NCI AUSTRALIA

# A path towards reproducible magnetotelluric (MT) time series processing on HPC

## The Australasian Leadership Computing Symposium 2023

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15 June 2023

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

Artist: Lynnice Letty Church – Tribes: Ngunnawal, Wiradjuri & Kamilaroi (ACT and NSW)
Gadi - "to search for" in Ngunnawal language - January 2020 for NCI Gadi Supercomputer

# The 2030 Geophysics Collection Project

- 2030 is an R&D project funded through a collaboration between AuScope, NCI, TERN and ARDC ( https://ardc.edu.au/project/2030-geophysics-collections/ )

- It seeks to:
  a. Make national-scale high-resolution geophysics datasets suitable for programmatic access in HPC environments;
  b. Lay the foundations for more rapid data processing by 2030 next-generation scalable, data intensive computation including Artificial Intelligence (AI) / Machine Learning (ML) and data assimilation.

- The project is about positioning Australian geophysical data collections to be capable of taking advantage of next generation technologies and computational infrastructures by 2030.

# What do we know about 2030 computing?

1. High-end computational power will be at exascale

2. Today's emerging collaborative platforms will continue to evolve as a mix of HPC and cloud

3. Data volumes will be measured in Zettabytes ($10^{21}$ bytes), which is about 10 times more than today

4. **It will be mandatory for data discovery, accessibility, interoperability and reusability to be fully machine-to-machine as envisaged by the FAIR principles in 2016**

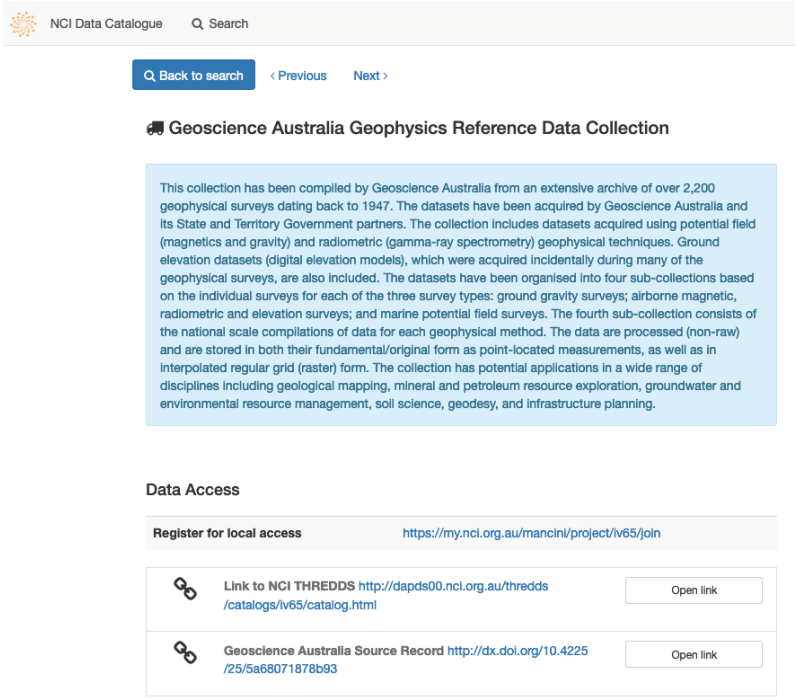
# What are the opportunities of 2030 computing?

1. So often today's research is undertaken on pre-canned, analysis-ready datasets (ARD) that are tuned towards the highest common denominator as determined by the data owner/publisher.
2. By 2030:
   a. Increased computational power co-located with fast-access storage systems will mean that geophysicists will be able to work on less processed data levels and then transparently develop their own derivative products.
   b. Researchers will be able to see the quality of their algorithms more rapidly: there will be multiple versions of open source software used as researchers fine tune individual algorithms to suit their specific requirements.
   c. We will be capable of more precise solutions and in hazards space and other relevant areas, analytics will be done in faster-than-real-time.

Landsat-8 image courtesy of the U.S. Geological Survey

Wyborn, L., Rees, N., Klump, J., Evans, B., Rawling, T., and Druken, K.: The Known Knowns, the Known Unknowns and the Unknown Unknowns of Geophysics Data Processing in 2030 , EGU General Assembly 2022, Vienna, Austria, 23–27 May 2022, EGU22-11012, https://doi.org/10.5194/egusphere-egu22-11012 , 2022.

# Expanding our geophysics data collections on HPC



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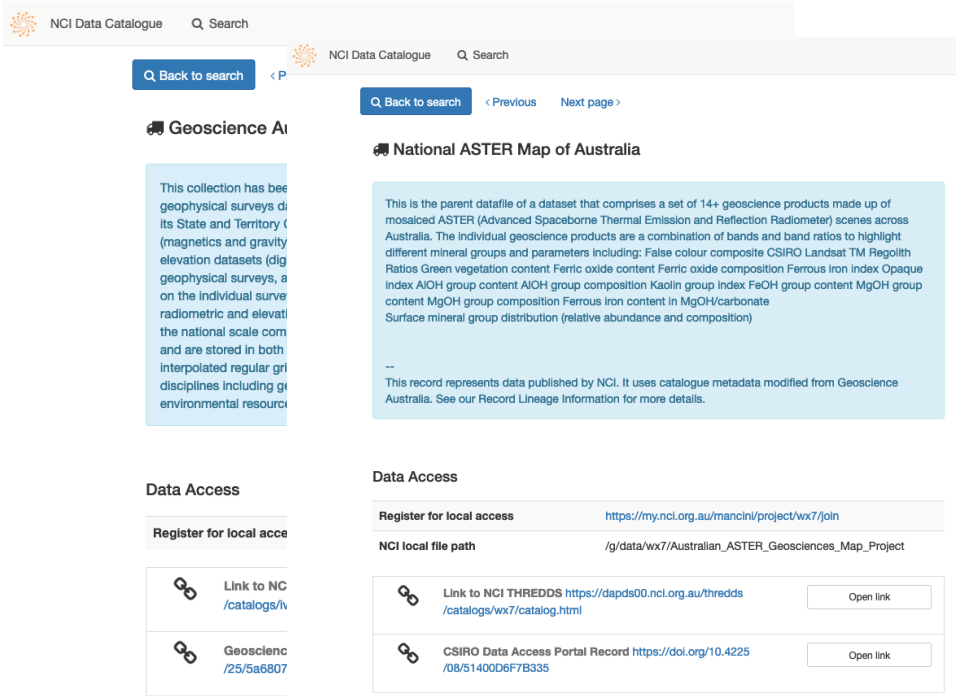

