

PetroChron Antarctica: a Geological Database for Interdisciplinary Use

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Key Points:

- PetroChron Antarctica is a new relational database containing petrological, geochemical and geochronological datasets from sampled rocks across Antarctica.
- Lithology and age of geolocated samples, along with computed chemical and physical rock properties, facilitate quantitative analysis and data integration for interdisciplinary use (e.g. geodynamics, oceanography, ice sheet dynamics, biodiversity and soil studies).
- The PetroChron Antarctica database is accessible online via a web portal, where data can be freely downloaded as comma-separated text (CSV) flat files or individual tables to be used in a relational database system.

Abstract

We present PetroChron Antarctica, a new relational database including petrological, geochemical and geochronological datasets along with computed rock properties from geological samples across Antarctica. The database contains whole-rock geochemistry with major/trace element and isotope analyses, geochronology from multiple isotopic systems and minerals for given samples, as well as an internally consistent rock classification based on chemical analysis and derived rock properties (i.e., chemical indices, density, p-velocity and heat production). A broad range of meta-information such as geographic location, petrology, mineralogy, age statistics and significance are also included and can be used to filter and assess the quality of the data. Currently, the database contains 11,559 entries representing 10,056 unique samples with varying amounts of geochemical and geochronological data. The distribution of rock types is dominated by mafic (36%) and felsic (33%) compositions, followed by intermediate (22%) and ultramafic (9%) compositions. Maps of age distribution and isotopic composition highlight major episodes of tectonic and thermal activity that define well known crustal heterogeneities across the continent, with the oldest rocks preserved in East Antarctica and more juvenile lithosphere characterising West Antarctica. PetroChron Antarctica allows spatial and temporal variations in geology to be explored at the continental scale and integrated with other Earth-cryosphere-biosphere-ocean datasets. As such, it provides a powerful resource ready for diverse applications including plate tectonic reconstructions, geological/geophysical maps, geothermal heat flow models, lithospheric and glacial isostasy, geomorphology, ice sheet reconstructions, biodiversity evolution, and oceanography.

Plain Language Summary

On a continent with less than 0.18% of outcrop, information such as the rock type, chemistry and age of Antarctic rock samples are critical inputs for understanding complex interactions between the lithosphere, cryosphere, biosphere, and ocean. We have created PetroChron Antarctica, a relational database containing a compilation of petrological, geochemical and geochronological data from geological samples across Antarctica. The database contains more than 10,000 samples, along with chemical indices and rock properties calculated from chemical analyses. PetroChron Antarctica contains spatial meta-information to enable visualisation and analysis of the database using an online interactive map, which highlights the variability in crustal geology at the continental scale and can be used for interdisciplinary scientific studies. PetroChron Antarctica is freely available through Zenodo and an ESRI Web Feature Service (<http://bit.ly/petrochron>).

1 Introduction

The Antarctic lithosphere was built over billions of years (e.g., Boger, 2011; Harley et al., 2013), and it is increasingly clear that this long and complex lithospheric evolution both records and influences interactions with the oceans and cryosphere (e.g., Burton-Johnson et al., 2020; Hochmuth et al., 2020; Paxman et al., 2020; Whitehouse et al., 2019). Understanding these interrelated processes critically depends on the ability to integrate large heterogeneous datasets from regional to continental scale (Stål et al., 2020). Antarctic datasets are typically poorly represented in global databases. In the Antarctic geosciences, dataset hosting and dissemination are mainly supported through the Scientific Committee on Antarctic Research (SCAR; <https://www.scar.org/resources/data/>) and NASA's Earth Science Data Systems Program

(<https://search.earthdata.nasa.gov/search>). However, geological datasets are poorly resolved compared with the burgeoning geophysical data streams. Where available, geological data are typically hosted within national databases (e.g., OZCHEM; Champion et al., 2007; Petlab; Strong et al., 2016) or individual publications and are therefore difficult to utilise.

Here we present PetroChron Antarctica, a new geological database that includes geochemical, geochronological and petrological datasets from Antarctic rock samples, compiled from existing databases and individual publications. We also generate compositionally-based classifications, geochemical indices and physical properties derived from the geochemical data where possible. This database builds upon the global whole-rock geochemistry compilation developed by Gard et al. (2019). A newly generated schema implemented to account for the newly incorporated data types and associated meta-information is described, including the data integration procedure. Finally, we relate some applications to highlight potential future uses of the database.

2 Existing initiatives and motivation for data augmentation and integration

The PetroChron Antarctica database incorporates various geochemical and geochronological datasets, together with related petrological information, from both global and national initiatives (Table 1). Whereas these collections are a valuable asset for the geoscience community and are incorporated in numerous regional and global studies, they are mostly organised around data types of interest (Fig. 1a) or localised in specific geographic areas where national campaigns have focused mapping and sampling efforts on accessible outcrop (Fig. 1b, c). This lack of integration between geochemical and geochronological data (and other rock-based data), along with a strong asymmetry in data density from these existing databases, demonstrates the need to augment and integrate additional Antarctic geological data streams. PetroChron Antarctica, therefore, incorporates standardised peer-reviewed academic publications and some unpublished data (Fig. 1d). Currently, the PetroChron Antarctica database contains 10,056 rock samples representing 11,559 data entries, of which around 40% are compiled from existing data repositories spanning over 80 years of research (Table 1). Whereas the existing databases are mostly located in West Antarctica, the distribution of geological data incorporated from individual publications is more widespread, and mostly located in East Antarctica (Fig. 1d; 72%).

