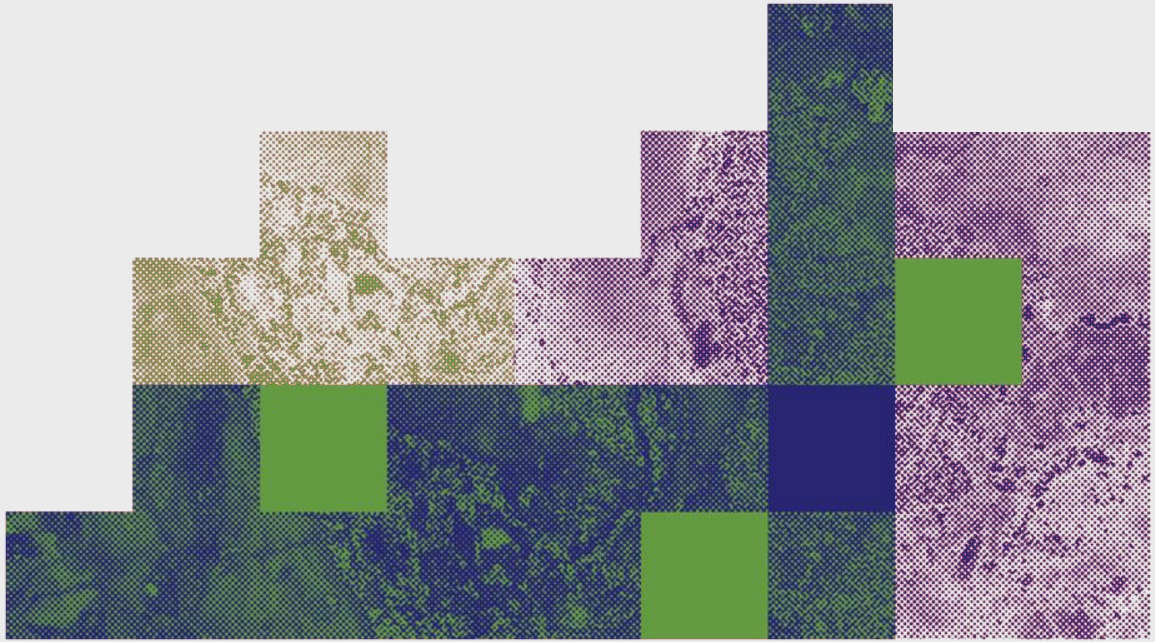
AuScope Geochemistry Network:

Providing a FAIR research vocabulary for geochemical data for the Australian and international geochemical community

Angus Nixon

On behalf of the AuScope Geochemistry Network (AGN)



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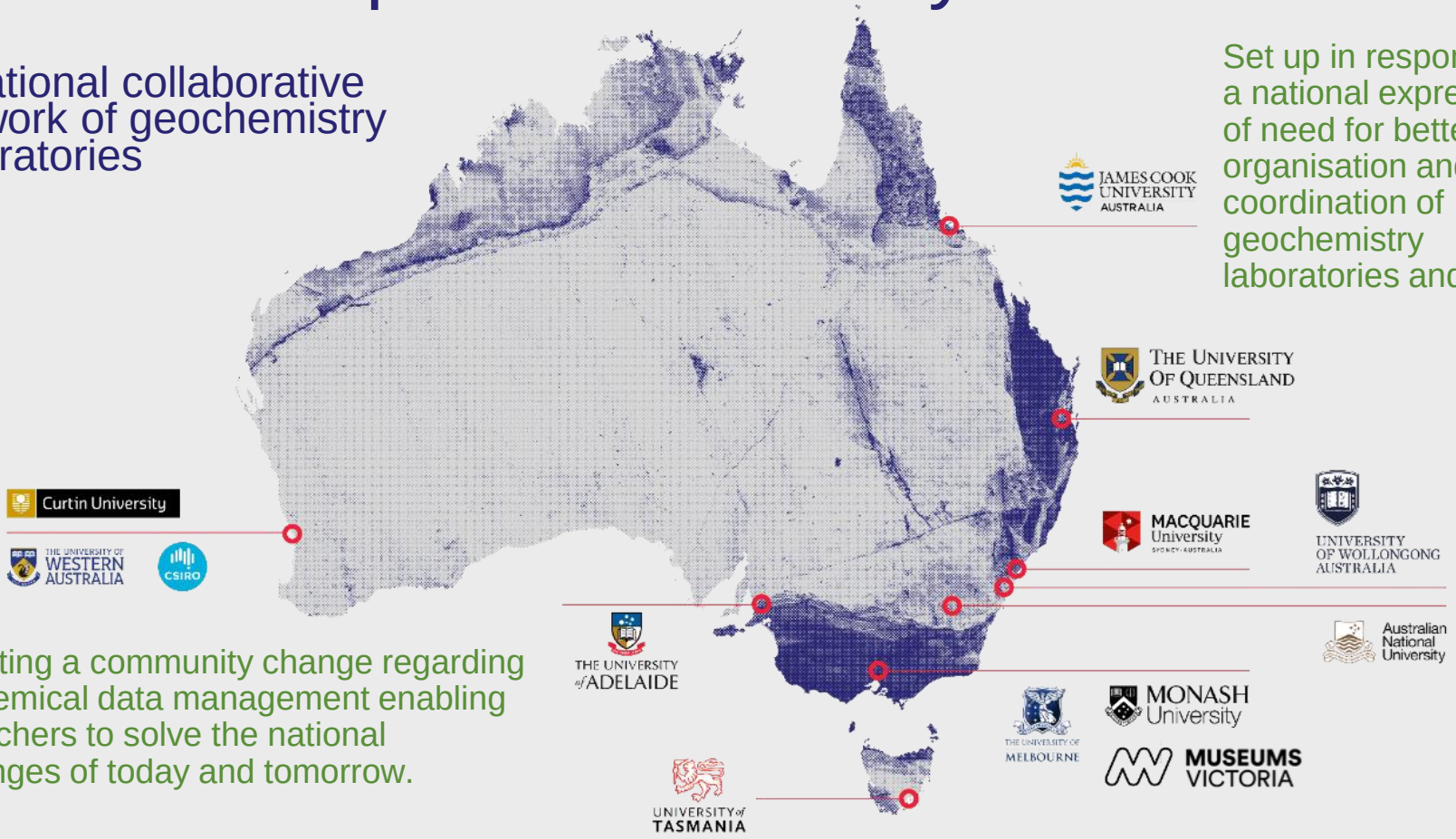
NCRIS National Research Infrastructure for Australia
An Australian Government Initiative