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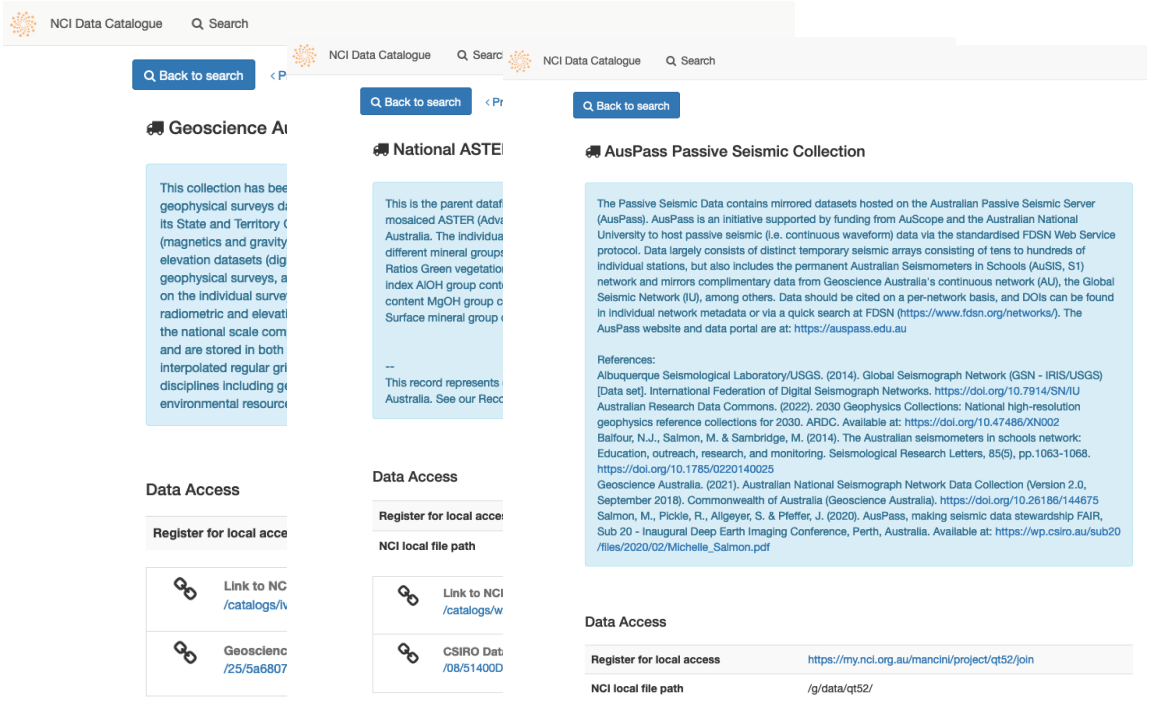

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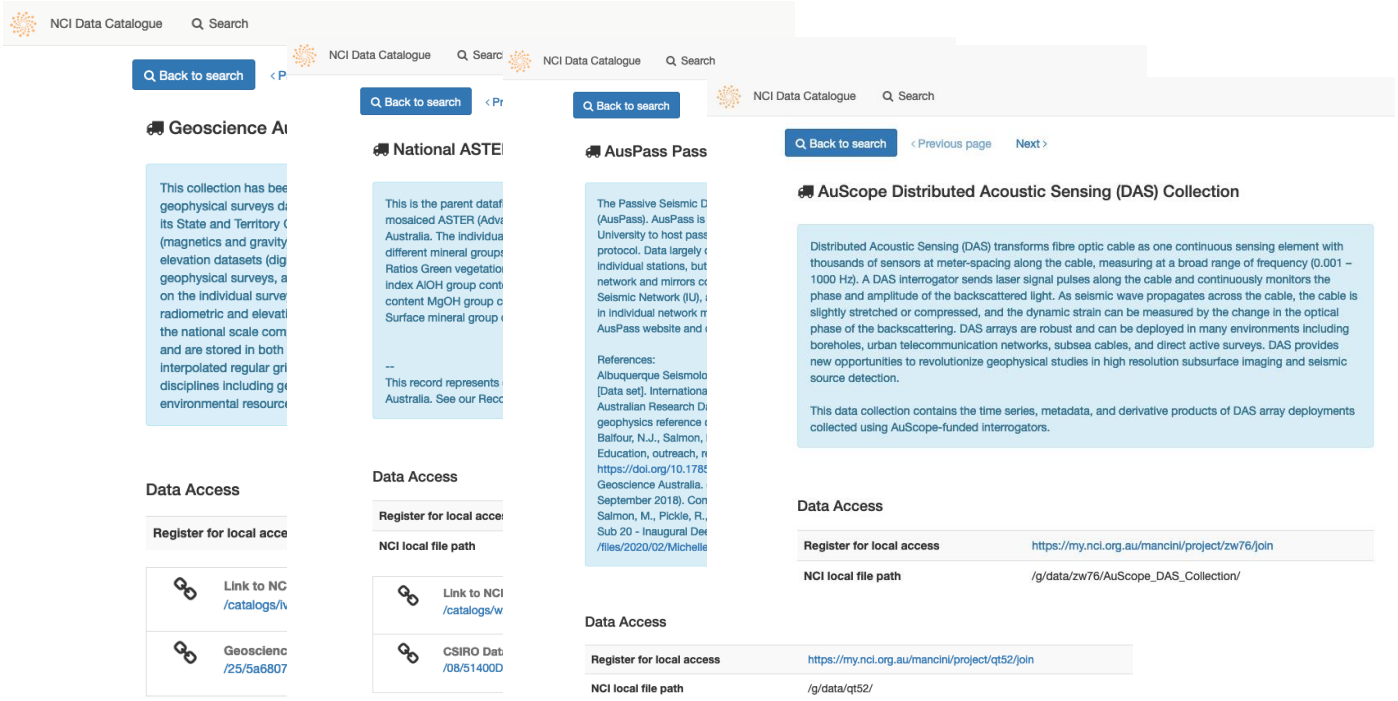