Data source	No. sample entries
Others (publications, unpublished...)	5,266
OZCHEM (Champion et al., 2007)	1,792
Petlab (Strong et al., 2016)	1,819
GEOROC (http://georoc.mpch-mainz.gwdg.de)	1,464
Burton-Johnson BAS compilation (in Gard et al., 2019)	1,074
DateView (Eglington, 2004)	144
Total	11,559

Table 1. Number of sample entries per data source. The Geochemistry of Rocks of the Oceans and Continents (GEOROC) data compilation contains chemical, isotope and limited age data for igneous rocks. National government collections include the Australian national whole-rock geochemical database (OZCHEM; Champion et al., 2007), the New Zealand national rock, mineral and geoanalytical database (Petlab; Strong et al., 2016) and the whole-rock geochemical data compilation from Burton-Johnson, British Antarctic Survey (BAS; included in Gard et al., 2019). Part of the geochronological database DateView (Eglington, 2004) is also included, but are not cited as such when the data have been modified or independently entered from individual publications.

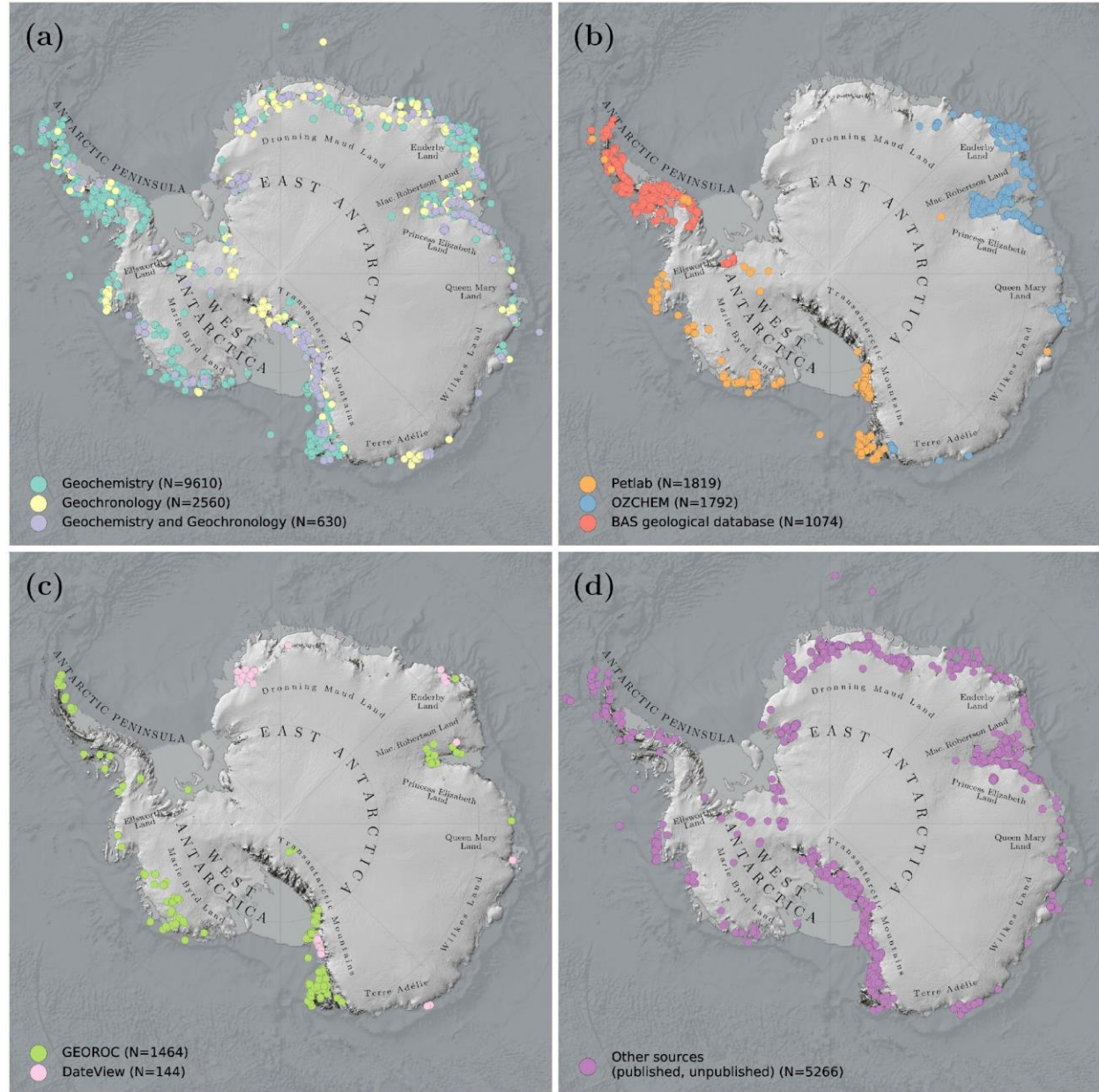


Figure 1. Spatial distribution of PetroChron Antarctica samples categorised by (a) data type, and data source including (b) national databases, (c) international compilations, and (d) international peer-reviewed publications.

