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Technical Note: The Linked Paleo Data framework – a common tongue for paleoclimatology

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Paleoclimatology is a highly collaborative scientific endeavor, increasingly reliant on online databases for data sharing. Yet, there is currently no universal way to describe, store and share paleoclimate data: in other words, no standard. Data standards are often regarded by scientists as mere technicalities, though they underlie much scientific and technological innovation, as well as facilitating collaborations between research groups. In this article, we propose a preliminary data standard for paleoclimate data, general enough to accommodate all the proxy and measurement types encountered in a large international collaboration (PAGES2K). We also introduce a vehicle for such structured data (Linked Paleo Data, or LiPD), leveraging recent advances in knowledge representations (Linked Open Data).

The LiPD framework enables guick guerying and extraction, and we expect that it will facilitate the writing of open-source, community codes to access, analyze, model and visualize paleoclimate observations. We welcome community feedback on this standard, and encourage paleoclimatologists to experiment with the format for their own purposes.

Introduction

Science is entering a data-intensive era, where insight is increasingly gained by extracting information from large volumes of data (Hey, 2012). This is particularly critical in paleoclimatology, as understanding past changes in climate system requires observations across large spatial and temporal scales. Paleoclimatic observations are typically limited to small geographic domains, so investigating large scales requires integrating many disparate studies and datasets. Observational work in paleoclimatology exemplifies the "long-tail" approach to data collection (Heidorn, 2008): the majority of observations are gathered by independent scientists with no formal language for describing their data and meta-data to each other - or to machines - in a standardized

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fashion. This results in a "Digital Tower of Babel", making the curation, access, re-use and valorization of paleoclimate data far more difficult than it should be, hindering scientific progress.

Recognizing the need for data sharing, paleoclimate investigators have made a major effort over the past decade to make their data available to the broader community, largely through online archiving systems like the World Data Center for Paleoclimatology and Pangaea. Nonetheless, the lack of consistent formatting and metadata standards (i.e. a common tongue) has made the re-use of such data needlessly laborintensive by preventing computers from participating in the task of making connections across datasets. As the number of records in these archives has grown, making connections manually has become more and more challenging, hampering integrative efforts at the very time they should be flourishing. Paleoclimatologists thus need a common tongue to describe their datasets to each other and to machines. Achieving this goal requires addressing two major hurdles: (1) the lack of an accepted data container for paleoclimate data; (2) the lack of a community standard for such data.

These two issues are clearly related, but somewhat distinct in practice. The data container must be universally readable, a condition satisfied by, for instance, netCDF files, which have been used for paleoclimate syntheses (Wahl et al., 2010). However, such files only allow for fixed schemas and require identical fields for all proxies. In reality, each proxy dataset may have a unique set of data and metadata properties. For broader applicability, we thus require a more flexible format. Further, to enhance the relevance of paleoclimate data to other fields, one would like this data container to be compatible with the Linked Data paradigm (Bizer et al., 2009), which allows for data-driven discovery between datasets that would otherwise be unlikely or impossible.

In this technical note, we present LiPD (Linked Paleo Data) a new, flexible linked-data container designed for paleoclimate data. Such a data container is a necessary first step towards a "semantic web of paleoclimatology" (Emile-Geay and Eshleman, 2013), and provides a straightforward framework in which communities and researchers can explicitly describe their data and metadata in common terms that the community, and

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A flexible container for paleoclimate data

Paleoclimate observations come in many varieties; standardizing the data and providing the framework to encode meaning to the parameters and metadata requires a flexible, and extensible format. The linked data variety of JavaScript Object Notation (JSON-LD), provides a lightweight, and human-readable solution to this problem. JSON-LD is almost infinitely customizable, here we present conventions for Linked Paleo Data (LiPD), which utilizes JSON-LD and provides a structure that is common to the overwhelming majority (if not all) of paleoclimate observational datasets. Despite their variety, all paleoclimate datasets, commonly comprised of both direct observations and inferred variability, share the same major features.

- 1. Some base metadata about the dataset (e.g.)
 - a. Identifiers (dataset name, version number, dataset DOI, investigators)
 - b. Archive¹ type

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- 2. Geographic metadata (e.g.,)
 - a. Latitude, longitude, elevation above or depth below sea level

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¹The archive is the medium in which the paleoclimatic signal is imprinted: e.g. coral aragonite, ice core, foraminiferal calcite in a sediment core, etc...

