

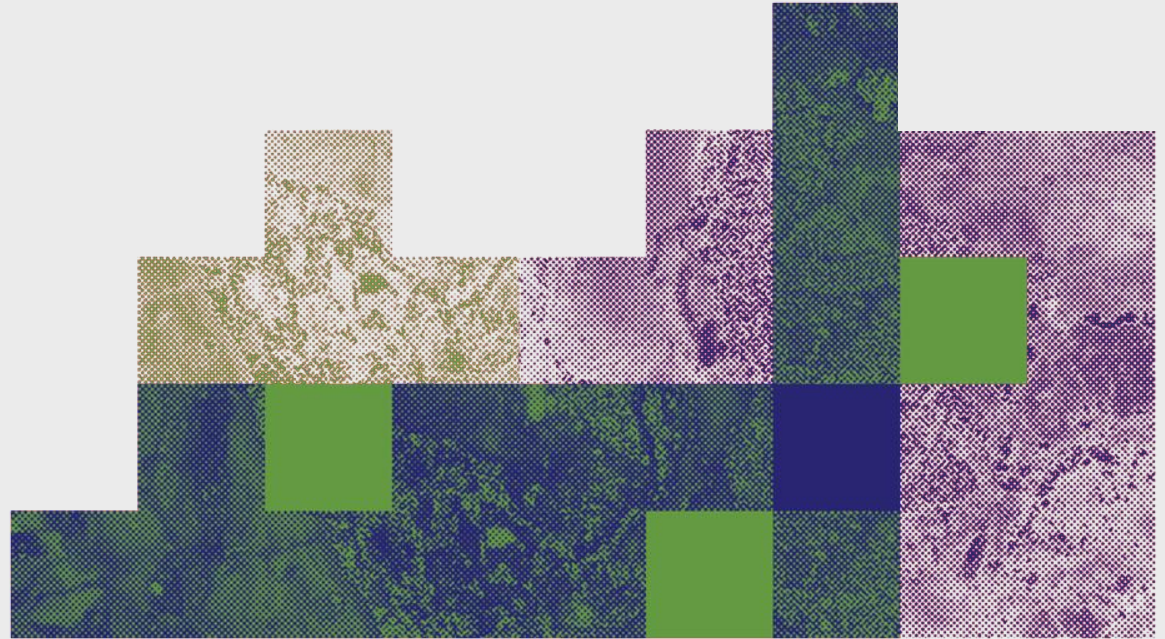


AuScope Geochemistry Network:

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

Angus Nixon

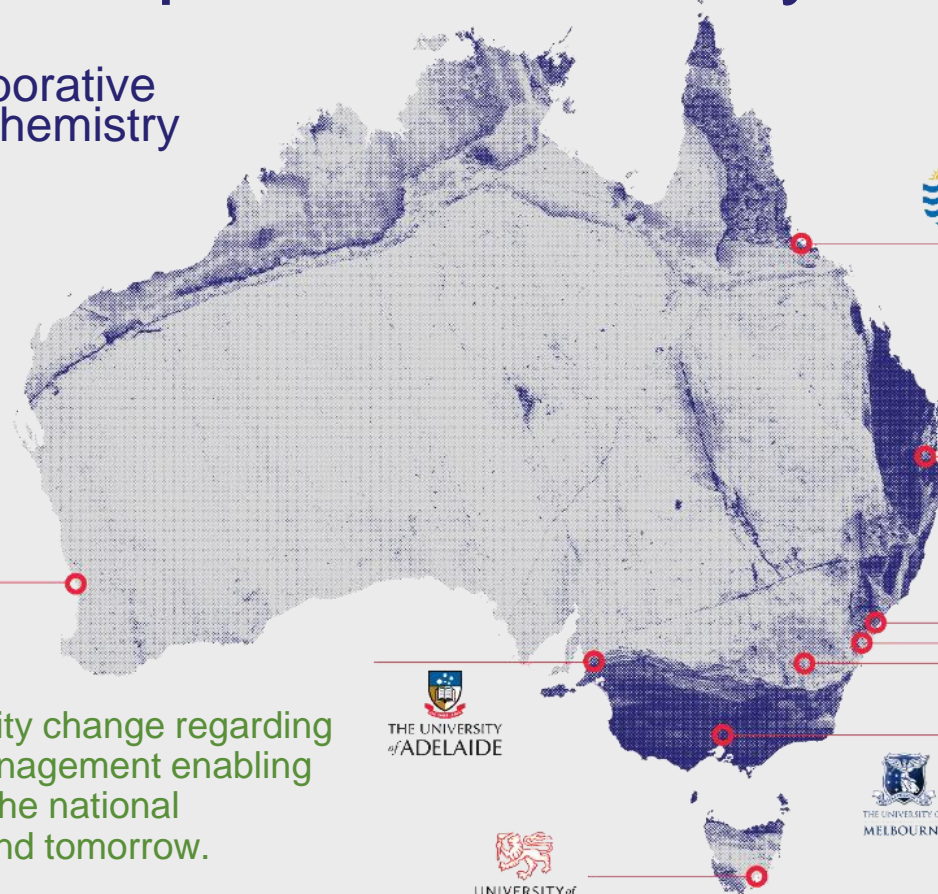
On behalf of the AuScope
Geochemistry Network (AGN)



The AuScope Geochemistry Network

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.



