera; Fred Jourdan; Erin L. Matchan; Sidney R. Hemming; Leah E. Morgan; Simon P. Kelley; William S. Cassata; Matt T. Heizler; Paulo M. Vasconcelos; Jeff A. Benowitz; Anthony A.P. Koppers; Darren F. Mark;

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Quaternary Geochronology

Volume 52, June 2019, Pages 77-87

Guidelines for reporting and archiving ^{210}Pb sediment chronologies to improve fidelity and extend data lifecycle

Colin J. Courtney Mustaphi, Janice Brahney, Marco A. Aquino-López, Simon Goring, Kiersten Orton, Alexandra Noronha, John Czaplewski, Quinn Asena, Sarah Paton, Johnny Panga Brushworth

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GEOSTANDARDS and GEOANALYTICAL RESEARCH

Original Article | Open Access

Community-Derived Standards for LA-ICP-MS U-(Th-)Pb Geochronology – Uncertainty Propagation, Age Interpretation and Data Reporting

Matthew S. A. Horstwood, Jan Košler, George Gehrels, Simon E. Jackson, Noah M. McLean, Chad Paton, Norman J. Pearson, Keith Sircombe, Paul Sylvester, Pieter Vermeesch, ... See all authors

First published: 01 February 2016 | https://doi.org/10.1111/j.1751-908X.2016.00379.x | Citations: 279

SECTIONS

DATA SCIENCE JOURNAL

Research Papers

Sample Identifiers and Metadata to Support Data Management and Reuse in Multidisciplinary Ecosystem Sciences

Authors: Joan E. Damerow, Charuleka Varadharajan, Kristin Boye, Eoin L. Brodie, Madison Burrus, K. Dana Chadwick, Robert Crystal-Ornelas, Hesham Elbashandy, Ricardo J. Eloy Alves, Kim S. Ely, Amy E. Goldman, Ted Haberman, Valerie Hendrix, Zarine Kakalia, Kenneth M. Kemner, Annie B. Kersting, Nancy Merino, Fianna O'Brien, Zach Perzan, Emily Robles, Patrick Sorensen, James C. Stegen, Ramona L. Walls, Pamela Weisenhorn, Mavrik Zavarin, Deborah Agarwal

Abstract

Physical samples are foundational entities for research across biological, Earth, and environmental sciences. Data generated from sample-based analyses are not only the basis of individual studies, but can also be integrated with other data to answer new and

Paleoceanography and Paleoclimatology

Feature Article | Free Access

PaCTS 1.0: A Crowdsourced Reporting Standard for Paleoclimate Data

D. Khider, J. Emile-Geay, N. P. McKay, Y. Gil, D. Garijo, V. Ratnakar, M. Alonso-Garcia, S. Bertrand, O. Bothe, P. Brewer, A. Bunn, M. Chevalier, L. Comas-Bru, A. Csank, E. Dassié, ... See all authors

First published: 03 September 2019 | https://doi.org/10.1029/2019PA003632 | Citations: 9

This article was corrected on 21 FEB 2020. See the end of the full text for details.

SECTIONS PDF TOOLS SHARE

Abstract

The progress of science is tied to the standardization of measurements, instruments, and data. This is especially true in the Big Data age, where analyzing large data volumes critically hinges on the data being standardized. Accordingly, the lack of community-sanctioned data standards in paleoclimatology has largely precluded the benefits of Big

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Quaternary Geochronology

Volume 39, April 2017, Pages 142-149

Research paper

Data reporting standards for publication of U-series data for geochronology and timescale assessment in the earth sciences

A. Dutton, K. Rubin, N. McLean, J. Bowring, E. Bard, R.L. Edwards, G.M. Henderson, M.R. Reid, D.A. Richards, K.W.W. Sims, J.D. Walker, Y. Yokoyama

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Abstract

Uranium-series data provide essential dating and tracer tools for a broad spectrum of geologic processes. Data reported in U-series geochronology studies often contain insufficient information to completely assess the data collected. It is

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With better standards we can move from ‘maps’ that average observations to knowledge graphs that portray individual research objects: Exploitation begins!