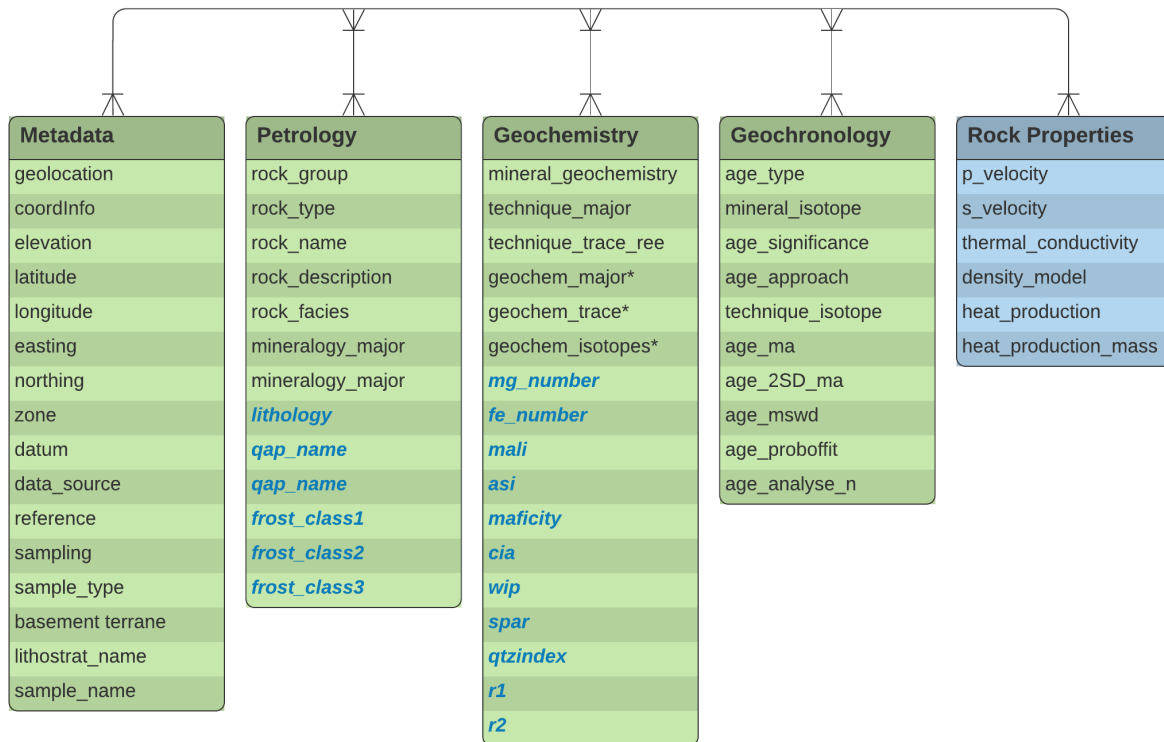
3 Database foundational framework

3.1 Data model

The database architecture follows the key concept described in Figure 2. We decided to use a simplified relational database structure including only five sub-tables (metadata, petrology, geochemistry, geochronology and rock properties) representing the core elements of sample-related information (Table 2). In an effort to meet the FAIR (findable, accessible, interoperable and reusable) data standard for inter- and intradisciplinary studies, we organise the different sub-tables around subdomains of knowledge used across the research community.

The minimalist relational model simplifies maintenance and minimizes file size. Indeed, complex relational models are usually not sustainable in the long term to support the expansion of datasets or fields to track provenance and modification. Our approach facilitates the extraction of the data from the database, the incorporation of the data into other databases with different schemas, and enables its use in various scientific workflows.

Figure 2. The PetroChron Antarctica data model using a simple five-table structure representing metadata information and sub-domains of knowledge (petrology, geochemistry, geochronology



and rock properties). Text in blue represents computed data based on chemical analyses. For readability purposes, chemical and isotopic elements are grouped by element types (i.e., major elements, trace elements, isotopes) as shown by the asterisks.

Table name	Table content description	Field Attribute	Field description
metadata	Contains metadata information related to the recorded data including the approximative location and spatial reference (name, geographic coordinates, datum...) of the sample, the source of the data (existing database, original paper reference), the type of sample and the technique used to collect it, the sample name and other geological information related to the terrane and/or stratigraphic unit the sample may belong to.	geolocation	Information on the sample location (geographic area, place name). Additional information may be included, such as sites number, distance. Note that SCAR Gazetteer place names were used in most cases to consistently populate location names
		coordinfo	Indicates the technique used to flag how geographic coordinates were recorded in the database
		data_source	Source of the data if the record was extracted from an existing database or data compilation
		sample_type	Type of the sample collected - e.g. veins, dyke, xenolith...
		sampling	Sampling technique used to collect sample - e.g. outcrop, dredge, core...
petrology	Comprises rock group, type, name, description, facies, mineralogy of the sample. Additional information are in chemical based classification (TAS, SIA granite type, frost classification). For further explanation, the reader is referred to Hasterok et al. (2018)	sample_name	Sample name as recorded by the author in the publication or existing database. Duplicate number may occur
		rock_group	High-level rock group of the sample (igneous, metamorphic and sedimentary rocks) assigned by original author/database
		rock_type	Standardised rock type - e.g. plutonic, volcanic, metavolcanic, metaplutonic, metasedimentary, clastic, assigned or inferred by the original author/database
		rock_name	Non-standardised rock name designated by the original author/database
		rock_description	Non-standardised detailed description of the rock sample from the original author/database