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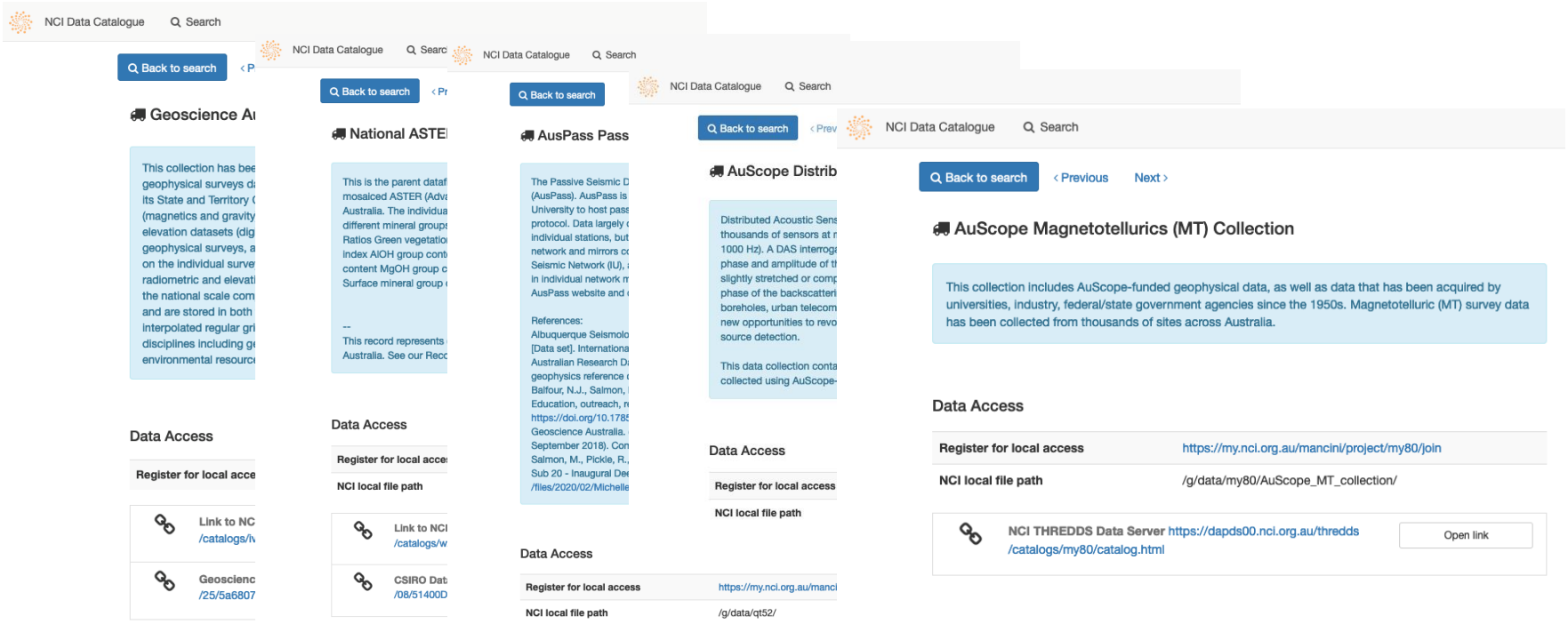


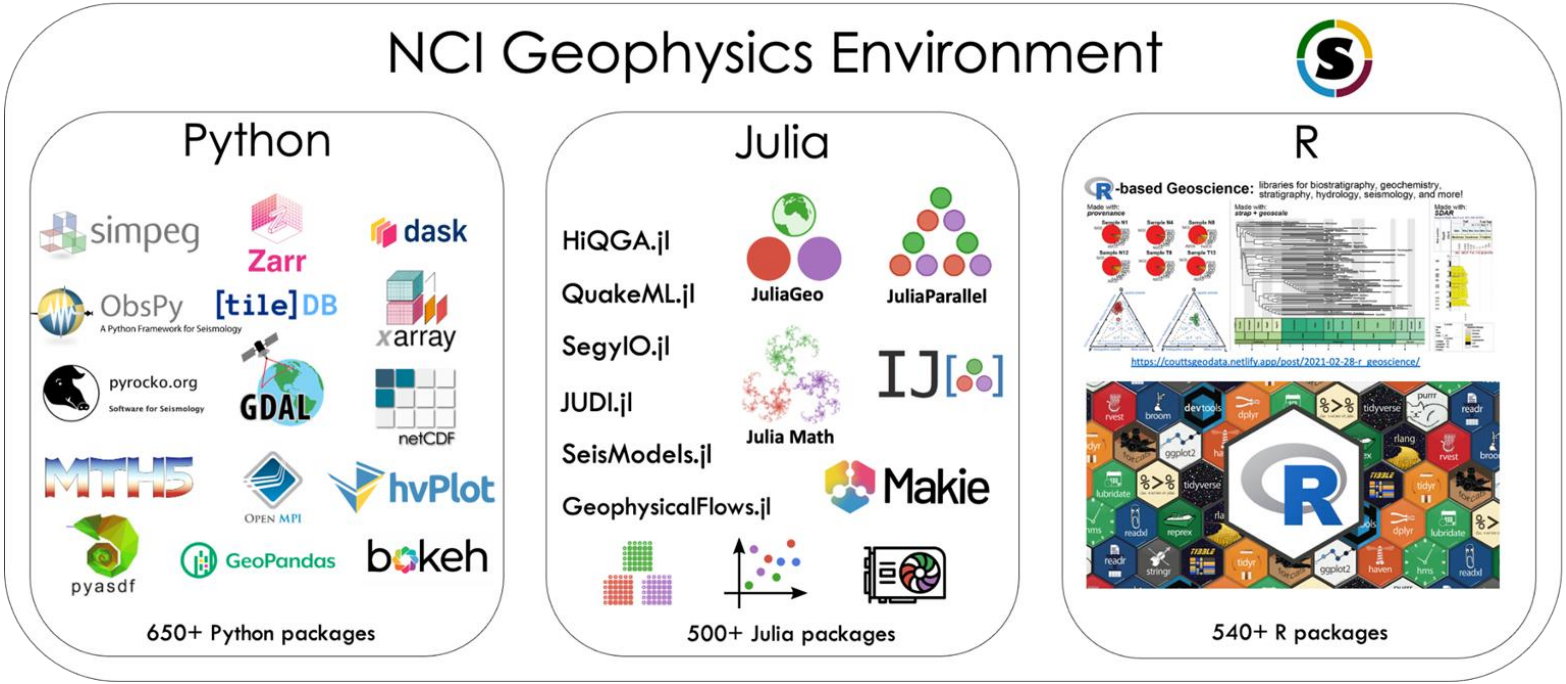
# Building up our geophysical software libraries on HPC

*The following geophysical software are available on the NCI platforms mostly under NCI project up99:*