 Curtin University

 THE UNIVERSITY OF WESTERN AUSTRALIA

 CSIRO

 JAMES COOK UNIVERSITY AUSTRALIA

 THE UNIVERSITY OF QUEENSLAND AUSTRALIA

 MACQUARIE UNIVERSITY SYDNEY AUSTRALIA



UNIVERSITY OF WOLLONGONG AUSTRALIA

 THE UNIVERSITY OF ADELAIDE



Australian National University

 THE UNIVERSITY OF MELBOURNE

 MONASH UNIVERSITY

 MUSEUMS VICTORIA

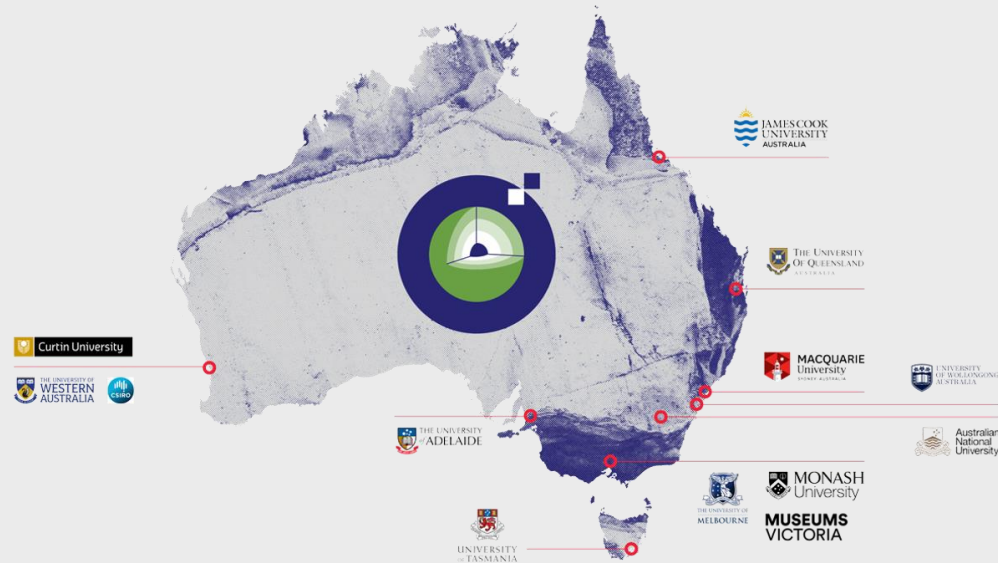
 UNIVERSITY OF TASMANIA

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

Project Overview

Objectives include:

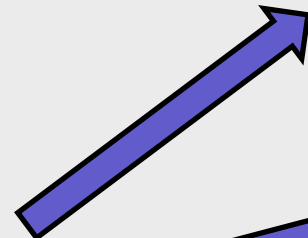
- Developing and maintaining a **FAIR data ecosystem** for the Australian Earth science community
- Establishing compatibility and engagement with **global resources** and **best practice**
- Integrating with **laboratory** and **research** workflows to capture data in the research pathway



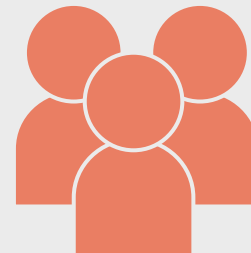
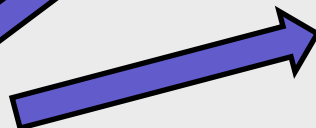
Improved Data Pipeline



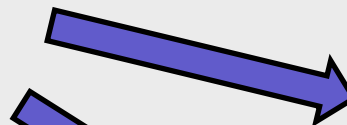
Securely store data
from lab to platform