	rock_facies	Metamorphic facies information
	mineralogy_major	List of major minerals present in the rock sample
	mineralogy_minor	List of minor minerals present in the rock sample
	lithology	Chemical based rock type following methods described in Hasterok et al. (2018)
	qap_name	Computed rock names based on the TAS igneous classification (Middlemost, 1994), including high-Mg volcanics (Le Bas & Streckeisen, 1991)
	sia_scheme	S-, I-, and A-type granite classification
	frost_class1	Magnesian or Ferroan (Frost et al., 2001)
	frost_class2	Calcic, calc-alkalic, alkali-calcic, alkalic (Frost et al., 2001)
	frost_class3	Metaluminous, peraluminous, peralkaline (Frost et al., 2001)
geochemistry		
	geochem_mineral	Mineral/fraction analysed - e.g., whole rock, zircon...
	geochem_tech_analysis	Analytical technique used for geochemical measurements
	geochem_major	Major element analyses - Includes major element oxides as well as volatile, carbonate and LOI content where available
	geochem_trace	Trace element analyses
	geochem_isotopes	Isotopic ratio analyses, including initial ratio
	mg_number	Magnesium number. Fe^{2+} estimated using $0.85 \times \text{FeOT}$
	fe_number	Iron number (Frost et al., 2001)
	mali	Modified alkali-lime index (Frost et al., 2001)
	asi	Alumina Saturation Index (ASI) (Frost et al., 2001)
	maficity	$n\text{Fe} + n\text{Mg} + n\text{Ti}$

	cia	Chemical index of alteration (Nesbitt & Young, 1989)
	wip	Weathering index of Parker (1970)
	spar	Modified from Debon and Le Fort (1983) to remove apatite
	qtzindex	Quartz Index (Debon & Le Fort, 1983)
	r1	R1R2 chemical variation diagram (De la Roche et al., 1980)
	r2	R1R2 chemical variation diagram (De la Roche et al., 1980)
geochronology	Includes age, age uncertainty and associated statistics of the age calculation (if provided in original reference/database). A set of metadata information related to the type of radiochronometer, the mineral dated, the approach and analytical technique used, and the significance of the age are populated.	age_type Radiochronometer used to estimate the rock sample age - Ar-Ar, U-Pb... age_mineral Mineral used for dating - e.g. mica, zircon... age_significance Significance of the calculated age - e.g. Crystallisation, Cooling... age_approach The approach used to calculate an age - e.g. Regression, Concordia, Discordia, Ar Plateau age_techgeochem The technique used to measure isotopic ratio used for dating - e.g. TIMS (single grain, multigrain), SHRIMP, Laser... age_ma Radiometric age in Ma age_2SD_ma Standard deviation - 95% or 2 sigma - in Ma age_mswd The calculated MSWD age_probffit The calculated probability of fit age_probchi2 The calculated probability of Chi2 test age_analyse_n Total number of analyses used to calculate an age
rock properties	List of physical rock properties including heat production, seismic velocity and density	p_velocity Empirically calculated seismic velocity based on chemical composition. The compositional empirical

		estimation computed from geochemical analysis. For further information on the computation, see Hasterok et al. (2018).		model used was V_p (km s^{-1}) $= 6.9 - 0.011C_{\text{SiO}_2} + 0.037C_{\text{MgO}} + 0.045C_{\text{CaO}}$. For discussion on the computation, the reader can refer to Hasterok and Webb (2017)
	s_velocity			Empirically calculated seismic velocity based on chemical composition. For further discussion on the computation, the reader can refer to Jennings et al. (2019)
	density_model			Rock density computed from chemical analyses using linear regression as described in Hasterok et al. (2018)
	thermal_conductivity			Empirically calculated thermal conductivity based on chemical composition. For further discussion on the computation, the reader can refer to Jennings et al. (2019).
	heat_production			Heat production mass multiplied by the density estimate (in kg.m^{-3}) (Rybach, 1988)
	heat_production_mass			Estimated from the chemical rock composition using the empirical formula $HP_{\text{mass}} = 10^{-5} * (9.67C_U + 2.56C_{\text{Th}} + 2.89C_{\text{K}_2\text{O}})$ where C are the concentrations of the Heat Producing Elements in ppm except K ₂ O in wt. % (Rybach, 1988).

Table 2. Description of table contents and detailed information of key field attributes.

3.2 Data compilation workflow

To ensure data consistency and enhance database reliability over PetroChron Antarctica's lifetime, we implemented several procedures written in a combination of programming languages (i.e., Python, PostgreSQL) for data standardisation to create a common data schema (Fig. 2, Table 2).

Collecting a useful Antarctic geological dataset starts with accurate sample location information. Historically (i.e., prior to GPS), this information was not readily recorded in a useful format, or it may have been lost in the process of transcribing notes or maps. In the case where accurate absolute spatial information is not provided in the original paper or dataset, geographic locations along with latitude and longitude from the SCAR Gazetteer is used (Secretariat SCAR, 1992 updated 2014). For each entry, an attribute identifies the source of the geographic coordinate (i.e., Geographic Coordinate Information). This approach allows us to retain 45% of the geological samples in PetroChron Antarctica that would previously have been excluded due to the lack of location information.

Lithology has a dominant control over the physical and chemical properties of rocks. We therefore categorise the database according to rock group (i.e., igneous, sedimentary, metamorphic) and rock type (e.g., plutonic, clastic, metavolcanic) where known or inferred. However, there are a variety of lithology names based on different criteria (mineralogical, textural, chemical). Thus, to achieve consistency and reproducibility and avoid any subjectivity in assigning rock names to samples, we include a computed lithology based on whole-rock geochemical data as described by Hasterok et al. (2018) and Gard et al. (2019).