The **A**uScope **G**eochemistry **N**etwork

A national collaborative network of geochemistry laboratories



Set up in response to a national expression of need for better organisation and coordination of geochemistry laboratories and data.

Motivating a community change regarding geochemical data management enabling researchers to solve the national challenges of today and tomorrow.

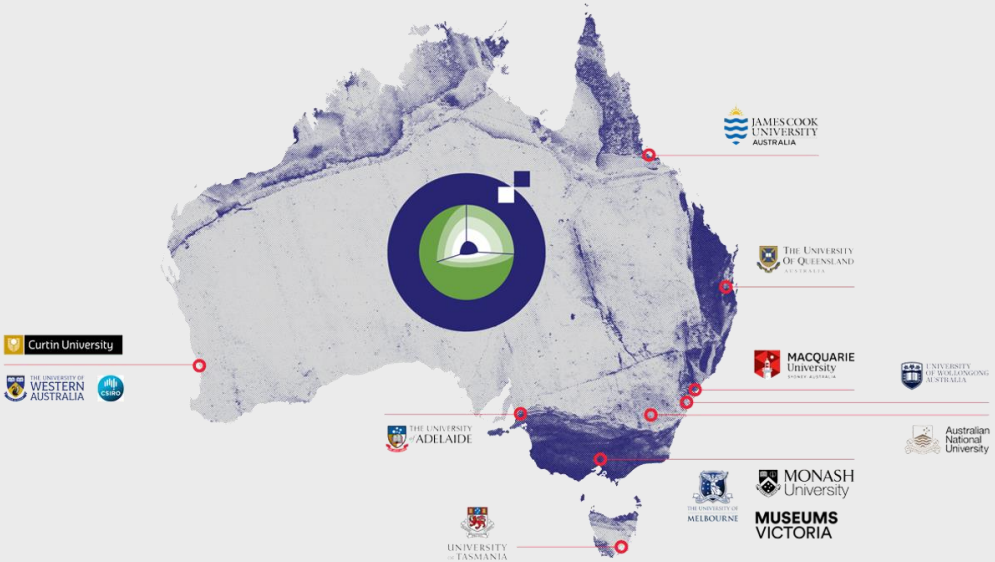
Project Overview

Objectives include:

- Developing and maintaining a **FAIR data ecosystem** for the Australian Earth science community

- Establishing compatibility and engagement with **global resources** and **best practice**

- Integrating with **laboratory** and **research** workflows to capture data in the research pathway



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Improved Data Pipeline

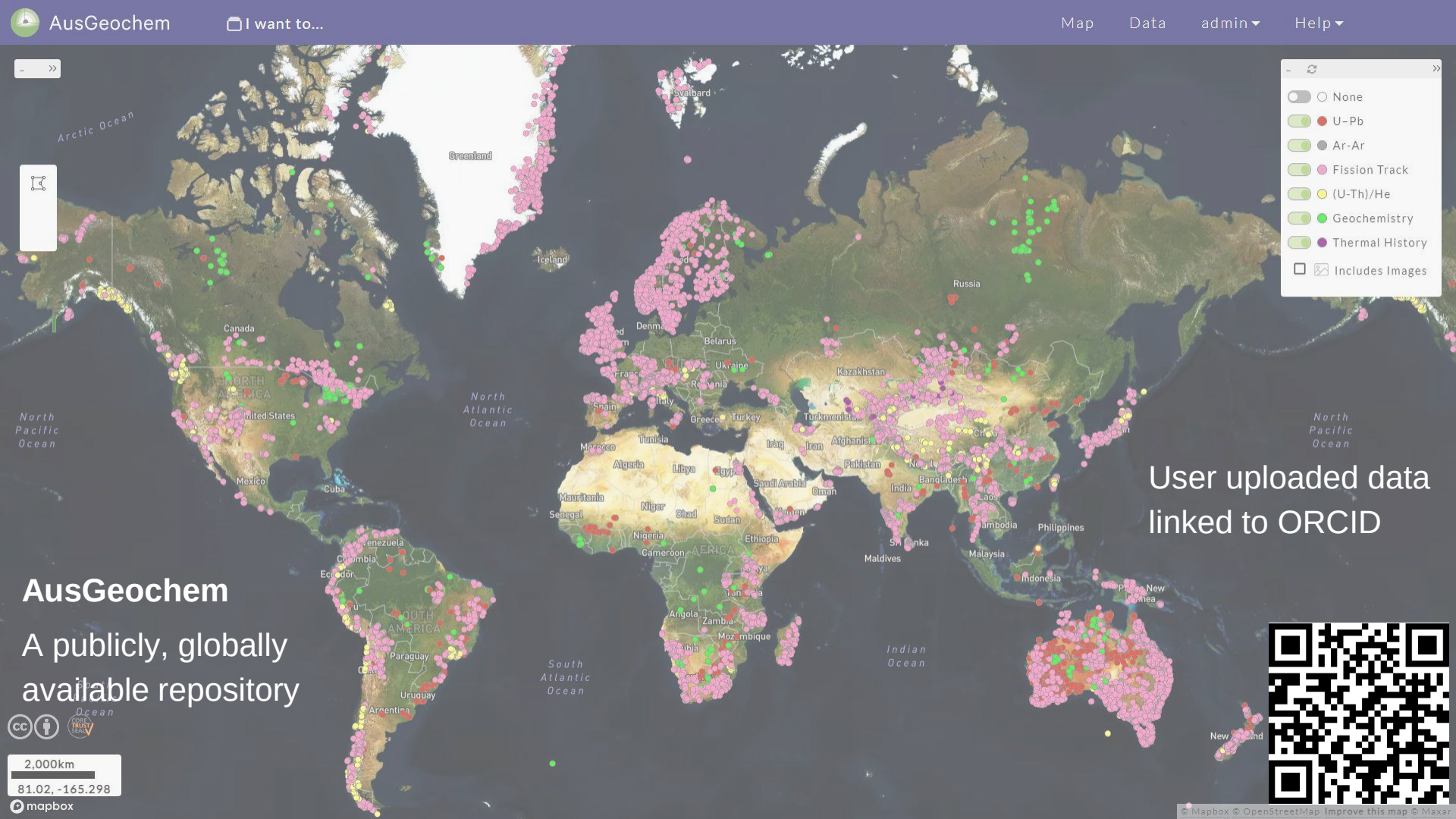
Securely store data from lab to platform