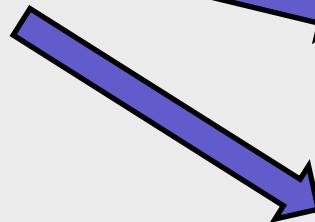
Publish and cite



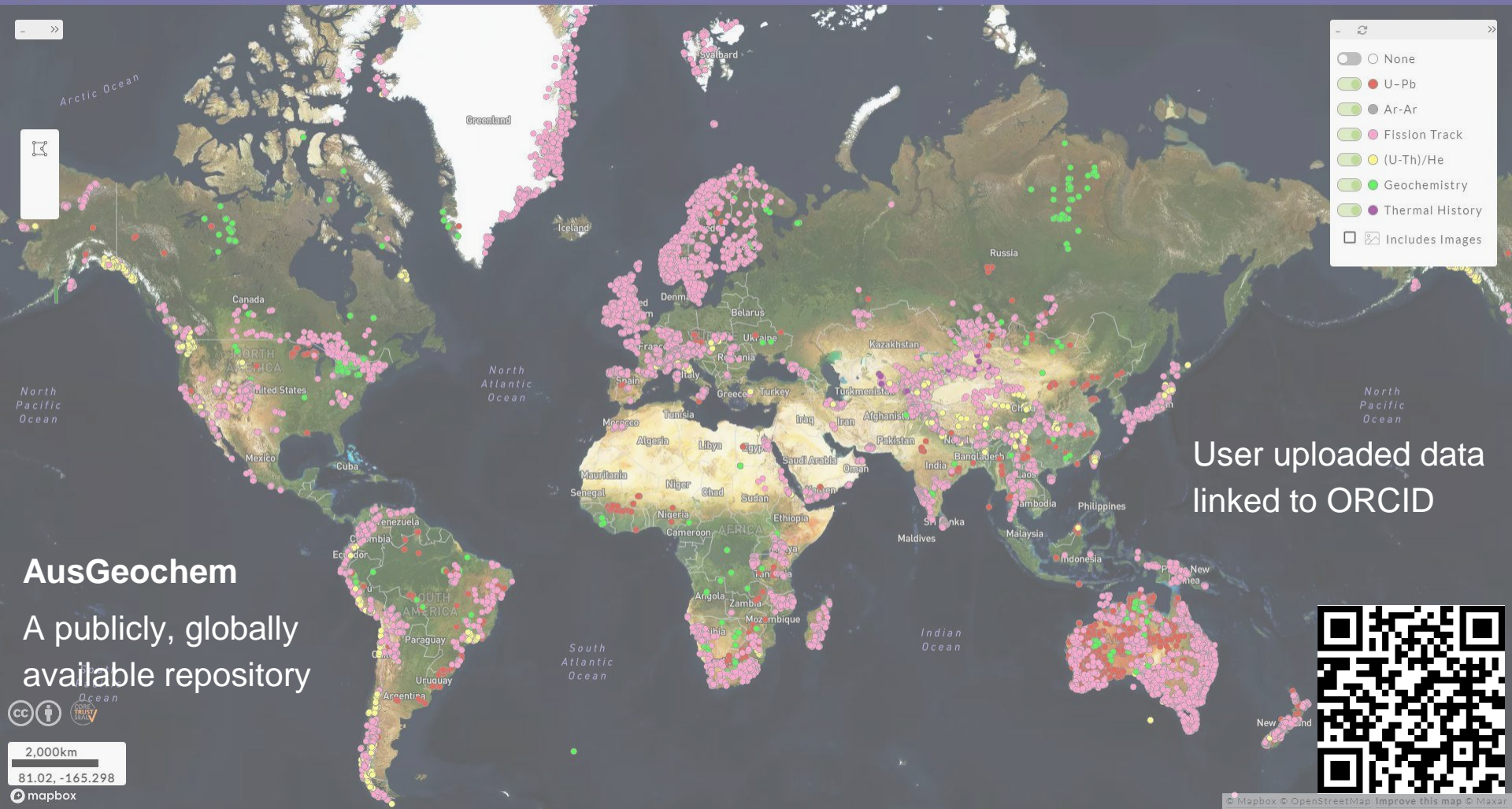
Share with
collaborators
and community



Explore and
interpret data



Connect with
databases



AusGeochem
 A publicly, globally
 available repository

User uploaded data
 linked to ORCID

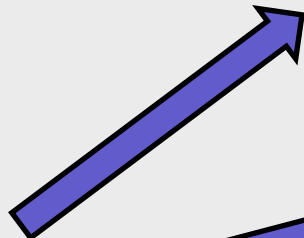
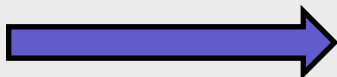
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 mapbox



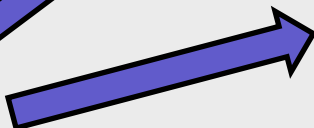
Improved Data Pipeline



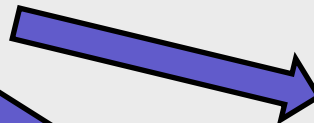
Securely store data
from lab to platform