**BIRRP**: The Bounded Influence Remote Reference Processing program
**EMTF**: Oregon State University robust single station, remote reference and multiple station MT timeseries data processing program
**OCCAM1DCSEM / DIPOLE1D**: Smooth one-dimensional models from CSEM and MT data
**OCCAM2DMT**: Occam's inversion for 2D MT modeling
**MARE2DEM**: parallel adaptive finite element code for 2D forward and inverse modeling for electromagnetic geophysics
**ModEM**: a flexible electromagnetic modelling and inversion program for 2D and 3D MT problems
https://my.nci.org.au/mancini/project/ModEM-geophys
**FEMTIC**: A 3-D Finite Element MagnetoTelluric Inversion code
**esys-escript**: a programming environment for implementing mathematical models in python using the finite element method (FEM).
**Firedrake**: an automated system for solving partial differential equations using the finite element method (FEM).
**jif3D**: a framework for joint inversion of different types of geophysical data in 3D.
**OpenQuake**: an open-source application that allows users to compute seismic hazard and seismic risk of earthquakes on a global scale.

https://opus.nci.org.au/x/KAIWC

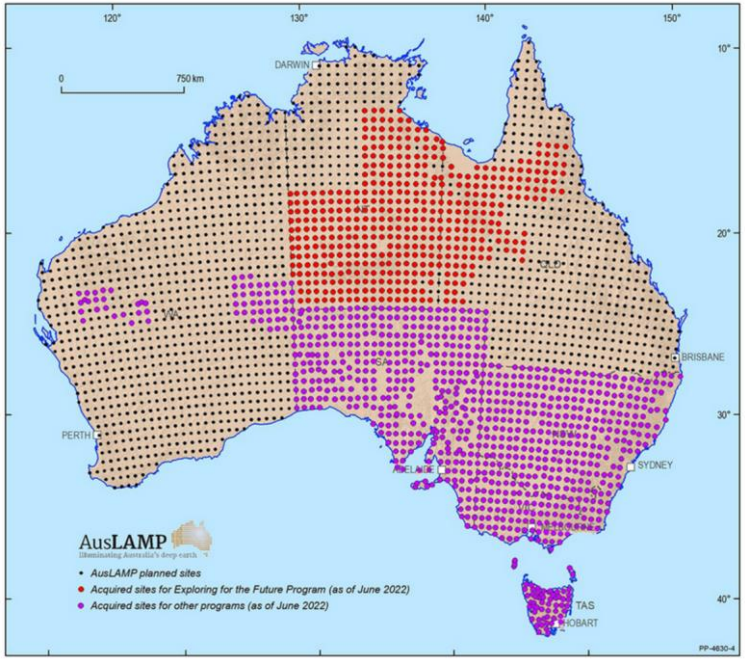
# Developing community driven specialised software environments




$ module use /g/data/up99/modulefiles
$ module load NCI-geophys/<version>

https://doi.org/10.6084/m9.figshare.21919584.v1

# National Scale Analysis: The Australian Lithospheric Architecture Magnetotelluric Project (AusLAMP)




https://www.ga.gov.au/about/projects/resources/auslamp

- A collaborative project between Geoscience Australia, the state and Northern Territory geological surveys, AuScope, universities and other research organisations.
- Aims to acquire long-period MT data at approximately 3000 sites across Australia.
- Dataset will be used to map electrical conductivity structure of the crust and upper mantle to improve the understanding of the geology and tectonic evolution of the Australian plate.
- Results may provide new information for identifying regions with mineral and energy resource potential.

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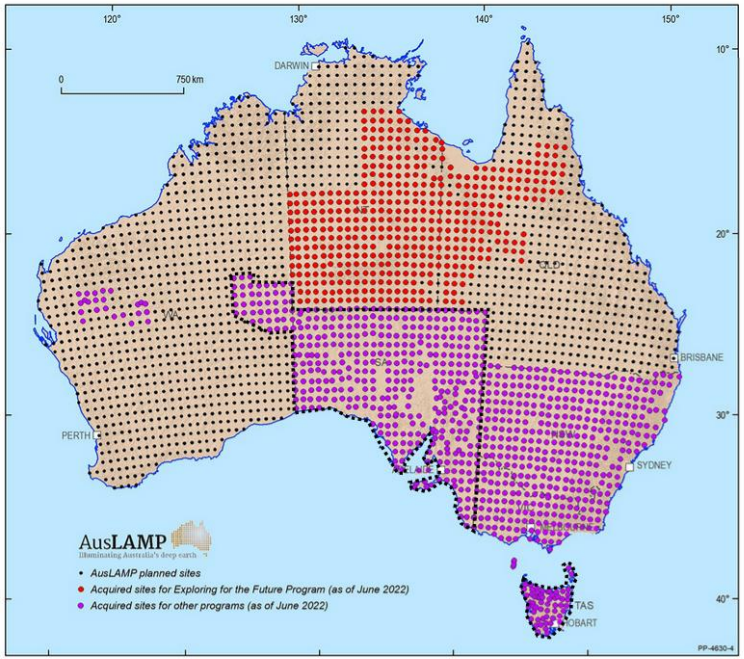


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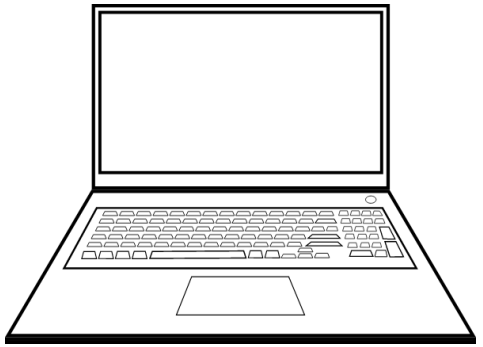

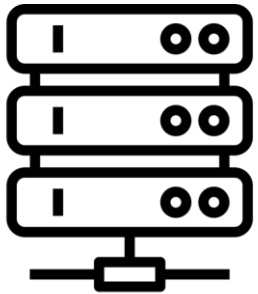

Local Server

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## Where is the AusLAMP MT time series data?

PR6-24 Earth Data Logger


https://www.gfz-potsdam.de/en/section/geophysical-imaging/infrastructure/geophysical-instrument-pool-potsdam-gipp/pool-components/depas-pool/recorder-/-earthdata-pr6-24

LEMI 424


https://www.isr.lviv.ua/lemi424.htm

University of Adelaide Orange Boxes

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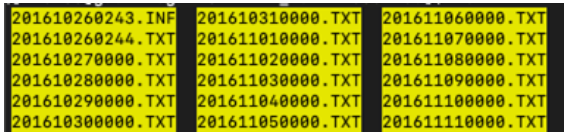
LEMI 424

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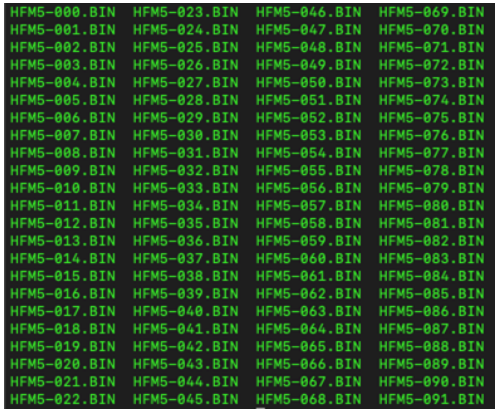