Publish and cite

Share with collaborators and community

Explore and interpret data

Connect with databases


AusGeochem
I want to...
Map
Data
admin
Help
None
U-Pb
Ar-Ar
Fission Track
(U-Th)/He
Geochemistry
Thermal History
Includes Images
User uploaded data linked to ORCID
AusGeochem
A publicly, globally available repository
2,000km
81.02, -165.298
mapbox
© Mapbox © OpenStreetMap Improve this map © Maxar

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- Models for storing data outputs
- Models for storing analytical parameters
- Attribution/citation/ID of materials and datasets
- Mechanism to acquire data from laboratories (minimal human input)

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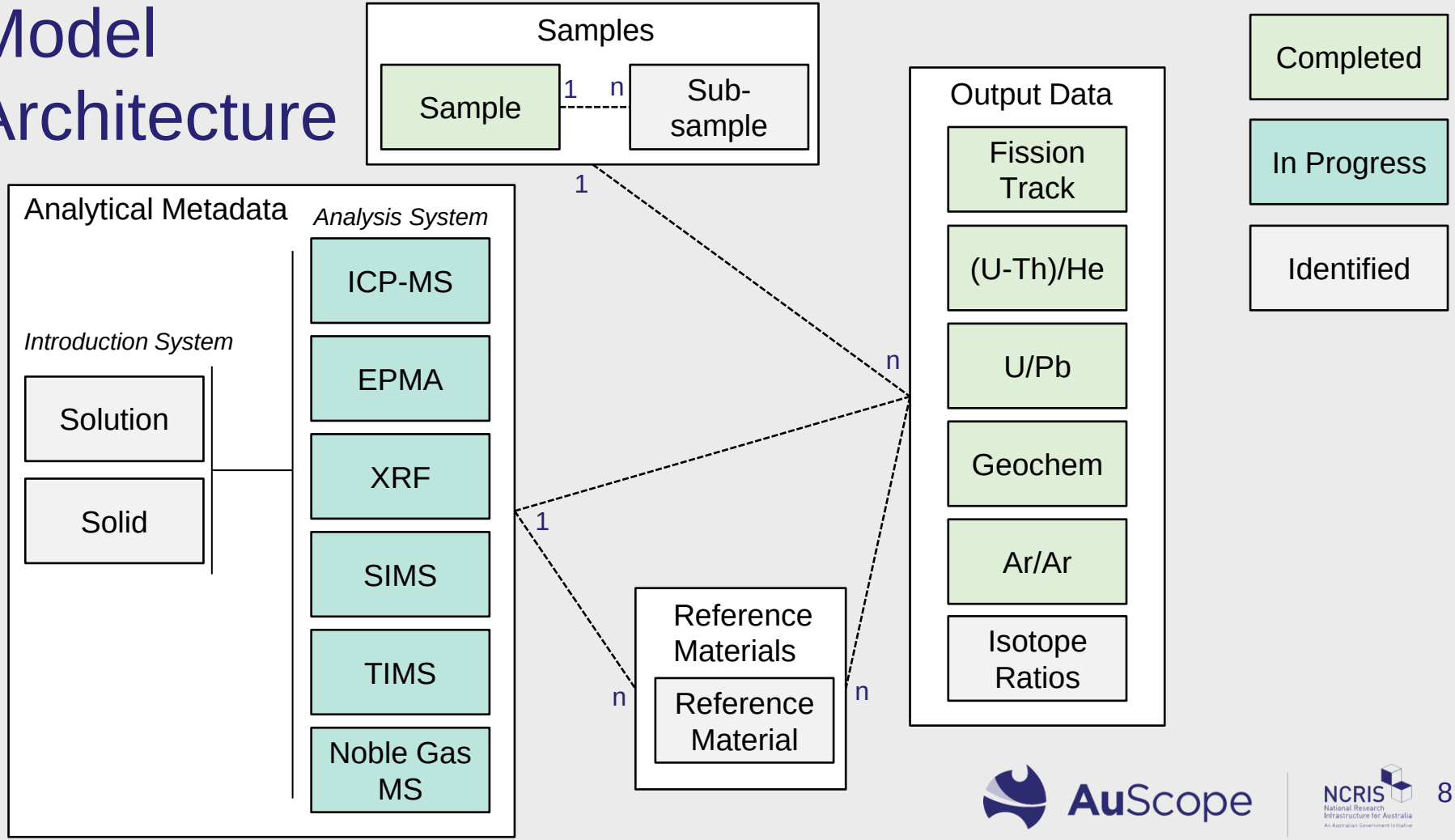
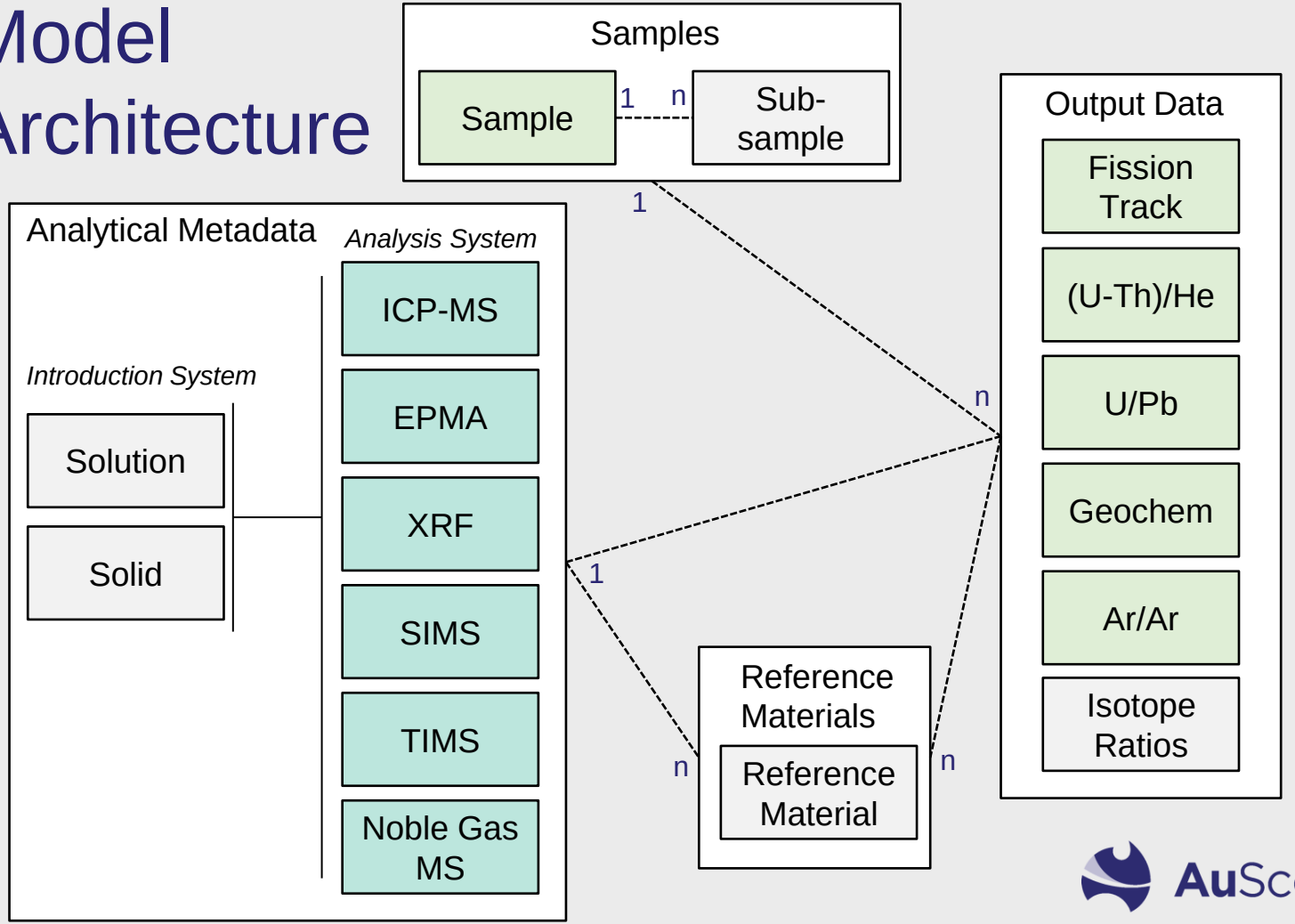
Model Architecture



Model Architecture



Multiple data types connected to sample materials

Data outputs can be connected to analytical metadata

Data and analytical sessions can be linked to reference materials

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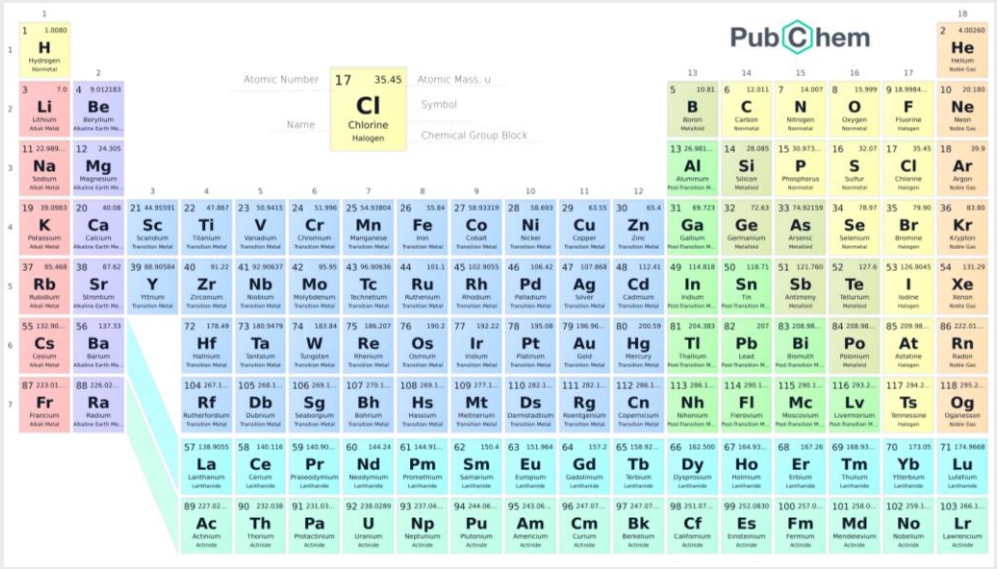
Example: Inorganic Geochemistry