Source: https://earthobservatory.nasa.gov/images/8733/william-smiths-geological-map-of-england

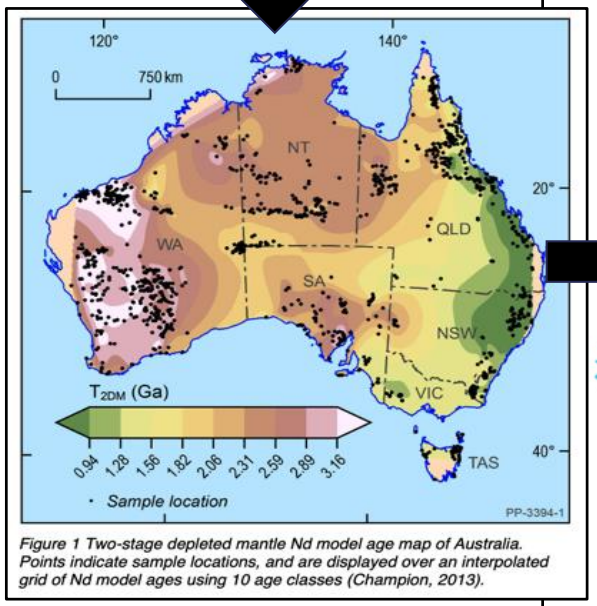
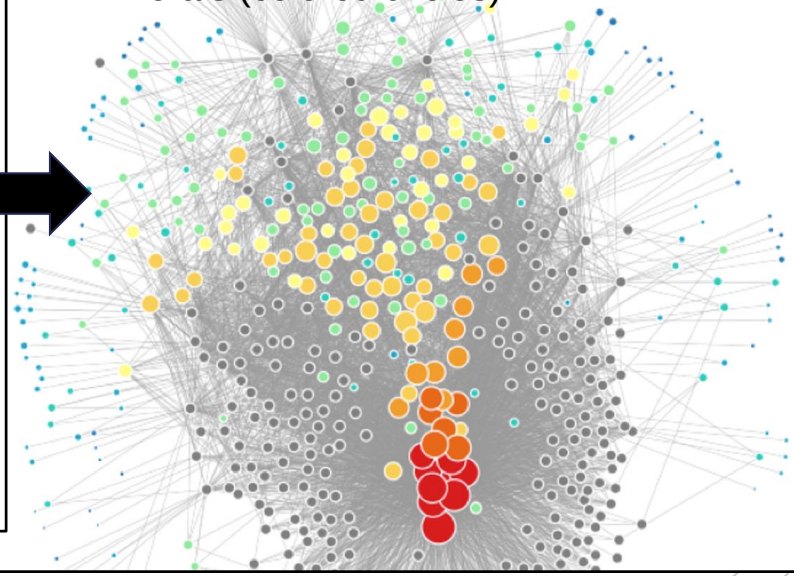


Figure 1 Two-stage depleted mantle Nd model age map of Australia. Points indicate sample locations, and are displayed over an interpolated grid of Nd model ages using 10 age classes (Champion, 2013).

Source: https://ecat.ga.gov.au/geonetwork/srv/eng/catalog.search#/metadata/133772

- The image/map of data has been the main means of communication of geoscientific data since William Smith’s map in 1815.
- Through the semantic web and knowledge graphs we can now visualise millions of individual words and data objects, not create visualisations of interpretations of millions of words and data objects.
- The new science predicted by Heidorn (2008) is here!!!

Network diagram of 400 carbon-bearing minerals (colored circles).