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LEMI 424

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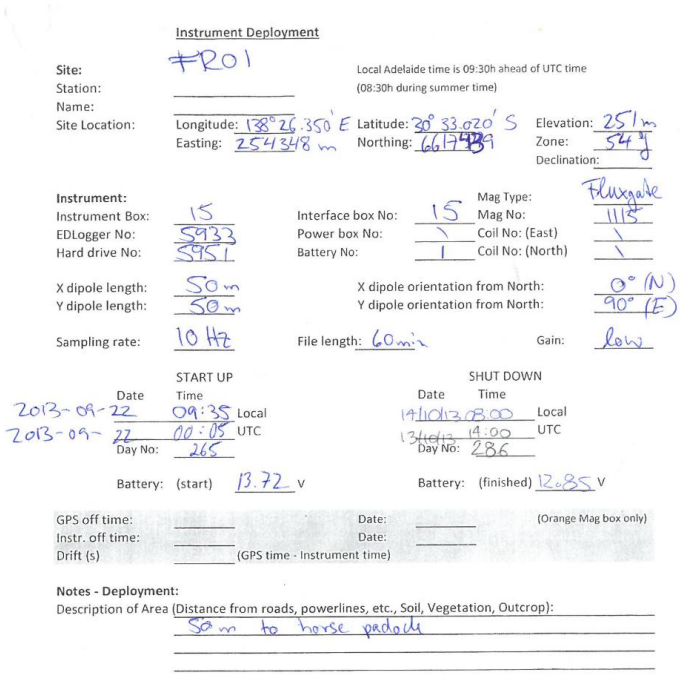
## Where is the AusLAMP MT time series metadata?

| 1 | Not Used | Not Used | Not Used | Not Used | Compulsory | Optional | Optional | Optional | Compulsory | Compulsory | Compulsory | Compulsory | Compulsory | Compulsory | Compulsory | Optional |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | Site Number | Coords Available | Deployed Date Entered | Pickedup Date Entered | Site Number | UTC Start Time Minute | UTC Start Time Second | Deployment Julian Day | Recording Method | MT Recorder Type/ Model | Magnetometer Type/ Model | Electrode Type/ Model | Power Source Type/ Model | Data Confidentiality | North Reference | Drift calculation end time - Time |
| 406 | SA333 | Coords | dep date | Retrival date | SA333 | 44 | 12 | 139 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 407 | SA333-2A | Coords | dep date | Retrival date | SA333-2A | 23 | 0 | 170 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 408 | SA333-2B | Coords | dep date | Retrival date | SA333-2B | 56 | 0 | 170 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 409 | SA334 | Coords | dep date | Retrival date | SA334 | 55 | 0 | 139 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 410 | SA335 | Coords | dep date | Retrival date | SA335 | 53 | 51 | 140 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 411 | SA336 | Coords | dep date | Retrival date | SA336 | 17 | 24 | 140 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 412 | SA337 | Coords | dep date | Retrival date | SA337 | 6 | 48 | 142 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 413 | SA338 | Coords | dep date | Retrival date | SA338 | 3 | 17 | 142 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 414 | SA339 | Coords | dep date | Retrival date | SA339 | 26 | 51 | 143 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 415 | SA340 | Coords | dep date | Retrival date | SA340 | 35 | 0 | 140 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 416 | SA340-2 | Coords | dep date | Retrival date | SA340-2 | 1 | 0 | 143 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 417 | SA341 | Coords | dep date | Retrival date | SA341 | 10 | 0 | 324 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 418 | SA342 | Coords | dep date | Retrival date | SA342 | 54 | 0 | 324 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 419 | SA344 | Coords | dep date | Retrival date | SA344 | 35 | 0 | 135 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 420 | SA344-2 | Coords | dep date | Retrival date | SA344-2 | 6 | 16 | 171 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 421 | SA345 | Coords | dep date | Retrival date | SA345 | 59 | 15 | 132 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 422 | SA346 | Coords | dep date | Retrival date | SA346 | 39 | 0 | 132 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 423 | SA347 | Coords | dep date | Retrival date | SA347 | 7 | 0 | 234 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 424 | SA348 | Coords | dep date | Retrival date | SA348 | 21 | 0 | 232 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 425 | SA349 | Coords | dep date | Retrival date | SA349 | | | 231 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 426 | SA350 | Coords | dep date | Retrival date | SA350 | 41 | 13 | 231 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 427 | SA351 | Coords | dep date | Retrival date | SA351 | 52 | 20 | 231 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |
| 428 | SA354 | Coords | dep date | Retrival date | SA354 | 18 | 52 | 79 | LP | Earth Data Recc | Bartington, Mo | SDEC (France), M | 12Volt 72 Amp/Hr Battery, Power Supply Charging - Solar Panel, 60Watt | Open | Magnetic North | |

# Can we process AusLAMP time series data at scale on HPC?

## Where is the AusLAMP MT time series metadata?



**Instrument Deployment**

**Site:** #R01
**Station:**
**Name:**
**Site Location:** Longitude: 138° 26.350' E Latitude: 30° 33.020' S Elevation: 251 m
Easting: 254348 m Northing: 6617489 Zone: 54 J
Declination:

Local Adelaide time is 09:30h ahead of UTC time
(08:30h during summer time)

**Instrument:**
Instrument Box: 15 Interface box No: 15 Mag Type: Fluxgate
EDLogger No: 5933 Power box No: \ Mag No: 1115
Hard drive No: 5951 Battery No: 1 Coil No: (East) \
Coil No: (North) \

X dipole length: 50 m X dipole orientation from North: 0° (N)
Y dipole length: 50 m Y dipole orientation from North: 90° (E)

Sampling rate: 10 Hz File length: 60 min Gain: low

| | START UP | | SHUT DOWN | |
|---|---|---|---|---|
| | Date | Time | Date | Time |
| 2013-09-22 | 09:35 | Local | 19/10/13 | 08:00 Local |
| 2013-09-22 | 00:05 | UTC | 13/10/13 | 14:00 UTC |
| Day No: | 265 | | Day No: | 286 |

Battery: (start) 13.72 V Battery: (finished) 12.85 V

GPS off time: Date: (Orange Mag box only)
Instr. off time: Date:
Drift (s) (GPS time - Instrument time)