- Measured concentrations of elements and compounds within geological samples

- Present from weight percent to parts per billion levels

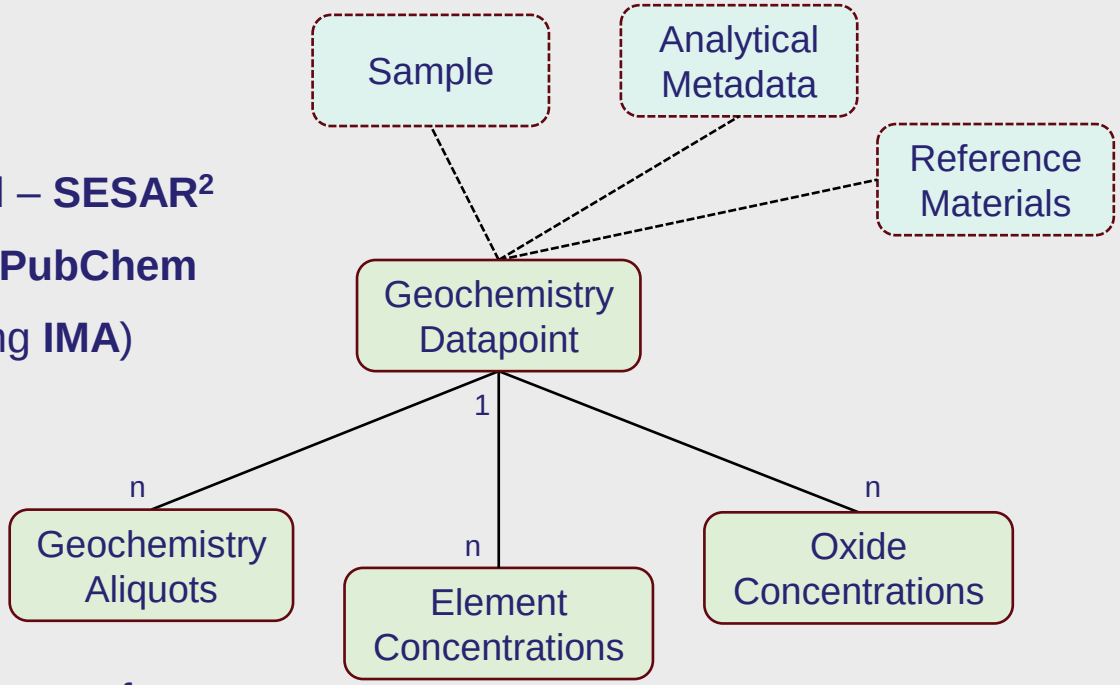


National Center for Biotechnology Information (2024)

Example: Inorganic Geochemistry

External Resources:

- Units – **QUDT**
- Analytical Scale + Analyte Material – **SESAR²**
- Elements + Oxides/Compounds – **PubChem**
- Mineral Type – **Mindat** (assimilating **IMA**)
- Samples – **IGSN** (user based)
- Analyst – **ORCID**

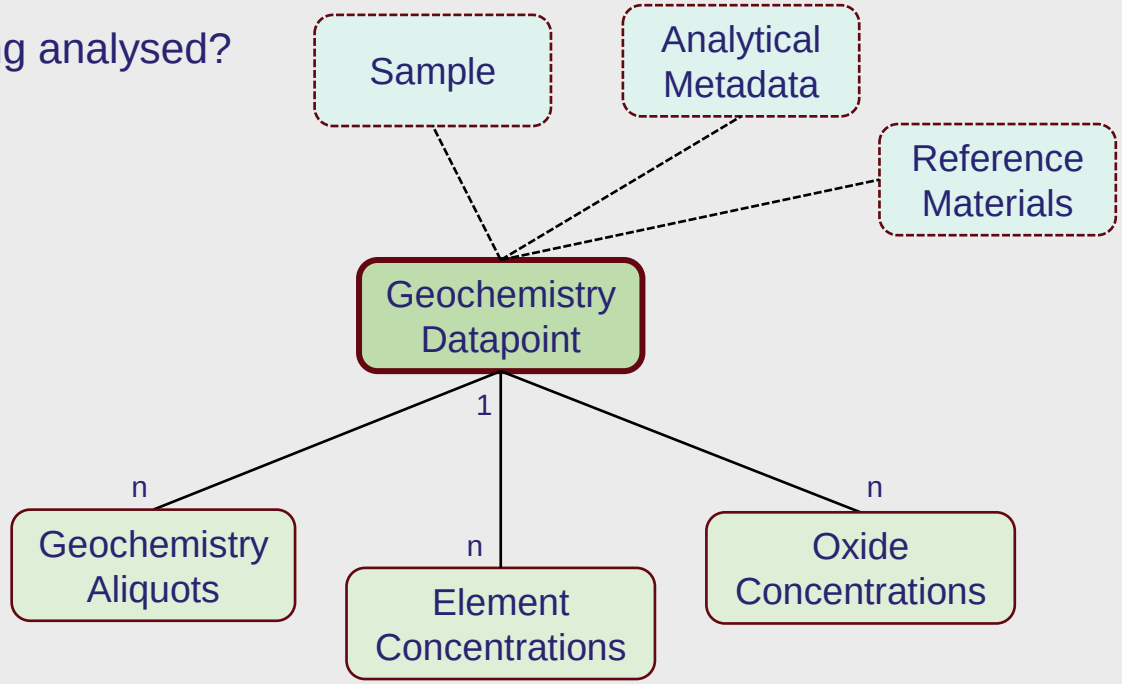


Models produced as custom SKOS formats for domain-specific applications

Example: Inorganic Geochemistry

What is being analysed, how is it being analysed?