Source: https://hazen.carnegiescience.edu/research/mineral-network-analysis

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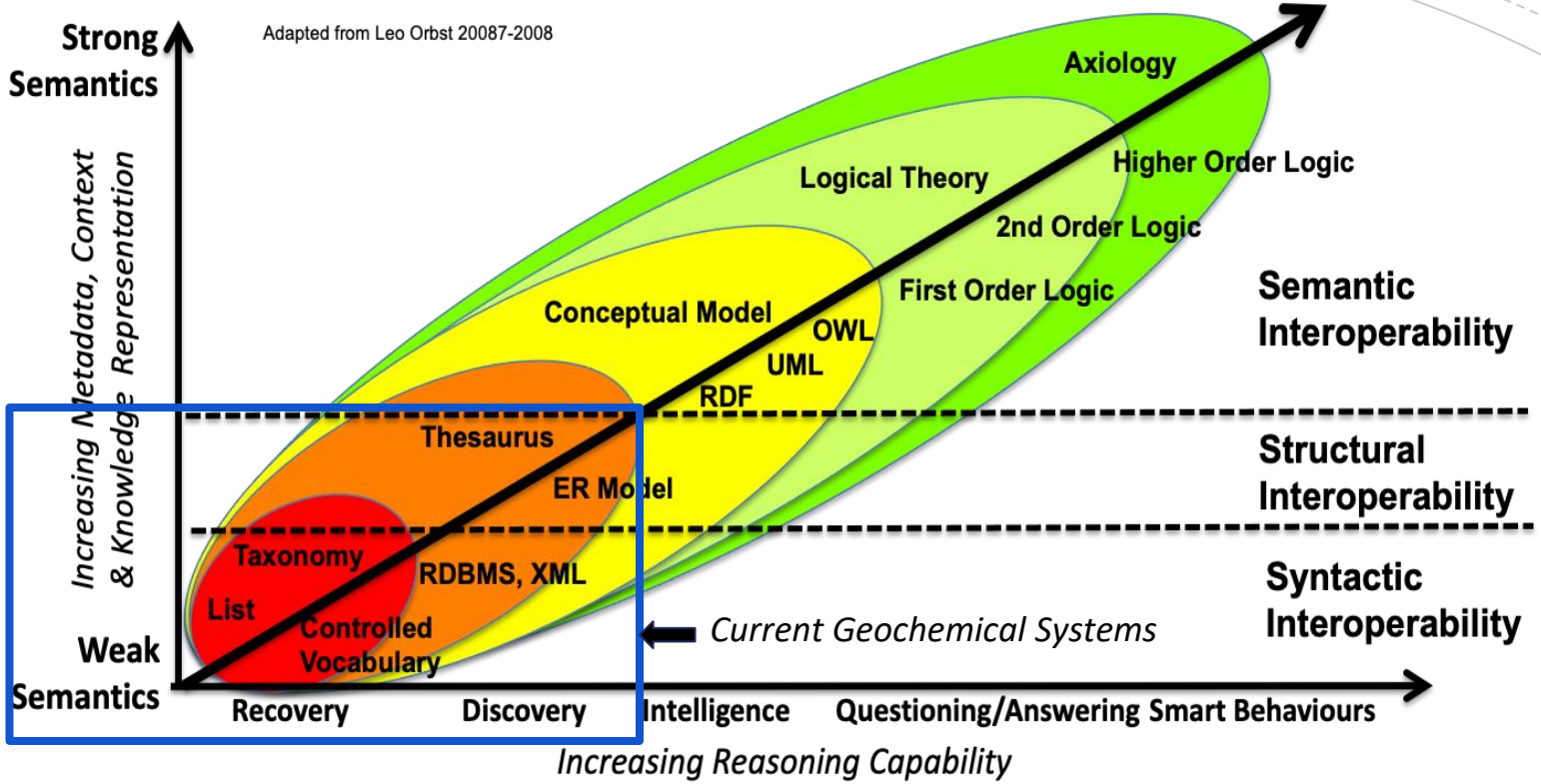
To get to the semantic web we need to raise the bar for geochemical data



- Most geochemical data systems only enable recovery and discovery of data by **humans:** the data are not programmatically accessible.
- Lack of vocabulary standards and ontologies means that they cannot be used for semantic reasoning and knowledge graphs.
- Many systems are designed for visualization of data within their systems, not for global sharing of knowledge at the data object level and are hard to use in AI and Machine Learning.

