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Towards FAIR Paleomagnetic Data Management Through Paleomagnetism.org 2.0

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Key Points:
- It is the second release of the Paleomagnetism.org paleomagnetic analysis and interpretation software
- It facilitates a workflow that aligns with modern FAIR Data Management protocols
- It integrates with a public data library that improves data sharing capabilities

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Abstract Scientific communities are placing an increasing emphasis on the implementation of data management protocols concerning data archiving and distribution. For instance, every proposal submitted to the European Horizon 2020 program, as well as to the National Science Foundation in the USA, requires a dedicated section that outlines project data management and accessibility. The widely adopted FAIR data guidelines identify core principles concerning modern data management conventions. The wide variety of data formats, the low data volume, and the general lack of a culture of data sharing makes that the paleomagnetic community rarely follows any of the FAIR principles. Most institutions define their own data formats and use in-house software to analyze their demagnetization data, which are critical to Paleomagnetic research. Efforts to overcome these problems exist in the form of the MagIC database for data archiving, and the online paleomagnetic data analysis and interpretation platform Paleomagnetism.org. In this contribution, we describe the second iteration of Paleomagnetism.org: an online multiplatform open-source environment for paleomagnetic data analysis. This update comprises a full overhaul of the application to satisfy the increasingly demanding data management requirements. The application now facilitates a workflow that aligns with FAIR guidelines by documenting data provenance. All data analyzed through the application are easily submitted to a public data library that distributes data and results through an HTTPS web service that lives up to modern data management standards.

Plain Language Summary All data that are used in research must be transparent to everyone in order to guarantee the reproducibility of scientific results. The FAIR guidelines describe a set of rules that dictate how data provenance and results should be documented. Paleomagnetism.org is an online application that allows for the interpretation and statistical analysis of paleomagnetic data. In this submission, we present the approach on how the application implements data management protocols following the FAIR guidelines.

1. Introduction

The FAIR acronym (Wilkinson et al., 2016) describes four fundamental principles concerning the Findability, Accessibility, Interoperability, and Reusability of data. They form a cornerstone of modern data infrastructures and are being increasingly adopted by scientific communities. In concrete terms, FAIR data mean that data sets are effortlessly searched and discovered, freely downloaded, shared, usable between multiple disciplines, and that derived results and the applied methodology are fully transparent. First, we discuss how the paleomagnetic community can benefit from embracing the FAIR principals and continue to describe how this philosophy is implemented on Paleomagnetism.org 2.0.

In the paleomagnetic community, the practice of publishing data through tables of statistical distributions is long lived and persistent. These distributions are often assumed to be Fisherian (Fisher, 1953), which is analogous to a Gaussian distribution (μ and σ) on a sphere centered around a mean vector $\vec{m}$ with a given true dispersion parameter κ. Paleomagnetic literature generally provides site mean directions that display estimated statistical parameters ($\vec{m}$, N, and k) of interpreted characteristic remanent magnetization (ChRM) directions from field specimens. These results support geological narratives but rarely includes the original demagnetization data on which these interpretations are based.

We identify two critical problems with this approach. Foremost, the published results are in fact interpretations of demagnetization data through visual inspection rather than the data themselves. Hence, they should be recognized as possibly subject to a methodological bias sensitive to user preference that influences the described outcome (e.g., when declaring whether a magnetic signal is considered primary or the consequence of a secondary later-stage overprint). On that perception alone, any interpretation should be published together with the data the result is based upon to make any methodical choices transparent for scrutiny by peers. Complimentary, why the data are treated in a particular way must be reviewed in context with respect to what is clarified textually in an associated manuscript. Secondly, the approach of only providing statistical descriptions becomes especially problematic when Fisherian statistics are forced on a non-Fisherian distributions.