**Notes - Deployment:**
Description of Area (Distance from roads, powerlines, etc., Soil, Vegetation, Outcrop):
50 m to horse paddock

# Converting MT time series (meta)data to international standards

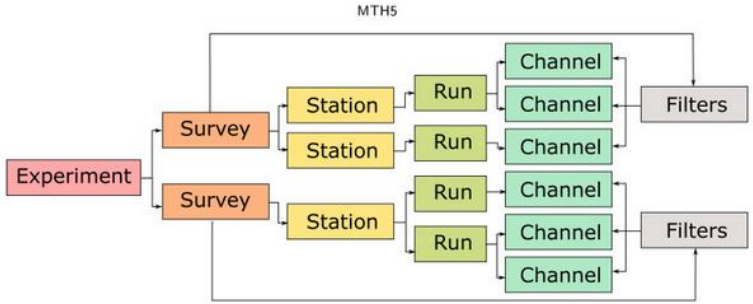
ELSEVIER

Computers & Geosciences
Volume 162, May 2022, 105102

Research paper

## MTH5: An archive and exchangeable data format for magnetotelluric time series data

Jared Peacock [a], Karl Kappler [b], Lindsey Heagy [c], Timothy Ronan [d], Anna Kelbert [e], Andrew Frassetto [d]



# MT_metadata

- Current version of MT_metadata has 355 attributes
  - 152 required parameters
  - 203 non mandatory parameters (but useful to have)

- For legacy AusLAMP metadata, we could not meet this standard as many of the required parameters were not recorded at the time of acquisition

- We did our best with what we had and worked on a Legacy AusLAMP MT_metadata profile that was a 72 element subset of the full MT_metadata standard

- Held regular meetings with the USGS based lead developer of MT_metadata and added in some revisions to the original standard (e.g., survey.funding_source.organization, survey.state, more options for station.release_license)

# Scaling up MT time series processing

The **M**agneto**T**ellurics **t**ime **s**eries **d**ata **p**ublication (**MTtsdp**) codes: https://github.com/nci/MTtsdp

| Processing Levels | Name | Description |
|---|---|---|
| Packed Raw Data | Raw Time Series | Telemetry data streamed from site loggers |
| Level 0 | Edited Time Series | Time ordered instrument recorded data (e.g., raw voltages, counts) at full resolution |
| Level 1 | Transformed Time Series | Level 0 data that have been transformed (e.g., calibrated, resampled, rotated, had noisy data removed, filters applied). |
| Level 2 | Derived frequency domain processed data | Geophysical parameters (e.g., impedance tensors) derived from frequency domain time series processing of Level 1 data |
| Level 3 | Derived modelling inputs and outputs | Level 2 parameters converted into input files for modelling and inversion algorithms with outputs mapped onto space-time grids. |

Rees, N., Evans, B., Heinson, G., Conway, D., Yang, R., Thiel, S., Robertson, K., Druken, K., Goleby, B., Wang, J., Wyborn, L. & Seillé, H., 2019. The Geosciences DeVL Experiment: new information generated from old magnetotelluric data of The University of Adelaide on the NCI High Performance Computing Platform, ASEG Extended Abstracts, 2019:1, 1-6, DOI: 10.1080/22020586.2019.12073015

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Rees, N., Evans, B., Heinson, G., Conway, D., Yang, R., Thiel, S., Robertson, K., Druken, K., Goleby, B., Wang, J., Wyborn, L. & Seillé, H., 2019. The Geosciences DeVL Experiment: new information generated from old magnetotelluric data of The University of Adelaide on the NCI High Performance Computing Platform, ASEG Extended Abstracts, 2019:1, 1-6, DOI: 10.1080/22020586.2019.12073015

# HPC has reduced processing times significantly

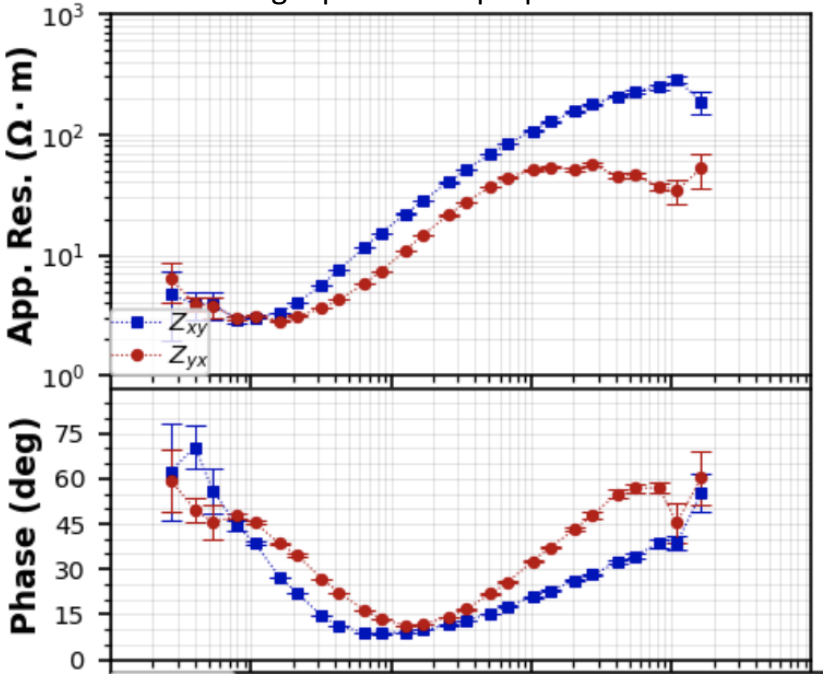
## Parallel I/O via NCI-geophys environment

- MTH5: HDF5 data container for magnetotelluric time series data
- MT_metadata: standardised time series and transfer function metadata for magnetotelluric data
- Tests conducted on the AusLAMP Musgraves Province time series data: https://dx.doi.org/10.25914/58gr-1550