- 3. Publication metadata (e.g.,)
 - a. DOI (which resolves the following information)
 - b. Authors, title, journal, publication date
- 4. Proxy data and metadata, including:
 - a. One or more tables of measurements, and their metadata
 - b. Parameter names, units, standards, and interpretations (including forward models)
 - 5. Geochronological data and metadata, which can include
 - a. Table(s) of radiometric dating measurements and associated metadata
 - b. Age model ensembles
 - c. Author interpretation and methodological choices

LiPD encodes these data and metadata into a structured hierarchy that allows explicit description of any aspect of the dataset at any level of the data (Fig. 1). LiPD serializes this hierarchy using JSON-LD, using nests of lists and key-value pairs. LiPD adopts the GeoJSON standard to describe the geospatial metadata of a given site like this:

```
"qeo":
      "type": "Feature",
      "geometry": {
            "type": "Point",
            "coordinates": [-17.82, 62.08, -1938]
      "properties": {
            "siteName": "RAPiD-12-1K, South Iceland Rise,
                               4313
```

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```
} ,
```

Note that the GeoJSON standard defaults to the WGS84 ellipsoid, and units of decimal degrees for latitude and longitude and meters above sea level for elevation. This standard readily accommodates polygonal geographic features and additional location metadata.

LiPD adopts the Linked Data extension of BibJSON (Johnson, 2013) to describe publication metadata, for example:

For the paleoData and chronData components of LiPD, which include tabular data, LiPD does not store the actual tabular data in the JSON-LD format, as this becomes increasingly verbose and inefficient with large data tables. Rather, the tabular data are stored in headerless comma separated value (CSV) files that are referenced and

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described by the JSON-LD file, using the W3C's CSV on the Web working groups recommendations, like this:

```
"paleoData": [{
        "paleoDataTableName": "data",
        "filename": "Atlantic0220Thornalley2009.csv",
5
         "columns": [{
               "number": 1,
               "parameter": "depth",
               "parameterType": "measured",
               "description": "depth below ocean floor",
10
               "units": "cm",
               "datatype": "csvw:NumericFormat",
               "notes": "depth refers to top of sample"
15
               "number": 2,
               "parameter": "year",
               "parameterType": "inferred",
               "description": "calendar year AD",
               "units": " AD",
20
               "datatype": "csvw:NumericFormat",
               "method": "linear interpolation"
               "number": 3,
               "parameter": "temperature",
               "parameterType": "inferred",
               "description": "sea-surface temperature inferred
                                              from Mq/Ca ratios",
```

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```
"datatype": "csvw:NumericFormat",
               "material": "foramifera carbonate",
               "calibration": {
                 "equation": "BAR2005: Mg/Ca=0.794*exp(0.10*SST)",
                 "reference": "Barker et~al., (2005),
5
                               Thornalley et~al., (2009)",
                 "uncertainty": 1.3
               "units": "deg C",
               "proxy": "Mq/Ca",
10
               "climateInterpretation": {
                     "parameter": "T",
                     "parameterDetail": "seaSurface",
                     "seasonality": "MJJ",
                     "interpDirection": "positive",
15
                     "basis": "Mq/Ca calibration to SST"
        }]
  }]
```

Describing the columns in the datatable in the LiPD framework allows explicit encoding of key metadata that are commonly lost or misunderstood in current data structures. For example, the "climateInterpretation" section above allows the scientist to explicitly describe the details of how the parameter "senses" climate. When encoded as above and explicitly defined and linked, the knowledge that this record is interpreted to record May through July sea surface temperature, and that those temperature estimates were derived from the Mg/Ca calibration equations of Barker et al. (2005) and Thornalley et al. (2009) becomes built into the dataset, and readable to both people and computers. It's gueryable, and linked to other datasets, and transparent when datasets are used in ways that are outside the published interpretations.

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and out of Matlab (as structured arrays), R (as lists) and Python (as dictionaries).

A preliminary data standard for paleoclimatology

The flexible container described in Sect. 2 can serialize any set of paleoenvironmental data with rich metadata. However this framework only becomes useful when a common vocabulary with explicit meanings is applied to the data. Developing this vocabulary requires buy-in from experts across the disparate domains of the paleogeosciences, and will be a gradual process of evolving standards. To begin this conversation, here we outline a preliminary metadata standards for required metadata, based on phase 2 of the Past Global Changes (PAGES) past two thousand years (2k) project. The following are the minimal metadata for every paleoArchive in the network. Many records include additional desirable data and metadata; an ongoing extended metadata table is available here. To illustrate this standard more concretely, we use the dataset of Thornalley et al. (2009) as an example (Fig. 2 and Table below).