The main source of uncertainty in paleomagnetic data comes from paleo-secular variation of the geomagnetic field (PSV) (e.g., Butler, 1992; Deenen et al., 2011; Tauxe & Kent, 2004). PSV is the stochastic wandering of the pole around the geographic north through time. Paleomagnetic studies thus aim to collect an amount of paleomagnetic readings from a geological unit (e.g., formation, pluton, flow sequence, etc.) that has the potential to yield data that sufficiently average the effects of PSV to levels lower than those of the studied signal (e.g., vertical axis rotations or paleolatitudinal shifts) (Deenen et al., 2011). When the scatter of a paleomagnetic data set is only derived from random measurement errors, such as for multiple directions obtained from lava site units that cooled on geologically instantaneous timescales, Fisher statistics provide an accurate approximation of the distribution of directions. However, when PSV is the main source of scatter, as is the case when averaging multiple lava sites or samples from sedimentary units, this produces a scatter that is up to two orders of magnitude larger than typical measurement uncertainties (Deenen et al., 2011) and is by approximation Fisherian around the pole. The position of a virtual magnetic pole, as a function of latitude (assuming a geocentric axial dipole), is recorded in situ at a site within a susceptible sample as a magnetic vector. Surmising the absence of active tectonics and sufficient time was sampled, the distribution of recorded virtual magnetic poles may thus be considered Fisherian with a mean vector centered on geographic north and with estimated polar dispersion parameter K. The resulting projection of this polar distribution to a set of magnetic directions becomes increasingly elongated with lower latitude. This ellipsoid has uncertainty on inclination ΔIx and declination ΔDx (Butler, 1992) that are independent, and the distribution can no longer be considered Fisherian (Creer, 1962; Cox, 1970; Deenen et al., 2011; Tauxe et al., 2008). Furthermore, ChRM directions in any rock may be affected by widely observed inclination flattening (King, 1955), which must be acknowledged and can be corrected for using the E/I method of Tauxe and Kent (2004) and other laboratory experiments (Hrouda, 1982; Kodama, 2012).

The consequence is that the typically published statistical parameters of a paleomagnetic directional set using Fisher statistics may not be representative of its true distribution. Essential information that is required to reproduce the original data set, even by approximation, is lost in the process. An applied fallback is to parametrically resample distributions by their estimated statistical parameters ($\vec{m}$, N, and k) (e.g., Koymans et al., 2016), but this is far from ideal considering the latitude-dependent relationship between the estimated directional dispersion k and polar dispersion K (Creer, 1962; Cox, 1970). The ongoing debate about how best to describe paleomagnetic data and how best to average such data sets to arrive at geologically meaningful directions that form the basis of (e.g., plate) tectonic interpretations highlights the importance of publishing the original data, including all decisions made between the initial measurement and the final geographical directional average.

We recognize that at the root of this problem lies the lack of proper tooling and data repositories that are available to the paleomagnetic community. While public databases like MagIC (Jarboe et al., 2012) and tools like PmagPY (Tauxe et al., 2016) and Paleomagnetism.org (Koymans et al., 2016) have existed for many years, they are unfortunately not leveraged to their full potential by the community. Perhaps owing to the sometimes steep learning curves and laborious task of converting data into the required formats, we therefore present an updated data treatment protocol for Paleomagnetism.org, whereby raw demagnetization data of a wide range of formats and metadata are entered at specimen level and which can be straightforwardly uploaded to a newly provided data library and exported as a MagIC database file.

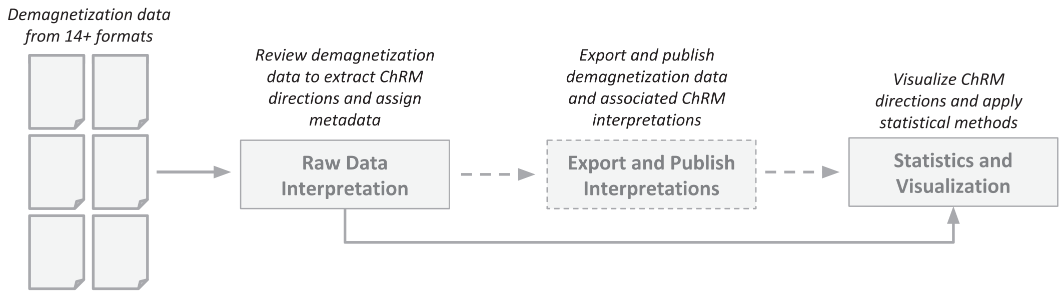

Figure 1. Schematic overview of a typical workflow in Paleomagnetism.org. Raw demagnetization data from many formats can be loaded and interpreted for ChRM directions. These directions can optionally be published and further used for statistical analysis.

2. Paleomagnetism.org Application

In the first released edition of Paleomagnetism.org, we introduced a simple user-to-user approach to share raw demagnetization data coupled with the associated interpreted directions through a custom file format that can be downloaded from an openly accessible online application. The second iteration of this software package follows a similar open-data philosophy but streamlines data analysis, metadata collection, publication, and data distribution following the workflow illustrated in Figure 1.