Sample Name
Comment
Geochemistry Analytical Technique
Analytical Session ID
Batch ID
Mount ID
Analysis Scale
Analyte Material
Mineral
Reference Material
Oxide Concentration Uncertainty Type
Elemental Concentration Uncertainty Type
Associated Literature
Laboratory
Analyst
Funding



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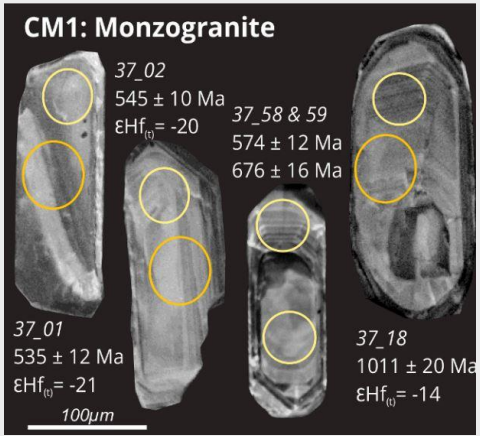
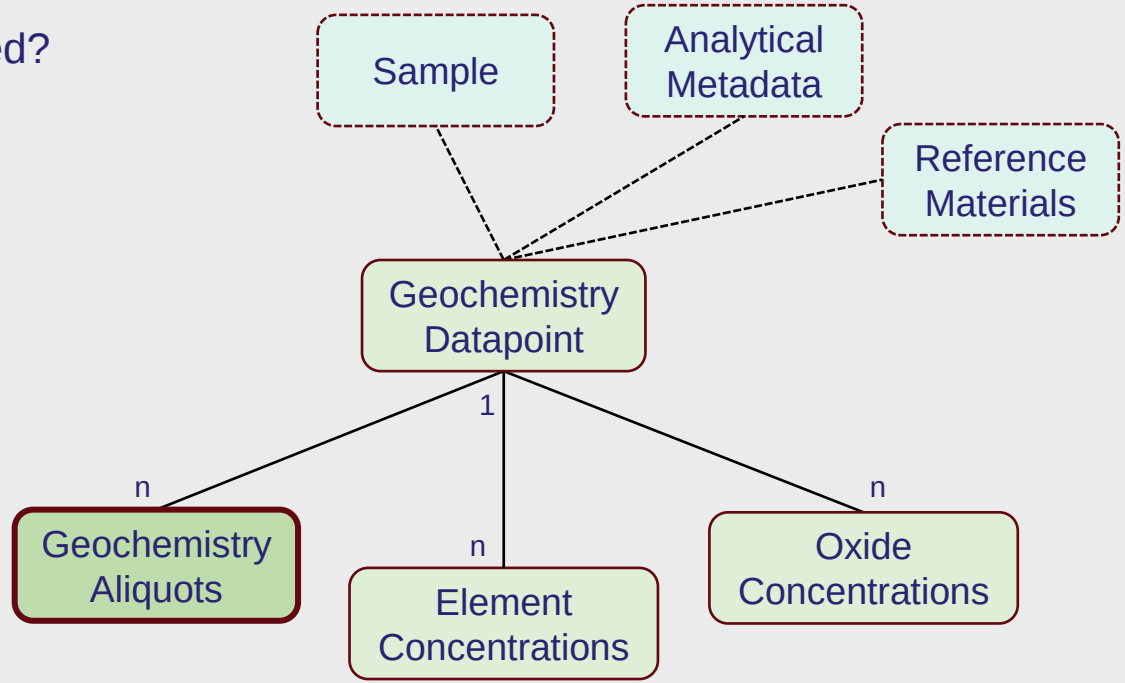
Example: Inorganic Geochemistry

Where in the sample is being analysed?

Sample Name
Aliquot ID
Spot ID
Grain Domain
Analysis Date & Time
Total wt%
Comment