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²https://en.wikipedia.org/wiki/BagIt

dataSetName name of the dataset; that is, an alphanumeric string that uniquely characterizes this record in the database, often based on site, authors, year and ancillary information example: RAPiD-12-1K.Thornalley.2009

archiveType example: marine sediments investigator example: David Thornalley

2. Geospatial metadata (in GeoJSON)

coordinates longitude, latitude, and elevation, in units of decimal degrees and meters above sea level; *example: "coordinates":* [–17.82, 62.08, –1938]

type geographic feature type (typically "point" or "polygon" *example: point* **siteName** *RAPiD-12-1K*

3. Publication metadata (in bibJSON)

DOI publication Digitial Object Identifier; example: 10.1038/nature07717

citation long publication string if DOI is unavailable; example: Thornalley, David JR, Harry Elderfield, and Nick McCave. "Holocene Oscillations in Temperature and Salinity of the Surface Subpolar North Atlantic." Nature 457, no. 7230 (2009): 711–14.

pubString short text citation; example: Thornalley et al., 2009

4. Paleo data metadata

paleoDataTableName short name of the paleoData table; example: data

filename measurement table filename (.csv);

example: Atlantic0220Thornalley2009.csv

chronology short name of chronology table used in this measurement table; *example: chronology*

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depth depth of sample/measurement

age/year best estimate age/year of sample/measurements

climate-sensitive parameter measurement interpreted in terms of past climate or environmental change *example: Mg/Ca*

paleoData column metadata metadata characterizing each column of the paleoDataTable

column column number; example: 3

parameter short parameter name example: SST

description longer description of the parameter *example: sea-surface temperature inferred from Mg/Ca ratios*

units example: deg C

climateInterpretation five parameters that allow for a concise description of how the climate-sensitive parameter is related to climate. This is required for at least one column in the PAGES 2k database, but may not be appropriate for all datasets.

parameter what aspect(s) of climate are recorded in this archive; *example:* temperature

parameterDetail provides detail on "climateInterpretationParameter" *example: sea surface*

seasonality example: May, June, July

interpretationDirection Do the values have a positive or negative relation to the inferred parameter *example: positive*

basis quote from paper or other argument that justifies the interpretation *example: regional core top calibration equation* (Barker et al., 2005)

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e:

parameter what aspect(s) of climate are recorded in this archive; *example:* temperature

parameterDetail provides detail on "climateInterpretationParameter" *example: sea surface*

seasonality example: May, June, July

interpretationDirection Do the values have a positive or negative relation to the inferred parameter *example: positive*

basis quote from paper or other argument that justifies the interpretation example: regional core top calibration equation (Barker et al., 2005)

Chronological metadata

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chronDataTableName short name of the chronData table; *example: chronology* **filename** chronology table filename (.csv);

example: Atlantic0220Thornalley2009Chronology.csv

chronology short name of chronology table used in this measurement table; *example: chronology*

chronData table columns columns required in chronology table, will vary by archive and geochronological methodology type – example for ¹⁴C age.

depth depth of sample/measurement

14CAge radiocarbon age

14CAgeUncertainty analytical radiocarbon age uncertainty

datedMaterial what was dated? (e.g., bulk sediment, terrestrial macrofossil, etc)

chronology column metadata metadata characterizing each column of the chronDataTable

column column number; example: 2

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parameter short parameter name example: 14CAge

description longer description of the parameter example: uncalibrated radiocarbon age

units example: 14C vr BP

errorLevel error level for uncertainty columns example: 14C yr BP

Discussion

The data container and preliminary data standard described here are extremely flexible, and can accommodate any paleoclimatic or paleoenvironmental data that are based on any expansion of dependent/independent variable pairs. This encompasses all paleoclimate and paleoenvironmental datasets that we can imagine. The challenge for developing a sufficiently broad paleodata framework has long been (1) defining all of the relevant terms for such a diverse community and (2) managing the appropriate level of detail (lumping vs. splitting) in the terminology. The framework presented here accommodates the first challenge by being accommodating the complexity and inevitable proliferation of terms, variables and interpretations inherent to the interdisciplinary field of paleoclimatology, and by assigning explicit meaning to the terms through the Linked Open Data framework. Implementation of these semantics will be an evolving, community-driven process. This is critical for two reasons: first, defining an ontology a priori has proven impossible to date; second, even if it were possible, such an ontology would be meaningless if it were not used. We will thus rely on usage and community discussion to reach agreement on terminology. The discussion may begin here, in the comments of this paper.