2.1. Version 1.0

It is the first Paleomagnetism.org application launched in September 2015 and has seen over 100,000 page visits since. Presently, it is used on a daily basis by multiple paleomagnetic laboratories worldwide. The ambition was to take a first step towards providing users with accessible software that promotes a standardized way of analyzing and sharing demagnetization data. To this end, we introduced an intuitive interface for the interpretation and subsequent statistical analysis of paleomagnetic data that are easily shared with, and reviewed by peers. As of today, the application accepts 16 different demagnetization data formats from laboratories worldwide.

In recent years, an increasing number of communities are starting to recognize that precise bookkeeping of data and its associated metadata are essential in lieu of core scientific principles that demand the reproducibility of results. In reality, we often find that (publicly funded) data are not made public or can no longer be found, accessed, or read by modern software. These data are then lost to the community, and as a consequence, published results based on the original data cannot be reproduced as per the original author. As a solution to this problem, we have introduced a new data library that serves as an optional public data repository that is completely integrated with the website.

Key specimen metadata in version 1.0 (e.g., age, lithology, and sampling location) could be added only in the statistics portal, for combinations of interpreted directions, rather than for the specimen data themselves. This incompatibility hampers inclusion of the Paleomagnetism.org 1.0 data in the MagIC database. Therefore, we redesigned the way metadata are collected on a specimen level and follow an approach that aligns with the FAIR philosophy.

2.2. Version 2.0

Because breaking changes had to be introduced to the application, the new version of Paleomagnetism.org is minted version 2.0 following proper semantic versioning protocol (https://semver.org). The previous version of the application has been deprecated but will remain accessible for the foreseeable future under http://old.paleomagnetism.org. Data from the previous application are forward compatible with the new application, but some extended metadata may need to be added inside the Interpretation portal, where raw data are interpreted. In this contribution, we will only discuss the new features that were added in the new release. For a user manual of the application, we refer to the publication of Koymans et al. (2016). Here, we limit ourselves to discussing the new philosophy assisted by the guiding FAIR principles: Findability, Accessibility, Interoperability, and Reusability.

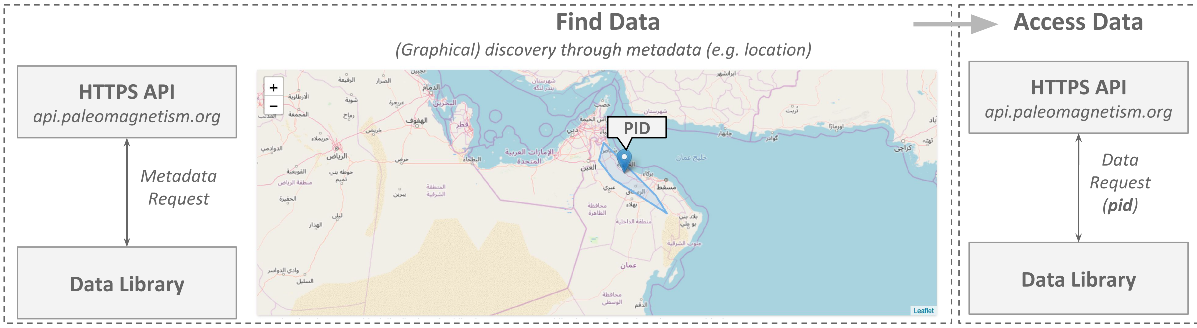

Figure 2. Schematic overview of how the HTTPS API aligns with the FAIR principles. With an initial query, metadata for all publications can be discovered from the web service and publications of interest can be found. From these metadata, the related identifiers (PID) can be extracted and used in consecutive queries to access and download the data themselves. This procedure is generally automated and handled by a machine, and the user is presented with a graphical interface for convenience.