The database structure is then focused on the integration of geochronological datasets with geochemical data. In the global whole-rock geochemical database of Gard et al. (2019), petrological information and geochemical analyses were linked to "estimated" crystallisation ages of the sample as presented in the original paper. A key difference in PetroChron Antarctica is that geochronological information is stored as a set of parameters including the age type (i.e., isotopic system), the mineral isotope (i.e., analysed mineral and/or whole rock), the age significance (e.g., crystallisation age), the age approach (e.g., Concordia age), and the analytical technique (e.g., SHRIMP; Fig. 2). This configuration significantly increases the flexibility to support geochronological data from multiple isotopic systems and minerals for a given sample, which potentially have different geological significances. The inclusion of age-related statistical information if applicable (e.g., Mean Squared Weighted Deviation – MSWD, and probability of fit) enables data to be manipulated through more complex statistical analyses and could also be useful for data quality assessment. Geochronological parameters generally follow the schema of the established geochronological database DateView (Eglington, 2004) for consistency and easy transfer between databases.

4 PetroChron Antarctica data and applications

4.1 Data statistics

Igneous rocks included in PetroChron Antarctica correspond to 60% of the total entries, followed by 39% for metamorphic rocks (Fig. 3a, b). Sedimentary rocks are poorly represented at only 1%. Igneous rocks are mainly represented by plutonic rocks (42%), whereas metamorphic rocks are dominated by metaplutonic varieties (20%). A large proportion (38%) of igneous rocks are mafic in composition, followed by those of felsic (29%) and intermediate

(24%) compositions (Fig. 3d). Metamorphic and sedimentary rocks are dominated by felsic compositions (42% and 39%, respectively). Overall, the compositional range across all sampled rocks recorded in PetroChron Antarctica compared with the global whole-rock geochemical database (Gard et al., 2019) is similar (Fig. 3c, 3d), when excluding samples marked as oceanic from the global dataset.

Computed properties in PetroChron Antarctica include lithology based on chemical classification (Fig. S1). There is a clear dominance of granitoid (32%) and gabbroic rocks (22%). Dioritic and syenitoid compositions (including geochemically equivalent volcanic rocks) are also a significant proportion of the igneous rocks (19% and 16%, respectively). Other computed geochemical indices include ASI, WIP, CIA or CPA that are often used in soil science as a proxy for alteration/weathering conditions of sampled rocks (see the full list of computed indices in Table 2). Petrophysical properties (density, P- and S-wave velocity, thermal conductivity and heat production) were computed from geochemical data, following the method described in Hasterok et al. (2018) and Jennings et al. (2019).