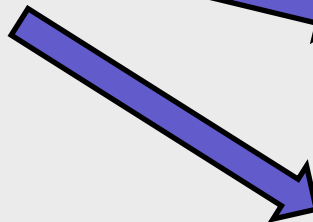
Publish and cite



Share with
collaborators
and community

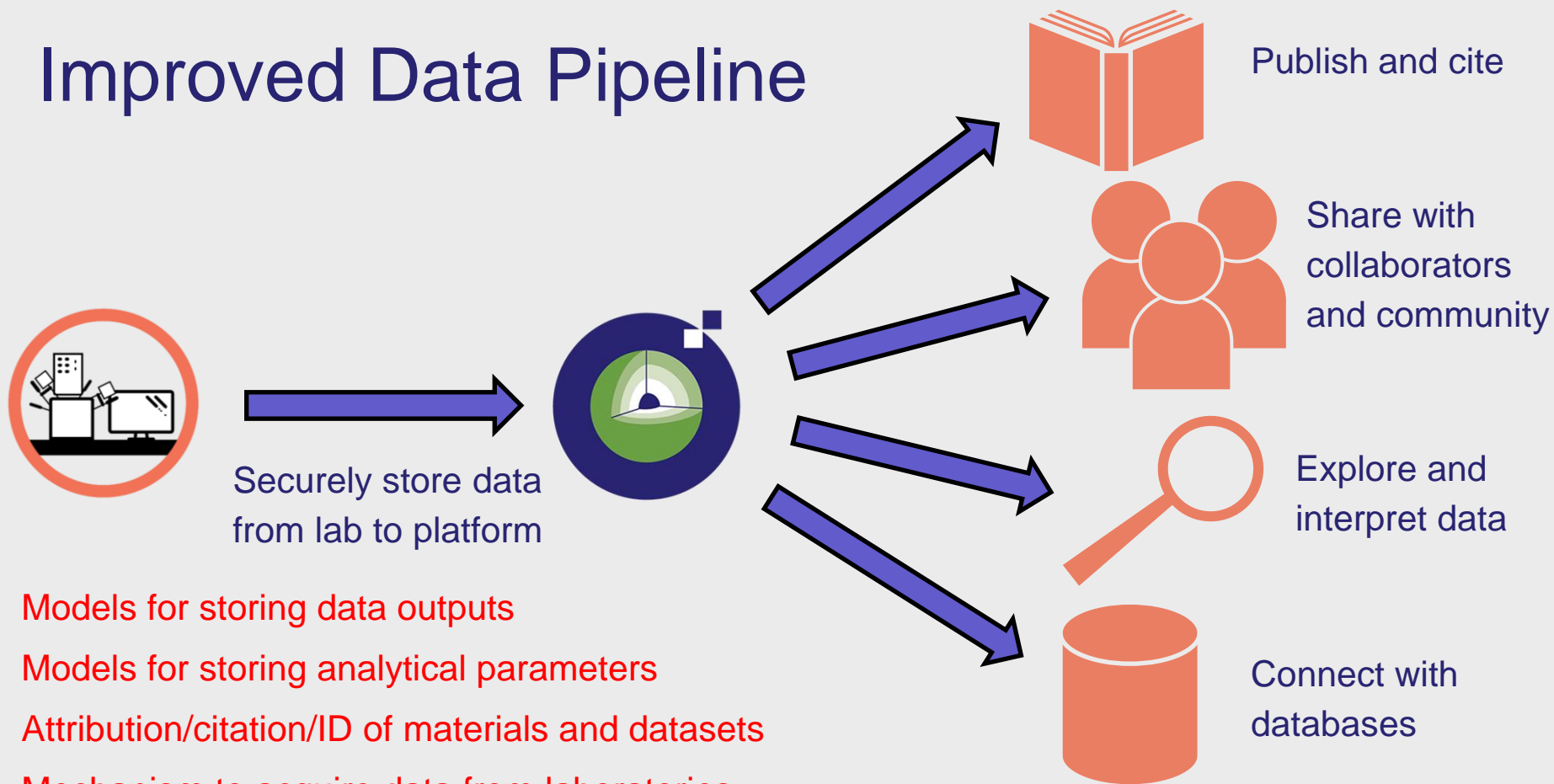


Explore and
interpret data



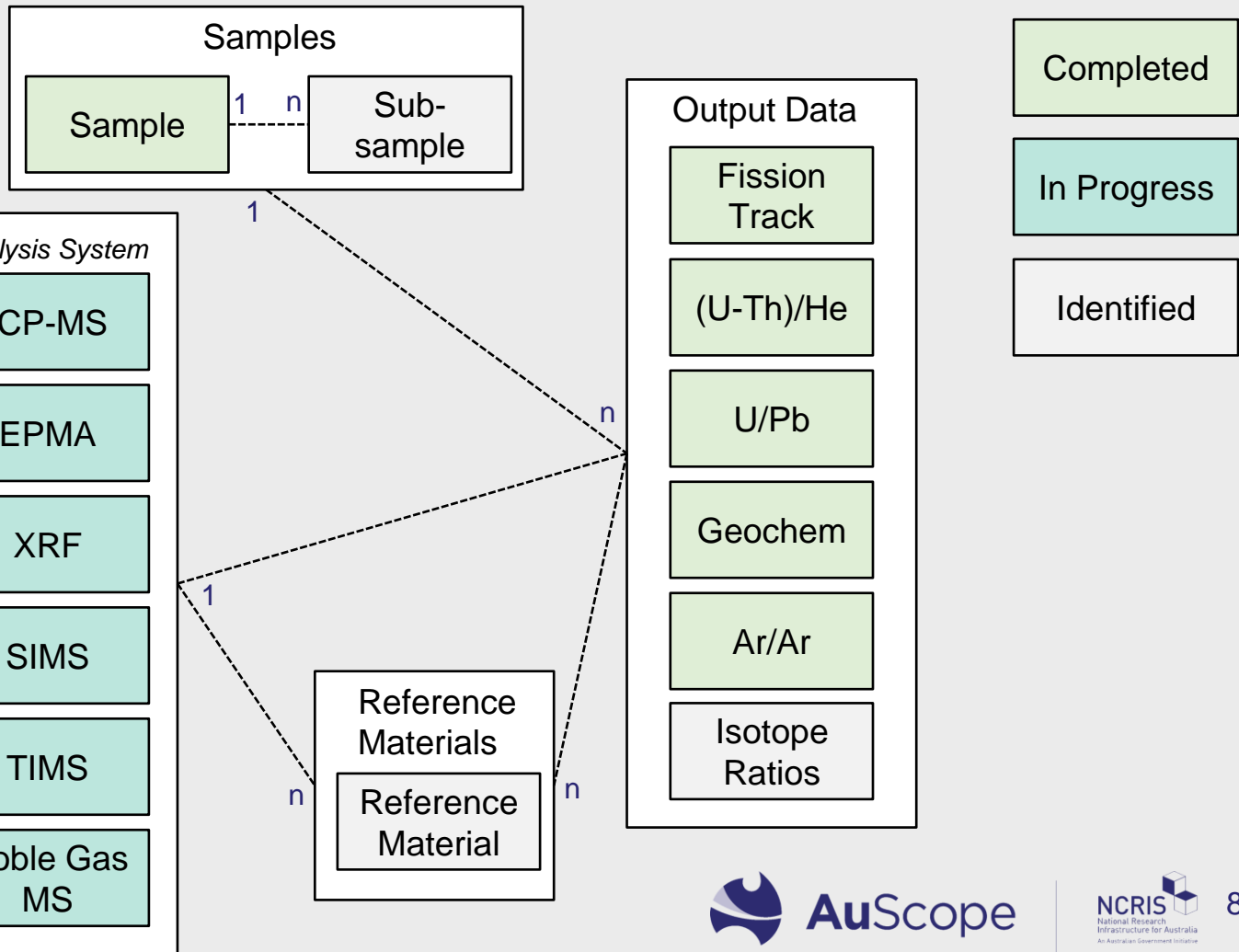
Connect with
databases

Improved Data Pipeline

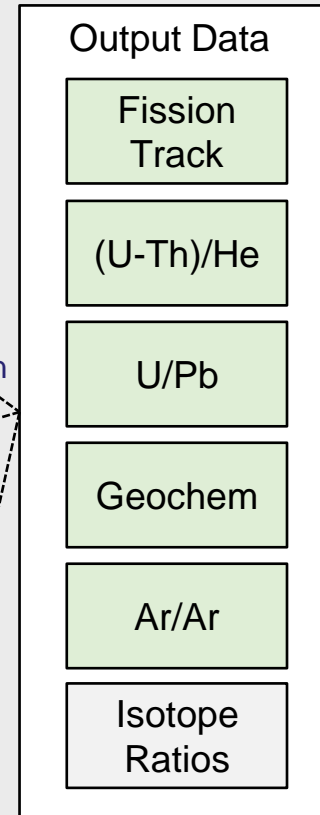
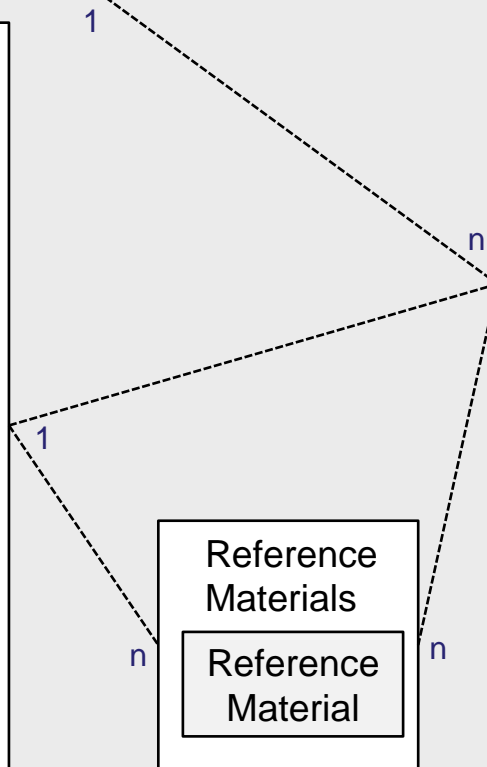
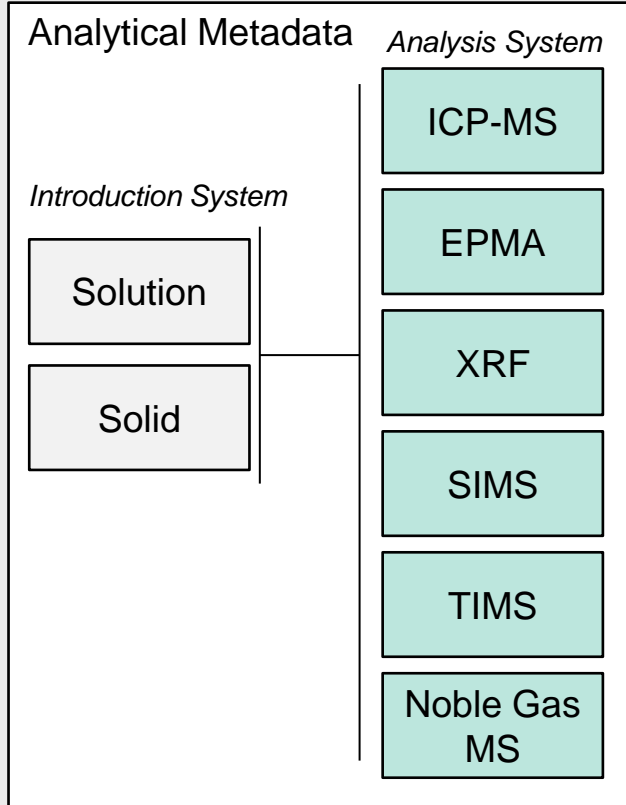
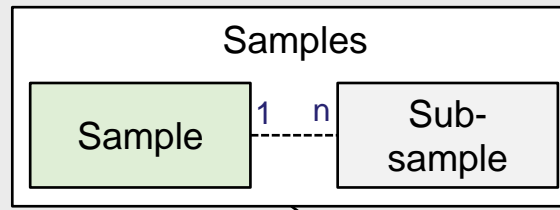


- Models for storing data outputs
- Models for storing analytical parameters
- Attribution/citation/ID of materials and datasets
- Mechanism to acquire data from laboratories (minimal human input)

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

Example: Inorganic Geochemistry

- Measured concentrations of elements and compounds within geological samples
- Present from weight percent to parts per billion levels