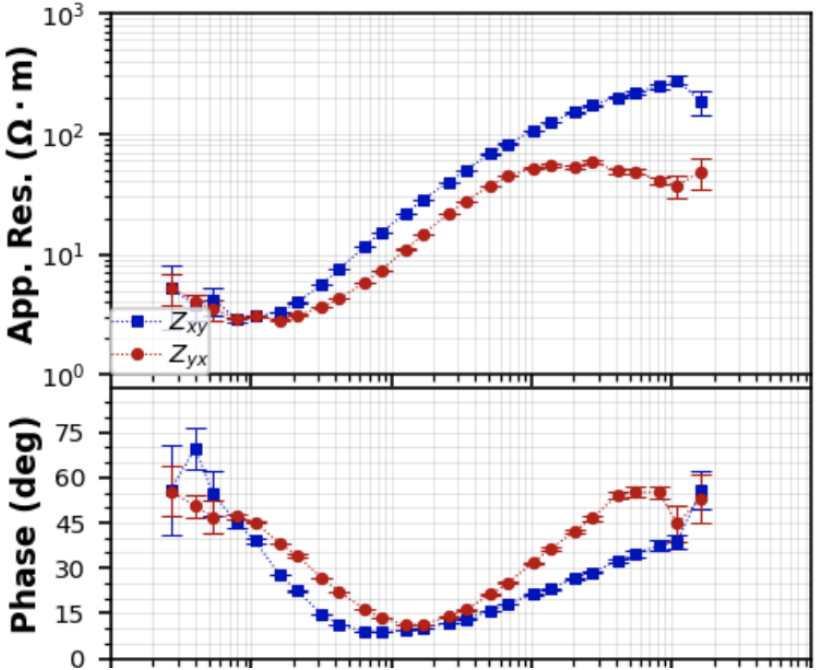
| Dataset of 93 stations | Serial I/O | MPI based Parallel I/O (96 cores) |
|---|---|---|
| Level 0: one mth5/mt_metadata file per station | ~ 5 hours 47 minutes | ~ 4 minutes |
| Level 1: one mth5/mt_metadata file per station | ~ 49 minutes | ~1 minute 13 seconds |
| Level 2: one EDI file per station | ~ 2 hours 30 minutes | ~ 2 minutes |

# Computational reproducibility

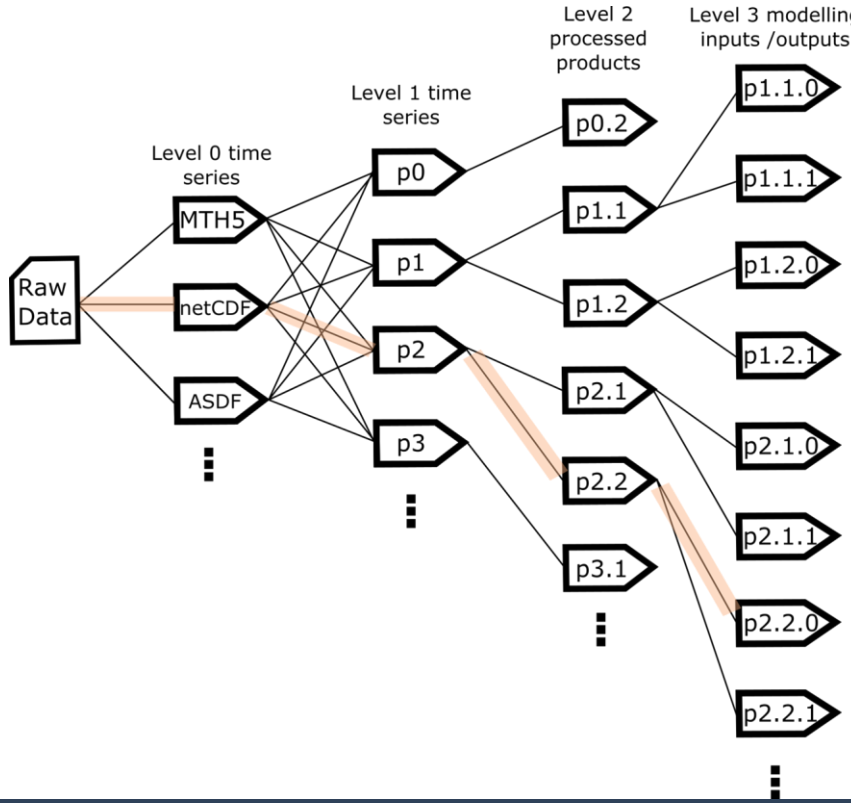
Original station WA72 processed using a personal laptop