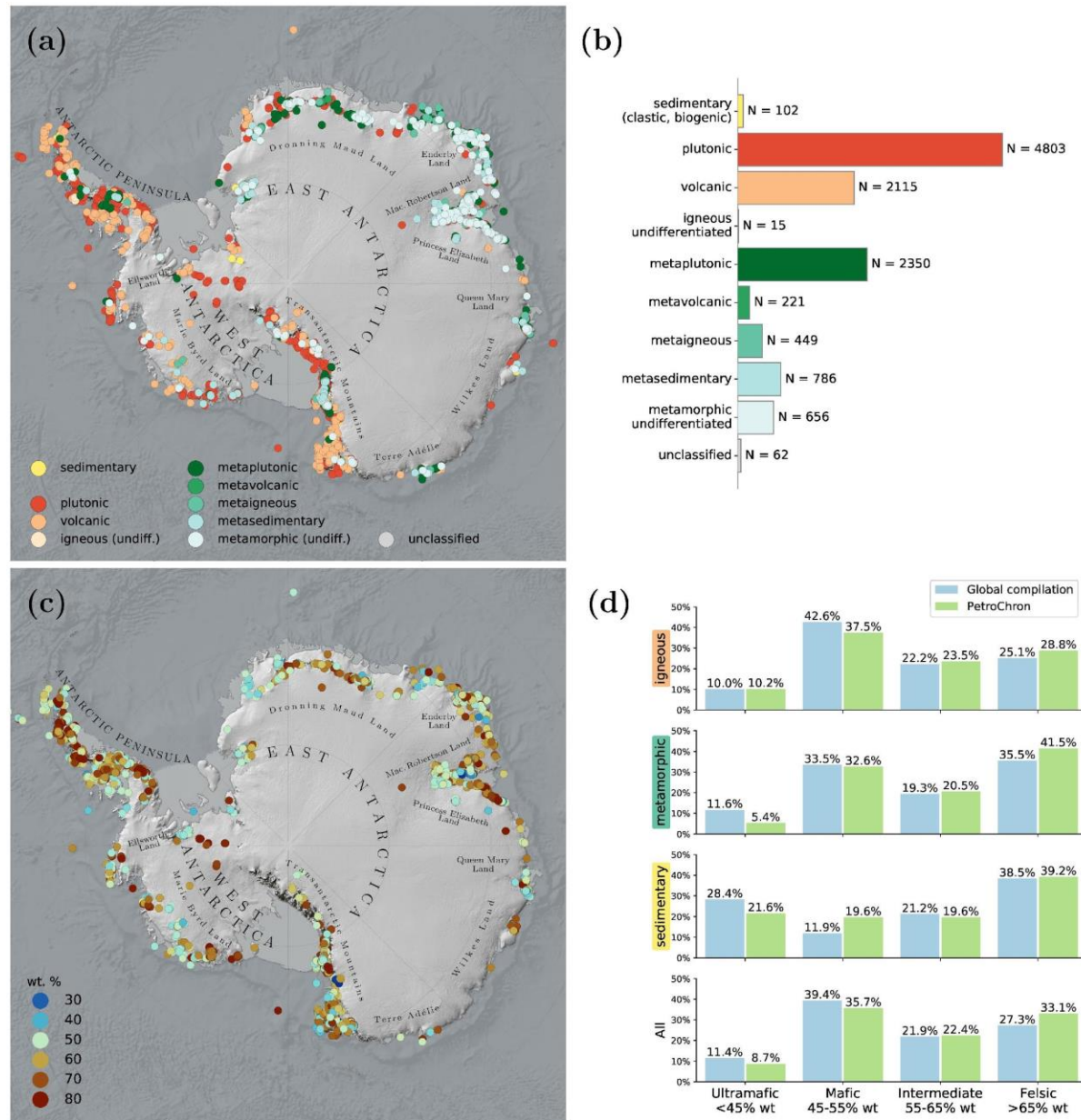


Figure 3. Sample rock type and composition. **(a)** Sample distribution coloured by rock type. **(b)** Bar chart representing rock type. **(c)** Compositional distribution coloured by SiO₂ wt% content. **(d)** Comparison of SiO₂ wt% content between the global whole-rock geochemical database (Gard et al., 2019) and PetroChron Antarctica.

4.2 Visualisations and applications

To illustrate the versatility and the utility of PetroChron Antarctica, we describe below some applications that could use interrelated datasets (i.e. geological, geochemical, and geochronological data associated with rock properties) to gain insights through map visualisation.

Figure 4 shows a set of maps illustrating some of the geochronological components of PetroChron Antarctica. For example, the “crystallisation age” map (Fig. 4a), based on zircon U-Pb isotopic data and typically interpreted to date high-temperature magmatic processes, highlights the dominance of Phanerozoic crust-forming events in the Antarctic Peninsula and Transantarctic Mountains (e.g., Allibone & Wysoczanski, 2002; Burgess et al., 2015; Goodge et al., 2012; Hagen-Peter & Cottle, 2016; Pankhurst et al., 1998; Riley et al., 2017; Zheng et al., 2018). In contrast, the majority of East Antarctic crust formed during the Proterozoic and Archean (Fig. 4a; e.g., Adachi et al., 2013; Boger et al., 2006; Corvino et al., 2008; Elburg et al., 2016; Elburg et al., 2015; Goodge & Fanning, 2010; Grew et al., 2012; Hokada et al., 2019; Liu et al., 2016; Maritati et al., 2019; Mikhalsky et al., 2017; Morrissey et al., 2017; Tsunogae et al., 2016; Tucker et al., 2017; Zhang et al., 2012), including some of the oldest rocks on Earth (c. 3.9 Ga in Enderby Land; e.g., Black et al., 1986).

A “metamorphic age” map (Fig. 4b) based on U-Pb and Sm-Nd isotopic data from zircon, monazite, garnet and whole-rock samples, show the predominance of late Neoproterozoic–Cambrian (~630–500 Ma) ages in the Transantarctic Mountains, Dronning Maud Land, MacRobertson Land and Princess Elizabeth Land (e.g., Baba et al., 2015; Bisnath et al., 2006; Board et al., 2005; De Vries Van Leeuwen et al., 2019; Goodge & Fanning, 2016; Halpin et al., 2007; Jacobs et al., 2003; Kawakami et al., 2017; Liu et al., 2018; Mikhalsky et al., 2013; Morrissey et al., 2016; Wang et al., 2016). These tectonothermal events record prolonged ocean closure, terrane accretion and collision-related processes related to Gondwana amalgamation and active margin tectonics (e.g., Boger, 2011; Fitzsimons, 2003; Goodge, 2020; Harley et al., 2013; Jacobs et al., 2015; Jordan et al., 2020; Mulder et al., 2019).

A map of “cooling ages” (Fig. 4c), recorded by low-temperature thermochronology across numerous minerals and whole-rock samples, is dominated by ages < 600 Ma (84% of ages recorded by FT, Ar-Ar, He). The youngest cooling ages (~140–30 Ma with a larger proportion of Paleogene ages) are located along the elevated Transantarctic Mountains (e.g., Fitzgerald & Stump, 1997; Foland et al., 1993; Gleadow & Fitzgerald, 1987; Prenzel et al., 2018; Zattin et al., 2014), whereas East Antarctica records a predominance of Late Carboniferous–Permian (~340–200 Ma) ages and to a lesser extent Cretaceous ages (e.g., Rolland et al., 2019; Sirevaag et al., 2018). The variability in spatial and temporal cooling patterns across Antarctica, although poorly documented, has fuelled debate about whether topographic relief evolved via continental-scale tectonic and/or climatic processes during the Phanerozoic (e.g., Maritati et al., 2020; Rolland et al., 2019).

Collectively, geochronological and isotopic data from across Antarctica reveal major episodes of tectonic and thermal activity, as well as denudation and deposition associated with complex crustal forming processes operating during at least three supercontinent cycles (i.e., Nuna, Rodinia, Gondwana/Pangea). This provides a valuable resource for testing possible links between plate tectonic configurations, major climatic and paleoenvironmental change and Antarctic landscape evolution.