PubChem

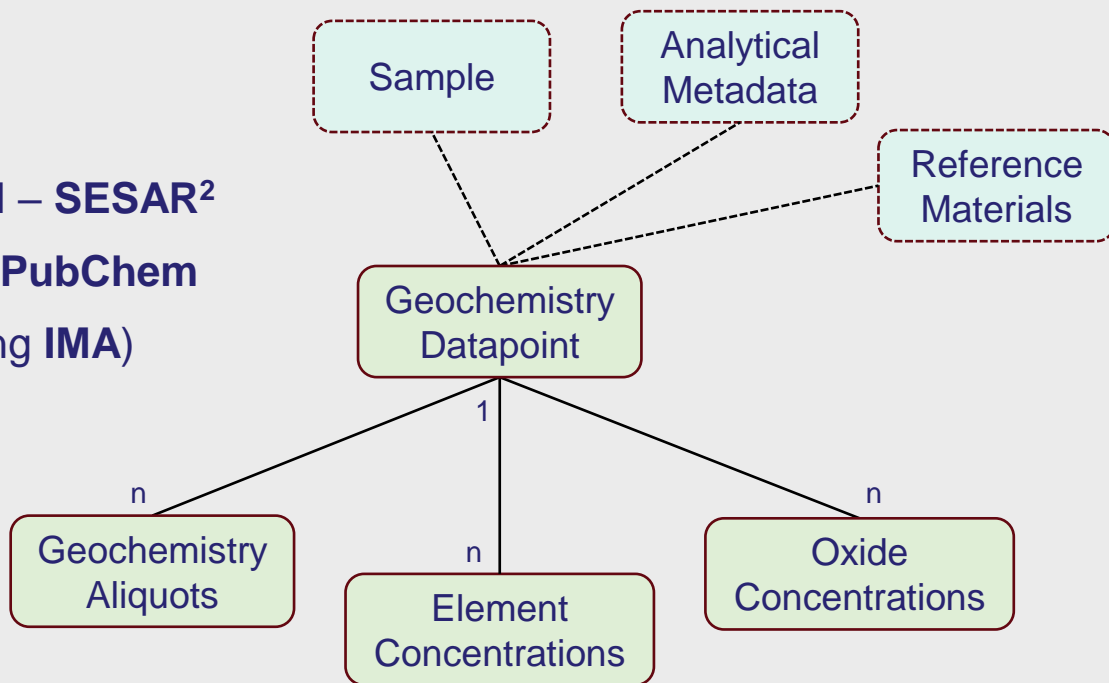
1												18																							
1	1.0080																	2	4.00260																
1	H																	2	He																
	Hydrogen																		Helium																
	Normal																		Gas																
Atomic Number		17		35.45																		Atomic Mass, u													
Name		Cl		Chlorine																		Symbol													
Chemical Group Block		Halogens																																	
3	7.0	4	9.012183																	10	20.180														
2	Li	Be																	10	Ne															
	Lithium	Beryllium																		Neon															
	Alkali Metal	Alkaline Earth Me.																		Noble Gas															
11	22.989	12	24.305																	18	39.9														
3	Na	Mg																	18	Ar															
	Sodium	Magnesium																		Argon															
	Alkali Metal	Alkaline Earth Me.																		Noble Gas															
19	39.0983	20	40.08	21	44.95591	22	47.887	23	50.9415	24	51.996	25	54.93804	26	55.84	27	58.93319	28	58.693	29	63.55	30	65.4	31	69.723	32	72.63	33	74.92159	34	78.97	35	79.90	36	83.80
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr																	
	Potassium	Calcium	Scandium	Titanium	Vanadium	Chromium	Manganese	Iron	Cobalt	Nickel	Copper	Zinc	Gallium	Germanium	Arsenic	Selenium	Bromine	Krypton																	
	Alkali Metal	Alkaline Earth Me.	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal																	
37	85.468	38	87.62	39	88.90584	40	91.22	41	92.90637	42	95.95	43	95.90636	44	101.1	45	102.9055	46	106.42	47	107.868	48	112.41	49	114.818	50	118.71	51	121.760	52	127.6	53	126.9045	54	131.29
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe																	
	Rubidium	Strontium	Yttrium	Zirconium	Niobium	Molybdenum	Technetium	Ruthenium	Rhodium	Palladium	Silver	Cadmium	Indium	Tin	Antimony	Tellurium	Iodine	Xenon																	
	Alkali Metal	Alkaline Earth Me.	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Noble Gas																	
55	132.96	56	137.33	72	178.49	73	180.9479	74	183.84	75	186.207	76	190.2	77	192.22	78	195.08	79	196.96	80	200.59	81	204.383	82	207	83	208.98	84	208.98	85	209.98	86	222.01		
6	Cs	Ba	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn																		
	Cesium	Barium	Hafnium	Tantalum	Tungsten	Rhenium	Osmium	Iridium	Platinum	Gold	Mercury	Thallium	Lead	Bismuth	Polonium	Astatine	Radon																		
	Alkali Metal	Alkaline Earth Me.	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal																		
87	223.01	88	226.02	104	261.1	105	268.1	106	269.1	107	279.1	108	293.1	109	277.1	110	282.1	111	284.1	112	286.1	113	286.1	114	290.1	115	290.1	116	293.1	117	294.2	118	295.2		
7	Fr	Ra	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og																		
	Francium	Radium	Rutherfordium	Dubnium	Seaborgium	Borhrium	Hassium	Moscovium	Darmstadtium	Roentgenium	Copernicium	Nihonium	Flerovium	Moscovium	Livermorium	Tennesseum	Oganesson																		
	Alkali Metal	Alkaline Earth Me.	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal	Transition Metal																		
57	138.905	58	140.116	59	140.90	60	144.24	61	144.91	62	150.4	63	151.964	64	157.2	65	158.92	66	162.500	67	164.93	68	167.26	69	168.93	70	173.05	71	174.9668						
	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu																				
	Lanthanum	Cerium	Praseodymium	Neodymium	Promethium	Samarium	Europium	Gadolinium	Terbium	Dysprosium	Holmium	Erbium	Thulium	Ytterbium	Lutetium																				
	Lanthanide	Lanthanide	Lanthanide	Lanthanide	Lanthanide	Lanthanide	Lanthanide	Lanthanide	Lanthanide	Lanthanide	Lanthanide	Lanthanide	Lanthanide	Lanthanide	Lanthanide																				
89	227.02	90	232.038	91	231.039	92	238.0289	93	237.04	94	244.06	95	243.06	96	247.07	97	247.07	98	251.07	99	252.0830	100	257.0	101	259.0	102	259.1	103	266.1						
	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr																				
	Actinide	Thorium	Protactinium	Uranium	Neptunium	Plutonium	Americium	Curium	Berkelium	Californium	Einsteinium	Fermium	Mendelevium	Nobelium	Lanthanum																				
	Actinide	Actinide	Actinide	Actinide	Actinide	Actinide	Actinide	Actinide	Actinide	Actinide	Actinide	Actinide	Actinide	Actinide	Actinide																				