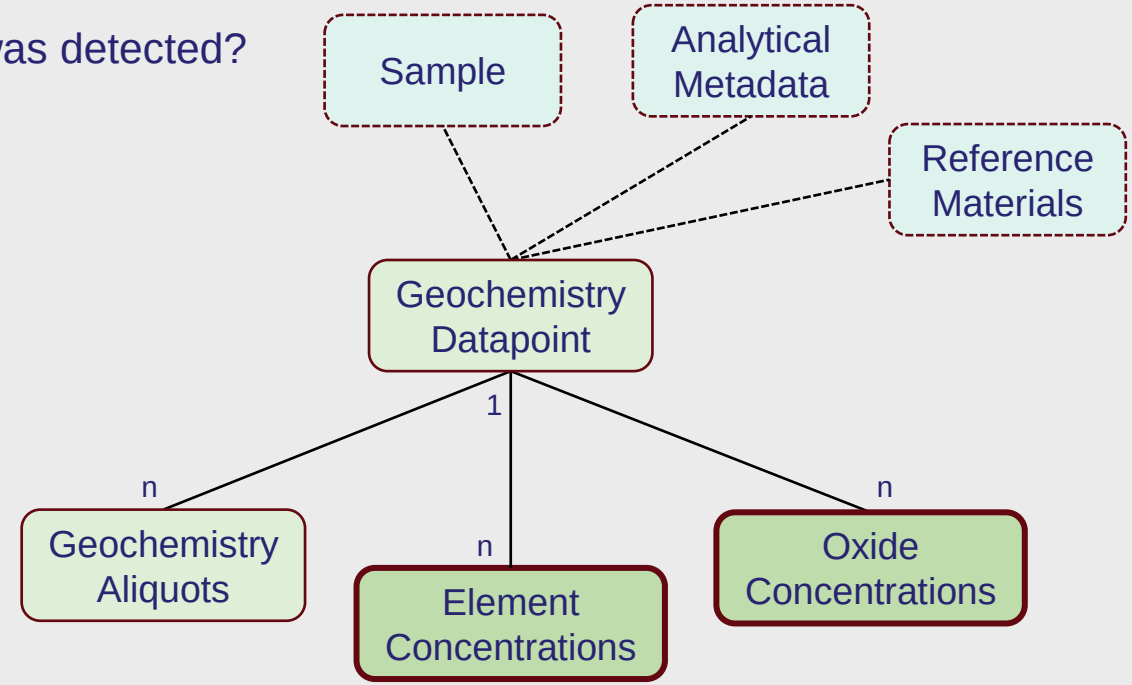


Blades et al., *Precambrian Research* (2021)

Example: Inorganic Geochemistry

What was analysed and how much was detected?

Aliquot ID
Spot ID
Element/Oxide
Concentration
Uncertainty
Measured Mass
Relative Operator



Example: Inorganic Geochemistry

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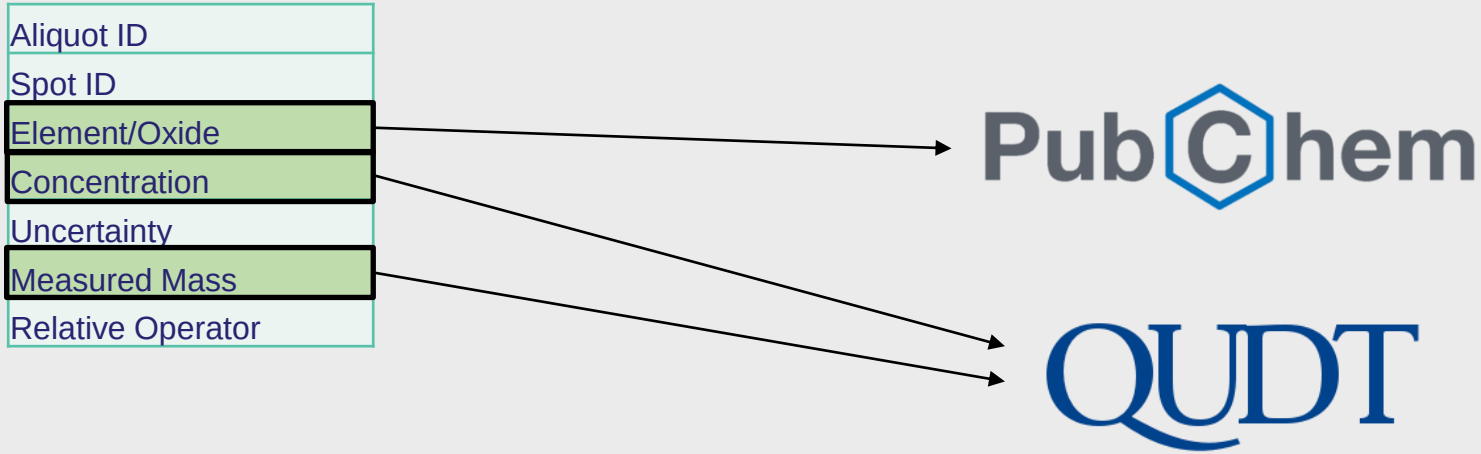

Vocabularies

ARDC Research Vocabularies Australia

- AGN vocabularies for Earth Science are available via RVA (v1.0)

  RDF, XML, JSON, JSON-LD, N-Triples, Turtle, Notation3, N-Quads, TriX, TriG

- 33 hierarchical concept schemes including uncertainty levels, analyte material, grain characteristics, and method-specific

- Support AGN (meta)data models

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https://vocabs.ardc.edu.au/viewById/689

Published Vocabularies

Uncertainty	Grain Aliquot Type	Fission Track Type
Analysis Scale	Crystal Fragmentation	FT Uranium Determination Method
Grain Domain	Detector Intensity Units	Grain Geometry
Relative Operator	Etchant	Grain Morphology
Data Reduction Software	eU Equation	Pit Relationship
Radioactive Decay Constant	FT Age Equation	rmr_0 Equation
Element	FT Age Population Type	Time-Temp. Model Approach
Chemical Species	FT Analytical Algorithm	Time-Temp. Model Constraint
Analyte Material	FT Analytical Software	Time-Temp. Model Path Type
Age Group	FT Characterisation Method	Time-Temp. Model Predicted Parameter
Geochemical Technique	FT Kinetic Indicator	Time-Temp. Model Type

Multiple Schemas Likely Multiple Schemas Single Schema

Schemas

Sample model and basic platform architecture Boone et al. (2022)

GEOSTANDARDS and GEOANALYTICAL RESEARCH

Original Article | Open Access

AusGeochem: An Open Platform for Geochemical Data Preservation, Dissemination and Synthesis

Samuel C. Boone, Hayden Dalton, Alexander Prent, Fabian Kohlmann, Moritz Theile, Yoann Gréau, Guillaume Florin, Wayne Noble, Sally-Ann Hodgekiss, Bryant Ware, David Phillips, Barry Kohn, Suzanne O'Reilly, Andrew Gleadow, Brent McInnes, Tim Rawling ... See fewer authors

First published: 29 January 2022 | https://doi.org/10.1111/ggr.12419 | Citations: 5