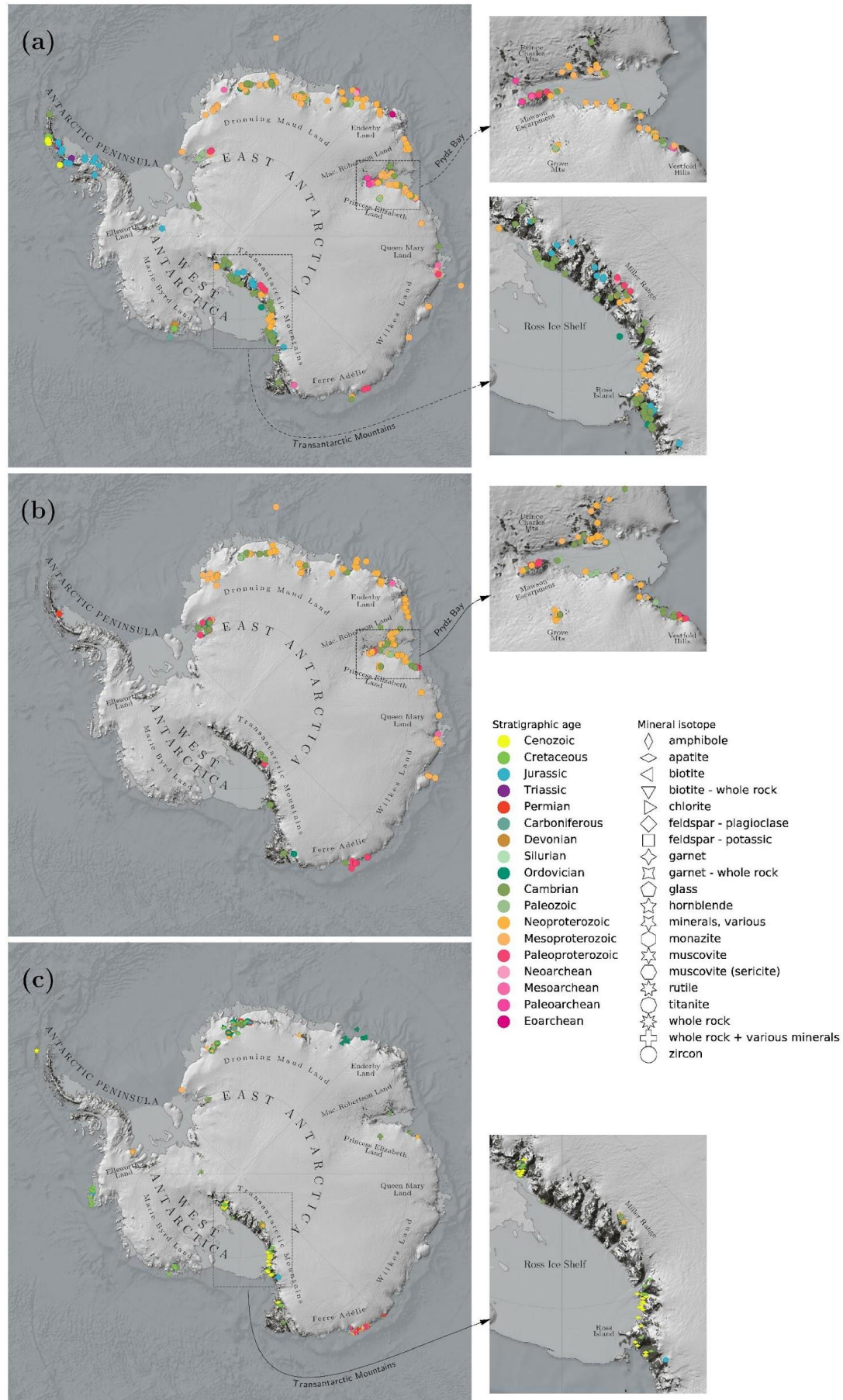


Figure 4. PetroChron Antarctica isotopic age/composition distributions. Maps of (a) zircon crystallisation ages; (b) metamorphic ages for different minerals/whole rock; (c) cooling ages for different minerals/whole rock. The colour scale follows the GeoMAP (© SCAR GeoMAP and GNS Science 2019) chronostratigraphic chart and highlights the variability in isotopic age within the mapped geological units. Dashed rectangles show the location of inset maps.

Figure 5 shows a map of rock properties computed from geochemical data across Antarctica. Density estimates peak at ~ 2630 and $\sim 2930 \text{ kg m}^{-3}$, and P-wave seismic velocity estimates peak at ~ 6.2 and $\sim 7.0 \text{ km s}^{-1}$, corresponding to felsic and mafic rock compositions, respectively. These values agree with the densities (2690 and 2950 kg m^{-3}) and velocities (~ 6.1 and 7.1 km s^{-1}) recorded in the global whole-rock geochemical database (Gard et al., 2019), when calculated from the same bin size. Antarctic heat production has a median value of $\sim 1.3 \text{ } \mu\text{W m}^{-3}$, with first and third quartiles at 0.6 and $2.4 \text{ } \mu\text{W m}^{-3}$ (Fig. 5c), which is higher than the value of $1.0 \text{ } \mu\text{W m}^{-3}$ estimated by Gard et al. (2019), who included oceanic samples. At a regional and local scale, crustal heat production shows a high degree of heterogeneity (Fig. 5c) due to the high variability of Antarctic local geology (Carson et al., 2014; Goodge, 2018) that can be integrated into geothermal heat flow models (Stål et al., 2021). This compositional variability clearly highlights the need to include robust and petrologically valid constraints from direct measurements in geophysical interpretations and numerical computations (Stål et al., 2020).