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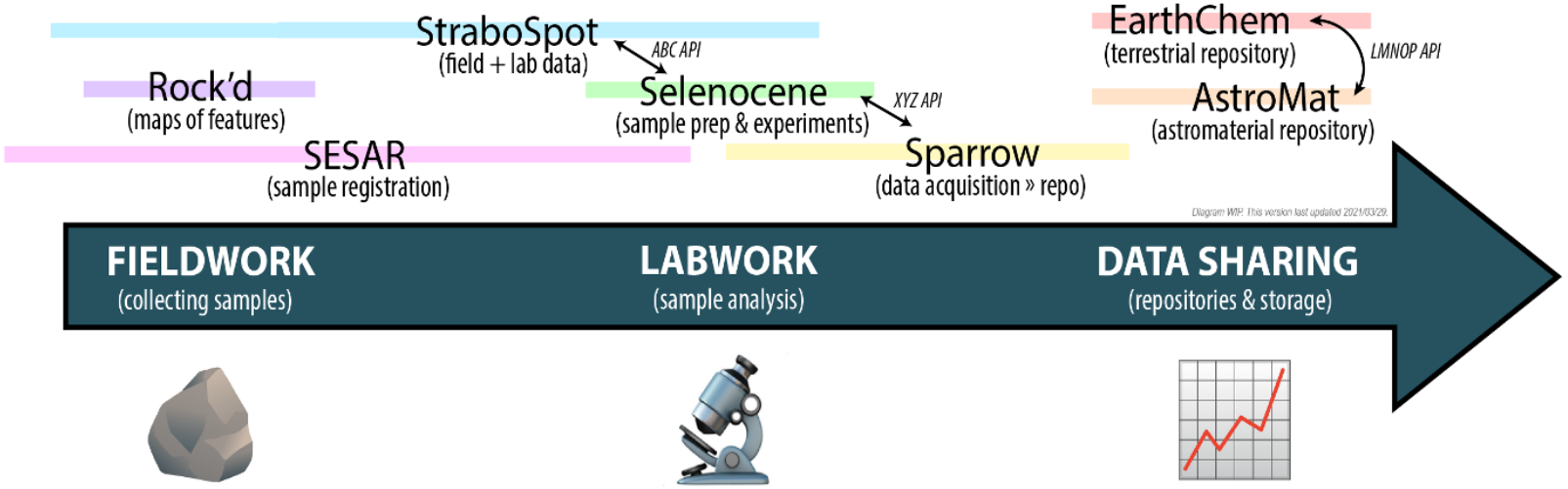
The Geochemical Ecosystem: we need agreed standards from field to laboratory to publication



A map of the US Geochemical Ecosystem - a series of multiple data systems covering aspects of geochemical data from field collection to to publication (from Beck Straus NASA)

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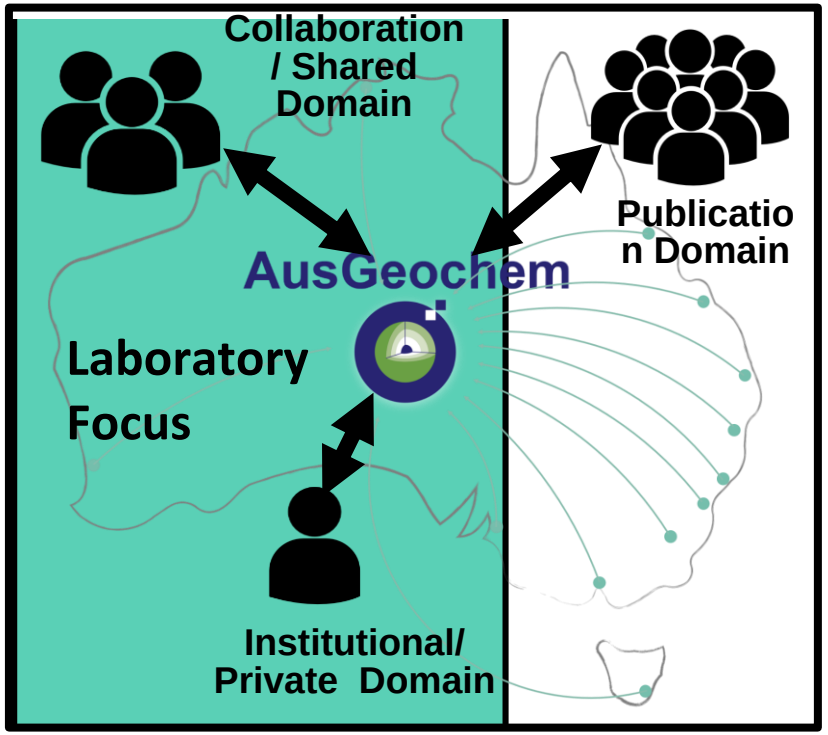
Do we compile at the laboratory or after publication?