3. FAIR Implemented on Paleomagnetism.org

- To make data Findable through metadata and unique persistent identifiers. Extensive metadata are now collected on the specimen level inside the Interpretation portal. This information must be attributed to each individual specimen (but can be applied to all specimens in a collection) by clicking the metadata field (or *key i*) and should be filled in as completely as possible. Values for some of the fields (e.g., lithology and geological type) must be selected from the semantic metadata vocabularies defined and required by the MagIC consortium.
- To make data Accessible, we introduce a public data library. All data that were interpreted with Paleomagnetism.org 2.0 can optionally be published in our web repository (Figure 1). We guarantee resources to review and host the data submitted by users and include it in the repository for the foreseeable future. To guarantee clear data provenance, only raw demagnetization data together with associated interpreted directions can be published through an integrated web form. All data accepted in the data library can be accessed through a public HTTPS web service or visually inspected through the website. An example of how data can be discovered and accessed through metadata is shown in Figure 2.
- To make data Interoperable, we apply common semantic vocabularies as defined by the MagIC consortium in our extended metadata model. By the use of rich and semantic metadata descriptions, identifiers at the specimen level, and a public web service, other research infrastructures can be easily integrated with our application to foster the interoperability between different geoscientific fields. The availability of a machine-readable web service allows integration of the submitted paleomagnetic data in larger pan-European research infrastructures (e.g., the European Plate Observing System (EPOS); Bailo et al., 2015).
- To make data Reusable by facilitating the publication of raw demagnetization data together with its associated interpreted magnetic components. In practice, this means that any researcher can review a published interpretation of a paleomagnetic data set by finding the referenced Paleomagnetism.org 2 data set through its metadata or persistent identifier on the website. This entry includes everything from raw demagnetization data to the interpreted statistical ChRM distributions. We feel that only at this level of granularity the community can live up to this core pillar of scientific integrity and guarantee the reproducibility of results.

4. MagIC Database Integration

A large effort was made to harmonize the interface between the application and the MagIC (https://earthref.org/MagIC) database. We made this integration through the collection of extended specimen metadata following MagIC defined semantic vocabularies. Data from any supported demagnetization format that were interpreted in our application can be exported to a standardized MagIC database input file. This file can then be uploaded to the MagIC database by registering on its respective website. The MagIC metadata model is optionally more extensive than what the Paleomagnetism.org application exports, but we consider that the most essential metadata are mapped in the integration. We hope that facilitating users with more user-friendly ways of integrating their data with larger data repositories will contribute significantly to proper data management in the community.

5. Data Library

Besides the interface with the well-established MagIC database, Paleomagnetism.org 2 offers to maintain an integrated data library for demagnetization data. Submitting data to the repository is convenient and takes a few clicks, alongside your input files. Our library contains a list of records where each entry is called a publication that may contain a single to many collections. A collection is defined as a coherent grouping of demagnetization data and interpretations derived from any number of paleomagnetic specimens. This grouping of specimens per collection is arbitrary and may be chosen by the user. Practically, a suitable collection of specimens may be, for example, a paleomagnetic site or a magnetostratigraphic section.

Every publication submitted to the Paleomagnetism.org 2 data library may be assigned additional metadata about the publisher (e.g., author, institution, description, and publication DOI) and referenced through its assigned persistent identifier. This identifier is a standard 256-bit unique value that can be resolved on the application to reference a particular digital object. Any collection and specimen within this specific publication can be referenced through the same persistent identifier with two indexed numbers appended at the end, delimited by dot characters, for instance:

27efedb6cfb0329332521fa5a59cbefee4c5a3016e552e6862a1b235d42c2066.0.1

The above example shows the persistent identifier belonging to data library publication `27ef...2066`. Within this publication, the first collection (index 0) is referenced after the first dot, followed by the second (index 1) specimen inside the collection. Once the persistent identifier is resolved on the application, the user is immediately presented with the metadata associated with that particular specimen. The specimen can then directly be loaded to the application and reviewed on the website. Alternatively, the data are available by programmatic access through the same identifier from the public HTTPS web service. A full collection or publication can be referenced by removing the last, or both, indices appended after the dot characters, respectively.

6. HTTPS Web Service

Web services have become the de facto standard for data sharing in a world that is increasingly relying on machine-to-machine communication. They form a cornerstone of existing scientific infrastructures, and many communities have already embraced this paradigm (e.g., the FDSNWS [https://www.fdsn.org] for digital seismology or standardized Web Feature and Web Map services, Michaelis & Ames, 2008). Web services are based on the HTTP(S) protocol and use a standard client-server model. A request is sent from the client with query options, and the server returns the requested resource respecting the clients' wishes. It is the most efficient and flexible way to distribute data to human and machine clients over the Internet.

The Paleomagnetism.org data library web service Application Programmatic Interface (API) is available under the subdomain https://api.paleomagnetism.org and returns a list of available records in the data library alongside publication metadata. Data from the API are always returned in JSON format and can be parsed by all modern programming languages. A typical workflow is to filter records by geographic location from which the remaining publication identifiers can be extracted. The API can then be queried with the particular identifiers to request the respective publications from the database for further processing.

7. Additional Features and Changes

In addition to the new data and metadata protocols described above, Paleomagnetism 2.0 includes several new features and changes. These minor modifications are briefly outlined below.