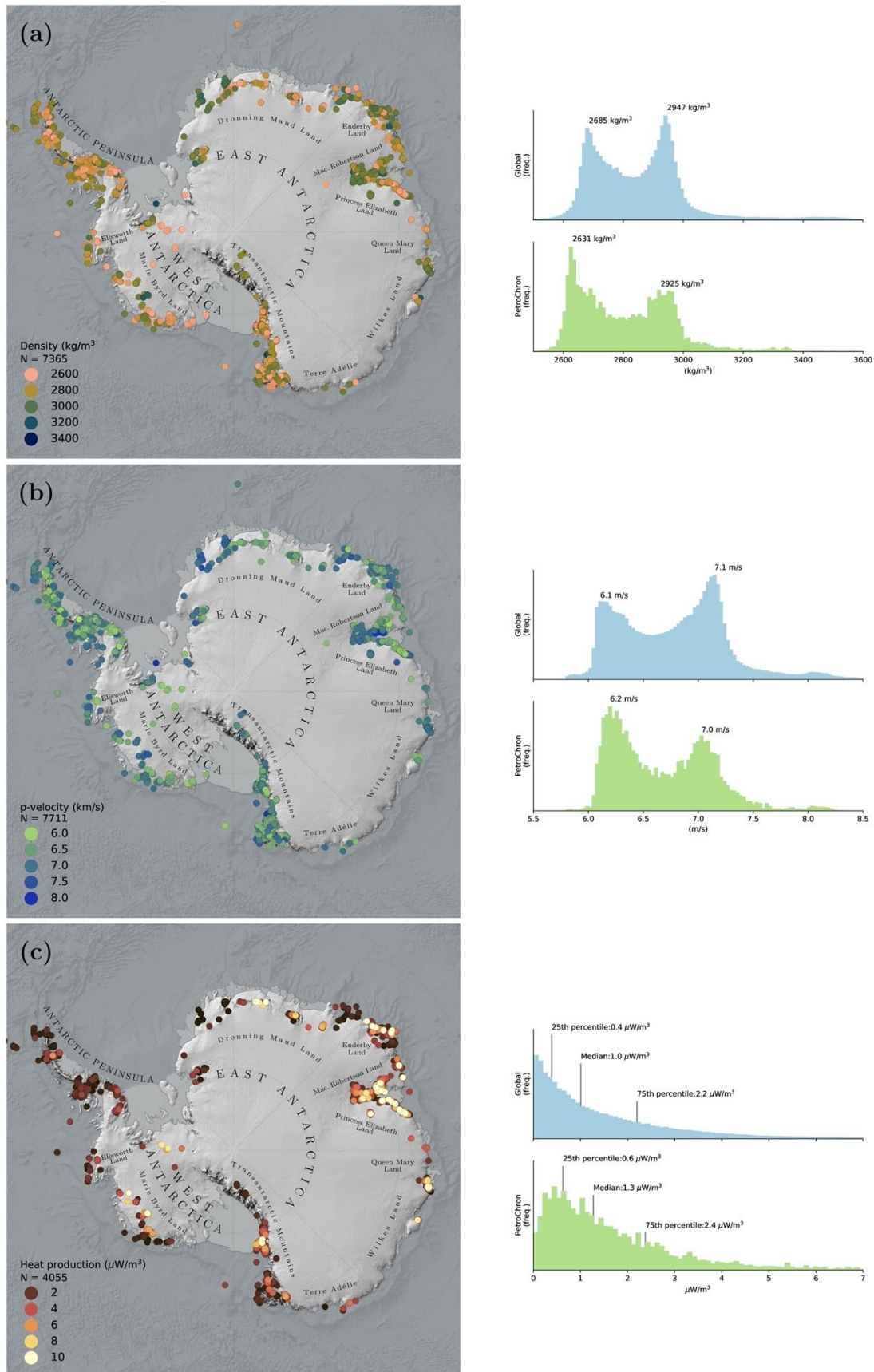


Figure 5. Computed physical property estimate distributions including (a) density; (b) P-wave velocity; and (c) heat production. Histograms compare distributions for the global whole-rock geochemical database (Gard et al., 2019) and PetroChron Antarctica.

5 Future work

We hope the PetroChron Antarctica database can be applied and integrated across Antarctic Earth-cryosphere-biosphere-ocean research. Future work will aim at expanding the database by incorporating not yet considered and newly published data, as well as correcting any errors and adding new data types including metamorphism, protolith and data-quality parameters. We also invite researchers to collaborate on our data compilation using the user input XLSX template (Table S1). Note that we make no claim on the accuracy of database entries or on ownership of these data.

Acknowledgments, and Data

- The PetroChron Antarctica database is available on Zenodo (<https://doi.org/10.5281/zenodo.5032026>) and through the PetroChron Antarctica web portal (an ESRI Web Feature Service; <http://bit.ly/petrochron>). The service copies the current data model and helps visualise the distribution of the data. The complete database file in a CSV format can be directly downloaded from the PetroChron Antarctica web portal and Zenodo, or as subset data tables that can be used in any Relational Database Management System (RDBMS) through Zenodo. Code to reproduce figures in this paper is available here: <https://github.com/TobbeTripitaka/PetroChron>
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