- Many geochemical databases capture data from the literature.
- In Australia, a straw poll estimated that no more than 10% of data from a publicly funded research laboratory ends up in the public domain: the rest remains 'trapped' in institutions or unpublished project reports
- Would it be more efficient to capture the primary version of the data as it is calibrated and QA/QC'ed in the laboratory?
- In Australia, the AuScope AusGeochem is targeting compilation at the laboratory, which helps enable compliance with the 2018 Australian Code for the Responsible Conduct of Research (including the guidelines for the Management of Data and Information in Research).



https://www.nhmrc.gov.au/about-us/publications/australian-code-responsible-conduct-research-2018

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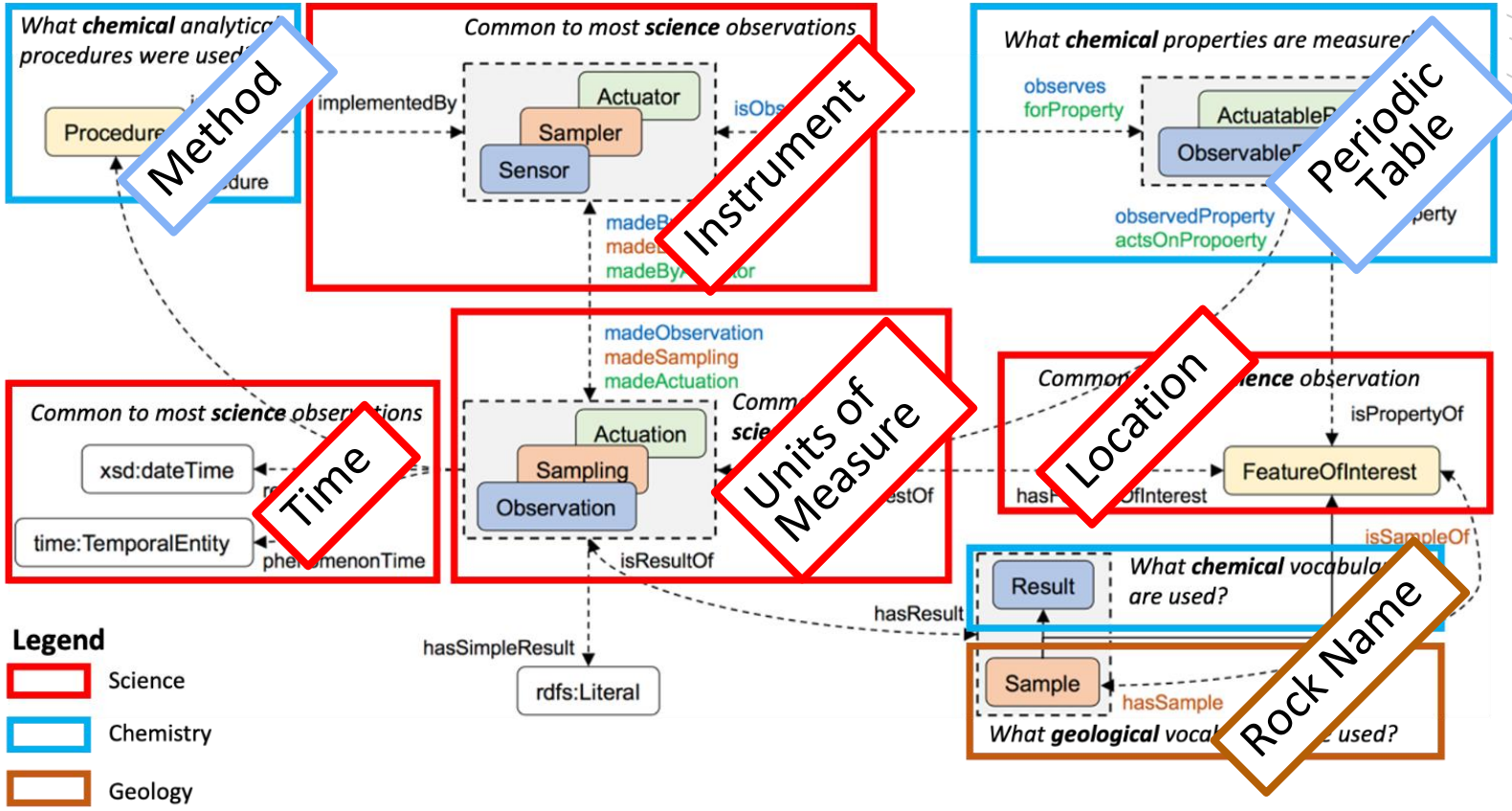
We should reuse components from other disciplines where possible



- For Geochemistry to link machine-to-machine with other disciplines we need to harmonise with global community standards such as:
  - Units of Measure, Time (CODATA, International Science Union)
  - Periodic Table (International Union of Pure and Applied Chemistry)
  - Rock names (International Union of Geosciences).
- For the rest, we need to develop within the geochemical community agreed minimum core variables and vocabularies for each geochemical data type/analytical technique.