The LiPD framework accommodates the second challenge by adopting a hierarchical structure, that starts with more general terminology and allowing further detail to be assigned deeper in the structure. Consider the example of two δ^{18} O datasets, one measured on a coral archive, and the other derived from foraminifera extracted from **CPD**

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a marine sediment core. On one hand, these two records are measuring the same parameter, and there are times when researchers might be interested in investigating all δ^{18} O regardless of the details of the archive on which they were measured. On the other hand, there are some important differences between the two measurements that users would like to include in the data repository. If we were to describe each parameter in a single term, we would have to decide whether to call them both " δ^{18} O", or to call one " δ^{18} O-skeletal aragonite" and the other " δ^{18} O-foraminfera > 120 µm size class". By taking advantage of JSON's capacity to build hierarchical metadata structures, we can encode an entire set of metadata at the appropriate level in the dataset as:

```
"parameter": "d180",
  "description": "d180 measured on skeletal aragonite",
  "units": "permil",
  "standard": "VSMOW",
  "material": "skeletal aragonite",
  "instrument": "Micromass Optima gas source
                 triple-collector mass spectrometer"
and:
"parameter": "d180",
"description": "d180 measured on G. bulloides > 120 microns",
"units": "permil",
"standard": "VSMOW",
"material": "foraminifera calcite",
"instrument": "Micromass Optima gas source
               triple-collector mass spectrometer"
```

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"species": "Globigerina bulloides"

This makes the commonalities and differences between the datasets explicit. Moreover, additional levels of metadata may be introduced into the descriptor to accommodate climate interpretation, calibration procedures or forward modeling as described above. The power of the hierarchical structure is that it allows the metadata to be placed at the appropriate level, avoiding logical contradictions in lumping and splitting that become necessary when trying to incorporate information from several levels into a single term - or when several users describe the same dataset in slightly different ways.

An important consideration for re-use and provenance tracking is **versioning**: each version of a LiPD record, or collection of LiPD records, should be associated with a unique identifier, which is crucial to reproducibility. We propose the following preliminary versioning scheme:

Individual records A number of the form I_1, I_2 , where I_1 is an integer associated with a publication (e.g.Thornalley et al., 2009) and I₂ is a counter updated every time a modification is made to the data or metadata.

Data compilations A number of the form C_1 , C_2 , C_3 , where C_1 is an integer associated with a publication (e.g.PAGES2k Consortium, 2013) and C_2 is a counter updated every time a record is added or removed, and C₃ is a counter updated every time a modification is made to the data or metadata in an individual record.

We are presently implementing a large-scale test of the LiPD framework by using it as the primary data archive for Phase 2 of the PAGES 2k global temperature database. Consequently, the described framework for describing the proxy data is fairly mature and field-tested. LiPD's relatively complex structure is in fact the simplest container we could devise that would accommodate the wide diversity of constraints provided by the > 5000 timeseries in the database. However, it may not be universal, and we welcome suggestions for increased generality.

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The standards for reporting and storing geochronological data are much less tested and will require far more community input. For instance, there seems to be no universal way of reporting radiocarbon, U/Th, or ²¹⁰Pb dates. Ideally, coordination between geochronologists would yield a universal standard for all radiometric age models; however, if there is to be any standard, it is more likely to first emerge within each subcommunity. We are confident that JSON-LD is flexible enough to encompass any possibility, but doing so in a way that allows research codes to easily read those chronologies and generate age models from them will likely require more work.

More generally, it is important to realize that the LiPD framework is not a rigid container that one must force paleoclimate data into, but rather a flexible system designed to wrap around a data set. We are keen to continue developing and expanding LiPD and the preliminary data standard with input from the community. We welcome any and all feedback on this framework, in particular potential problems that we have not foreseen.

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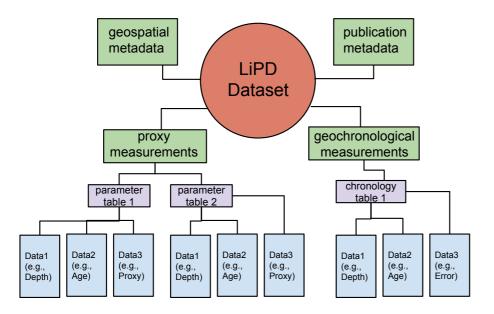


Figure 1. Schematic data model example of Linked PaleoData.

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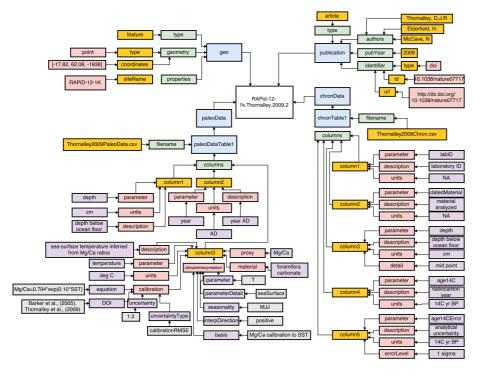


Figure 2. Data model for RAPiD-12-1k example used in the technical note.

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