A geospatial platform for the tectonic interpretation of low-temperature thermochronology Big Data

Samuel C. Boone, Fabian Kohlmann, Wayne Noble, Moritz Theile, Romain Beucher, Barry Kohn, Stijn Glorie, Martin Danišík, Renjie Zhou, Malcolm McMillan, Angus Nixon, Andrew Gleadow, Xiaodong Qin, Dietmar Müller & Brent McInnes

Scientific Reports **13**, Article number: 8581 (2023) | Cite this article

2643 Accesses | **1** Citations | **18** Altmetric | Metrics

Fission Track and (U-Th)/He Boone et al. (2023)

International Standards

- AGN is a member of the OneGeochemistry project working to build and promote **standards** and **interoperability**

- Aim to publish machine-actionable schemas for AGN through this project

- Continued governance of standards to be facilitated as part of OneGeochemistry working groups?

Summary

- AGN is an Australian collaboration creating resources for **open data and analytical metadata infrastructure** for geochemistry

- Partnerships with **labs** and **universities** to produce reporting standards

- Vocabularies openly accessible and globally available

  Research Vocabularies Australia

- Schema to be published in collaboration with **OneGeochemistry**

Thank you!

ausgeochem.auscope.org.au

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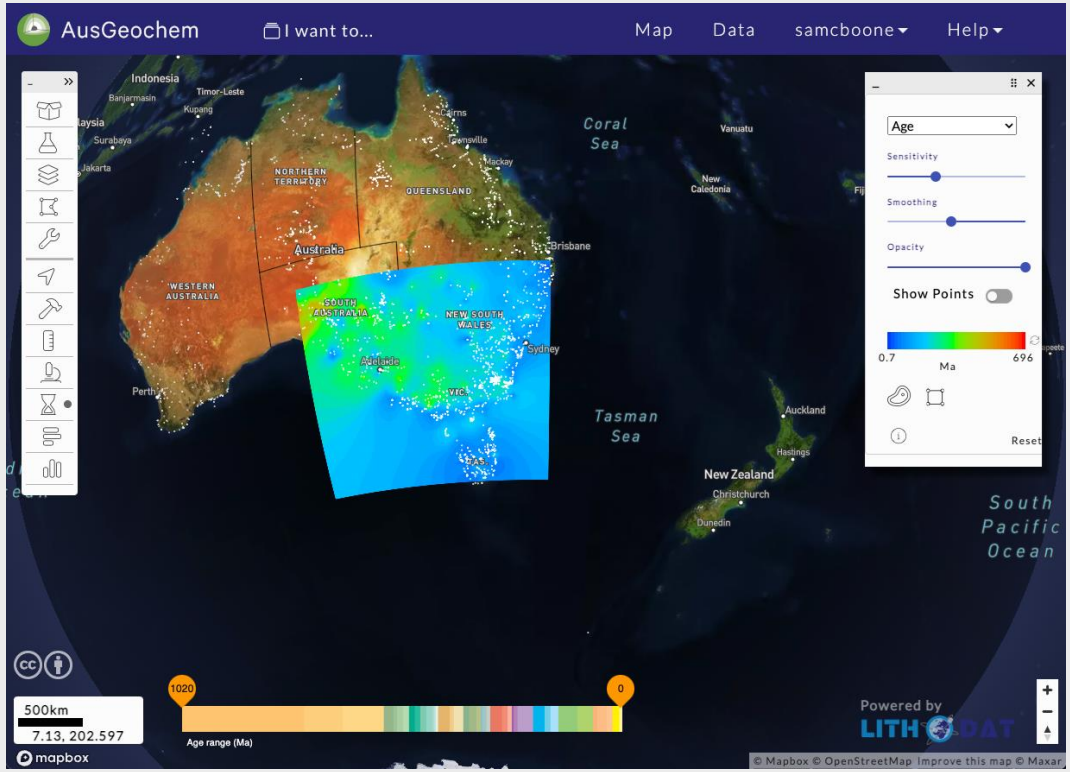
RVA Vocabularies



https://vocabs.ardc.edu.au/viewById/689

auscope.org.au | @auscope

AuScope | NCRIS National Research Infrastructure for Australia

References

- Blades, M. L., Collins, A. S., Foden, J., Payne, J. L., Stüwe, K., Abu-Alam, T., Makroum, F. & Hassan, M. (2021). Age and hafnium isotope evolution of Sudanese Butana and Chad illuminates the Stenian to Ediacaran evolution of the south and east Sahara. *Precambrian Research*, 362, 106323. doi: https://doi.org/10.1016/j.precamres.2021.106323
- Boone, S.C., Dalton, H., Prent, A., Kohlmann, F., Theile, M., Gréau, Y., Florin, G., Noble, W., Hodgekiss, S.-A., Ware, B., Phillips, D., Kohn, B., O'Reilly, S., Gleadow, A., McInnes, B., Rawling, T., 2022. AusGeochem: An open platform for geochemical data preservation, dissemination and synthesis. *Geostandards and Geoanalytical Research*, 46(2), 245-259. doi: https://doi.org/10.1111/ggr.12419
- Boone, S.C., Kohlmann, F., Noble, W., Theile, M., Beucher, R., Kohn, B., Glorie, S., Danišík, M., Zhou, R., McMillan, M., Nixon, A., Gleadow, A., Qin, X., Müller, D., McInnes, B., 2023. A geospatial platform for the tectonic interpretation of low-temperature thermochronology Big Data. *Scientific Reports*, 13(1), 8581. doi: https://doi.org/10.1038/s41598-023-35776-3
- National Center for Biotechnology Information (2024). Periodic Table of Elements. Retrieved October 24, 2024 from https://pubchem.ncbi.nlm.nih.gov/periodic-table/