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Upcoming events: aimed at raising awareness

CODATA WORLD DATA SYSTEM **Virtual SciDataCon 2021**

About | Call for Sessions | Contact | Progra

Session Title: The OneGeochemistry Initiative: Mobilising a Global Network of FAIR Geochemical Data to Support Research into the Grand Challenge of an Environmentally Sustainable Future

Session Organisers: Lesley Wyborn , Kirsten Elger , Alexander Prent , Kerstin Lehnert

21 Oct 2021
13:00 14:30 UTC

Session Description:

Register for the session: https://us02web.zoom.us/meeting/register/tZwtdOivrzkuGdUVxHAs

Geochemical data are fundamental for understanding past, present, and future processes in natural systems, from the interior of the Earth to its surface environments on land, in the oceans and in the air, to the entire solar system. Currently, despite the pervasive acquisition and analysis of geochemical data in the last century, it is hard to harness this wealth of data as existing practices have resulted in geochemical databases that are located in either personal, institutional, national, or programmatic silos. Due to lack of standards that are especially challenging to develop in long-tail communities, like geochemistry, much of this existing data is not interoperable and reusable: very little is open and accessible online. To create a global network of reusable geochemical data the International Geochemistry Community needs to come together to define the required,

OneGeochemistry: a Proposed International Framework to Enable Online Interchange of Globally Distributed Geochemical Data

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eResearch Australasia 2021 Conference 11 - 15 October
AeRO

14 October, 2021:
4:10 - 4:50 pm AEDT

Geochemical data are fundamental to understanding past, present, and future processes in natural systems, from the interior of the Earth to its surface environments on land, in the oceans and in the air, to the entire solar system. Currently, despite the pervasive acquisition and analysis of geochemical data in the last century, it is hard to harness this wealth of data as existing practices have resulted in geochemical databases that are located in either personal, institutional, national, or programmatic silos. Due to lack of standards that are especially challenging to develop in long-tail communities, like geochemistry, much of this existing data is not interoperable and reusable: very little is open and accessible online. To create a global network of reusable geochemical data the International Geochemistry Community needs to come together to define the required, fragmented over thousands of databases accessible online and where it is, the lack reuse without considerable human effort

A mapping of the global landscape identi time Digital Earth, AuScope Geochemistry Network, EPOS); each deals with various parts of the geochemical ecosystem ranging from collection /description of samples in the field, through laboratory analysis, to publication of the results and their longer term accessibility in online databases.

GOLDSCHMIDT® Hawai'i 2022

geochemical society

1. Session Proposal: Modern Geochemical Data Systems, Modelling Platforms and Data Standards: creating new opportunities to address scientific problems.

2. Workshop Proposal: Earth Science meets Data Science: what are our needs for geochemical data, services and analytical capabilities in the 21st century?

3. Workshop Proposal: Standards for the Publication of Geochemical Data - Fostering the Conversation

EGU General Assembly 2022

Vienna | Austria

3–8 April 2022

1. Great Debate: Where is my data, where did it come from and how was it obtained? Improving Access to Geoanalytical Research Data

2. Session Proposal: Making Geoanalytical Data FAIR: Managing Data from Field to Laboratory to Archive to Publication

- *All promote the need for global community agreement on Minimum Core Variables for each data type, analytical technique*
- ***None promote a specific database***

OneGeochemistry

Conclusions

1. OneGeochemistry is NOT a single database, single dashboard, single system or a system of systems
2. OneGeochemistry is seeks to address an urgent need to define the building blocks for a global framework including minimum core variables, vocabularies, machine readability of data, vocabularies, machine readability of data, etc., particularly for validation of data in publications.
3. OneGeochemistry is focused on FAIR data where data is also Fully AI Ready, reusable for modern AI/ML techniques
4. But above all whilst OneGeochemistry seeks global sharing of data through community-led standardisation, it still needs to allow for:
    i. Deeper domain specialisation and innovation;
    ii. The development of new techniques; and
    iii. Constant improvement and evolution of existing techniques.

OneGeochemistry

An invitation to participate!

Contact any of the current participants to join the initiative!

- Kerstin Lehnert (EarthChem, Astromat, Osiris-Rex) lehnert@ldeo.columbia.edu
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