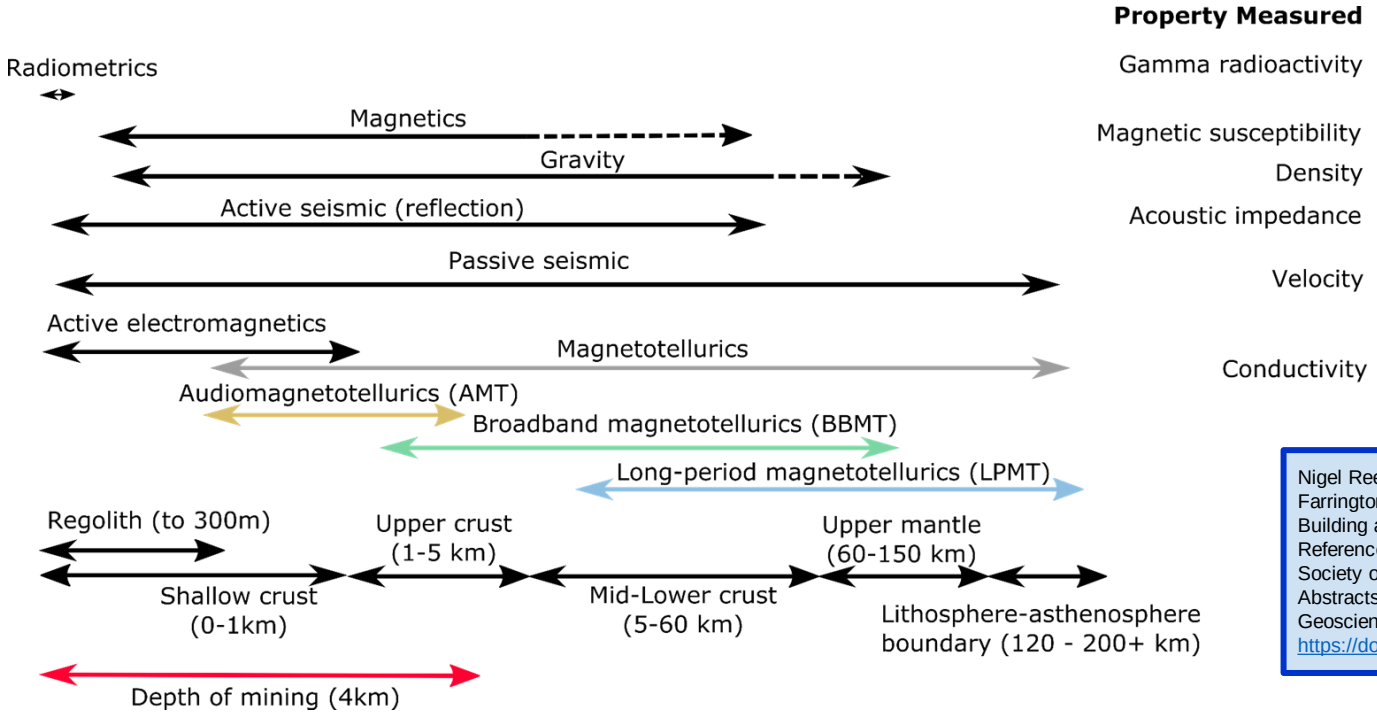

Processing station WA72 using the MTtsdp automations on HPC



# Transparent provenance between processing levels



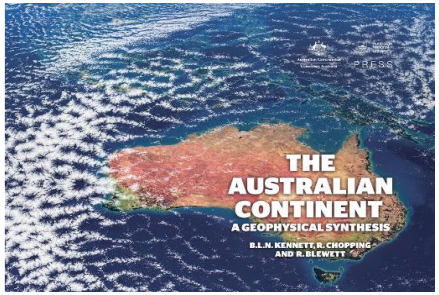
# 2030 ambition: Multiphysics Analysis but starting with PS and MT




Nigel Rees, Lesley Wyborn, Ben Evans, Rebecca Farrington, Tim Rawling, Rui Yang, & Yue Sun. (2023). Building a National High-Resolution Geophysics Reference Collection for 2030 Computation. Australian Society of Exploration Geophysicists Extended Abstracts, Volume 2023, 4th Australasian Exploration Geoscience Conference, Brisbane, 2023. https://doi.org/10.5281/zenodo.7980192

Types of geophysical data collected in Australia, the physical property measured and the depth of the crust that is sampled: also shown is the depth of current mining. Figure modified from original of Richard Chopping (GSWA).

# Can we create a collaborative National High Resolution Geophysics Data Platform?




Brian Kennett, Richard Chopping and Richard Blewett, 2018. The Australian Continent, a Geophysical synthesis. Available on https://press.anu.edu.au/publications/australian-continent#tabanchor

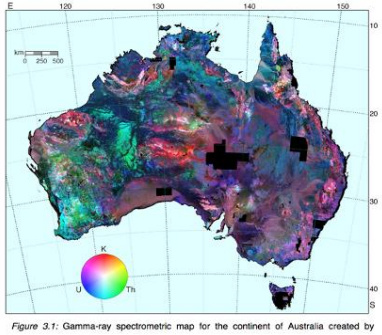


*Figure 3.1:* Gamma-ray spectrometric map for the continent of Australia created by

Radiometrics

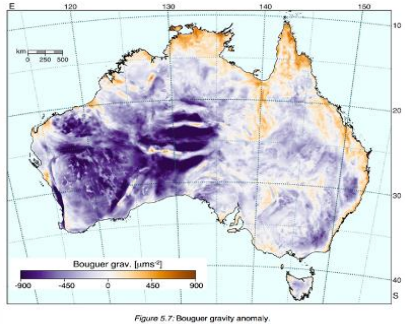



*Figure 5.7:* Bouguer gravity anomaly.

Bouger Gravity

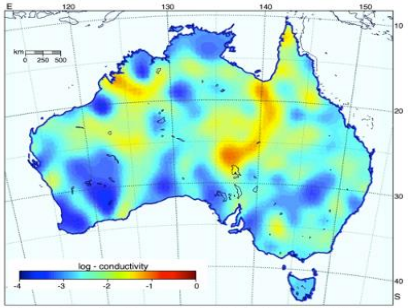



*Figure 10.3:* Logarithm of electrical conductivity [S/m] at a depth of 52 km.

Electrical Conductivity at 52 km

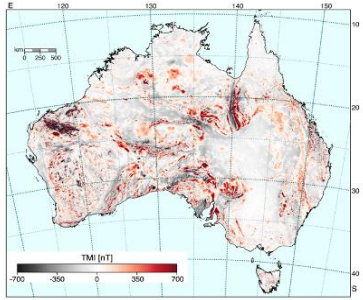



*Figure 4.6:* Total magnetic intensity across the Australian continent.

Total Magnetic Intensity

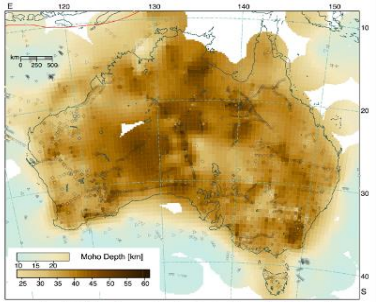



*Figure 7.16:* Moho surface across Australia utilising the full range of seismic information

Moho Depth

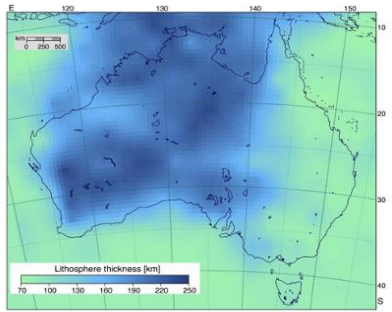



*Figure 8.9:* Estimate of thickness of the lithosphere across the Australian region.

Thickness of the lithosphere

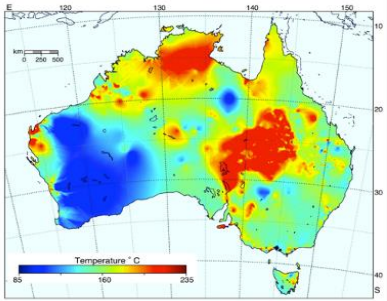



*Figure 11.2:* OZtemp estimate of the temperature distribution at 5 km depth across the Australian continent.

Temperature at 5km

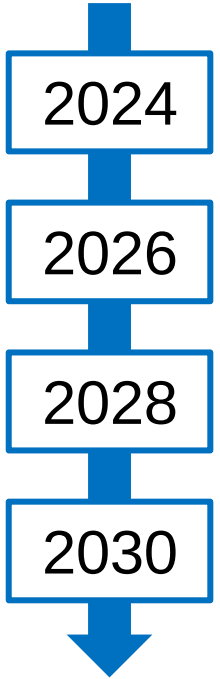
# Preparing for 2030: we no longer have the gift of time

Photo by Nathan Dumlao on Unsplash

We need to make up our minds today if we want to scale up.

If so we need to:

- Find all the rawer forms of critical geophysical datasets (and their collectors!) and work on ensuring all metadata, data and vocabularies are FAIR and machine actionable.
- Start working now on more automated systems that capture provenance through each successive processing level.
- Make less processed forms of data more accessible and able to be aggregated into seamless national high-resolution datasets.
- Ensure that whatever we do, it is always scalable to the future and can maximise benefits from new compute, data and software technologies as they come on line.



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