7.1. Naming and Importing

Files exported from the Interpretation and Statistics portal have been renamed from *.dir* to *.col* and *.pmag* to *.pub*, respectively. The content of the files is a human-readable JSON that can be viewed and edited with any text editor or programming language.

The data import for the statistics portal was changed because metadata are no longer collected per site but per magnetic direction. The new default input is a formatted *.csv* file that is described on the Statistics portal home tab and can be made with Excel or an alternative text processor. The historical add site is also implemented for convenience and allows users to apply metadata to all magnetic directions.

Since the release of Paleomagentism.org in 2015, we have added the following data formats to the Interpretation portal: Black Mountain Lab, California Institute of Technology (Caltech), Cenieh, Geological Survey of Norway, University of Barcelona, University of Helsinki, University of Oxford, University of Oslo, MagIC, BCN2G, Agico JR5, and JR6.

7.2. Key Bindings

Some changes to key bindings were made, and more shortcuts were implemented for user convenience. For every portal, the available key commands can be found under the *settings* tab. For example, data export from the statistics portal of all selected collections is now triggered by typing *key s*. Similarly, collections can be deleted from memory by pressing *key q*.

7.3. Component Grouping

Every intepretation is assigned to a manageable group that is by default defined as *ChRM*. An arbitrary group name can be chosen and be used to distinguish between high and low temperature components. All components that belong to a single group will be added to a separate collection when loaded in the statistics portal.

7.4. Coordinate Systems

Directions are now stored in specimen coordinates, and the coordinates reference frame can be switched using the keyboard (*key 8*). In the case of directions that exist exclusively in geographic corrected domain, the shown specimen coordinates will be unchanged from geographic coordinates and should be considered unrepresentative.

7.5. Geography Portal

A part of the statistics portal has been moved to the new Geography portal. Under the Geography portal, paleomagnetic data can be tested against global apparent polar wander paths (Besse & Courtillot, 2002; Kent & Irving, 2010; Torsvik et al., 2012) rotated in the coordinates of the main plates, as described in van Hinsbergen et al. (2015). In addition, the magnetostratigraphy module was also added to this portal and is configured to automatically construct a binary column based on the polarity of the magnetic directions.

As a novelty, we developed a new tool to upload rotation files from GPlates plate reconstruction software (Boyden et al., 2011; Gurnis et al., 2012). This is a powerful feature that integrates arbitrary custom plate models from a well-established community standard, which can be used to verify geological reconstructions using paleomagnetic data. This tool enables the user to predict the paleomagnetic direction and paleolatitude for a location on any element of a GPlates reconstruction at a given time, provided the element is connected through the rotation tree to South Africa (plate ID 701; see Li et al., 2017). This allows for testing and iterating tectonic reconstructions to in situ paleomagnetic data (see, for instance, van Hinsbergen et al., 2019, for extensive application to the Mediterranean region).

7.6. CTMD Module

We have removed the common true mean direction (CTMD) test (McFadden & McElhinny, 1990) in favor of the x-, y-, and z-coordinate bootstrap (Tauxe, 2010). The CTMD test classifies the equivalence of two Fisherian distributions based on the angle between their mean directions and dispersion parameters. This decision was made because the CTMD test is based on a collection's statistical distribution, while in the application, the original components are always available and should be used.

7.7. Other

Finally, we note the redesign of the application with performance improvements. The source code has been fully rewritten to facilitate future developments on the application and is available on GitHub at https://github.com/Jollyfant/PMAG2. Every version release of the software is attributed a DOI, so a particular version can be referenced, which is important in case of bug fixes that affect the reproducibility of results.

A fully detailed change log with all changes is available on the website.

8. Conclusion

In this contribution, we present the second iteration of Paleomagnetism.org. We put an emphasis on streamlining the user experience and workflow from initial data interpretation to its final distribution. Our ambition is to assist the paleomagnetic community in following modern data management protocols guided by the FAIR principles. We establish this through (1) improved metadata descriptions for specimens, (2) a free, online data library exposed through an HTTPS web service, and (3) integration with the widely adopted MagIC database. Demagnetization data analyzed in the Interpretation portal can be bundled to a collection that can be freely shared with colleagues or exported to a MagIC database file. Multiple collections can be bundled to a data publication and added to our collective data library, which will be hosted under our domain and is freely accessible. This publication, including any collection or specimen within it, can always be referenced or viewed through its unique persistent identifier and will be curated by the Paleomagnetism.org team.

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