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**

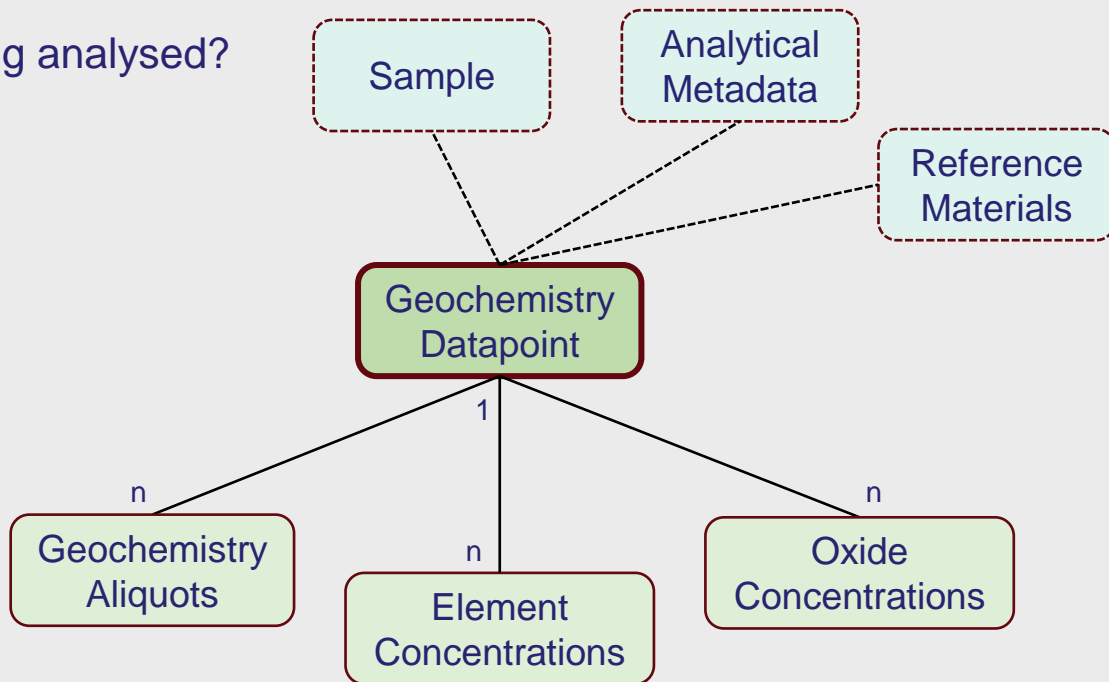


Models produced as custom SKOS formats for domain-specific applications

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



Example: Inorganic Geochemistry

What is being analysed, how is it being analysed?

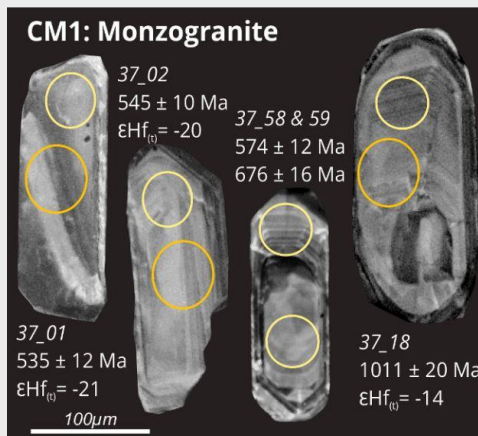
Sample Name
Comment
Geochemistry Analytical Technique
Analytical Session ID
Batch ID
Mount ID
Analysis Scale
Analyte Material
Mineral
Reference Material
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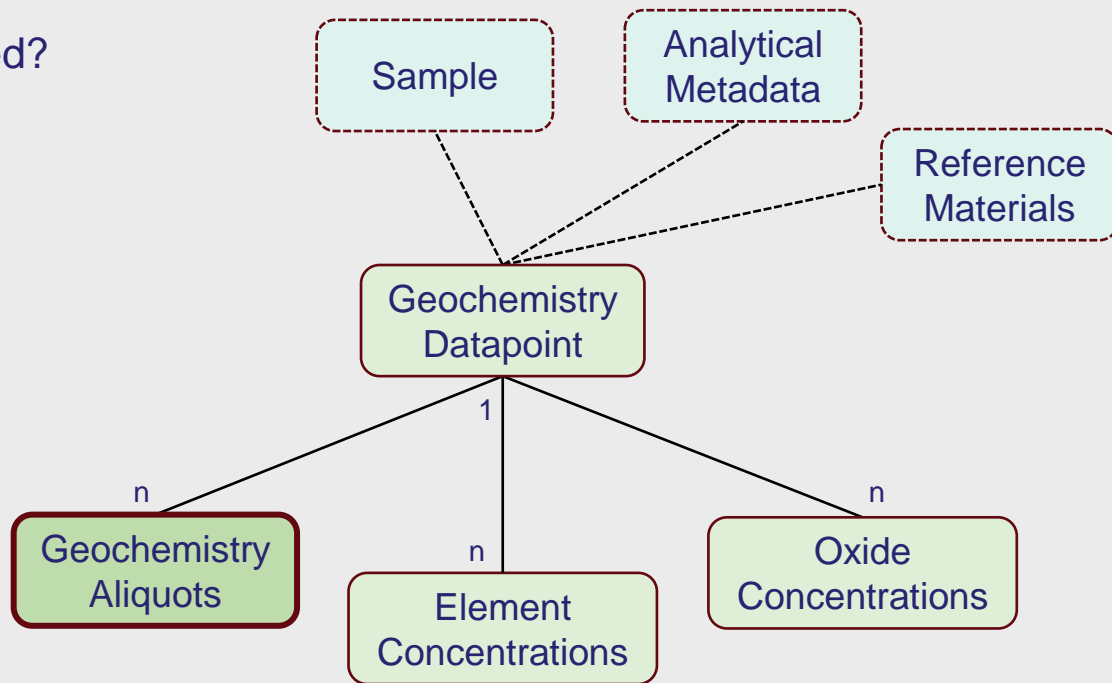
Example: Inorganic Geochemistry

Where in the sample is being analysed?

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



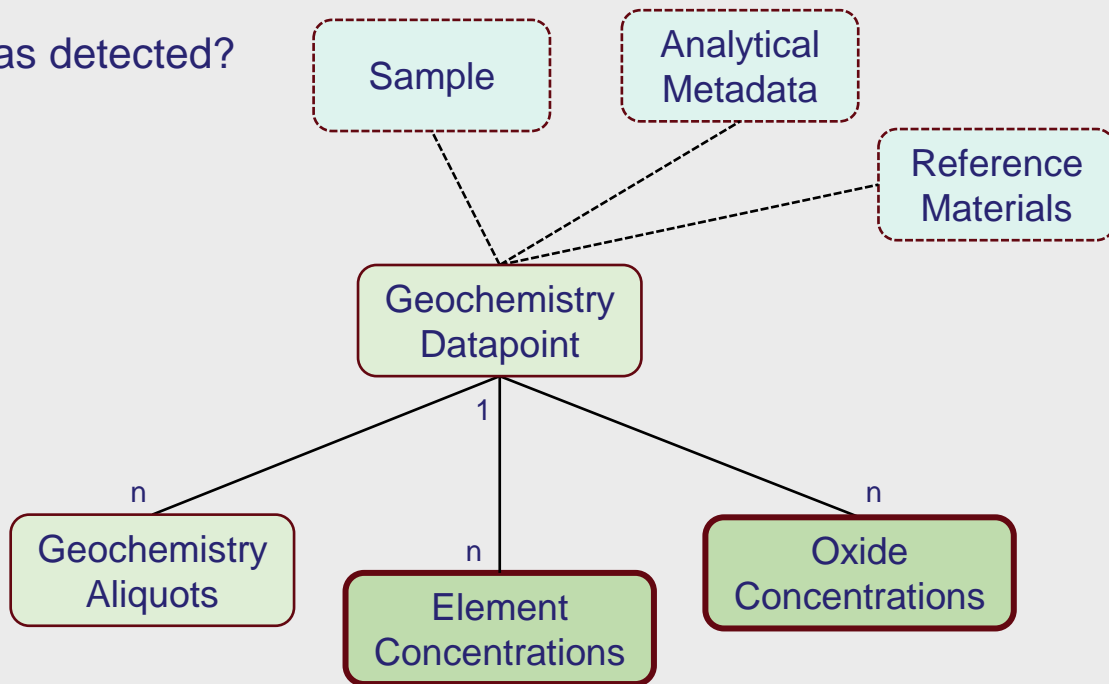
Blades et al., *Precambrian Research* (2021)



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

What was analysed and how much was detected?

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

Pub  hem

QUDT

Vocabularies



- 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



Vocabularies



- 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



<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	r_{m_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

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 Danišik](#), [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**

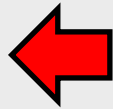
Thank you!

ausgeochem.auscope.org.au

Dr. Angus Nixon

AGN Geochemistry Model Leader

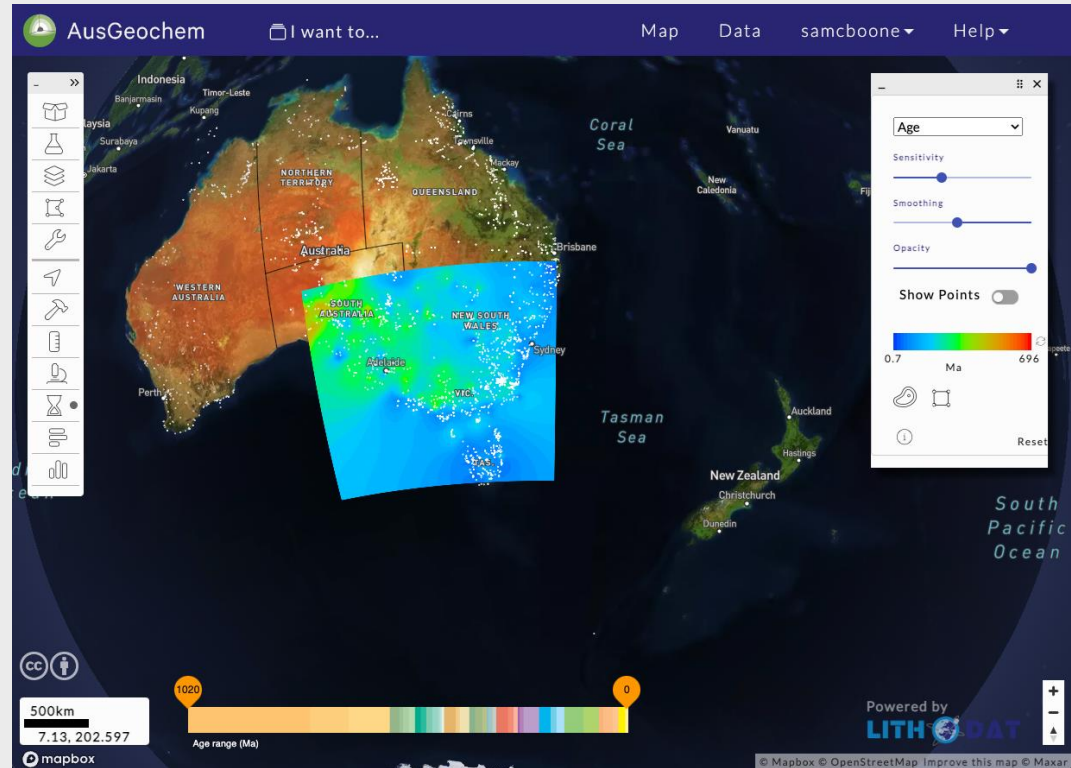
angus.nixon@adelaide.edu.au



RVA Vocabularies

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

auscope.org.au | [@auscope](https://twitter.com/auscope)



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- 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., Daniščík, 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/>